WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 09:38 AM EST

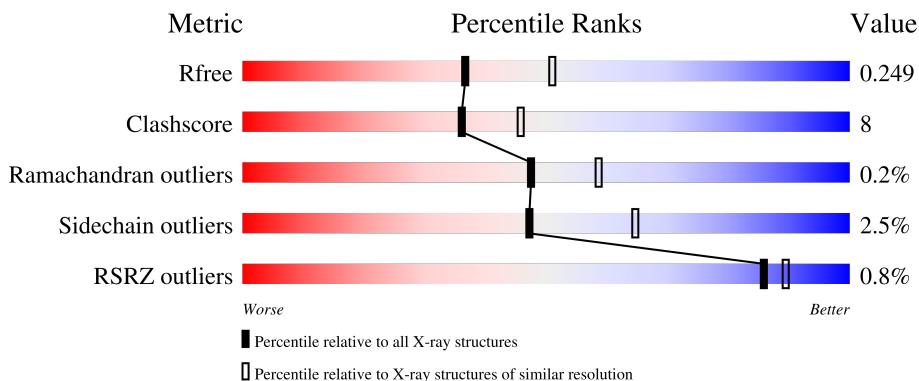|		
PDB ID	:	4FFI
Title	:	Crystal Structure of Levan Fructotransferase D54N mutant from Arthrobacter ureafaciens in complex with levanbiose
Authors	:	Park, J.; Rhee, S.
Deposited on	:	2012-06-01
Resolution	:	2.30 Å(reported)

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.
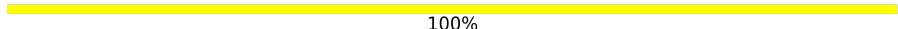
Metric	Percentile Ranks	Value
Rfree		0.249
Clashscore		8
Ramachandran outliers		0.2%
Sidechain outliers		2.5%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
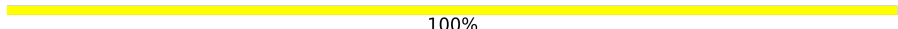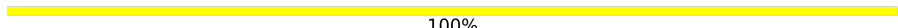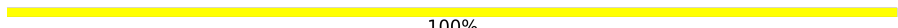
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	81% 15%
1	B	492	78% 17%
1	C	492	85% 12%
1	D	492	81% 15%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
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.
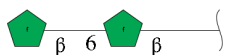
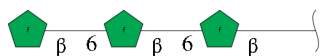

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	2	23	12	11	0	0	0

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

- 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 34	C 18	O 16	0	0	0

- Molecule 4 is water.

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

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 o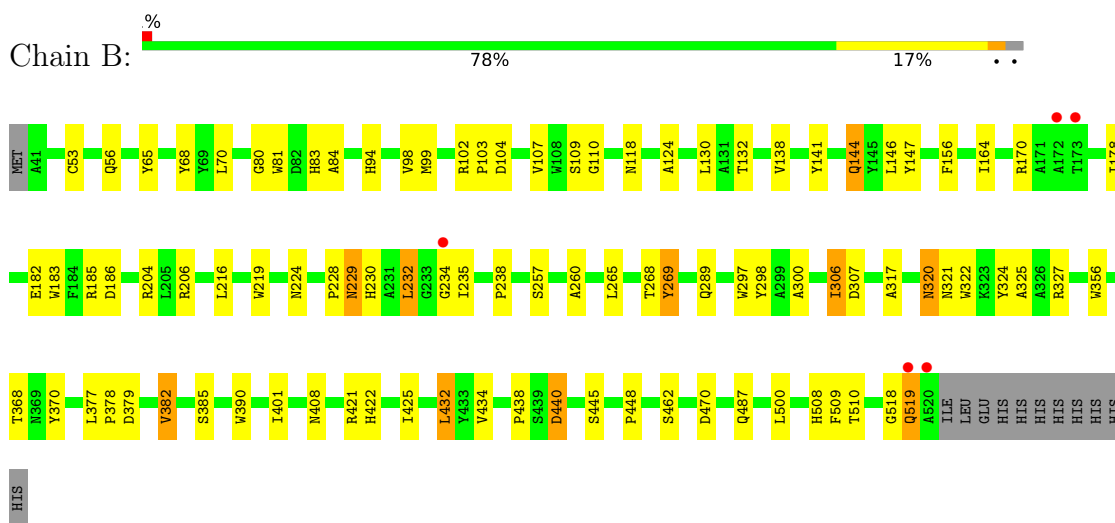r more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Levan fructotransferase
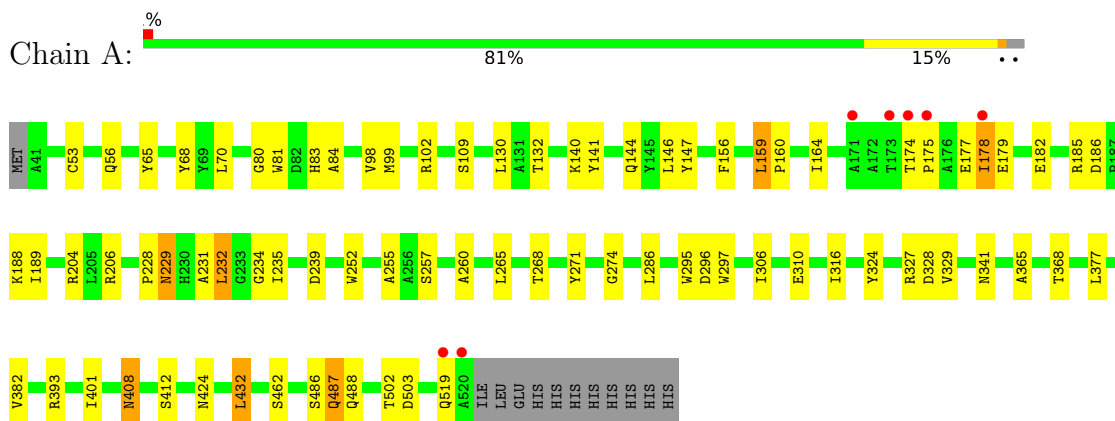
Chain A:

• Molecule 1: Levan fructotransferase

Chain B:

• Molecule 1: Levan fructotransferase

Chain C:

S257 M258 I263 T268 D277 H282 D285 W297 Y298 W322 T331 S334 T362 T376 R393 E398 I401 N408 S412 H422 T423 N424 I425 L432 P438 L446 S462 R466 D470 Q487 T496 D503 Q519

ALA ILE LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Levan fructotransferase

Chain D:

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

Chain E:

FRU1 FRU2

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

Chain F:

FRU1 FRU2

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

Chain G:

FRU1 FRU2

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

Chain I:

FRU1 FRU2

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

Chain J:

FRU1
FRU2
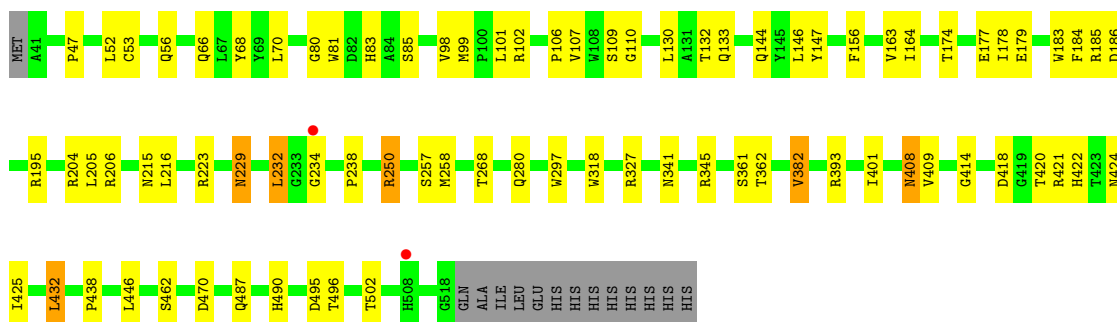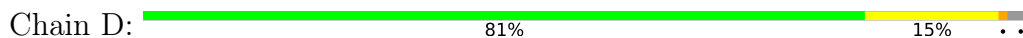
• Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

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 44.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.30) 92.9 (44.40-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.00 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.251 0.216 , 0.249	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)	0.34 , 34.9	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.33	0/3863	0.63	1/5312 (0.0%)
1	B	0.32	0/3863	0.64	1/5312 (0.0%)
1	C	0.33	0/3858	0.64	1/5305 (0.0%)
1	D	0.34	0/3849	0.64	1/5293 (0.0%)
All	All	0.33	0/15433	0.64	4/21222 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	432	LEU	N-CA-C	-6.06	94.65	111.00
1	D	432	LEU	N-CA-C	-5.91	95.06	111.00
1	B	432	LEU	N-CA-C	-5.86	95.17	111.00
1	A	432	LEU	N-CA-C	-5.82	95.29	111.00

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	60	0
1	B	3739	0	3491	62	0
1	C	3734	0	3486	46	0
1	D	3725	0	3478	63	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
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	234	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 8.

All (234) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:146:LEU:HD23	1:D:146:LEU:C	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:215:ASN:O	1:C:216:LEU:HB2	2.07	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
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: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:D:109:SER:HB2	1:D:186:ASP:OD1	2.09	0.52
1:A:174:THR:HG23	1:A:177:GLU:OE2	2.10	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:306:ILE:HD13	1:B:306:ILE:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:518:GLY:C	1:B:519:GLN:OE1	2.49	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:B:56:GLN:HB2	1:B:68:TYR:HB2	1.95	0.49
1:A:146:LEU:HD23	1:A:146:LEU:C	2.33	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: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: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: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:B:146:LEU:HD23	1:B:146:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:146:LEU:C	1:C:146:LEU:HD23	2.37	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: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: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: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:D:80:GLY:HA2	1:D:107:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:144:GLN:N	1:D:144:GLN:CD	2.70	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
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:A:486:SER:C	1:A:487:GLN:HG3	2.39	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:206:ARG:HA	1:A:234:GLY:HA2	2.03	0.40
1:A:310:GLU:OE2	1:A:310:GLU:HA	2.22	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%)	47	58
1	B	478/492 (97%)	446 (93%)	30 (6%)	2 (0%)	34	42
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%)	47	58

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%)	372 (98%)	9 (2%)	49	66
1	B	381/393 (97%)	367 (96%)	14 (4%)	34	48
1	C	381/393 (97%)	374 (98%)	7 (2%)	59	75
1	D	380/393 (97%)	372 (98%)	8 (2%)	53	70
All	All	1523/1572 (97%)	1485 (98%)	38 (2%)	47	65

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ARG
1	A	159	LEU
1	A	178	ILE
1	A	229	ASN
1	A	232	LEU
1	A	297	TRP
1	A	328	ASP
1	A	408	ASN
1	A	487	GLN
1	B	104	ASP
1	B	144	GLN
1	B	229	ASN
1	B	230	HIS
1	B	232	LEU
1	B	297	TRP
1	B	306	ILE
1	B	307	ASP

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Mol	Chain	Res	Type
1	B	320	ASN
1	B	382	VAL
1	B	408	ASN
1	B	440	ASP
1	B	448	PRO
1	B	519	GLN
1	C	98	VAL
1	C	101	LEU
1	C	232	LEU
1	C	250	ARG
1	C	297	TRP
1	C	408	ASN
1	C	487	GLN
1	D	229	ASN
1	D	232	LEU
1	D	250	ARG
1	D	297	TRP
1	D	382	VAL
1	D	408	ASN
1	D	446	LEU
1	D	487	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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	289	GLN
1	A	408	ASN
1	A	424	ASN
1	A	479	ASN
1	A	519	GLN
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

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Mol	Chain	Res	Type
1	C	133	GLN
1	C	144	GLN
1	C	282	HIS
1	C	341	ASN
1	C	391	ASN
1	C	408	ASN
1	C	422	HIS
1	C	424	ASN
1	C	487	GLN
1	C	519	GLN
1	D	66	GLN
1	D	74	GLN
1	D	133	GLN
1	D	180	ASN
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	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	1.44	1 (9%)	10,18,18	1.19	1 (10%)
2	FRU	E	2	2	11,11,12	1.59	2 (18%)	15,15,18	1.27	2 (13%)
2	FRU	F	1	2	11,12,12	1.34	0	10,18,18	0.86	0
2	FRU	F	2	2	11,11,12	1.45	2 (18%)	15,15,18	1.13	2 (13%)
2	FRU	G	1	2	11,12,12	1.47	2 (18%)	10,18,18	1.12	1 (10%)
2	FRU	G	2	2	11,11,12	1.55	1 (9%)	15,15,18	1.38	3 (20%)
3	FRU	H	1	3	11,12,12	1.78	3 (27%)	10,18,18	1.16	0
3	FRU	H	2	3	11,11,12	1.44	2 (18%)	15,15,18	1.13	1 (6%)
3	FRU	H	3	3	11,11,12	1.37	1 (9%)	15,15,18	1.27	3 (20%)
2	FRU	I	1	2	11,12,12	1.16	1 (9%)	10,18,18	1.40	2 (20%)
2	FRU	I	2	2	11,11,12	1.57	2 (18%)	15,15,18	1.31	2 (13%)
2	FRU	J	1	2	11,12,12	1.57	4 (36%)	10,18,18	1.39	1 (10%)
2	FRU	J	2	2	11,11,12	1.45	2 (18%)	15,15,18	1.14	1 (6%)
2	FRU	K	1	2	11,12,12	1.57	4 (36%)	10,18,18	1.06	1 (10%)
2	FRU	K	2	2	11,11,12	1.63	2 (18%)	15,15,18	1.30	3 (20%)
2	FRU	L	1	2	11,12,12	1.18	1 (9%)	10,18,18	1.49	2 (20%)
2	FRU	L	2	2	11,11,12	1.63	2 (18%)	15,15,18	1.44	2 (13%)
2	FRU	M	1	2	11,12,12	1.65	2 (18%)	10,18,18	1.50	1 (10%)
2	FRU	M	2	2	11,11,12	1.56	2 (18%)	15,15,18	1.11	1 (6%)
2	FRU	N	1	2	11,12,12	1.50	2 (18%)	10,18,18	1.34	2 (20%)
2	FRU	N	2	2	11,11,12	1.47	1 (9%)	15,15,18	1.28	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	FRU	C4-C3	-3.72	1.43	1.53
2	L	2	FRU	C4-C3	-3.54	1.43	1.53
2	M	2	FRU	C4-C3	-3.49	1.43	1.53
2	G	2	FRU	C4-C3	-3.47	1.43	1.53
2	E	2	FRU	C4-C3	-3.45	1.43	1.53
2	F	2	FRU	C4-C3	-3.36	1.44	1.53
2	I	2	FRU	C4-C3	-3.35	1.44	1.53
3	H	1	FRU	O4-C4	-3.29	1.35	1.43
3	H	3	FRU	C4-C3	-3.24	1.44	1.53
2	N	2	FRU	C4-C3	-3.19	1.44	1.53
2	J	2	FRU	C4-C3	-3.18	1.44	1.53
3	H	2	FRU	O4-C4	-3.13	1.35	1.43
2	M	1	FRU	O3-C3	-3.12	1.36	1.42
3	H	1	FRU	O5-C2	-2.97	1.38	1.43
2	J	1	FRU	O3-C3	-2.72	1.37	1.42
3	H	1	FRU	C4-C3	-2.60	1.41	1.52
2	N	1	FRU	O3-C3	-2.51	1.37	1.42
2	K	1	FRU	O3-C3	-2.46	1.37	1.42
2	G	1	FRU	O3-C3	-2.42	1.37	1.42
2	E	1	FRU	O3-C3	-2.41	1.37	1.42
2	L	2	FRU	O3-C3	-2.24	1.37	1.43
2	I	2	FRU	O3-C3	-2.16	1.37	1.43
2	N	1	FRU	C4-C3	-2.15	1.43	1.52
2	M	1	FRU	C4-C3	-2.14	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	FRU	O2-C2	-2.14	1.37	1.40
2	K	1	FRU	C4-C3	-2.13	1.43	1.52
2	K	1	FRU	O4-C4	-2.12	1.38	1.43
2	J	1	FRU	O2-C2	-2.12	1.37	1.40
3	H	2	FRU	C4-C3	-2.12	1.47	1.53
2	E	2	FRU	O3-C3	-2.11	1.38	1.43
2	J	1	FRU	O4-C4	-2.05	1.38	1.43
2	J	2	FRU	O3-C3	-2.05	1.38	1.43
2	L	1	FRU	O3-C3	-2.05	1.38	1.42
2	G	1	FRU	C4-C5	-2.02	1.47	1.53
2	K	2	FRU	O3-C3	-2.01	1.38	1.43
2	I	1	FRU	O3-C3	-2.01	1.38	1.42
2	F	2	FRU	O3-C3	-2.01	1.38	1.43
2	J	1	FRU	C4-C3	-2.01	1.44	1.52
2	M	2	FRU	O3-C3	-2.00	1.38	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	FRU	O1-C1-C2	3.53	119.38	111.86
2	J	1	FRU	O1-C1-C2	3.27	118.82	111.86
2	L	2	FRU	O5-C5-C6	3.24	116.22	109.21
2	L	1	FRU	O1-C1-C2	3.13	118.51	111.86
2	I	1	FRU	O1-C1-C2	3.11	118.48	111.86
2	I	2	FRU	O5-C5-C6	2.91	115.50	109.21
2	G	2	FRU	O6-C6-C5	2.78	120.82	111.29
3	H	3	FRU	O6-C6-C5	2.71	120.60	111.29
2	G	2	FRU	O5-C5-C6	2.61	114.86	109.21
2	G	1	FRU	O1-C1-C2	2.61	117.41	111.86
2	J	2	FRU	O6-C6-C5	2.59	120.18	111.29
2	K	2	FRU	O6-C6-C5	2.49	119.84	111.29
2	F	2	FRU	O1-C1-C2	2.49	119.83	111.29
2	M	2	FRU	O6-C6-C5	2.46	119.75	111.29
2	K	2	FRU	O5-C5-C6	2.43	114.46	109.21
2	N	1	FRU	O4-C4-C3	-2.33	105.17	112.15
2	K	2	FRU	C1-C2-C3	-2.32	109.50	115.09
2	L	1	FRU	O4-C4-C3	-2.28	105.32	112.15
2	N	2	FRU	O1-C1-C2	2.28	119.12	111.29
2	N	2	FRU	C1-C2-C3	-2.27	109.61	115.09
2	N	1	FRU	O6-C6-C5	2.27	119.08	111.29
2	G	2	FRU	O1-C1-C2	2.27	119.06	111.29
2	N	2	FRU	O6-C6-C5	2.24	118.98	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	FRU	O6-C6-C5	2.19	118.82	111.29
2	I	1	FRU	O4-C4-C3	-2.15	105.70	112.15
2	L	2	FRU	O1-C1-C2	2.14	118.62	111.29
2	K	1	FRU	O1-C1-C2	2.13	116.40	111.86
3	H	3	FRU	C3-C4-C5	2.10	106.71	102.64
2	E	1	FRU	O1-C1-C2	2.08	116.29	111.86
3	H	2	FRU	O5-C2-C1	-2.07	104.73	109.21
2	I	2	FRU	O6-C6-C5	2.04	118.30	111.29
3	H	3	FRU	O1-C1-C2	2.04	118.30	111.29
2	E	2	FRU	O1-C1-C2	2.04	118.28	111.29
2	E	2	FRU	O6-C6-C5	2.01	118.20	111.29

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
3	H	2	FRU	C4-C5-C6-O6
2	E	1	FRU	O5-C5-C6-O6
2	N	1	FRU	O5-C5-C6-O6
3	H	2	FRU	O5-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

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Mol	Chain	Res	Type	Atoms
2	J	2	FRU	O1-C1-C2-O5
2	M	2	FRU	O1-C1-C2-O5
2	G	1	FRU	C4-C5-C6-O6
2	G	1	FRU	O1-C1-C2-O5
3	H	3	FRU	C4-C5-C6-O6
2	G	1	FRU	O1-C1-C2-O2
2	J	1	FRU	O5-C5-C6-O6
2	M	1	FRU	O5-C5-C6-O6
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	2	FRU	2	0
2	E	2	FRU	1	0
2	M	1	FRU	3	0
2	I	1	FRU	1	0
2	E	1	FRU	1	0
2	G	1	FRU	2	0

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

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	480/492 (97%)	-0.28	7 (1%)	73	79	11, 23, 37, 55	0
1	B	480/492 (97%)	-0.31	5 (1%)	82	86	12, 22, 36, 58	0
1	C	479/492 (97%)	-0.42	2 (0%)	92	95	9, 20, 29, 48	0
1	D	478/492 (97%)	-0.40	2 (0%)	92	95	8, 21, 33, 42	0
All	All	1917/1968 (97%)	-0.35	16 (0%)	86	89	8, 21, 34, 58	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	GLN	3.3
1	B	173	THR	3.0
1	A	519	GLN	2.8
1	B	172	ALA	2.8
1	A	173	THR	2.8
1	A	171	ALA	2.8
1	C	234	GLY	2.8
1	A	520	ALA	2.7
1	D	234	GLY	2.4
1	A	178	ILE	2.4
1	B	234	GLY	2.4
1	D	508	HIS	2.3
1	B	520	ALA	2.3
1	C	519	GLN	2.2
1	A	175	PRO	2.2
1	A	174	THR	2.2

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

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	L	1	12/12	0.74	0.25	59,62,63,64	0
2	FRU	I	1	12/12	0.80	0.17	46,49,49,50	0
2	FRU	L	2	11/12	0.84	0.18	54,58,60,60	0
2	FRU	F	2	11/12	0.89	0.23	37,39,41,43	0
2	FRU	K	2	11/12	0.89	0.17	42,43,44,45	0
2	FRU	F	1	12/12	0.91	0.10	23,28,32,37	0
2	FRU	E	2	11/12	0.92	0.11	34,34,36,37	0
2	FRU	G	2	11/12	0.92	0.15	33,35,35,40	0
2	FRU	N	2	11/12	0.92	0.15	30,31,33,35	0
3	FRU	H	3	11/12	0.92	0.19	33,38,41,43	0
2	FRU	M	2	11/12	0.93	0.15	26,30,34,35	0
2	FRU	J	2	11/12	0.93	0.12	28,30,31,34	0
2	FRU	I	2	11/12	0.93	0.14	45,48,49,49	0
3	FRU	H	2	11/12	0.94	0.11	33,34,35,36	0
2	FRU	G	1	12/12	0.94	0.15	34,35,36,38	0
2	FRU	J	1	12/12	0.96	0.11	21,23,26,28	0
3	FRU	H	1	12/12	0.96	0.10	18,21,26,30	0
2	FRU	K	1	12/12	0.96	0.09	25,29,34,39	0
2	FRU	N	1	12/12	0.96	0.09	19,22,24,27	0
2	FRU	E	1	12/12	0.97	0.13	24,30,32,32	0
2	FRU	M	1	12/12	0.97	0.12	21,23,25,27	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-charide. Each fit is shown from different orientation to approximate a three-dimensional view.
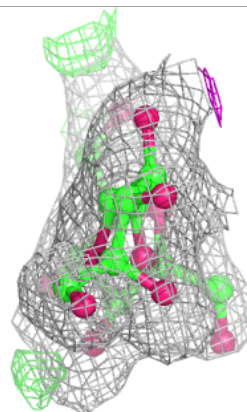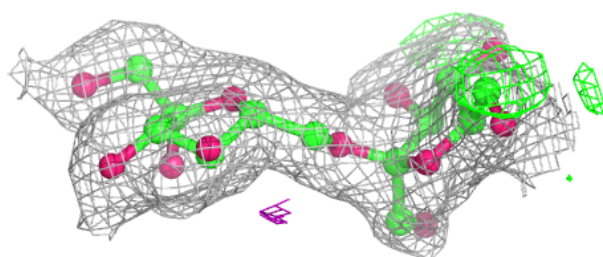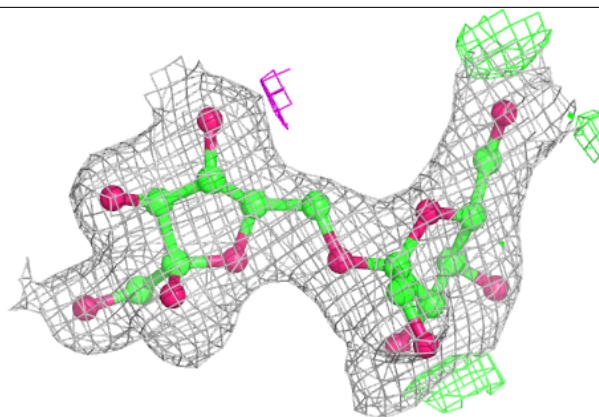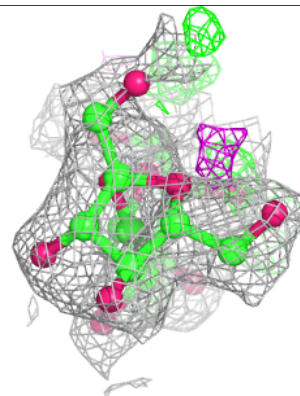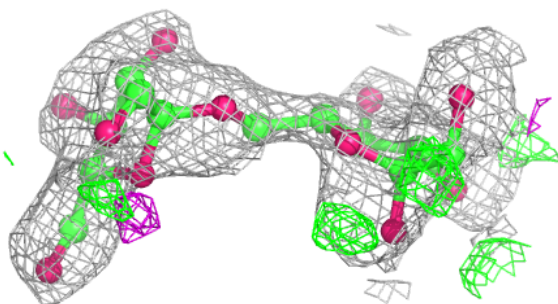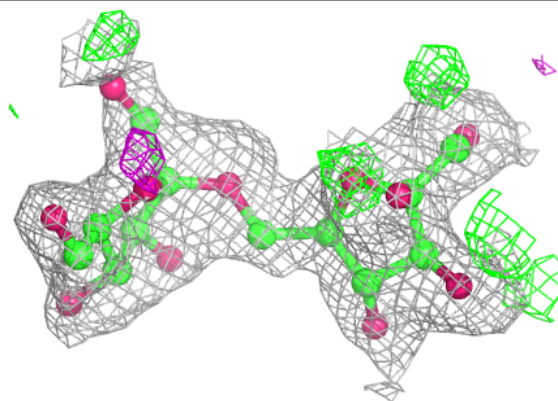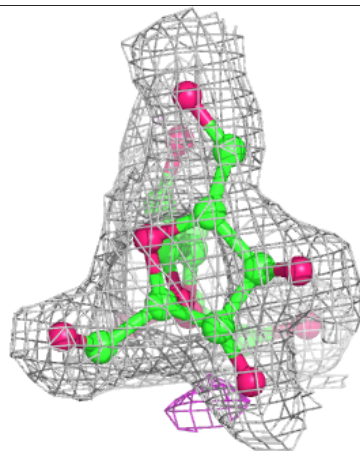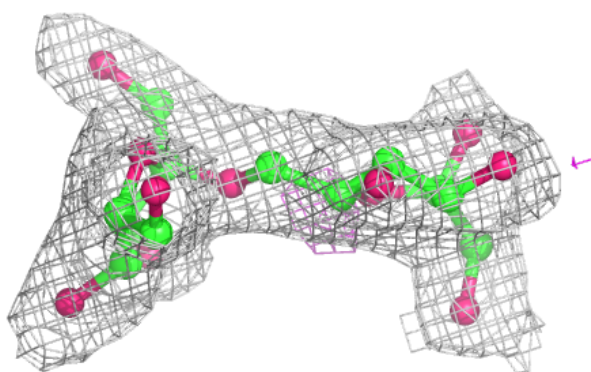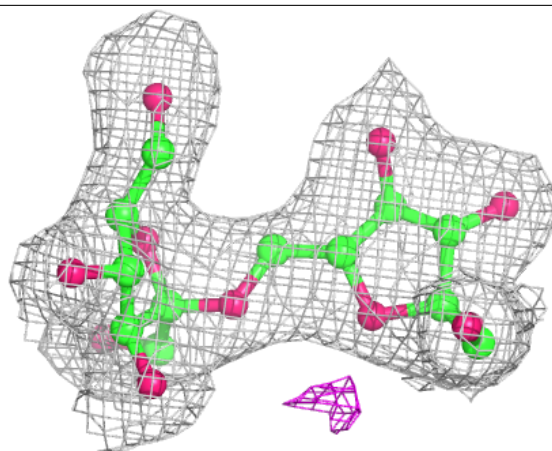
Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
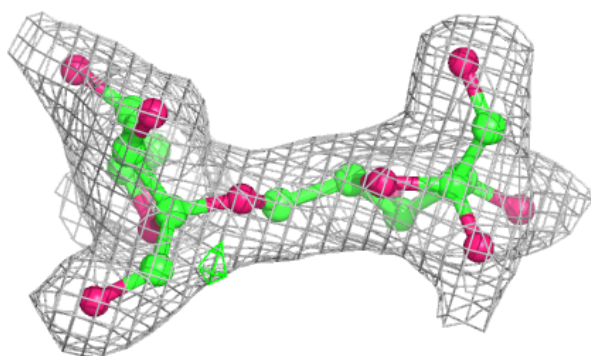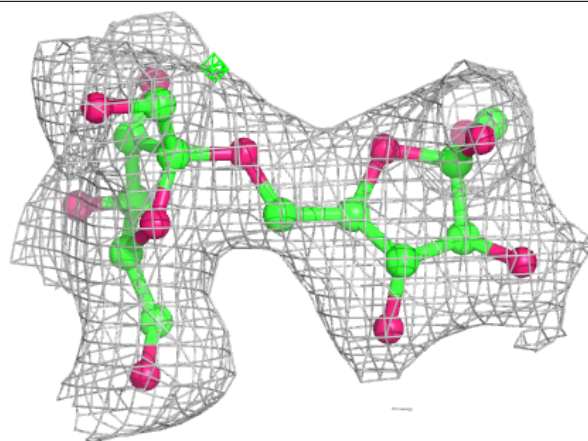
Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
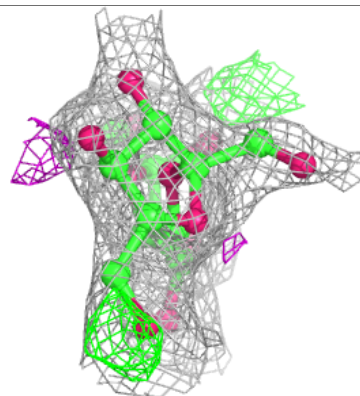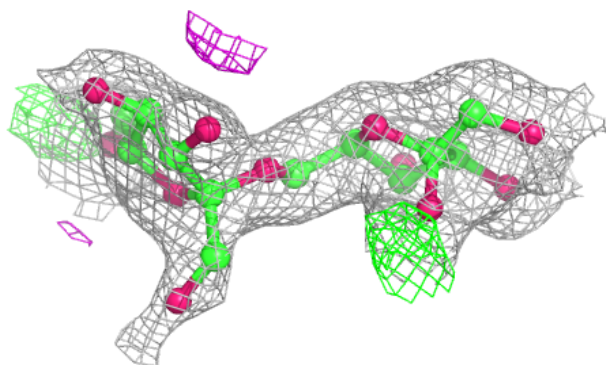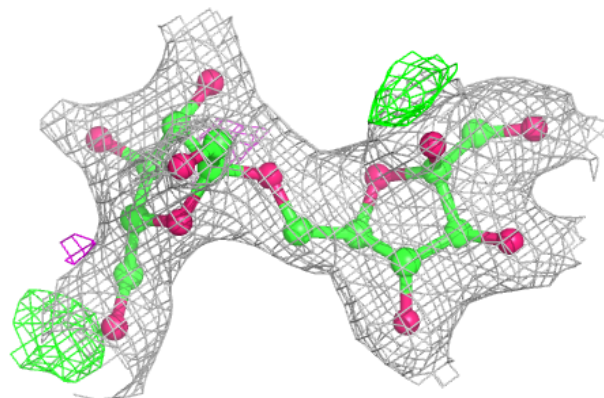
Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
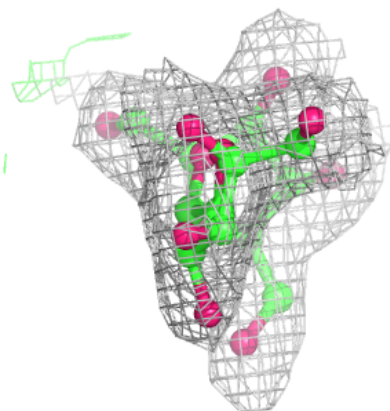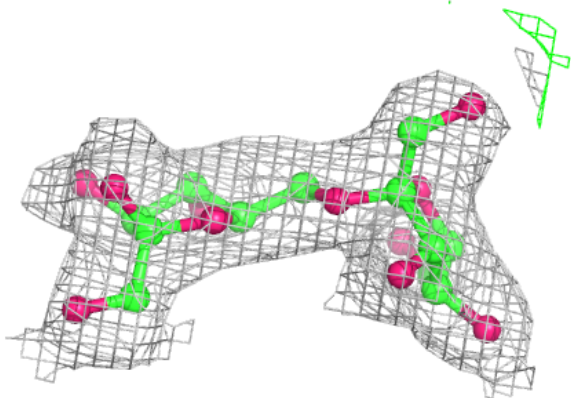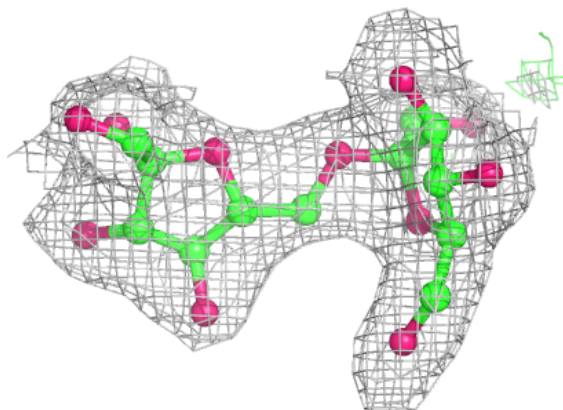
Electron density around Chain I:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
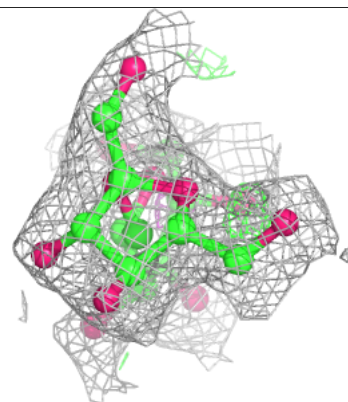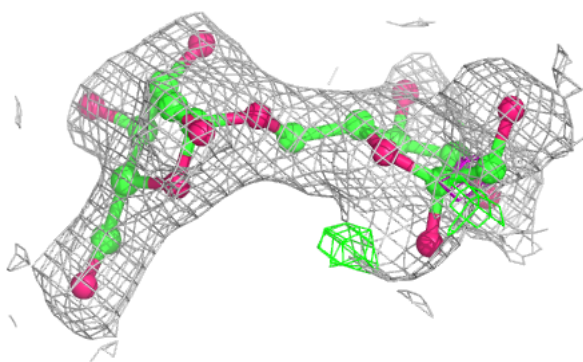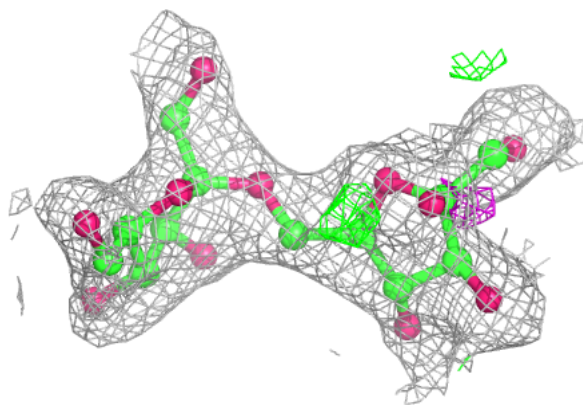
Electron density around Chain J:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
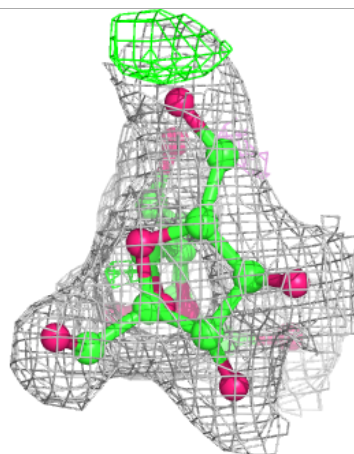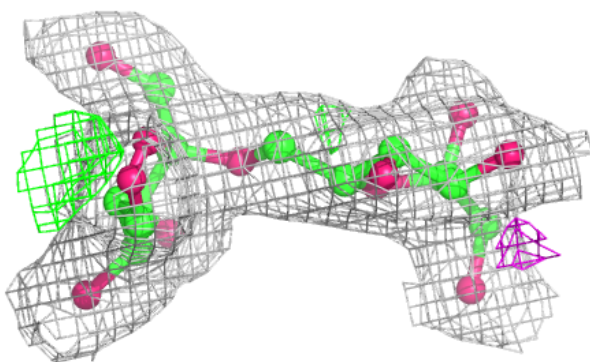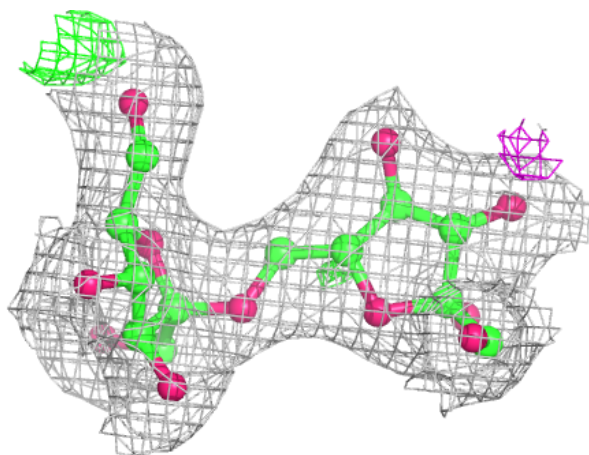
Electron density around Chain K:

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

Electron density around Chain L:

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

Electron density around Chain M:

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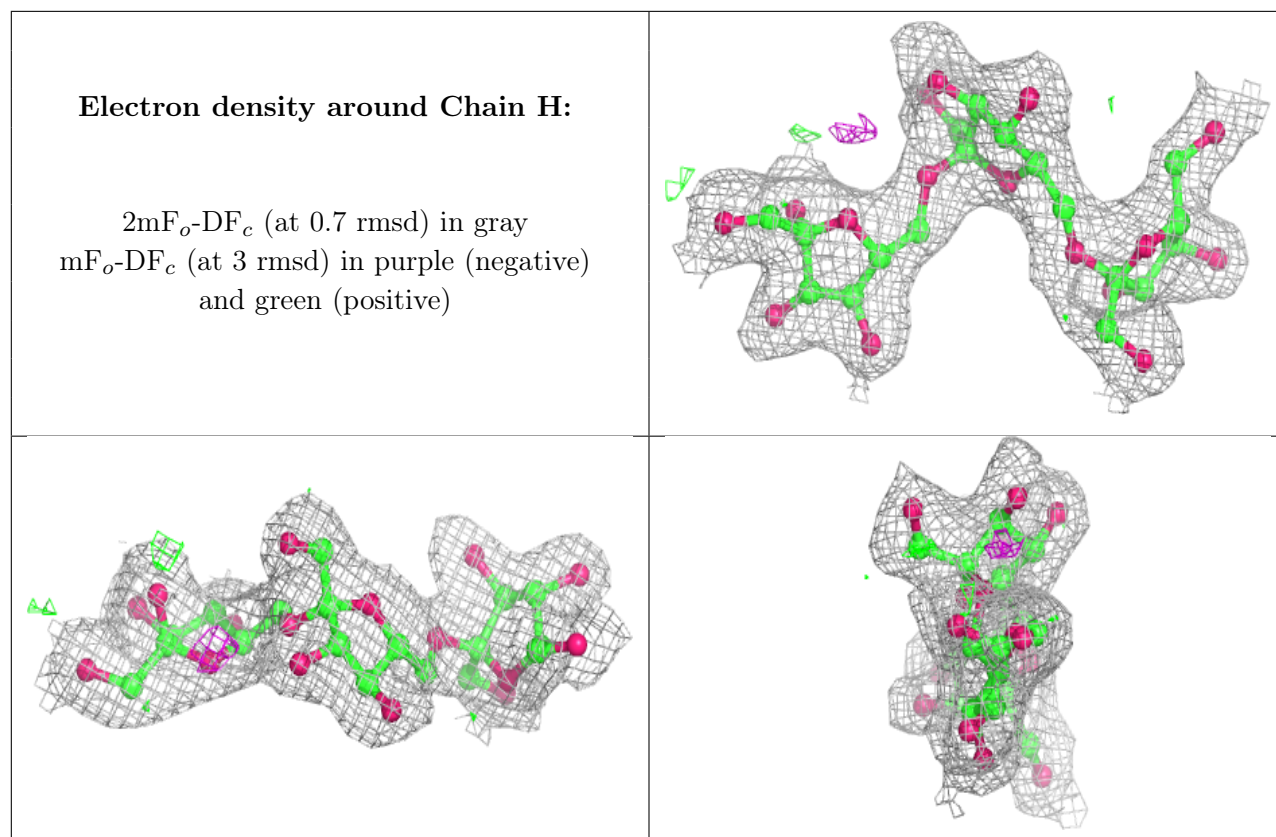mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
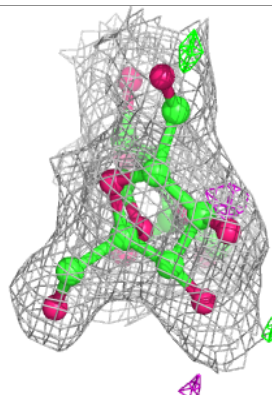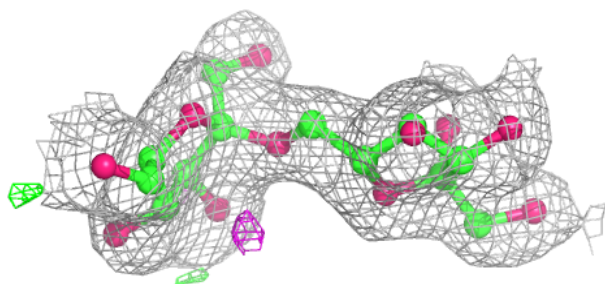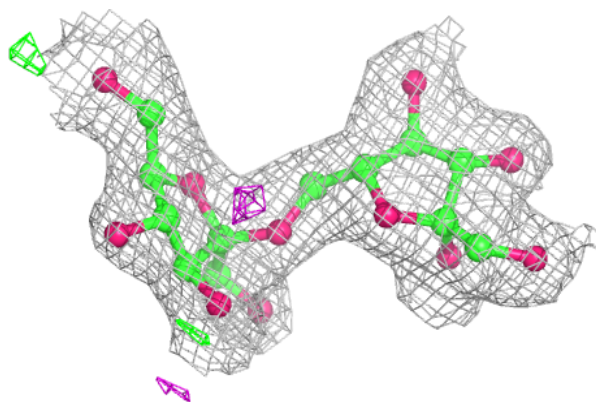
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.