



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:27 PM UTC

PDB ID : 4I9E / pdb_00004i9e
Title : Crystal structure of Aspartyl phosphate phosphatase F from Bacillus subtilis
Authors : Marina, A.; Gallego, F.
Deposited on : 2012-12-05
Resolution : 2.40 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

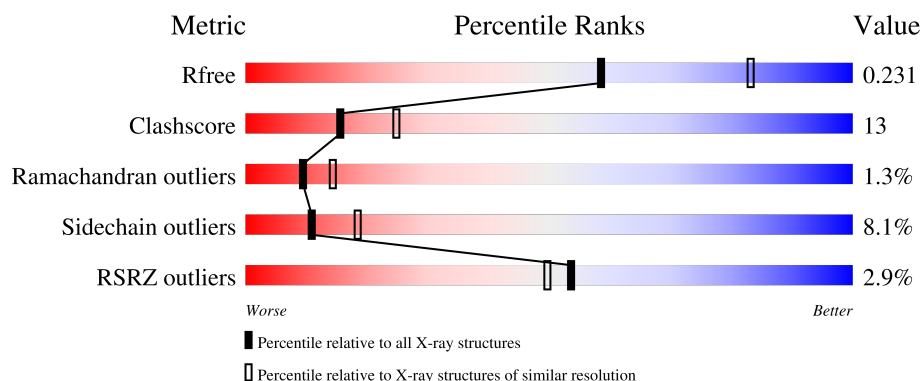
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	383	2% 74% 21% ••
1	B	383	4% 69% 26% 5%•
2	C	2	50% 50%
2	D	2	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6873 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.

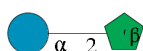
- Molecule 1 is a protein called Response regulator aspartate phosphatase F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	2	0
			3245	2106	518	605	16			
1	B	383	Total	C	N	O	S	0	6	0
			3276	2124	527	608	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P71002
A	0	ALA	-	expression tag	UNP P71002
B	-1	GLY	-	expression tag	UNP P71002
B	0	ALA	-	expression tag	UNP P71002

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



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

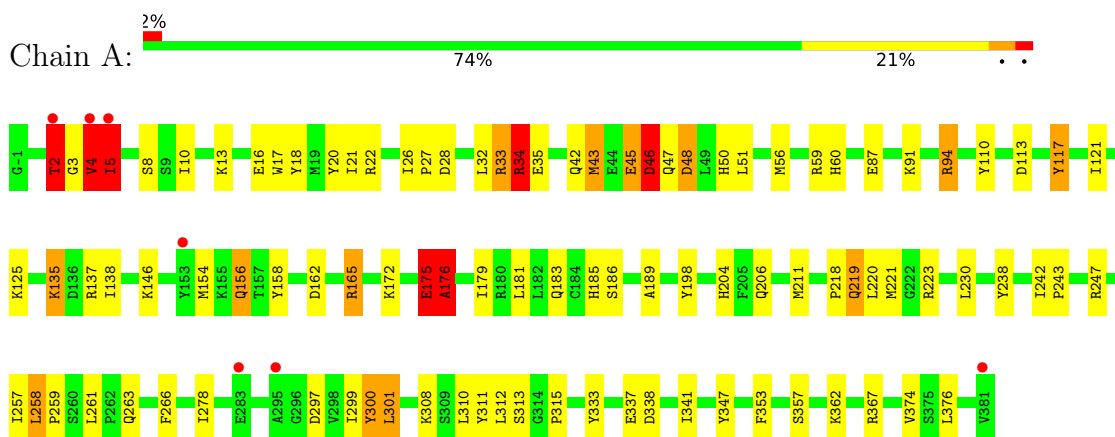
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	132	Total	O	0	0
			132	132		

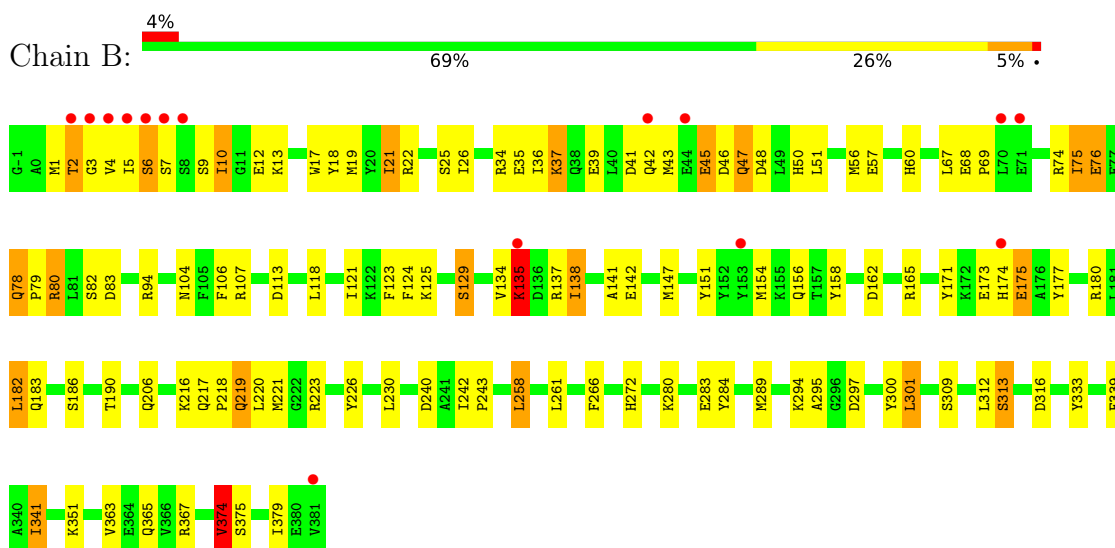
3 Residue-property plots

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: Response regulator aspartate phosphatase F



- Molecule 1: Response regulator aspartate phosphatase F



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



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

Chain D:

100%

GLC1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.21Å 97.21Å 203.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.21 – 2.40 84.19 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (84.21-2.40) 99.9 (84.19-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.240 0.192 , 0.231	Depositor DCC
R_{free} test set	2383 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6873	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.14	3/3324 (0.1%)	1.22	16/4463 (0.4%)
1	B	1.05	4/3356 (0.1%)	1.18	14/4504 (0.3%)
All	All	1.09	7/6680 (0.1%)	1.20	30/8967 (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	A	0	4
1	B	0	4
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	SER	CA-CB	6.95	1.67	1.53
1	B	242	ILE	CA-CB	6.25	1.62	1.54
1	A	242	ILE	CA-CB	6.03	1.57	1.54
1	B	21	ILE	CA-CB	5.65	1.60	1.54
1	B	141	ALA	CA-CB	-5.45	1.44	1.53
1	A	189	ALA	CA-CB	-5.03	1.45	1.53
1	A	59	ARG	CA-C	5.02	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	SER	N-CA-C	-11.55	98.06	114.12
1	A	175	GLU	N-CA-C	9.34	124.10	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLN	N-CA-C	-7.38	103.86	114.12
1	A	4	VAL	N-CA-C	7.35	124.63	109.34
1	A	266	PHE	N-CA-C	7.18	118.90	111.14
1	A	156	GLN	N-CA-C	-7.01	99.10	109.62
1	A	5	ILE	N-CA-C	7.00	123.89	109.34
1	B	333	TYR	N-CA-C	6.49	118.43	111.36
1	B	46	ASP	N-CA-C	-6.43	98.78	109.46
1	B	129	SER	N-CA-CB	-6.30	102.19	110.88
1	A	45	GLU	N-CA-C	-6.28	97.42	110.80
1	B	156	GLN	N-CA-C	-6.27	100.21	109.62
1	A	238	TYR	N-CA-C	6.22	118.06	111.28
1	B	25	SER	CA-C-N	6.06	125.18	120.33
1	B	25	SER	C-N-CA	6.06	125.18	120.33
1	A	198	TYR	N-CA-C	6.04	117.87	111.28
1	A	176	ALA	N-CA-C	6.03	123.63	110.80
1	B	266	PHE	N-CA-C	5.87	117.37	110.97
1	B	374	VAL	N-CA-CB	-5.77	102.74	112.44
1	B	339	PHE	N-CA-C	5.73	117.52	111.28
1	B	162	ASP	N-CA-C	5.72	117.52	111.28
1	B	2	THR	CB-CA-C	-5.28	101.57	110.43
1	A	300	TYR	N-CA-C	5.26	117.93	111.82
1	B	78	GLN	CA-C-N	5.25	125.23	120.03
1	B	78	GLN	C-N-CA	5.25	125.23	120.03
1	A	338	ASP	N-CA-C	-5.21	105.51	111.14
1	A	117	TYR	N-CA-C	5.17	116.72	111.14
1	A	301	LEU	N-CA-C	-5.16	105.55	111.07
1	A	34	ARG	N-CA-C	5.14	116.69	111.14
1	A	261	LEU	N-CA-C	5.10	120.41	113.16

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	GLU	Peptide
1	A	176	ALA	Peptide
1	A	2	THR	Peptide
1	A	4	VAL	Peptide
1	B	134	VAL	Peptide
1	B	3	GLY	Peptide
1	B	47	GLN	Peptide
1	B	5	ILE	Peptide

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	3245	0	3154	90	0
1	B	3276	0	3168	97	0
2	C	23	0	21	1	0
2	D	23	0	21	0	0
3	A	174	0	0	6	0
3	B	132	0	0	2	0
All	All	6873	0	6364	174	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 13.

All (174) 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:A:175:GLU:HG3	1:A:176:ALA:H	1.14	1.09
1:A:16:GLU:OE2	3:A:660:HOH:O	1.70	1.08
1:A:21:ILE:HD12	1:A:56:MET:CE	1.85	1.06
1:A:4:VAL:HG12	1:A:5:ILE:HG23	1.35	1.06
1:A:175:GLU:CG	1:A:176:ALA:H	1.69	1.04
1:B:48:ASP:HB3	1:B:106:PHE:HZ	1.21	1.02
1:A:21:ILE:HD12	1:A:56:MET:HE1	1.04	1.01
1:A:175:GLU:HG3	1:A:176:ALA:N	1.69	0.99
1:A:367:ARG:HE	1:B:367[B]:ARG:NH1	1.60	0.98
1:B:47:GLN:HG2	1:B:50:HIS:CD2	1.99	0.97
1:A:2:THR:HG23	1:A:3:GLY:HA2	1.50	0.94
1:B:124:PHE:HB3	1:B:147:MET:HE1	1.52	0.91
1:A:21:ILE:CD1	1:A:56:MET:HE1	1.99	0.89
1:B:137:ARG:NH2	1:B:173:GLU:OE2	2.05	0.88
1:B:218:PRO:HA	1:B:221:MET:HE3	1.55	0.88
1:A:2:THR:HG23	1:A:3:GLY:CA	2.05	0.87
1:B:47:GLN:HG2	1:B:50:HIS:HD2	1.40	0.85
1:B:2:THR:C	1:B:223:ARG:HH21	1.87	0.82
1:B:17:TRP:HE1	1:B:60:HIS:HD2	1.24	0.82
1:B:10:ILE:HD12	1:B:36:ILE:HG23	1.60	0.82
1:B:48:ASP:HB3	1:B:106:PHE:CZ	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:CD1	1:B:36:ILE:HG23	2.11	0.80
1:A:4:VAL:CG1	1:A:5:ILE:HG23	2.12	0.76
1:A:87:GLU:OE1	1:A:91:LYS:HE3	1.87	0.73
1:B:121:ILE:HD11	1:B:154:MET:HE1	1.71	0.72
1:A:337:GLU:OE2	1:A:367:ARG:NH1	2.23	0.71
1:A:46:ASP:O	1:A:50:HIS:HD2	1.74	0.70
1:B:68:GLU:HB2	1:B:69:PRO:HD3	1.72	0.70
1:A:367:ARG:NE	1:B:367[B]:ARG:NH1	2.39	0.69
1:A:117:TYR:HB3	1:A:154:MET:HE3	1.75	0.69
1:A:17:TRP:HE1	1:A:60:HIS:HD2	1.41	0.68
1:A:263:GLN:HG3	1:A:300:TYR:OH	1.94	0.68
1:B:174[B]:HIS:ND1	1:B:177:TYR:CD2	2.63	0.67
1:A:158:TYR:CD2	1:B:154:MET:HE3	2.29	0.67
1:A:94:ARG:HD3	1:A:135:LYS:NZ	2.09	0.67
1:A:16:GLU:OE1	3:A:628:HOH:O	2.13	0.66
1:B:45:GLU:H	1:B:45:GLU:CD	2.04	0.66
1:B:174[B]:HIS:CE1	1:B:177:TYR:HE2	2.14	0.65
1:A:315:PRO:HG2	1:A:347:TYR:OH	1.95	0.65
1:B:174[B]:HIS:HD1	1:B:177:TYR:HD2	1.45	0.64
1:B:137:ARG:HH22	1:B:173:GLU:CD	2.06	0.64
1:B:78:GLN:HB2	1:B:79:PRO:HD2	1.80	0.63
1:A:185:HIS:HD2	1:A:204:HIS:ND1	1.96	0.63
1:B:47:GLN:CG	1:B:50:HIS:HD2	2.12	0.62
1:B:124:PHE:HB3	1:B:147:MET:CE	2.28	0.62
1:B:217:GLN:HG2	1:B:220:LEU:HD12	1.81	0.62
1:B:174[B]:HIS:ND1	1:B:177:TYR:CE2	2.68	0.61
1:A:4:VAL:HG12	1:A:5:ILE:CG2	2.23	0.61
1:A:175:GLU:CG	1:A:176:ALA:N	2.37	0.60
1:B:217:GLN:HG3	3:B:520:HOH:O	2.00	0.60
1:B:219:GLN:HB3	3:B:520:HOH:O	2.01	0.60
1:A:158:TYR:HD2	1:B:154:MET:CE	2.14	0.60
1:B:147:MET:HE3	1:B:151:TYR:HE2	1.65	0.60
1:A:121:ILE:O	1:A:125:LYS:HG2	2.01	0.60
1:A:258:LEU:N	1:A:259:PRO:CD	2.65	0.59
1:A:333:TYR:O	1:A:337:GLU:HG3	2.02	0.59
1:A:21:ILE:CD1	1:A:56:MET:CE	2.69	0.59
1:A:3:GLY:N	1:A:223:ARG:NH1	2.50	0.59
1:A:154:MET:HE2	1:B:158:TYR:HD2	1.68	0.59
1:A:181:LEU:HD23	1:A:211:MET:HE1	1.85	0.58
1:B:43:MET:O	1:B:45:GLU:HG3	2.04	0.58
1:B:17:TRP:HE1	1:B:60:HIS:CD2	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:OE1	1:A:91:LYS:CE	2.52	0.58
1:B:341:ILE:HG13	1:B:363:VAL:HG21	1.85	0.57
1:A:46:ASP:O	1:A:50:HIS:CD2	2.57	0.57
1:A:4:VAL:HG23	1:A:223:ARG:HH22	1.69	0.57
1:B:21:ILE:HD11	1:B:60:HIS:CD2	2.40	0.56
1:B:218:PRO:CA	1:B:221:MET:HE3	2.30	0.56
1:A:2:THR:CG2	1:A:3:GLY:HA2	2.30	0.55
1:B:21:ILE:HG13	1:B:56:MET:CE	2.36	0.55
1:A:158:TYR:CD2	1:B:154:MET:CE	2.90	0.55
1:B:18:TYR:O	1:B:22:ARG:HG3	2.07	0.55
1:B:313:SER:HB3	1:B:316:ASP:HB2	1.87	0.55
1:A:179:ILE:O	1:A:183:GLN:HG3	2.07	0.54
1:B:138:ILE:O	1:B:142:GLU:HG2	2.07	0.54
1:A:2:THR:HG23	1:A:3:GLY:HA3	1.88	0.53
1:A:16:GLU:HG3	1:A:32:LEU:HD11	1.91	0.53
1:A:18:TYR:O	1:A:22:ARG:HG3	2.09	0.53
1:A:17:TRP:HE1	1:A:60:HIS:CD2	2.24	0.53
1:A:175:GLU:HG2	1:A:176:ALA:H	1.70	0.52
1:B:2:THR:CA	1:B:223:ARG:HH21	2.21	0.52
1:A:362:LYS:NZ	3:A:552:HOH:O	2.42	0.52
1:B:21:ILE:HG13	1:B:56:MET:HE2	1.91	0.52
1:B:26:ILE:HD11	1:B:67:LEU:HD12	1.91	0.52
1:B:104:ASN:HD22	1:B:123:PHE:HD1	1.55	0.52
1:A:4:VAL:CG2	1:A:223:ARG:HH22	2.23	0.52
1:A:43:MET:HG2	1:A:45:GLU:HB2	1.92	0.51
1:B:142:GLU:OE2	1:B:171:TYR:OH	2.25	0.51
1:A:10:ILE:HD11	1:A:43:MET:HE1	1.91	0.51
1:A:218:PRO:HA	1:A:221:MET:HE3	1.91	0.51
1:A:162:ASP:OD1	1:A:165:ARG:NH1	2.43	0.50
1:B:26:ILE:HD11	1:B:67:LEU:CD1	2.42	0.50
1:A:154:MET:CE	1:B:158:TYR:HD2	2.23	0.50
1:A:20:TYR:CD2	1:A:28:ASP:HB3	2.47	0.49
1:B:12:GLU:OE2	1:B:107:ARG:NH2	2.43	0.49
1:B:258:LEU:HD12	1:B:295:ALA:HB2	1.94	0.49
1:B:121:ILE:CD1	1:B:154:MET:HE1	2.42	0.49
1:A:219[A]:GLN:NE2	1:A:220:LEU:HG	2.27	0.49
1:B:297:ASP:O	1:B:301:LEU:HB2	2.13	0.49
1:B:147:MET:HE3	1:B:151:TYR:CE2	2.46	0.49
1:A:367:ARG:HH11	1:A:367:ARG:HG2	1.78	0.49
1:B:363:VAL:O	1:B:367[B]:ARG:HG3	2.13	0.48
1:A:137:ARG:NH2	3:A:610:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:CE	1:B:158:TYR:CD2	2.96	0.48
1:A:158:TYR:HD2	1:B:154:MET:HE2	1.78	0.48
1:A:156:GLN:NE2	1:B:158:TYR:H	2.12	0.48
1:A:16:GLU:HG3	1:A:32:LEU:CD1	2.44	0.48
1:B:230:LEU:O	1:B:230:LEU:HD23	2.13	0.48
1:A:87:GLU:CD	1:A:91:LYS:HE3	2.39	0.48
1:B:124:PHE:CB	1:B:147:MET:HE1	2.34	0.47
1:B:174[B]:HIS:ND1	1:B:177:TYR:HD2	2.04	0.47
1:A:10:ILE:CD1	1:A:43:MET:HE1	2.45	0.47
1:B:45:GLU:HB2	1:B:47:GLN:HG3	1.97	0.47
1:A:17:TRP:CZ2	1:A:33:ARG:HB2	2.49	0.47
1:A:46:ASP:HB3	1:A:48:ASP:HB2	1.96	0.47
1:A:243:PRO:O	1:A:247:ARG:HG3	2.13	0.47
1:A:13:LYS:NZ	3:A:504:HOH:O	2.48	0.47
1:B:34:ARG:O	1:B:37:LYS:HB3	2.15	0.47
1:B:1:MET:HE2	1:B:223:ARG:HG2	1.96	0.47
1:A:219[B]:GLN:HE21	1:A:257:ILE:HD12	1.79	0.46
1:A:94:ARG:HD3	1:A:135:LYS:HZ1	1.80	0.46
1:A:26:ILE:HB	1:A:27:PRO:HD3	1.97	0.46
1:A:8:SER:OG	1:A:110:TYR:HA	2.16	0.46
1:A:34:ARG:NH1	1:A:35:GLU:OE2	2.49	0.46
1:A:310:LEU:HD23	1:A:311:TYR:CZ	2.50	0.46
1:B:118:LEU:HG	1:B:374:VAL:HG22	1.98	0.46
1:B:75:ILE:O	1:B:78:GLN:HG2	2.16	0.45
3:A:521:HOH:O	1:B:125:LYS:HE3	2.15	0.45
1:B:18:TYR:HD1	1:B:56:MET:HE1	1.81	0.45
1:B:2:THR:C	1:B:223:ARG:NH2	2.67	0.45
1:A:48:ASP:OD2	1:A:146:LYS:HE3	2.16	0.45
1:B:9:SER:O	1:B:13:LYS:HG3	2.17	0.45
1:A:5:ILE:H	1:A:5:ILE:HG13	1.64	0.44
1:A:219[A]:GLN:H	1:A:219[A]:GLN:HG3	1.55	0.44
1:B:341:ILE:HD11	1:B:367[B]:ARG:NH2	2.32	0.44
1:A:367:ARG:HE	1:B:367[B]:ARG:HH11	1.53	0.44
1:B:258:LEU:HA	1:B:261:LEU:HD12	1.98	0.44
1:A:156:GLN:HE22	1:B:158:TYR:H	1.65	0.44
1:A:353:PHE:O	1:A:357:SER:HB3	2.19	0.43
1:B:138:ILE:HD13	1:B:138:ILE:HA	1.82	0.43
1:A:3:GLY:H	1:A:223:ARG:NH1	2.16	0.43
1:A:299:ILE:HG21	2:C:1:GLC:H62	2.01	0.43
1:B:272:HIS:CE1	1:B:284:TYR:CE2	3.07	0.43
1:B:74:ARG:NH2	1:B:76:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HD11	1:B:220:LEU:HD13	2.00	0.43
1:B:80:ARG:HB3	1:B:83:ASP:OD2	2.19	0.42
1:A:308:LYS:O	1:A:313:SER:HB3	2.19	0.42
1:B:121:ILE:HD11	1:B:154:MET:CE	2.44	0.42
1:B:74:ARG:O	1:B:75:ILE:C	2.61	0.42
1:A:172:LYS:HB3	1:A:172:LYS:HE2	1.20	0.42
1:B:186:SER:O	1:B:190:THR:HG23	2.20	0.42
1:A:154:MET:HE3	1:B:158:TYR:CD2	2.54	0.42
1:A:310:LEU:HD23	1:A:311:TYR:CE2	2.55	0.42
1:B:18:TYR:CD1	1:B:56:MET:HE1	2.55	0.42
1:B:300:TYR:O	1:B:301:LEU:C	2.63	0.42
1:B:174[B]:HIS:CE1	1:B:175:GLU:OE2	2.73	0.42
1:B:309:SER:HA	1:B:313:SER:HB2	2.01	0.42
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.93	0.41
1:B:39:GLU:HA	1:B:42:GLN:HE21	1.85	0.41
1:B:174[B]:HIS:ND1	1:B:175:GLU:OE2	2.52	0.41
1:B:180:ARG:NH1	1:B:183:GLN:OE1	2.52	0.41
1:A:42:GLN:O	1:A:42:GLN:HG3	2.20	0.41
1:B:226:TYR:CD2	1:B:226:TYR:C	2.98	0.41
1:A:45:GLU:O	1:A:46:ASP:C	2.62	0.41
1:B:230:LEU:HD23	1:B:230:LEU:C	2.46	0.41
1:A:43:MET:CG	1:A:45:GLU:HB2	2.51	0.41
1:A:94:ARG:CD	1:A:135:LYS:NZ	2.80	0.41
1:A:341:ILE:HD13	1:A:341:ILE:HA	1.91	0.41
1:B:240:ASP:O	1:B:243:PRO:HD2	2.20	0.40
1:B:21:ILE:CG1	1:B:56:MET:HE2	2.51	0.40
1:B:280:LYS:O	1:B:283:GLU:HB3	2.22	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	383/383 (100%)	363 (95%)	15 (4%)	5 (1%)	9	14
1	B	387/383 (101%)	363 (94%)	18 (5%)	6 (2%)	7	11
All	All	770/766 (100%)	726 (94%)	33 (4%)	11 (1%)	9	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	176	ALA
1	B	4	VAL
1	B	135[A]	LYS
1	B	135[B]	LYS
1	B	7	SER
1	A	297	ASP
1	A	46	ASP
1	A	43	MET
1	B	6	SER
1	B	75	ILE

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	342/342 (100%)	320 (94%)	22 (6%)	16	28
1	B	342/342 (100%)	306 (90%)	36 (10%)	6	10
All	All	684/684 (100%)	626 (92%)	58 (8%)	11	16

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	5	ILE
1	A	33	ARG
1	A	34	ARG
1	A	46	ASP

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Mol	Chain	Res	Type
1	A	48	ASP
1	A	51	LEU
1	A	94	ARG
1	A	113	ASP
1	A	135	LYS
1	A	165	ARG
1	A	186	SER
1	A	206	GLN
1	A	219[A]	GLN
1	A	219[B]	GLN
1	A	230	LEU
1	A	258	LEU
1	A	278	ILE
1	A	301	LEU
1	A	312	LEU
1	A	374	VAL
1	A	376	LEU
1	B	10	ILE
1	B	19	MET
1	B	35	GLU
1	B	37	LYS
1	B	41	ASP
1	B	45	GLU
1	B	51	LEU
1	B	57	GLU
1	B	76	GLU
1	B	80	ARG
1	B	82	SER
1	B	94	ARG
1	B	113	ASP
1	B	129	SER
1	B	135[A]	LYS
1	B	135[B]	LYS
1	B	138	ILE
1	B	165	ARG
1	B	175	GLU
1	B	182	LEU
1	B	206	GLN
1	B	216	LYS
1	B	219	GLN
1	B	258	LEU
1	B	289[A]	MET

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Mol	Chain	Res	Type
1	B	289[B]	MET
1	B	294	LYS
1	B	301	LEU
1	B	312	LEU
1	B	313	SER
1	B	341	ILE
1	B	351	LYS
1	B	365	GLN
1	B	374	VAL
1	B	375	SER
1	B	379	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	50	HIS
1	A	60	HIS
1	A	61	ASN
1	A	78	GLN
1	A	104	ASN
1	A	156	GLN
1	A	185	HIS
1	A	206	GLN
1	A	217	GLN
1	A	235	GLN
1	B	42	GLN
1	B	50	HIS
1	B	60	HIS
1	B	61	ASN
1	B	78	GLN
1	B	104	ASN
1	B	156	GLN
1	B	206	GLN
1	B	263	GLN
1	B	270	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	C	1	2	11,11,12	0.84	0	15,15,17	0.86	0
2	FRU	C	2	2	11,12,12	0.82	0	10,18,18	0.96	0
2	GLC	D	1	2	11,11,12	0.39	0	15,15,17	1.16	2 (13%)
2	FRU	D	2	2	11,12,12	1.27	1 (9%)	10,18,18	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/19/22	0/1/1/1
2	FRU	C	2	2	-	2/5/24/24	0/1/1/1
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	FRU	D	2	2	-	2/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	FRU	O2-C2	2.81	1.45	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	C1-C2-C3	2.25	112.92	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	C6-C5-C4	-2.18	107.68	113.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

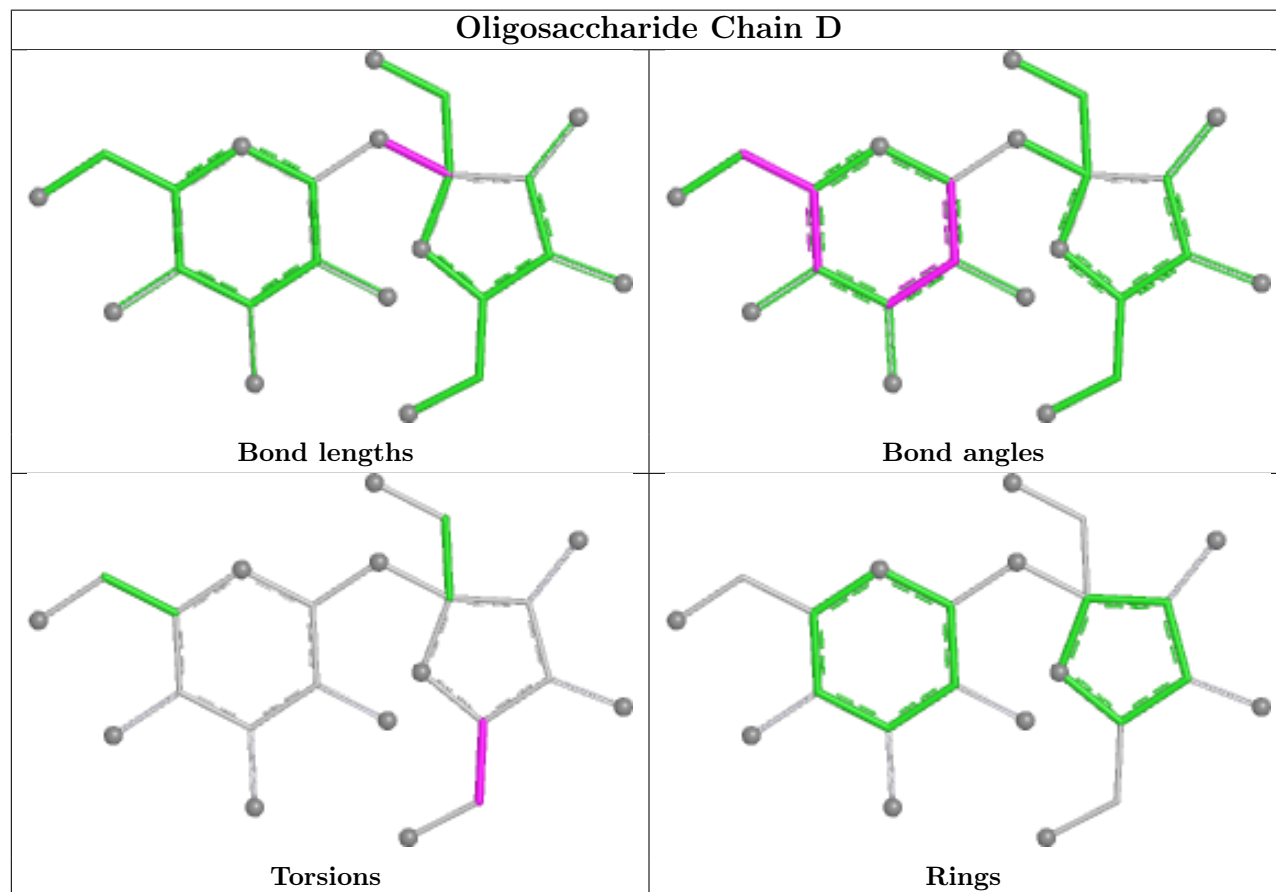
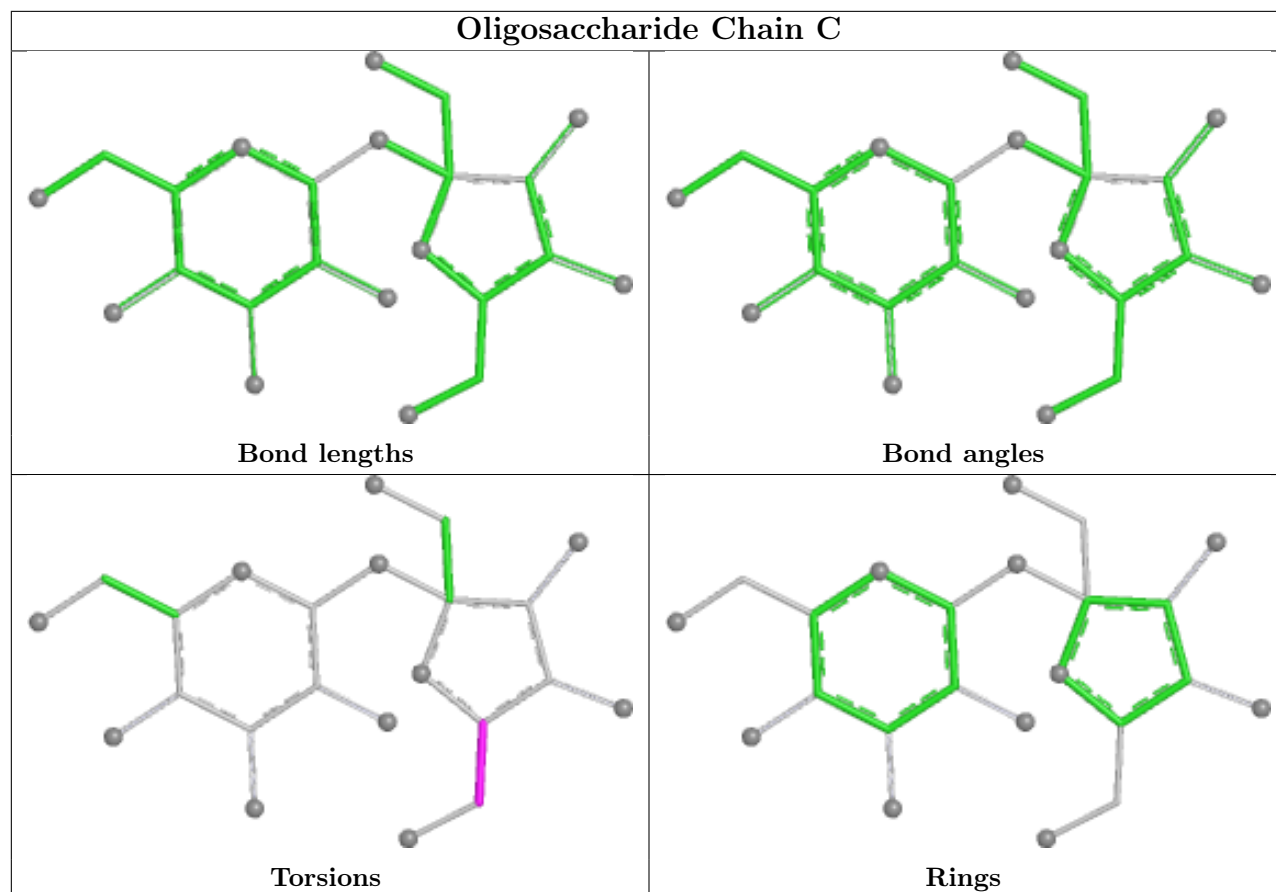
Mol	Chain	Res	Type	Atoms
2	C	2	FRU	C4-C5-C6-O6
2	C	2	FRU	O5-C5-C6-O6
2	D	2	FRU	O5-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	1	0

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



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	383/383 (100%)	-0.16	7 (1%) 67 63	14, 43, 68, 89	2 (0%)
1	B	383/383 (100%)	0.01	15 (3%) 43 39	15, 47, 80, 102	6 (1%)
All	All	766/766 (100%)	-0.08	22 (2%) 53 50	14, 45, 76, 102	8 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	SER	4.4
1	B	5	ILE	3.7
1	B	7	SER	3.6
1	B	153[A]	TYR	3.3
1	A	5	ILE	3.3
1	B	135[A]	LYS	3.2
1	B	71[A]	GLU	2.9
1	A	381	VAL	2.8
1	B	174[A]	HIS	2.8
1	A	283	GLU	2.4
1	B	42	GLN	2.4
1	B	70	LEU	2.4
1	B	4	VAL	2.4
1	A	4	VAL	2.3
1	A	2	THR	2.2
1	B	381	VAL	2.2
1	B	3	GLY	2.2
1	A	153[A]	TYR	2.2
1	B	2	THR	2.1
1	B	44	GLU	2.1
1	A	295	ALA	2.0
1	B	8	SER	2.0

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

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

6.3 Carbohydrates [i](#)

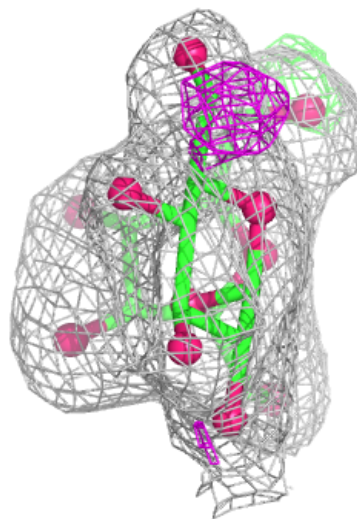
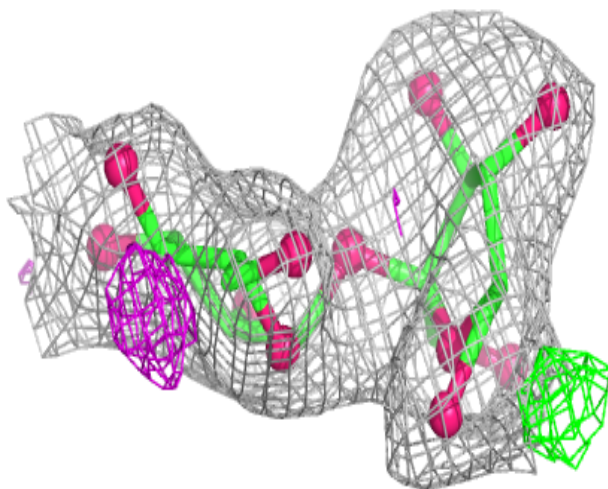
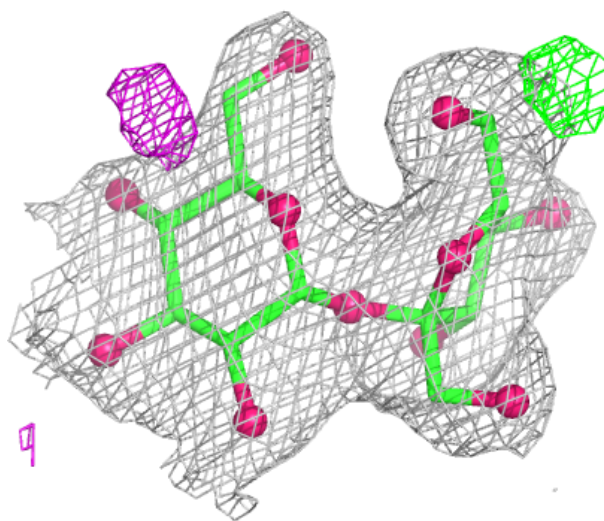
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

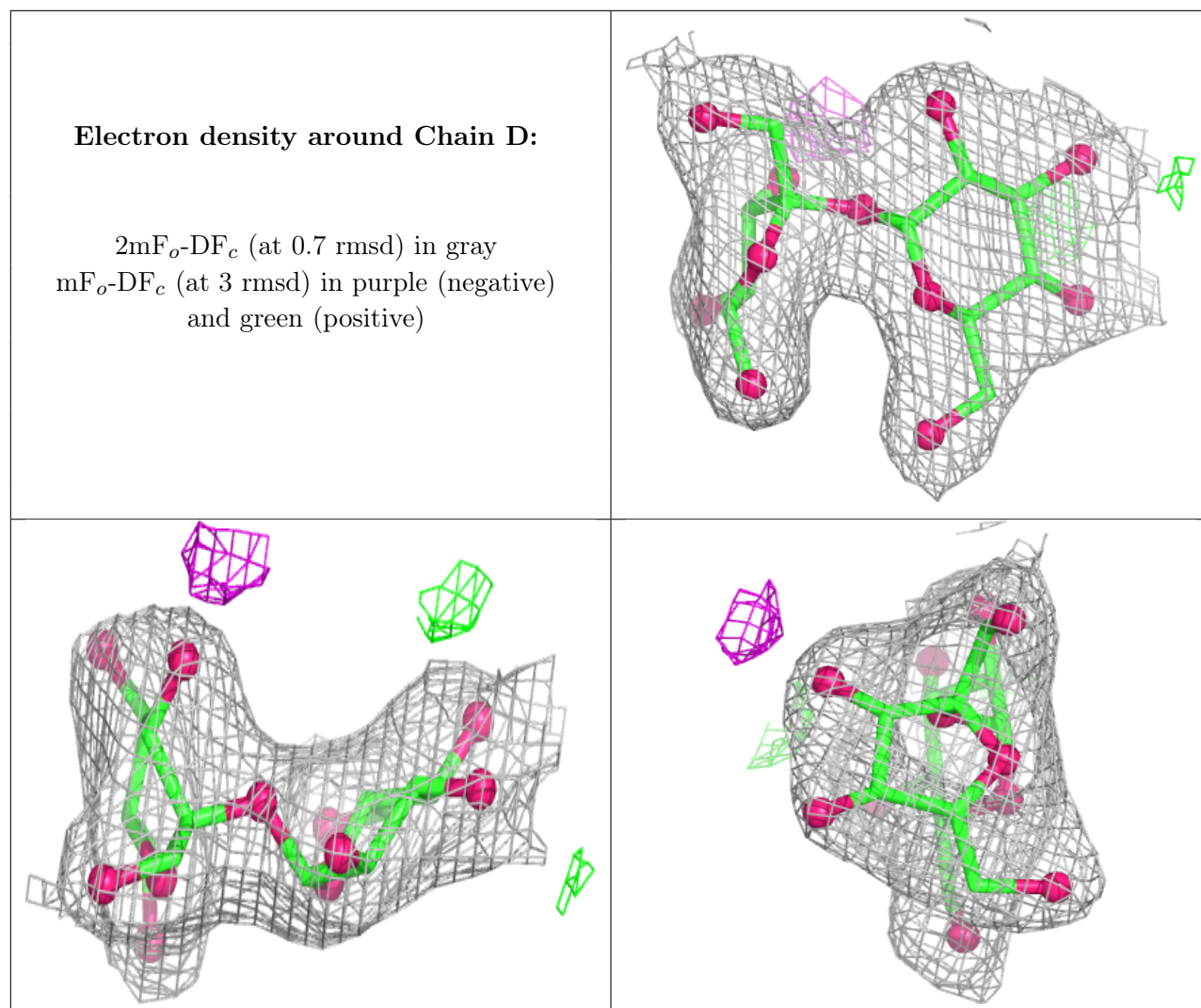
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FRU	C	2	12/12	0.89	0.09	45,55,61,66	0
2	GLC	C	1	11/12	0.93	0.08	44,47,50,55	0
2	FRU	D	2	12/12	0.93	0.08	45,49,50,57	0
2	GLC	D	1	11/12	0.97	0.06	40,46,47,48	0

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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.