



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:28 AM UTC

PDB ID : 7ZNR / pdb_00007znr
Title : Inactive D62N mutant of BT1760 Endo-acting levanase from *Bacteroides thetaiotaomicron* VPI-5482
Authors : Basle, A.; Bolam, D.
Deposited on : 2022-04-21
Resolution : 2.65 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

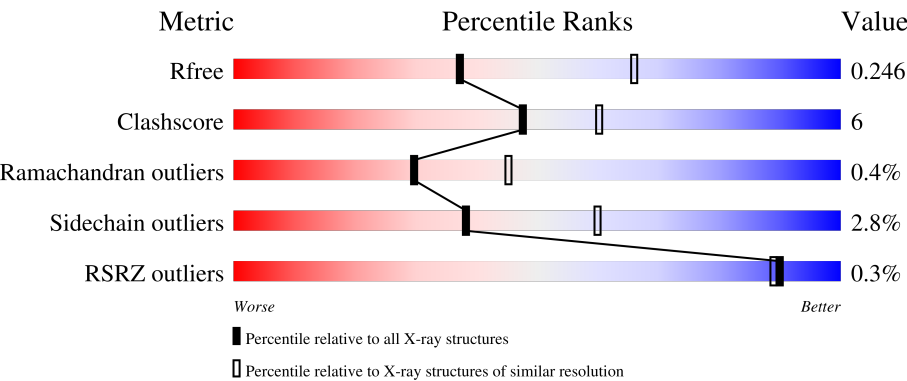
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



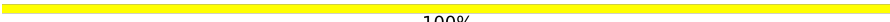
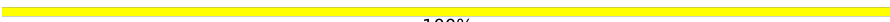
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	523	80%12%• 7%
1	B	523	76%15%• 7%
2	C	5	40%60%
2	D	5	60%40%
2	E	5	60%40%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
4	G	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	E	3	X	-	-	-
2	FRU	E	5	X	-	-	-
4	FRU	G	1	X	-	-	-
4	FRU	G	2	X	-	-	-
5	SO4	B	604	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15118 atoms, of which 7029 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 Sucrose-6-phosphate hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	S	0	0	0
			7327	2476	3427	645	759	20			
1	B	487	Total	C	H	N	O	S	0	0	0
			7327	2476	3427	645	759	20			

There are 2 discrepancies between the modelled and reference sequences:

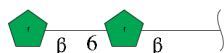
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASN	ASP	engineered mutation	UNP A0A0P0F2Q3
B	42	ASN	ASP	engineered mutation	UNP A0A0P0F2Q3

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



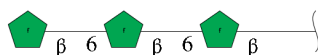
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	H	O	0	0	0
			100	30	44	26			
2	D	5	Total	C	H	O	0	0	0
			100	30	44	26			
2	E	5	Total	C	H	O	0	0	0
			100	30	44	26			

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



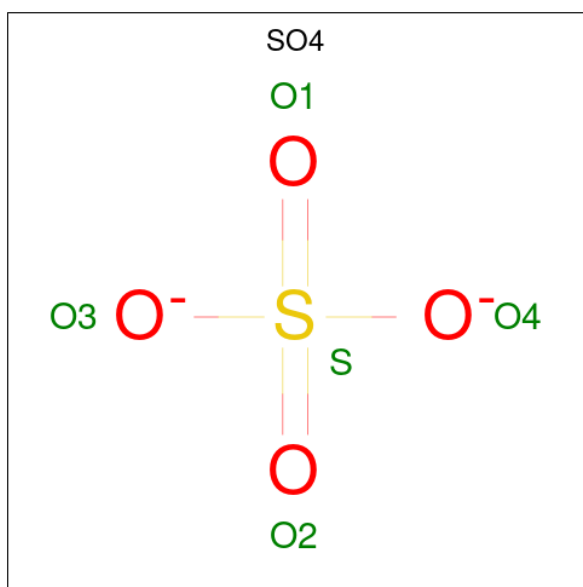
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	H	O	0	0	0
			40	12	17	11			

- Molecule 4 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	H	O	0	0	0
			59	18	26	15			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

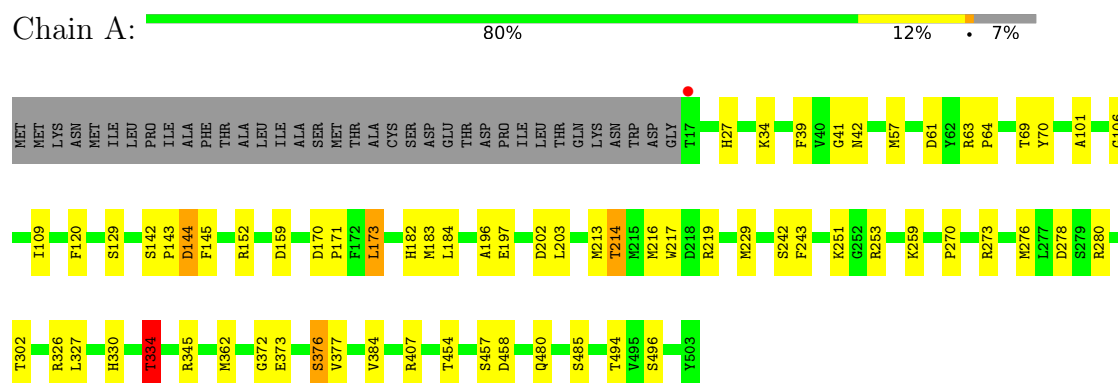
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	1	Total O 1 1	0	0

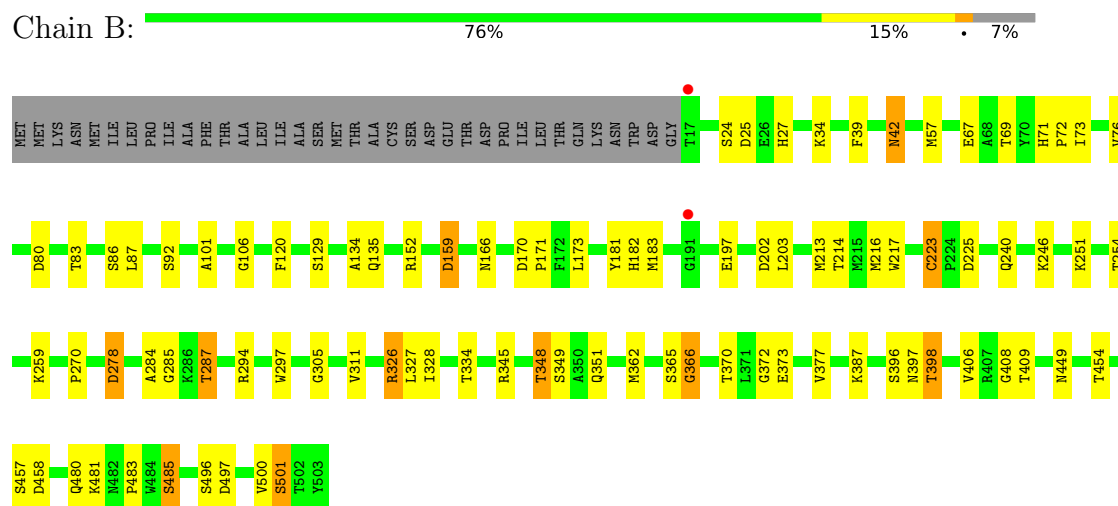
3 Residue-property plots [i](#)

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

- Molecule 1: Sucrose-6-phosphate hydrolase



- Molecule 1: Sucrose-6-phosphate hydrolase



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

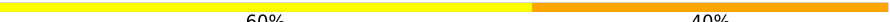


- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain D:  60% 40%

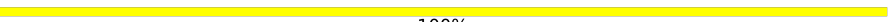
FRU1
FRU2
FRU3
FRU4
FRU5

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

Chain E:  60% 40%

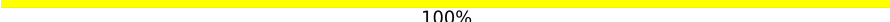
FRU1
FRU2
FRU3
FRU4
FRU5

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

Chain F:  100%

FRU1
FRU2

- Molecule 4: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain G:  100%

FRU1
FRU2
FRU3

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.72Å 174.72Å 215.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.87 – 2.65 67.87 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (67.87-2.65) 99.9 (67.87-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0352, REFMAC 5.8.0352	Depositor
R, R_{free}	0.191 , 0.246 0.191 , 0.246	Depositor DCC
R_{free} test set	2381 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15118	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: SO4, 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	0.67	0/4006	1.17	12/5431 (0.2%)
1	B	0.63	0/4006	1.12	12/5431 (0.2%)
All	All	0.65	0/8012	1.15	24/10862 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	THR	CA-CB-OG1	-10.71	93.53	109.60
1	A	278	ASP	CA-CB-CG	9.42	122.02	112.60
1	B	278	ASP	CA-CB-CG	9.39	121.99	112.60
1	B	480	GLN	CB-CA-C	-8.60	95.45	109.72
1	B	409	THR	CA-CB-OG1	-6.92	99.22	109.60
1	B	454	THR	CB-CA-C	6.87	121.47	109.80
1	A	454	THR	CB-CA-C	6.47	120.80	109.80
1	A	214	THR	CB-CA-C	6.34	121.12	109.46
1	A	458	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	159	ASP	N-CA-CB	-6.00	100.35	110.49
1	A	144	ASP	CA-C-N	-5.98	113.62	122.83
1	A	144	ASP	C-N-CA	-5.98	113.62	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	THR	CA-CB-OG1	-5.98	100.63	109.60
1	A	334	THR	CB-CA-C	5.69	119.24	109.51
1	B	348	THR	CA-CB-OG1	-5.65	101.13	109.60
1	B	458	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	214	THR	CA-CB-OG1	-5.55	101.27	109.60
1	B	370	THR	CB-CA-C	5.47	119.72	109.71
1	B	25	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	159	ASP	N-CA-CB	-5.41	101.35	110.49
1	B	223	CYS	CB-CA-C	-5.37	107.39	111.20
1	A	57	MET	N-CA-C	-5.09	103.81	110.53
1	A	145	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	80	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	345	ARG	Sidechain
1	B	152	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	345	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3900	3427	3665	35	0
1	B	3900	3427	3665	49	0
2	C	56	44	52	6	0
2	D	56	44	52	4	0
2	E	56	44	52	2	0
3	F	23	17	22	0	0
4	G	33	26	30	0	0
5	A	30	0	0	0	0
5	B	30	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	0	0	0
6	B	1	0	0	0	0
All	All	8089	7029	7538	87	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (87) 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:42:ASN:HD21	2:D:3:FRU:H11	1.43	0.84
1:A:253:ARG:HH11	1:A:253:ARG:HG2	1.45	0.79
1:B:287:THR:HG23	1:B:294:ARG:HH11	1.48	0.78
1:B:397:ASN:OD1	1:B:449:ASN:ND2	2.18	0.77
1:A:219:ARG:HH21	2:E:3:FRU:H4	1.60	0.66
1:A:109:ILE:CG2	1:A:173:LEU:HD23	2.26	0.66
1:A:242:SER:O	1:A:280:ARG:NH2	2.29	0.65
1:B:42:ASN:HD21	2:D:3:FRU:C1	2.09	0.65
1:A:253:ARG:HG2	1:A:253:ARG:NH1	2.11	0.65
1:B:254:THR:HA	5:B:601:SO4:O4	1.97	0.64
1:A:63:ARG:NH2	1:A:302:THR:OG1	2.30	0.64
1:B:120:PHE:CD1	1:B:173:LEU:HD11	2.33	0.64
1:B:294:ARG:HG2	1:B:327:LEU:HD22	1.80	0.64
1:A:142:SER:OG	1:A:144:ASP:O	2.14	0.64
1:B:396:SER:OG	1:B:398:THR:HG23	2.03	0.59
1:B:225:ASP:OD2	1:B:287:THR:HB	2.03	0.58
1:A:229:MET:HE1	1:A:327:LEU:HD23	1.86	0.58
2:C:2:FRU:H61	2:C:3:FRU:C6	2.33	0.58
1:B:287:THR:CG2	1:B:294:ARG:HH11	2.15	0.57
1:A:61:ASP:OD2	1:A:63:ARG:NH1	2.37	0.56
1:A:330:HIS:HB2	1:A:334:THR:HG22	1.88	0.56
2:C:2:FRU:H61	2:C:3:FRU:H62	1.88	0.55
1:A:106:GLY:HA3	1:A:120:PHE:O	2.08	0.54
1:B:326:ARG:HH12	1:B:328:ILE:CD1	2.21	0.52
1:B:311:VAL:HG12	1:B:311:VAL:O	2.09	0.52
1:A:109:ILE:HG22	1:A:173:LEU:HD23	1.92	0.52
1:A:109:ILE:HG21	1:A:173:LEU:HD23	1.93	0.51
1:B:69:THR:HA	1:B:101:ALA:O	2.10	0.51
1:A:251:LYS:HG2	1:A:270:PRO:HB3	1.92	0.51
1:B:305:GLY:N	5:B:604:SO4:O4	2.36	0.51
1:B:351:GLN:HB2	1:B:500:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASN:HD21	2:C:3:FRU:H11	1.77	0.49
1:B:408:GLY:HA2	1:B:483:PRO:HG2	1.93	0.49
1:B:106:GLY:HA3	1:B:120:PHE:O	2.13	0.49
1:B:246:LYS:HE3	1:B:278:ASP:O	2.12	0.48
1:A:69:THR:HA	1:A:101:ALA:O	2.13	0.48
1:B:120:PHE:CD2	1:B:183:MET:HE1	2.48	0.48
1:B:182:HIS:HD2	1:B:197:GLU:OE2	1.97	0.48
1:B:213:MET:HG2	1:B:259:LYS:HA	1.96	0.47
1:B:76:VAL:HG12	1:B:86:SER:HA	1.96	0.47
1:A:120:PHE:CD2	1:A:183:MET:HE1	2.50	0.47
1:B:216:MET:O	1:B:217:TRP:C	2.57	0.46
1:B:27:HIS:O	1:B:34:LYS:NZ	2.44	0.46
1:A:27:HIS:O	1:A:34:LYS:NZ	2.44	0.46
1:A:63:ARG:HA	1:A:64:PRO:HA	1.79	0.46
1:B:181:TYR:CD2	1:B:203:LEU:HD21	2.49	0.46
1:B:311:VAL:O	1:B:311:VAL:CG1	2.64	0.46
1:B:287:THR:CG2	1:B:294:ARG:HD2	2.46	0.45
1:B:251:LYS:HG2	1:B:270:PRO:HB3	1.99	0.45
1:B:202:ASP:O	1:B:203:LEU:HB2	2.16	0.45
1:A:182:HIS:HD2	1:A:197:GLU:OE2	1.99	0.45
1:B:42:ASN:OD1	1:B:223:CYS:SG	2.75	0.45
1:B:351:GLN:HB2	1:B:500:VAL:HG23	1.97	0.45
1:A:202:ASP:O	1:A:203:LEU:HB2	2.15	0.45
1:A:213:MET:HG2	1:A:259:LYS:HA	1.97	0.45
1:B:377:VAL:O	1:B:485:SER:HA	2.17	0.45
1:B:135:GLN:HE22	2:D:1:FRU:H11	1.82	0.45
1:A:376:SER:OG	1:A:407:ARG:NH1	2.50	0.44
1:A:377:VAL:O	1:A:485:SER:HA	2.18	0.44
1:A:384:VAL:HA	1:A:480:GLN:HB2	1.98	0.44
1:A:216:MET:O	1:A:217:TRP:C	2.61	0.44
1:A:42:ASN:HD21	2:C:3:FRU:C1	2.31	0.43
1:B:285:GLY:HA2	1:B:297:TRP:O	2.19	0.43
1:B:387:LYS:O	1:B:500:VAL:HA	2.18	0.43
1:A:41:GLY:O	1:A:42:ASN:C	2.62	0.43
1:B:406:VAL:HG12	1:B:406:VAL:O	2.19	0.43
1:A:372:GLY:O	1:A:373:GLU:C	2.62	0.43
1:A:70:TYR:CE2	2:C:4:FRU:H11	2.54	0.43
1:B:349:SER:O	1:B:501:SER:HA	2.18	0.42
1:A:170:ASP:N	1:A:171:PRO:CD	2.82	0.42
1:A:273:ARG:O	1:A:276:MET:HE2	2.18	0.42
1:B:134:ALA:HB3	1:B:166:ASN:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLY:O	1:B:373:GLU:C	2.61	0.42
1:A:243:PHE:HB2	2:E:5:FRU:H4	2.02	0.42
1:B:170:ASP:N	1:B:171:PRO:CD	2.82	0.42
1:B:365:SER:O	1:B:366:GLY:C	2.63	0.42
1:B:71:HIS:N	1:B:72:PRO:CD	2.83	0.41
1:A:184:LEU:HA	1:A:196:ALA:O	2.21	0.41
1:B:240:GLN:NE2	2:D:1:FRU:H61	2.36	0.41
1:B:216:MET:HE3	1:B:216:MET:HB3	1.98	0.41
1:B:57:MET:HB3	1:B:73:ILE:HG23	2.03	0.41
1:B:86:SER:C	1:B:87:LEU:HD12	2.46	0.41
1:A:34:LYS:HE2	1:A:39:PHE:CE2	2.55	0.41
1:B:34:LYS:HE2	1:B:39:PHE:CE2	2.56	0.41
1:B:42:ASN:OD1	1:B:284:ALA:HB1	2.21	0.40
1:B:481:LYS:HE3	5:B:606:SO4:O3	2.22	0.40
2:C:2:FRU:C6	2:C:3:FRU:H62	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:604:SO4:O1	5:B:604:SO4:O4[7_455]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	485/523 (93%)	449 (93%)	35 (7%)	1 (0%)	43	60
1	B	485/523 (93%)	448 (92%)	34 (7%)	3 (1%)	21	34
All	All	970/1046 (93%)	897 (92%)	69 (7%)	4 (0%)	30	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	SER
1	B	159	ASP
1	A	143	PRO
1	B	366	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/444 (93%)	405 (98%)	8 (2%)	50	71
1	B	413/444 (93%)	398 (96%)	15 (4%)	31	51
All	All	826/888 (93%)	803 (97%)	23 (3%)	38	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	SER
1	A	173	LEU
1	A	214	THR
1	A	334	THR
1	A	362	MET
1	A	376	SER
1	A	457	SER
1	A	496	SER
1	B	24	SER
1	B	42	ASN
1	B	67	GLU
1	B	83	THR
1	B	92	SER
1	B	287	THR
1	B	334	THR
1	B	348	THR
1	B	362	MET
1	B	398	THR
1	B	457	SER
1	B	485	SER

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Mol	Chain	Res	Type
1	B	496	SER
1	B	497	ASP
1	B	501	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	182	HIS
1	A	272	ASN
1	A	306	ASN
1	A	474	ASN
1	B	42	ASN
1	B	182	HIS
1	B	194	HIS
1	B	272	ASN
1	B	293	ASN
1	B	306	ASN
1	B	351	GLN
1	B	449	ASN
1	B	474	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FRU	C	1	2	11,12,12	1.67	2 (18%)	10,18,18	1.89	3 (30%)
2	FRU	C	2	2	11,11,12	0.87	0	15,15,18	2.03	3 (20%)
2	FRU	C	3	2	11,11,12	0.51	0	15,15,18	1.25	1 (6%)
2	FRU	C	4	2	11,11,12	1.11	1 (9%)	15,15,18	1.29	1 (6%)
2	FRU	C	5	2	11,11,12	1.15	0	15,15,18	2.21	7 (46%)
2	FRU	D	1	2	11,12,12	0.74	0	10,18,18	1.25	1 (10%)
2	FRU	D	2	2	11,11,12	0.56	0	15,15,18	1.38	2 (13%)
2	FRU	D	3	2	11,11,12	0.61	0	15,15,18	1.22	2 (13%)
2	FRU	D	4	2	11,11,12	0.96	0	15,15,18	1.40	2 (13%)
2	FRU	D	5	2	11,11,12	1.49	2 (18%)	15,15,18	2.41	6 (40%)
2	FRU	E	1	2	11,12,12	1.28	2 (18%)	10,18,18	1.39	2 (20%)
2	FRU	E	2	2	11,11,12	1.38	1 (9%)	15,15,18	3.37	10 (66%)
2	FRU	E	3	2	11,11,12	1.13	0	15,15,18	2.79	7 (46%)
2	FRU	E	4	2	11,11,12	0.44	0	15,15,18	1.34	2 (13%)
2	FRU	E	5	2	11,11,12	0.72	0	15,15,18	1.66	3 (20%)
3	FRU	F	1	3	11,12,12	1.73	3 (27%)	10,18,18	1.68	2 (20%)
3	FRU	F	2	3	11,11,12	1.05	1 (9%)	15,15,18	3.21	7 (46%)
4	FRU	G	1	4	11,11,12	1.31	3 (27%)	15,15,18	3.81	11 (73%)
4	FRU	G	2	4	11,11,12	1.06	1 (9%)	15,15,18	2.06	5 (33%)
4	FRU	G	3	4	11,11,12	1.27	1 (9%)	15,15,18	1.78	4 (26%)

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	C	1	2	-	3/5/24/24	0/1/1/1
2	FRU	C	2	2	-	1/4/20/24	0/1/1/1
2	FRU	C	3	2	-	2/4/20/24	0/1/1/1
2	FRU	C	4	2	-	1/4/20/24	0/1/1/1
2	FRU	C	5	2	-	0/4/20/24	0/1/1/1
2	FRU	D	1	2	-	3/5/24/24	0/1/1/1
2	FRU	D	2	2	-	2/4/20/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	D	3	2	-	2/4/20/24	0/1/1/1
2	FRU	D	4	2	-	2/4/20/24	0/1/1/1
2	FRU	D	5	2	-	3/4/20/24	0/1/1/1
2	FRU	E	1	2	-	5/5/24/24	0/1/1/1
2	FRU	E	2	2	-	3/4/20/24	0/1/1/1
2	FRU	E	3	2	1/1/4/4	2/4/20/24	0/1/1/1
2	FRU	E	4	2	-	0/4/20/24	0/1/1/1
2	FRU	E	5	2	1/1/4/4	4/4/20/24	0/1/1/1
3	FRU	F	1	3	-	3/5/24/24	0/1/1/1
3	FRU	F	2	3	-	1/4/20/24	0/1/1/1
4	FRU	G	1	4	1/1/4/4	4/4/20/24	0/1/1/1
4	FRU	G	2	4	1/1/4/4	4/4/20/24	0/1/1/1
4	FRU	G	3	4	-	4/4/20/24	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	FRU	O2-C2	3.95	1.47	1.40
3	F	1	FRU	O5-C2	3.68	1.49	1.43
2	D	5	FRU	C4-C5	3.14	1.61	1.53
3	F	1	FRU	C4-C5	2.72	1.59	1.53
4	G	3	FRU	C1-C2	2.70	1.60	1.51
2	D	5	FRU	C6-C5	2.61	1.60	1.51
4	G	1	FRU	C3-C2	2.33	1.58	1.53
3	F	2	FRU	C4-C5	2.27	1.58	1.53
2	E	2	FRU	C1-C2	2.26	1.59	1.51
4	G	1	FRU	C1-C2	2.25	1.59	1.51
4	G	1	FRU	O6-C6	2.17	1.51	1.42
4	G	2	FRU	C3-C2	2.14	1.58	1.53
3	F	1	FRU	O4-C4	2.12	1.48	1.43
2	E	1	FRU	O2-C2	2.11	1.44	1.40
2	C	4	FRU	O5-C5	-2.09	1.40	1.45
2	E	1	FRU	C1-C2	2.03	1.57	1.52
2	C	1	FRU	C4-C5	2.02	1.58	1.53

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	FRU	O5-C2-C1	-7.22	93.96	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	FRU	C1-C2-C3	6.65	130.80	115.10
4	G	1	FRU	O5-C5-C6	6.54	123.04	109.22
2	E	2	FRU	O5-C2-C1	5.98	121.86	109.22
4	G	1	FRU	O5-C2-C1	5.87	121.64	109.22
2	E	2	FRU	O5-C2-C3	-5.82	93.60	105.15
2	C	5	FRU	C1-C2-C3	-5.42	102.30	115.10
2	C	2	FRU	O5-C2-C1	-5.39	97.83	109.22
4	G	1	FRU	C3-C4-C5	-5.32	92.33	102.61
2	E	3	FRU	O4-C4-C3	-4.74	96.62	111.82
2	D	5	FRU	C6-C5-C4	4.67	126.12	115.10
3	F	2	FRU	O4-C4-C5	4.61	124.33	111.08
2	E	2	FRU	O3-C3-C2	4.53	124.08	111.08
2	E	5	FRU	C1-C2-C3	-4.51	104.44	115.10
3	F	2	FRU	O4-C4-C3	-4.35	97.87	111.82
2	E	3	FRU	C3-C4-C5	4.32	110.95	102.61
2	E	2	FRU	O4-C4-C5	4.27	123.34	111.08
2	E	3	FRU	O3-C3-C2	4.24	123.27	111.08
3	F	2	FRU	C6-C5-C4	4.22	125.05	115.10
3	F	2	FRU	O5-C5-C6	-4.15	100.44	109.22
4	G	3	FRU	O1-C1-C2	4.09	125.26	111.33
2	C	1	FRU	O4-C4-C5	3.96	122.47	111.08
2	E	3	FRU	O5-C5-C6	3.93	117.52	109.22
4	G	2	FRU	O5-C5-C6	-3.90	100.97	109.22
2	C	2	FRU	O5-C5-C6	-3.88	101.02	109.22
2	E	3	FRU	C4-C3-C2	-3.86	95.15	102.61
4	G	1	FRU	O5-C5-C4	-3.83	97.56	105.15
2	D	5	FRU	O4-C4-C5	3.72	121.78	111.08
2	D	5	FRU	O4-C4-C3	-3.72	99.90	111.82
4	G	1	FRU	C6-C5-C4	3.69	123.80	115.10
2	D	2	FRU	O5-C2-C1	3.68	116.99	109.22
2	E	2	FRU	O6-C6-C5	3.56	123.47	111.33
3	F	1	FRU	O4-C4-C5	3.50	121.13	111.08
2	E	2	FRU	O3-C3-C4	-3.41	100.87	111.82
2	C	4	FRU	C3-C4-C5	3.38	109.14	102.61
2	E	4	FRU	O1-C1-C2	-3.30	100.09	111.33
4	G	1	FRU	O3-C3-C2	3.27	120.48	111.08
4	G	2	FRU	O3-C3-C2	3.21	120.29	111.08
4	G	1	FRU	O5-C2-C3	-3.17	98.87	105.15
2	D	5	FRU	C3-C4-C5	3.14	108.68	102.61
2	C	3	FRU	O5-C5-C6	-3.11	102.64	109.22
2	E	3	FRU	O5-C2-C3	3.03	111.18	105.15
2	C	1	FRU	O5-C5-C6	-2.95	100.85	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	FRU	O5-C5-C4	-2.88	99.43	105.15
2	E	3	FRU	O1-C1-C2	-2.78	101.86	111.33
2	C	2	FRU	O3-C3-C2	2.76	119.00	111.08
4	G	2	FRU	C1-C2-C3	-2.75	108.60	115.10
4	G	2	FRU	O5-C2-C3	-2.71	99.77	105.15
2	D	4	FRU	O5-C2-C1	-2.69	103.52	109.22
2	E	1	FRU	O1-C1-C2	2.66	117.55	111.67
2	E	2	FRU	C6-C5-C4	2.65	121.35	115.10
3	F	2	FRU	O3-C3-C2	2.64	118.66	111.08
2	D	4	FRU	C3-C4-C5	2.62	107.67	102.61
4	G	3	FRU	C3-C4-C5	2.61	107.65	102.61
2	C	5	FRU	O4-C4-C3	-2.57	103.58	111.82
2	D	3	FRU	O3-C3-C4	2.57	120.06	111.82
3	F	2	FRU	C1-C2-C3	-2.54	109.10	115.10
2	E	2	FRU	O1-C1-C2	2.50	119.85	111.33
3	F	1	FRU	O4-C4-C3	-2.50	104.67	112.16
2	C	5	FRU	O3-C3-C4	2.47	119.74	111.82
2	E	5	FRU	O3-C3-C2	2.47	118.18	111.08
4	G	3	FRU	O5-C2-C1	2.46	114.41	109.22
2	D	5	FRU	O6-C6-C5	2.46	119.69	111.33
2	E	4	FRU	C1-C2-C3	-2.45	109.31	115.10
2	D	5	FRU	O5-C5-C4	-2.45	100.30	105.15
2	C	1	FRU	O2-C2-O5	-2.44	104.63	109.33
2	D	1	FRU	O2-C2-O5	-2.44	104.64	109.33
2	D	2	FRU	O3-C3-C2	2.27	117.59	111.08
4	G	1	FRU	O6-C6-C5	-2.24	103.71	111.33
4	G	2	FRU	C6-C5-C4	2.23	120.37	115.10
2	C	5	FRU	O4-C4-C5	2.23	117.49	111.08
2	E	2	FRU	C1-C2-C3	2.23	120.36	115.10
4	G	1	FRU	O1-C1-C2	2.22	118.91	111.33
4	G	1	FRU	O4-C4-C5	2.20	117.41	111.08
2	D	3	FRU	O1-C1-C2	-2.20	103.86	111.33
2	C	5	FRU	C6-C5-C4	2.19	120.27	115.10
2	E	1	FRU	O2-C2-O5	-2.18	105.14	109.33
2	C	5	FRU	O5-C5-C6	2.16	113.78	109.22
4	G	3	FRU	O3-C3-C2	2.13	117.20	111.08
2	E	5	FRU	O5-C2-C3	2.05	109.22	105.15
2	C	5	FRU	C3-C4-C5	2.01	106.49	102.61

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
2	E	3	FRU	C2
2	E	5	FRU	C2
4	G	1	FRU	C2
4	G	2	FRU	C2

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	FRU	O1-C1-C2-C3
2	C	1	FRU	O1-C1-C2-O2
2	C	1	FRU	O1-C1-C2-O5
2	D	1	FRU	O1-C1-C2-C3
2	D	1	FRU	O1-C1-C2-O2
2	D	1	FRU	O1-C1-C2-O5
2	E	1	FRU	O1-C1-C2-C3
2	E	1	FRU	O1-C1-C2-O2
2	E	2	FRU	O1-C1-C2-C3
2	E	2	FRU	O1-C1-C2-O5
3	F	1	FRU	O1-C1-C2-O2
4	G	1	FRU	O1-C1-C2-O5
4	G	1	FRU	O5-C5-C6-O6
2	E	3	FRU	O1-C1-C2-O5
4	G	1	FRU	C4-C5-C6-O6
2	D	3	FRU	O5-C5-C6-O6
2	E	1	FRU	O5-C5-C6-O6
4	G	2	FRU	O5-C5-C6-O6
4	G	3	FRU	O5-C5-C6-O6
2	D	3	FRU	C4-C5-C6-O6
2	E	3	FRU	O1-C1-C2-C3
4	G	1	FRU	O1-C1-C2-C3
4	G	2	FRU	O1-C1-C2-C3
4	G	2	FRU	C4-C5-C6-O6
4	G	3	FRU	C4-C5-C6-O6
2	E	5	FRU	O5-C5-C6-O6
2	E	5	FRU	C4-C5-C6-O6
2	D	5	FRU	O1-C1-C2-O5
2	D	4	FRU	C4-C5-C6-O6
2	D	2	FRU	O1-C1-C2-O5
2	E	1	FRU	C4-C5-C6-O6
2	D	2	FRU	O1-C1-C2-C3
2	D	5	FRU	O1-C1-C2-C3

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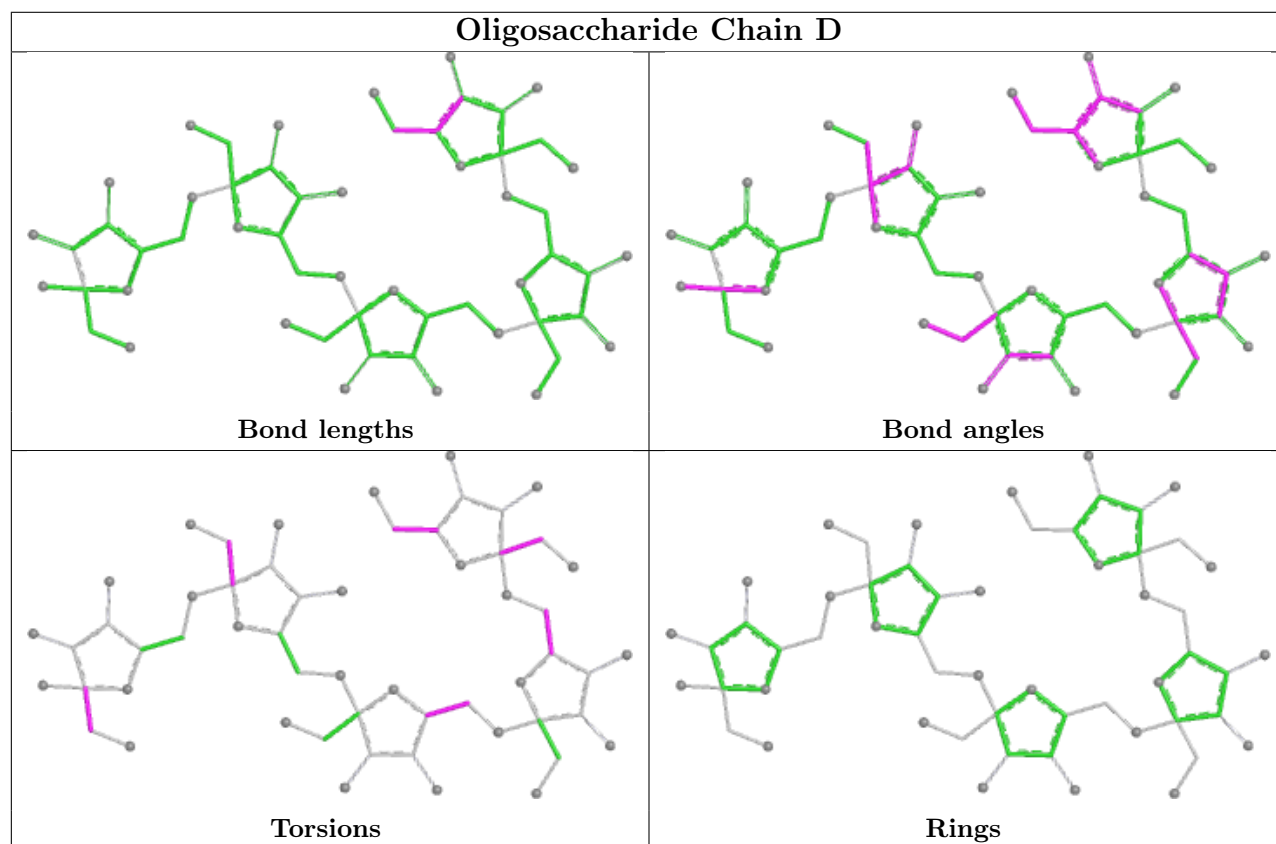
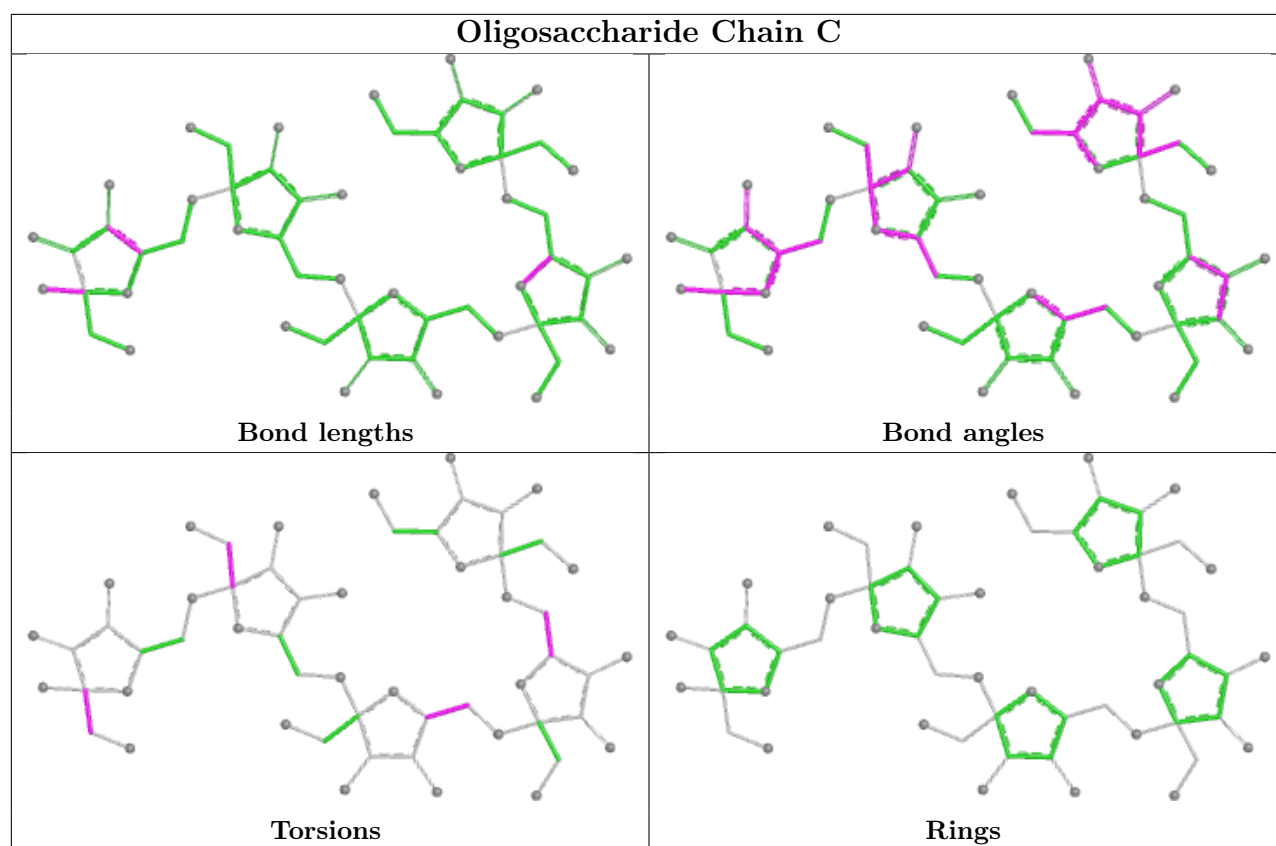
Mol	Chain	Res	Type	Atoms
2	D	4	FRU	O5-C5-C6-O6
4	G	3	FRU	O1-C1-C2-C3
4	G	3	FRU	O1-C1-C2-O5
2	E	5	FRU	O1-C1-C2-O5
3	F	1	FRU	O1-C1-C2-C3
4	G	2	FRU	O1-C1-C2-O5
2	E	1	FRU	O1-C1-C2-O5
3	F	1	FRU	O1-C1-C2-O5
2	E	5	FRU	O1-C1-C2-C3
2	E	2	FRU	O5-C5-C6-O6
2	C	2	FRU	O1-C1-C2-O5
3	F	2	FRU	O5-C5-C6-O6
2	D	5	FRU	C4-C5-C6-O6
2	C	3	FRU	C4-C5-C6-O6
2	C	3	FRU	O5-C5-C6-O6
2	C	4	FRU	O5-C5-C6-O6

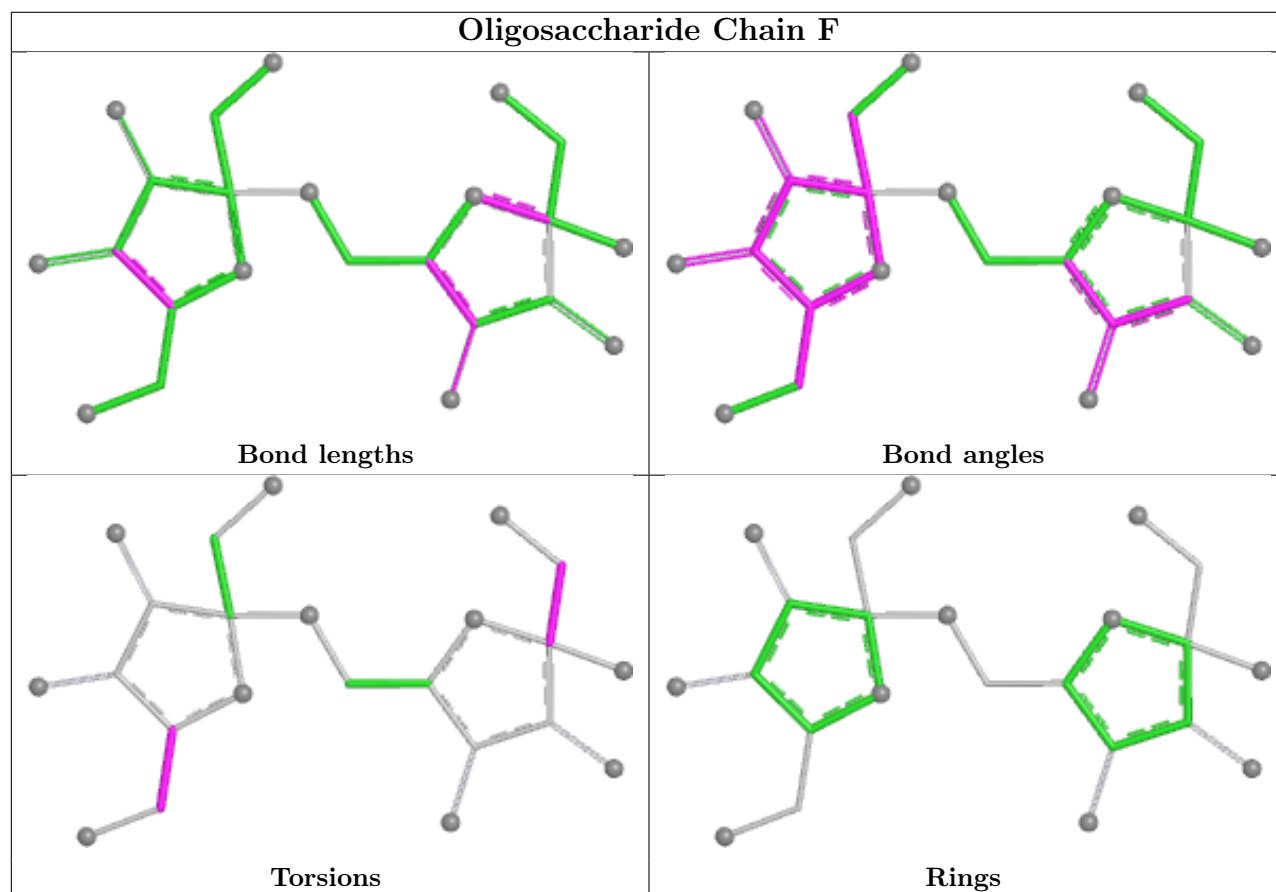
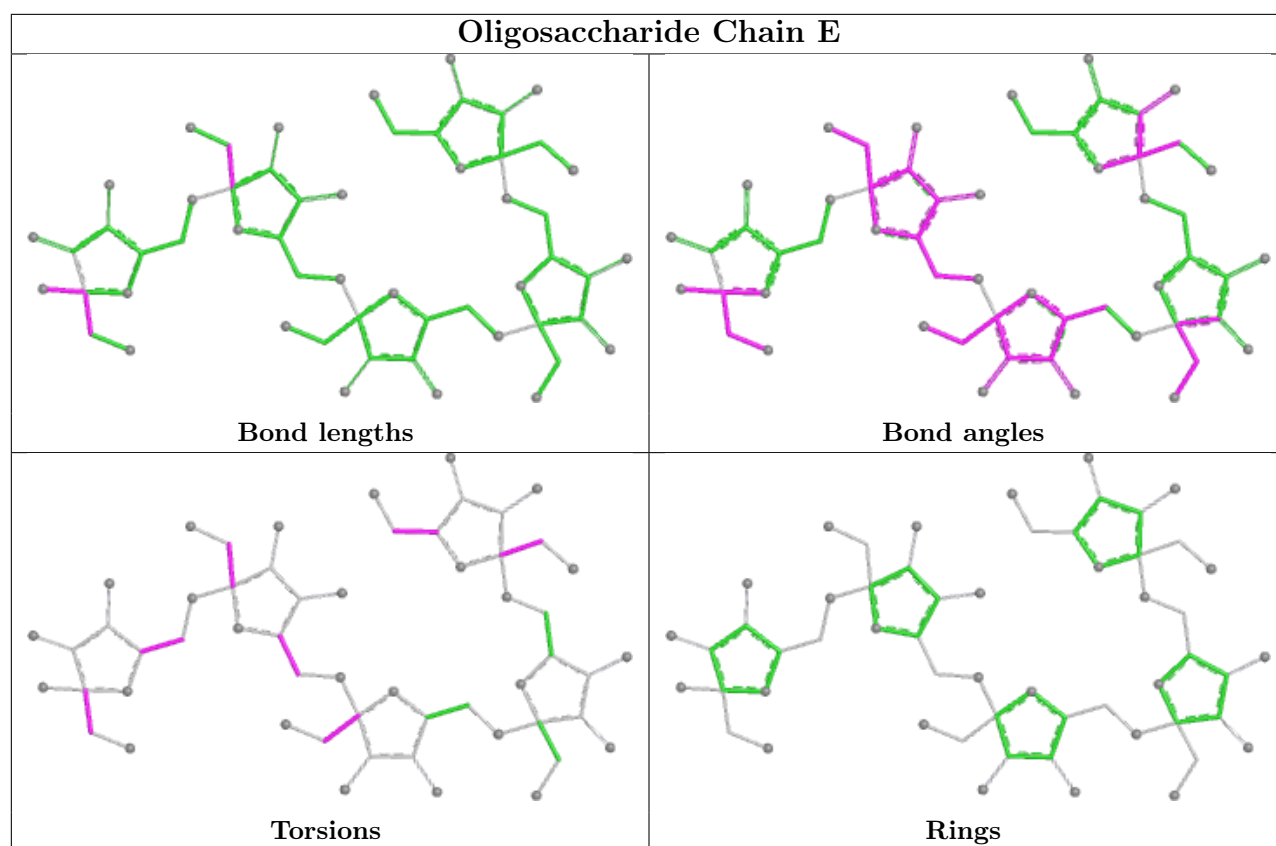
There are no ring outliers.

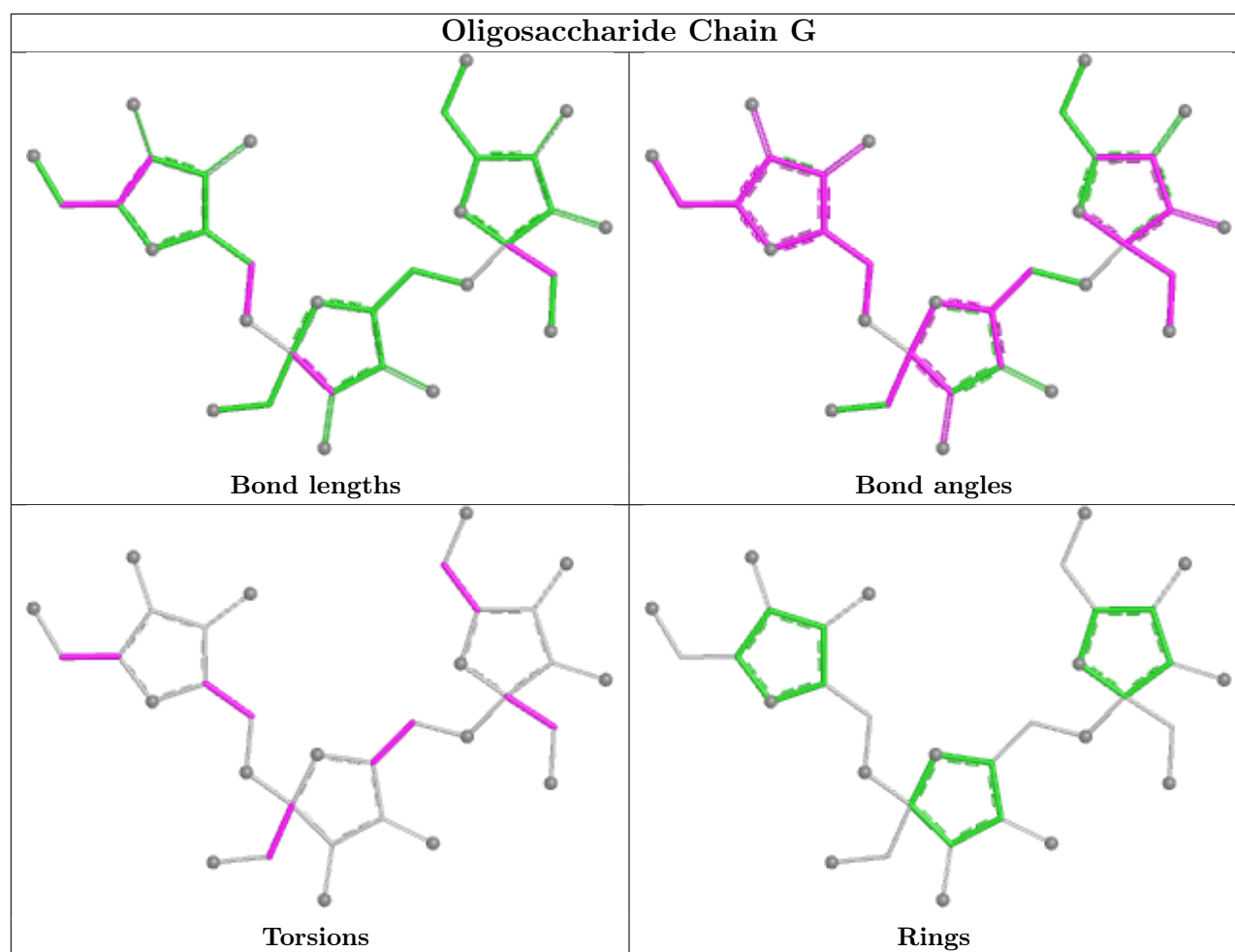
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	FRU	5	0
2	D	3	FRU	2	0
2	C	4	FRU	1	0
2	D	1	FRU	2	0
2	C	2	FRU	3	0
2	E	3	FRU	1	0
2	E	5	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.







5.6 Ligand geometry [i](#)

12 ligands 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	$\# Z > 2$
5	SO4	A	601	-	4,4,4	0.13	0	6,6,6	0.20	0
5	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.21	0
5	SO4	A	604	-	4,4,4	0.32	0	6,6,6	0.16	0
5	SO4	A	605	-	4,4,4	0.32	0	6,6,6	0.17	0
5	SO4	B	603	-	4,4,4	0.28	0	6,6,6	0.12	0
5	SO4	B	604	-	4,4,4	0.26	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	B	605	-	4,4,4	0.28	0	6,6,6	0.19	0
5	SO4	A	602	-	4,4,4	0.20	0	6,6,6	0.21	0
5	SO4	A	606	-	4,4,4	0.24	0	6,6,6	0.23	0
5	SO4	B	601	-	4,4,4	0.35	0	6,6,6	0.13	0
5	SO4	B	602	-	4,4,4	0.22	0	6,6,6	0.17	0
5	SO4	B	606	-	4,4,4	0.27	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	604	SO4	1	1
5	B	601	SO4	1	0
5	B	606	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	487/523 (93%)	-0.49	1 (0%) 91 90	34, 51, 76, 92	0
1	B	487/523 (93%)	-0.09	2 (0%) 88 87	46, 68, 94, 112	0
All	All	974/1046 (93%)	-0.29	3 (0%) 90 89	34, 61, 88, 112	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	GLY	2.4
1	A	17	THR	2.3
1	B	17	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FRU	G	1	11/12	0.74	0.20	60,84,97,103	0
2	FRU	E	1	12/12	0.76	0.16	89,108,114,131	0
4	FRU	G	3	11/12	0.79	0.16	74,105,116,119	0
2	FRU	E	2	11/12	0.81	0.13	70,105,115,120	0
2	FRU	D	5	11/12	0.84	0.15	54,68,79,86	0
3	FRU	F	2	11/12	0.84	0.13	59,72,88,89	0

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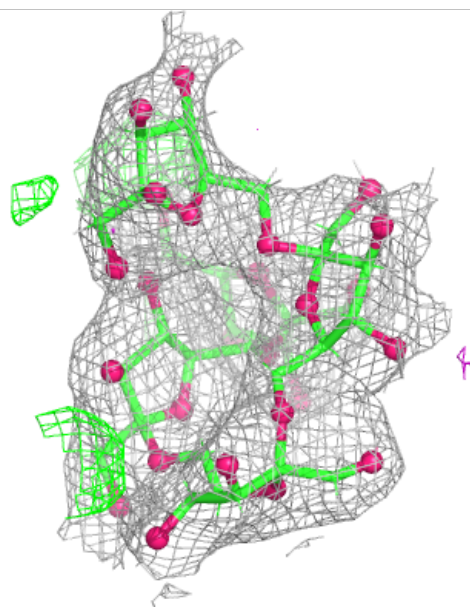
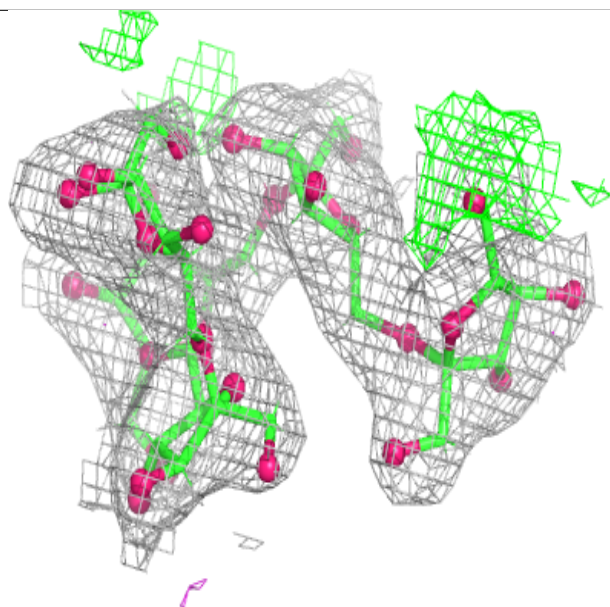
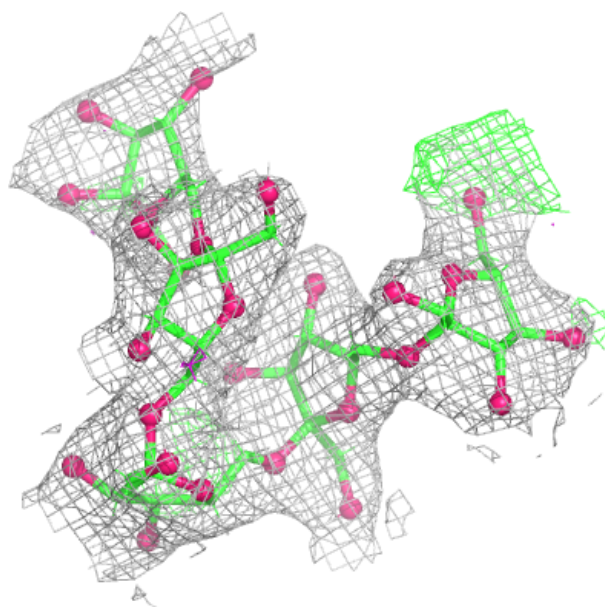
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FRU	C	1	12/12	0.86	0.15	77,89,97,100	0
2	FRU	D	1	12/12	0.87	0.12	68,106,114,120	0
3	FRU	F	1	12/12	0.89	0.14	65,84,102,123	0
2	FRU	C	5	11/12	0.90	0.09	42,46,51,61	0
2	FRU	E	5	11/12	0.90	0.11	56,99,106,112	0
4	FRU	G	2	11/12	0.91	0.10	64,87,97,106	0
2	FRU	E	3	11/12	0.93	0.10	53,67,79,82	0
2	FRU	E	4	11/12	0.95	0.08	63,84,106,111	0
2	FRU	D	3	11/12	0.96	0.07	59,66,69,70	0
2	FRU	D	2	11/12	0.96	0.09	60,76,109,118	0
2	FRU	D	4	11/12	0.97	0.06	59,63,67,71	0
2	FRU	C	3	11/12	0.98	0.06	36,47,54,54	0
2	FRU	C	4	11/12	0.98	0.05	40,43,45,47	0
2	FRU	C	2	11/12	0.98	0.05	53,61,72,75	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.

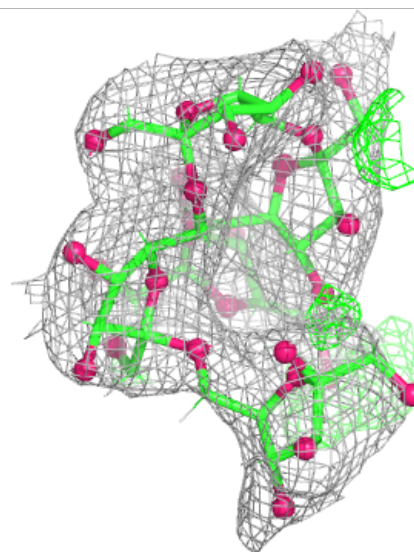
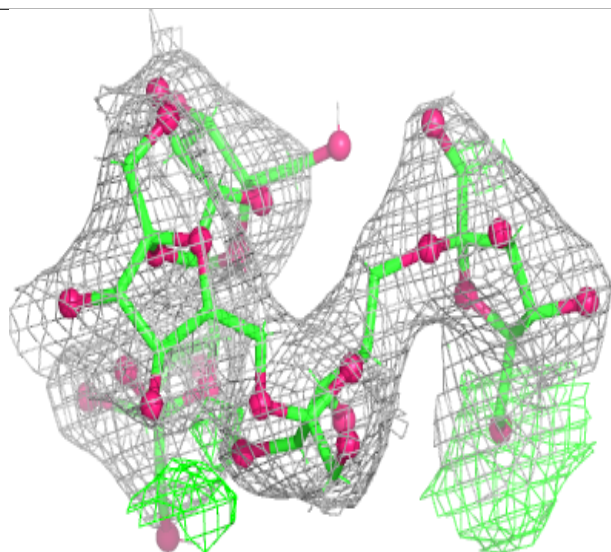
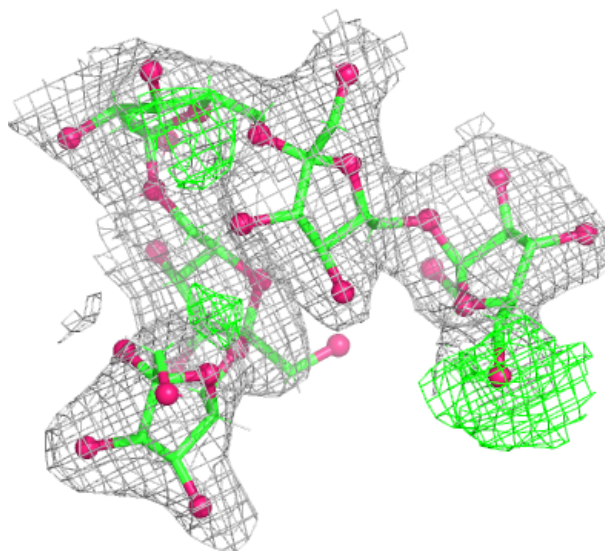
Electron density around Chain C:

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



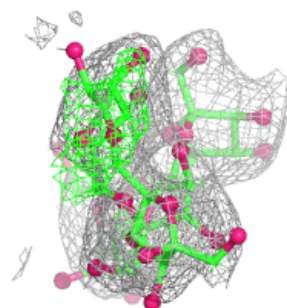
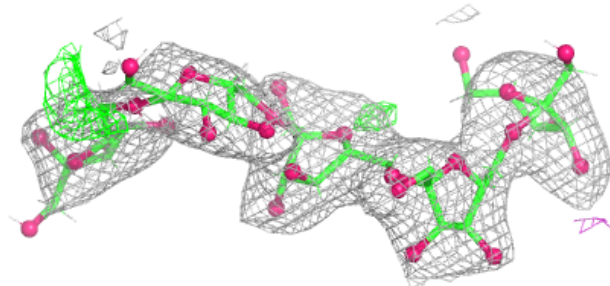
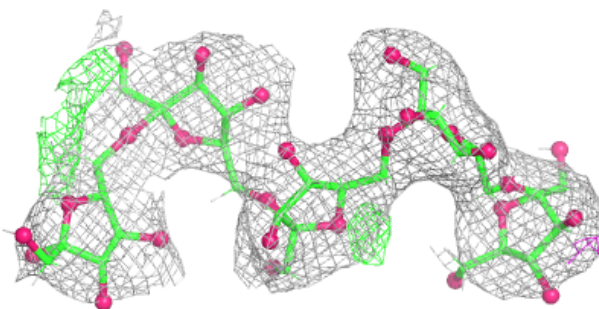
Electron density around Chain D:

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



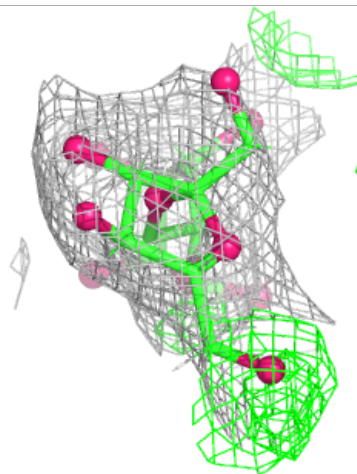
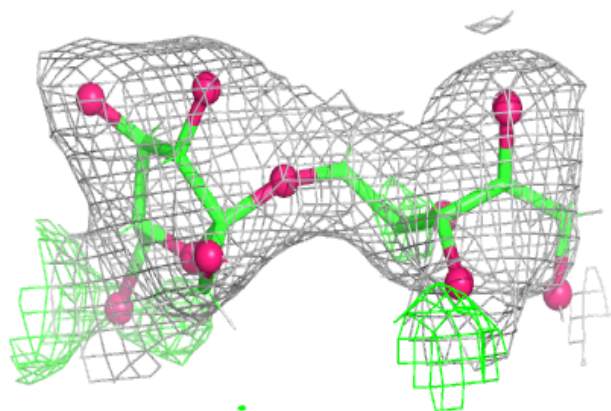
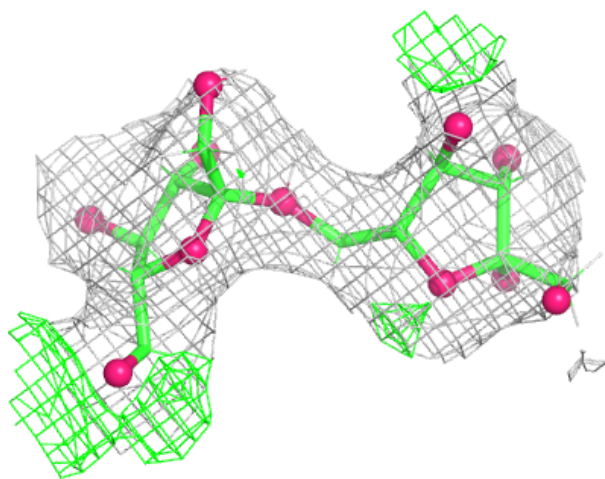
Electron density around Chain E:

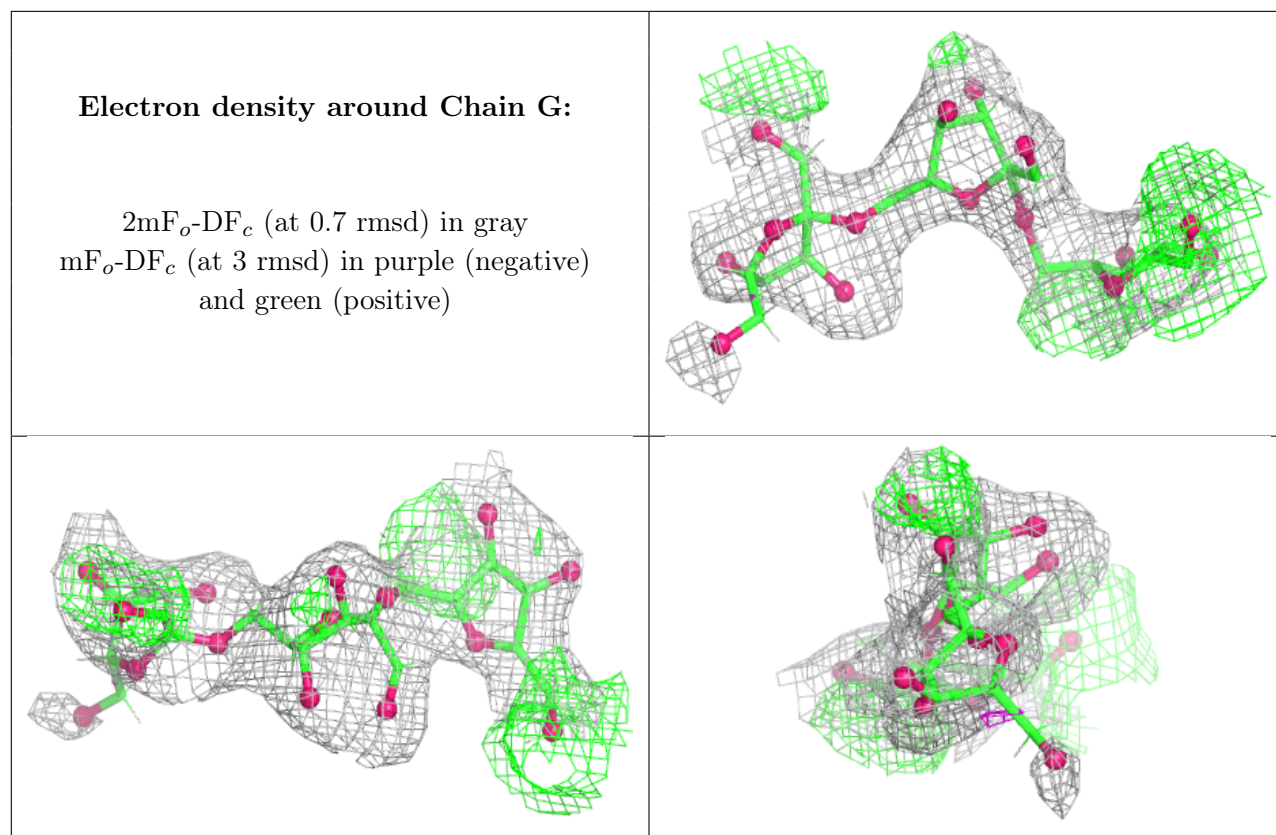
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
5	SO4	B	603	5/5	0.70	0.12	78,113,134,158	0
5	SO4	B	601	5/5	0.84	0.08	86,106,128,133	0
5	SO4	B	602	5/5	0.84	0.06	79,102,109,115	0
5	SO4	A	604	5/5	0.84	0.13	99,115,120,125	0
5	SO4	B	605	5/5	0.84	0.10	102,103,119,131	0
5	SO4	A	603	5/5	0.85	0.11	70,79,113,128	0
5	SO4	A	606	5/5	0.87	0.13	70,103,117,124	0
5	SO4	B	606	5/5	0.88	0.10	89,98,121,130	0
5	SO4	A	605	5/5	0.89	0.11	92,93,110,139	2
5	SO4	B	604	5/5	0.90	0.14	84,87,99,110	3
5	SO4	A	601	5/5	0.93	0.09	66,75,80,80	0
5	SO4	A	602	5/5	0.94	0.10	68,77,94,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.