Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 12:07 AM EDT

PDB ID	:	5TIB
Title	:	Gasdermin-B C-terminal domain containing the polymorphism residues Arg299:Ser306 fused to maltose binding protein
Authors	:	Chao, K.; Herzberg, O.
Deposited on	:	2016-10-01
Resolution	:	2.60 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:

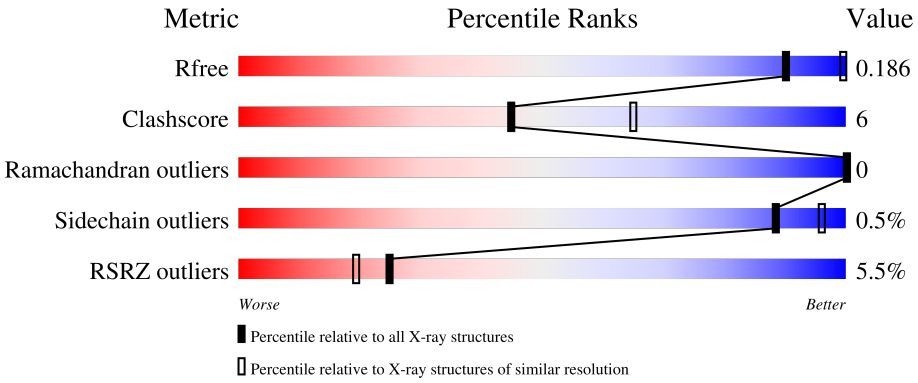
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	557	90% 6%
1	B	557	9% 77% 18% 5%
2	C	2	100%
2	D	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8238 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 Sugar ABC transporter substrate-binding protein,Gasdermin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4056	2600	661	782	13			
1	B	530	Total	C	N	O	S	0	0	0
			3845	2464	635	734	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	see remark 999	UNP A0A178SBV6
A	83	ALA	LYS	see remark 999	UNP A0A178SBV6
A	172	ALA	GLU	see remark 999	UNP A0A178SBV6
A	173	ALA	ASN	see remark 999	UNP A0A178SBV6
A	239	ALA	LYS	see remark 999	UNP A0A178SBV6
A	362	ALA	LYS	see remark 999	UNP A0A178SBV6
A	363	ALA	ASP	see remark 999	UNP A0A178SBV6
A	367	ASN	-	linker	UNP A0A178SBV6
A	368	ALA	-	linker	UNP A0A178SBV6
A	369	ALA	-	linker	UNP A0A178SBV6
A	370	ALA	-	linker	UNP A0A178SBV6
A	1299	ARG	GLY	see remark 999	UNP Q8TAX9
A	1306	SER	PRO	see remark 999	UNP Q8TAX9
B	82	ALA	ASP	see remark 999	UNP A0A178SBV6
B	83	ALA	LYS	see remark 999	UNP A0A178SBV6
B	172	ALA	GLU	see remark 999	UNP A0A178SBV6
B	173	ALA	ASN	see remark 999	UNP A0A178SBV6
B	239	ALA	LYS	see remark 999	UNP A0A178SBV6
B	362	ALA	LYS	see remark 999	UNP A0A178SBV6
B	363	ALA	ASP	see remark 999	UNP A0A178SBV6
B	367	ASN	-	linker	UNP A0A178SBV6
B	368	ALA	-	linker	UNP A0A178SBV6
B	369	ALA	-	linker	UNP A0A178SBV6
B	370	ALA	-	linker	UNP A0A178SBV6

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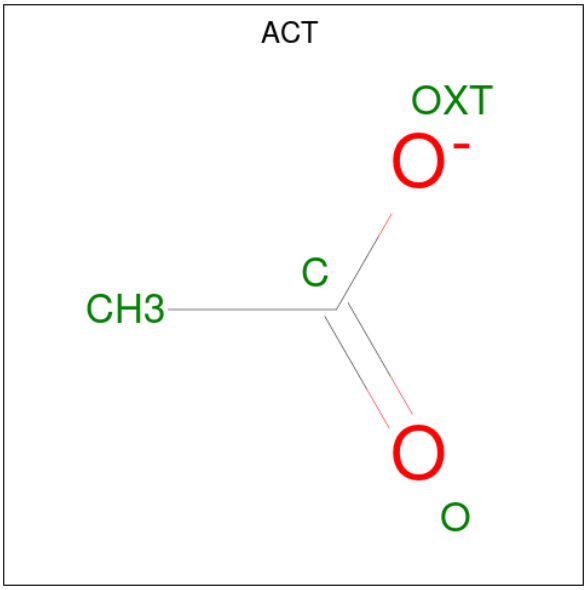
Chain	Residue	Modelled	Actual	Comment	Reference
B	1299	ARG	GLY	see remark 999	UNP Q8TAX9
B	1306	SER	PRO	see remark 999	UNP Q8TAX9

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is water.

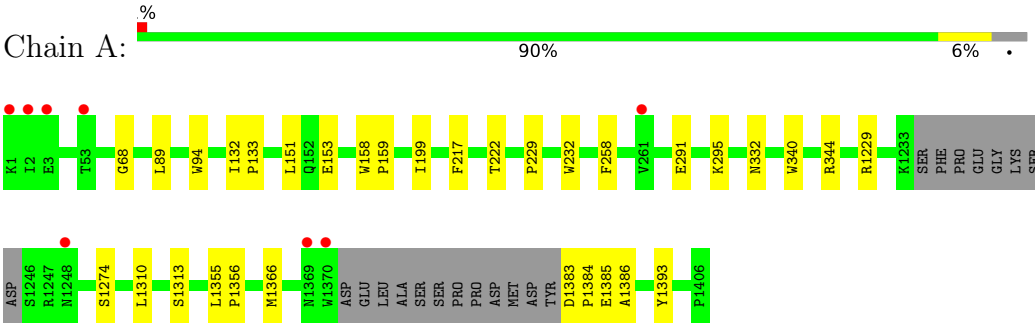
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	232	Total O 232 232	0	0
5	B	54	Total O 54 54	0	0

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.

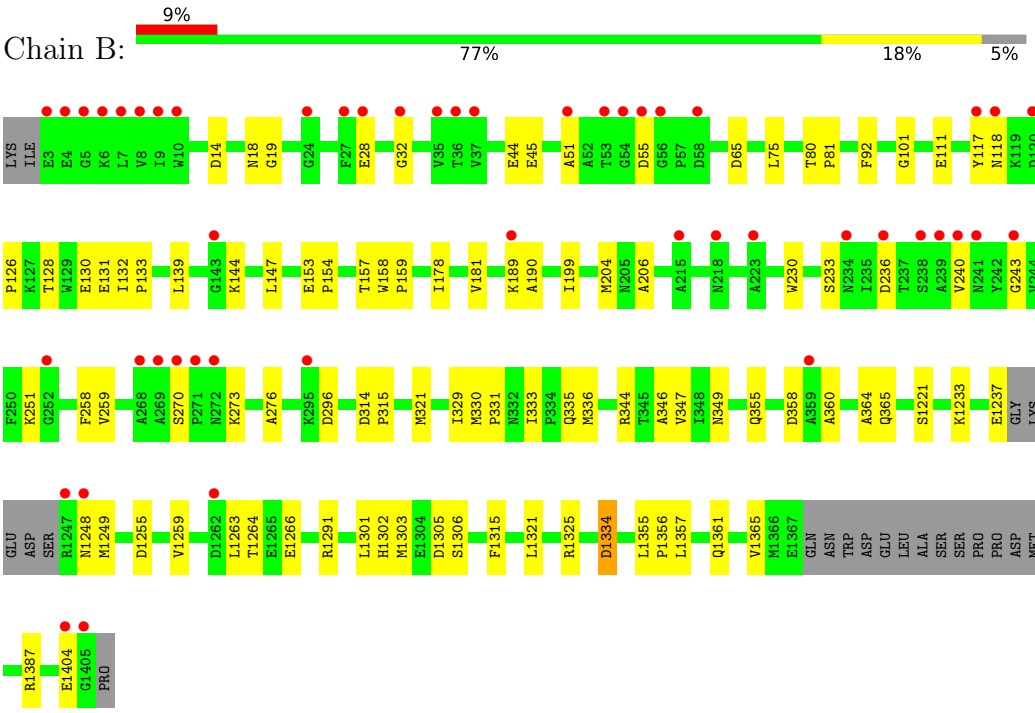
• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B

Chain A:



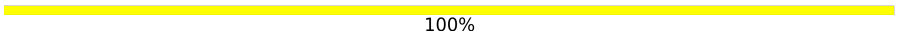
• Molecule 1: Sugar ABC transporter substrate-binding protein,Gasdermin-B

Chain B:



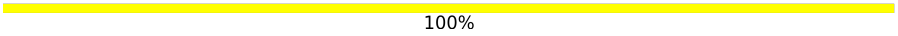
• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.06Å 104.06Å 252.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.19 – 2.60 36.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.19-2.60) 100.0 (36.41-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.184 , 0.233 0.191 , 0.186	Depositor DCC
R_{free} test set	2168 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8238	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 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GLC, NA

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	0.93	1/4136 (0.0%)	0.77	0/5617
1	B	0.67	0/3924	0.72	0/5362
All	All	0.81	1/8060 (0.0%)	0.75	0/10979

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1385	GLU	CD-OE1	5.04	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4056	0	3993	18	0
1	B	3845	0	3599	84	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	4	0	3	0	0
4	A	1	0	0	0	0
5	A	232	0	0	1	0
5	B	54	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8238	0	7637	101	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 6.

All (101) 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:1301:LEU:HG	1:B:1315:PHE:CE2	2.26	0.71
1:B:355:GLN:NE2	1:B:360:ALA:HA	2.07	0.70
1:B:331:PRO:HG2	1:B:336:MET:HE2	1.79	0.65
1:B:139:LEU:O	1:B:144:LYS:HB2	1.97	0.65
1:B:28:GLU:O	1:B:32:GLY:N	2.30	0.64
1:B:1315:PHE:CE1	1:B:1321:LEU:HB2	2.33	0.63
1:B:178:ILE:HD11	1:B:333:ILE:HD12	1.80	0.63
1:B:65:ASP:HB3	1:B:330:MET:HE3	1.81	0.63
1:B:130:GLU:OE1	1:B:130:GLU:N	2.29	0.62
1:B:189:LYS:NZ	1:B:358:ASP:OD2	2.32	0.62
1:B:154:PRO:HA	1:B:157:THR:CG2	2.30	0.62
1:A:153:GLU:CD	1:A:344:ARG:HH12	2.04	0.61
1:B:154:PRO:HA	1:B:157:THR:HG22	1.83	0.61
1:B:1248:ASN:OD1	1:B:1249:MET:N	2.33	0.61
1:B:117:TYR:CE2	1:B:125:PRO:HG3	2.37	0.59
1:B:157:THR:HG21	1:B:347:VAL:HG11	1.85	0.59
1:B:1301:LEU:HD11	1:B:1315:PHE:CD2	2.38	0.58
1:B:331:PRO:CG	1:B:336:MET:HE2	2.33	0.58
1:B:1301:LEU:CD1	1:B:1315:PHE:CD2	2.87	0.58
1:B:118:ASN:ND2	1:B:240:VAL:HG13	2.20	0.57
1:B:178:ILE:HD12	1:B:335:GLN:HG2	1.86	0.57
1:B:270:SER:O	1:B:273:LYS:HD2	2.04	0.57
1:B:331:PRO:HD2	1:B:336:MET:CE	2.35	0.56
1:B:19:GLY:N	1:B:296:ASP:OD2	2.35	0.56
1:A:1274:SER:HB2	1:A:1310:LEU:HB2	1.89	0.55
1:B:331:PRO:CG	1:B:336:MET:CE	2.85	0.55
1:B:132:ILE:N	1:B:133:PRO:CD	2.70	0.55
1:B:1255:ASP:O	1:B:1259:VAL:HG23	2.07	0.54
1:A:1384:PRO:HB3	1:B:101:GLY:HA3	1.89	0.54
1:B:18:ASN:HB2	1:B:296:ASP:OD2	2.08	0.54
1:B:51:ALA:HB3	1:B:75:LEU:HD13	1.90	0.54
1:B:1365:VAL:O	1:B:1365:VAL:HG12	2.06	0.54
1:A:158:TRP:N	1:A:159:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:HG2	1:B:45:GLU:HG3	1.88	0.53
1:B:117:TYR:CD2	1:B:125:PRO:HG3	2.43	0.53
1:B:273:LYS:O	1:B:276:ALA:N	2.42	0.53
1:B:1237:GLU:CB	1:B:1334:ASP:OD2	2.57	0.52
1:B:117:TYR:CE1	1:B:243:GLY:HA3	2.44	0.52
1:B:181:VAL:O	1:B:365:GLN:NE2	2.43	0.52
1:B:233:SER:O	1:B:236:ASP:HB2	2.10	0.52
1:B:331:PRO:CD	1:B:336:MET:CE	2.88	0.52
1:B:178:ILE:HG22	1:B:178:ILE:O	2.09	0.52
1:B:331:PRO:HB2	1:B:336:MET:HE2	1.91	0.51
1:B:126:PRO:CB	1:B:131:GLU:OE1	2.59	0.51
1:B:1291:ARG:NH1	1:B:1305:ASP:OD1	2.44	0.51
1:B:314:ASP:OD1	1:B:315:PRO:HD2	2.11	0.51
1:B:130:GLU:O	1:B:133:PRO:HD2	2.11	0.50
1:B:178:ILE:HG22	1:B:1221:SER:OG	2.12	0.50
1:B:14:ASP:O	1:B:230:TRP:HB2	2.12	0.50
1:B:1355:LEU:N	1:B:1356:PRO:CD	2.75	0.49
1:B:199:ILE:HG21	1:B:206:ALA:HB2	1.94	0.49
1:B:1303:MET:O	1:B:1306:SER:CB	2.61	0.48
1:B:1264:THR:HG22	1:B:1266:GLU:H	1.78	0.48
1:B:128:THR:HG22	1:B:249:THR:OG1	2.14	0.47
1:B:158:TRP:N	1:B:159:PRO:CD	2.77	0.47
1:B:132:ILE:HD13	1:B:147:LEU:HD22	1.97	0.47
1:B:190:ALA:HB1	1:B:251:LYS:HE3	1.96	0.47
1:A:1383:ASP:HB3	1:A:1386:ALA:HB3	1.97	0.46
1:A:153:GLU:OE1	1:A:344:ARG:NH1	2.47	0.46
1:B:153:GLU:OE1	1:B:344:ARG:NH1	2.49	0.46
1:B:331:PRO:HB2	1:B:336:MET:CE	2.45	0.46
1:B:1302:HIS:HB3	5:B:1618:HOH:O	2.15	0.46
1:A:132:ILE:N	1:A:133:PRO:CD	2.79	0.46
1:A:68:GLY:HA3	1:A:332:ASN:O	2.16	0.46
1:A:1355:LEU:N	1:A:1356:PRO:CD	2.78	0.45
1:A:1366:MET:CE	1:A:1393:TYR:HB2	2.46	0.45
1:B:349:ASN:HB3	1:B:355:GLN:HB2	1.98	0.45
1:B:199:ILE:HA	1:B:204:MET:O	2.16	0.45
1:A:291:GLU:OE2	1:A:295:LYS:HE2	2.16	0.45
1:B:51:ALA:HA	1:B:55:ASP:O	2.16	0.45
1:B:92:PHE:HD2	5:B:1636:HOH:O	2.00	0.45
1:B:331:PRO:HG2	1:B:336:MET:CE	2.45	0.45
1:B:331:PRO:HD2	1:B:336:MET:HE1	1.97	0.44
1:B:331:PRO:CB	1:B:336:MET:HE2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:OE1	1:B:44:GLU:N	2.49	0.44
1:B:1233:LYS:HG2	1:B:1387:ARG:CZ	2.48	0.44
1:B:1303:MET:O	1:B:1306:SER:HB2	2.18	0.44
1:B:259:VAL:HB	1:B:329:ILE:HA	2.01	0.43
1:A:151:LEU:HD13	1:A:199:ILE:HD11	1.99	0.43
1:A:1229:ARG:HD3	5:A:1752:HOH:O	2.19	0.43
1:B:273:LYS:O	1:B:276:ALA:HB3	2.19	0.43
1:B:1357:LEU:O	1:B:1361:GLN:HG3	2.19	0.43
1:B:131:GLU:C	1:B:133:PRO:HD2	2.38	0.43
1:B:346:ALA:HB2	1:B:364:ALA:HB2	2.01	0.42
1:A:217:PHE:HA	1:A:222:THR:HG22	2.01	0.42
1:B:28:GLU:O	1:B:32:GLY:CA	2.68	0.42
1:B:178:ILE:CG2	1:B:1221:SER:OG	2.67	0.42
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.42
1:B:321:MET:HB2	1:B:321:MET:HE2	1.98	0.42
1:B:65:ASP:OD1	1:B:330:MET:HE1	2.20	0.42
1:B:1263:LEU:HD21	1:B:1325:ARG:HD3	2.01	0.41
1:B:1383:ASP:OD1	1:B:1384:PRO:HD2	2.21	0.41
1:B:111:GLU:HG3	5:B:1611:HOH:O	2.20	0.41
1:B:245:THR:OG1	1:B:246:VAL:N	2.54	0.41
1:B:314:ASP:HA	1:B:315:PRO:HD3	1.93	0.41
1:B:80:THR:N	1:B:81:PRO:HD3	2.36	0.40
1:A:1310:LEU:O	1:A:1313:SER:HB2	2.21	0.40
1:B:189:LYS:NZ	1:B:358:ASP:CG	2.75	0.40
1:A:89:LEU:HD22	1:A:94:TRP:CZ2	2.56	0.40
1:A:340:TRP:CE3	1:A:340:TRP:HA	2.56	0.40
1:B:28:GLU:O	1:B:32:GLY:HA2	2.21	0.40

There are no symmetry-related clashes.

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	527/557 (95%)	521 (99%)	6 (1%)	0	100	100
1	B	524/557 (94%)	515 (98%)	9 (2%)	0	100	100
All	All	1051/1114 (94%)	1036 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	411/451 (91%)	410 (100%)	1 (0%)	93	98
1	B	358/451 (79%)	355 (99%)	3 (1%)	81	92
All	All	769/902 (85%)	765 (100%)	4 (0%)	88	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	PHE
1	B	258	PHE
1	B	1334	ASP
1	B	1404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	1248	ASN
1	A	1302	HIS
1	A	1361	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	12,12,12	0.63	0	17,17,17	1.18	2 (11%)
2	GLC	C	2	2	11,11,12	1.22	1 (9%)	15,15,17	0.60	0
2	GLC	D	1	2	12,12,12	0.87	0	17,17,17	0.90	1 (5%)
2	GLC	D	2	2	11,11,12	0.65	0	15,15,17	1.21	1 (6%)

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	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	C2-C3	3.46	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	GLC	C1-O5-C5	3.13	116.44	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GLC	O1-C1-O5	-2.67	102.36	110.38
2	C	1	GLC	O2-C2-C3	-2.62	104.29	110.35
2	D	1	GLC	C3-C4-C5	2.12	114.03	110.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

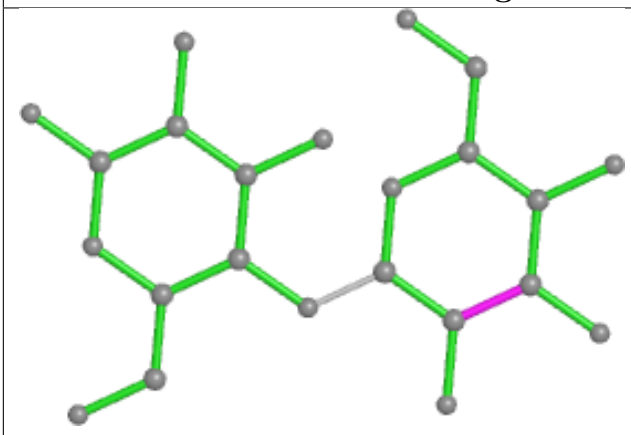
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

There are no ring outliers.

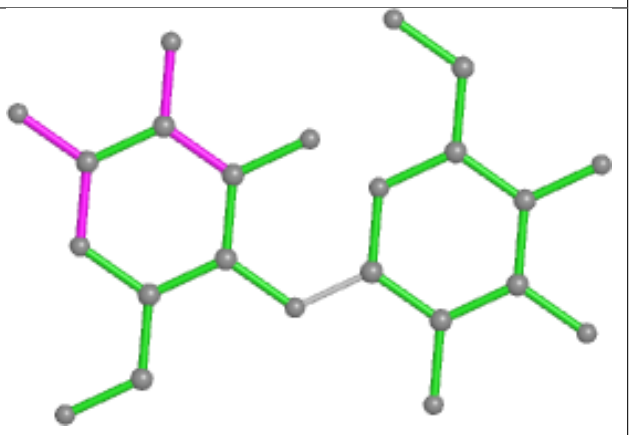
No monomer is involved in short contacts.

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

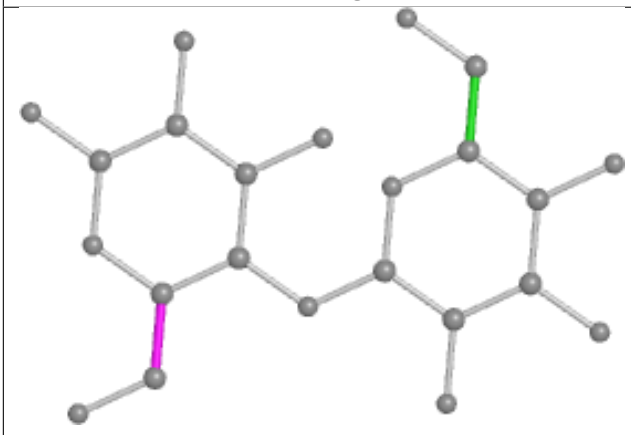
Oligosaccharide Chain C



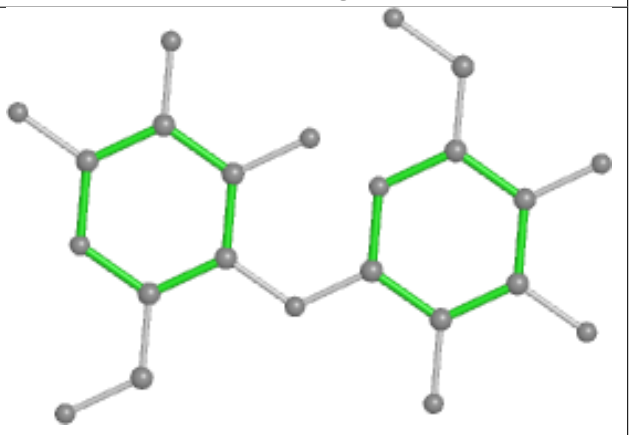
Bond lengths



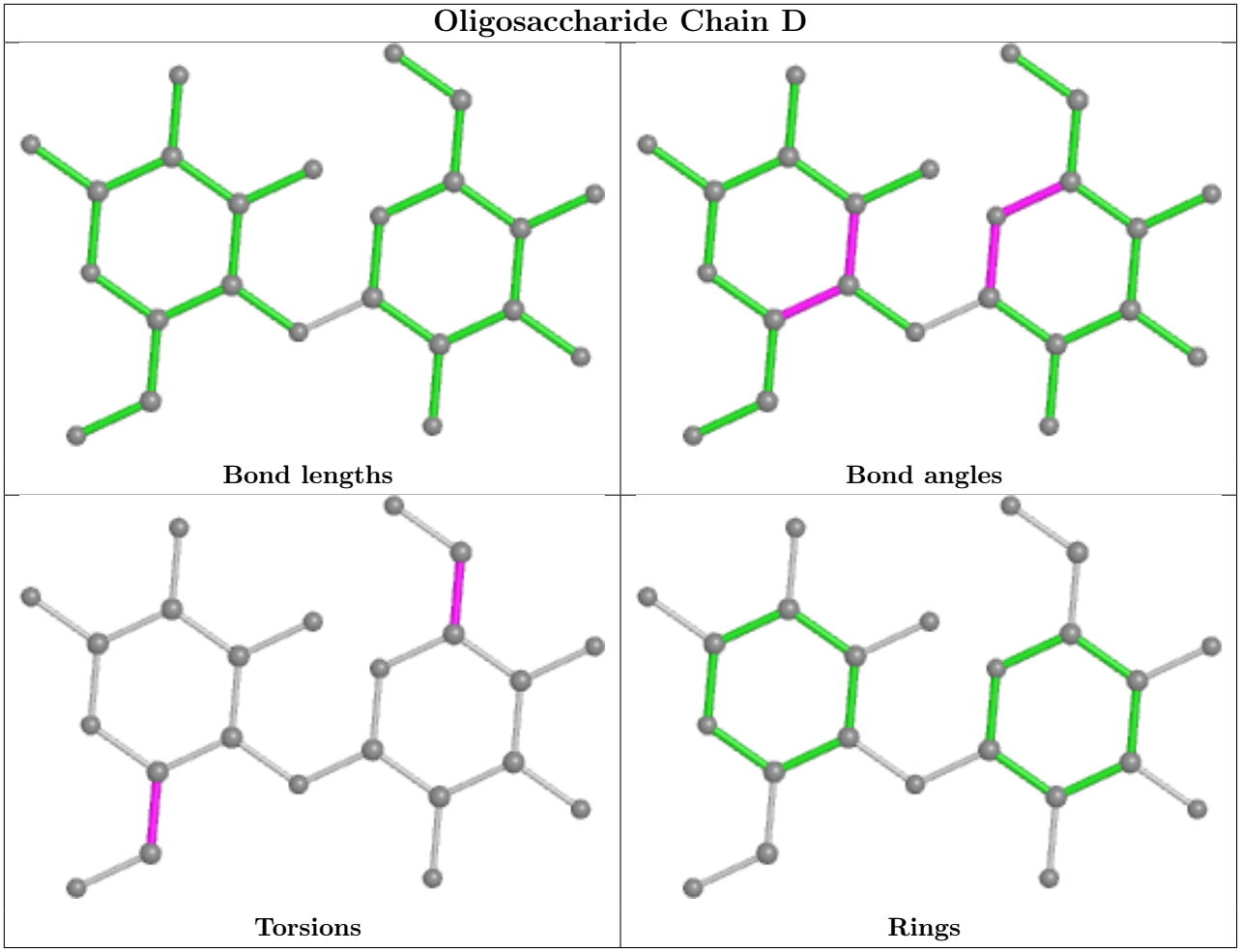
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
3	ACT	A	1502	-	3,3,3	0.78	0	3,3,3	0.82	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	533/557 (95%)	-0.32	8 (1%) 73 70	16, 29, 55, 97	0
1	B	530/557 (95%)	0.37	50 (9%) 8 5	30, 63, 95, 110	0
All	All	1063/1114 (95%)	0.03	58 (5%) 25 19	16, 45, 87, 110	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	5.5
1	B	5	GLY	4.8
1	B	272	ASN	4.7
1	B	1405	GLY	4.6
1	B	32	GLY	4.5
1	B	36	THR	4.5
1	B	243	GLY	4.4
1	B	268	ALA	4.2
1	B	35	VAL	4.2
1	B	4	GLU	4.0
1	B	239	ALA	3.8
1	B	55	ASP	3.7
1	B	120	ASP	3.6
1	B	1404	GLU	3.6
1	A	1	LYS	3.6
1	A	53	THR	3.6
1	B	236	ASP	3.5
1	B	9	ILE	3.4
1	B	241	ASN	3.3
1	B	215	ALA	3.2
1	B	269	ALA	3.2
1	B	1248	ASN	3.2
1	B	54	GLY	3.1
1	B	271	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	8	VAL	3.1
1	B	24	GLY	3.1
1	B	117	TYR	3.1
1	B	240	VAL	3.0
1	B	189	LYS	2.8
1	B	56	GLY	2.8
1	B	238	SER	2.8
1	A	261	VAL	2.7
1	B	270	SER	2.7
1	B	1247	ARG	2.7
1	B	143	GLY	2.6
1	B	1262	ASP	2.6
1	B	223	ALA	2.5
1	B	252	GLY	2.5
1	B	37	VAL	2.5
1	A	1248	ASN	2.5
1	A	2	ILE	2.4
1	A	1370	TRP	2.4
1	B	295	LYS	2.3
1	B	359	ALA	2.3
1	B	27	PHE	2.2
1	B	6	LYS	2.2
1	B	234	ASN	2.2
1	B	3	GLU	2.2
1	A	3	GLU	2.1
1	B	118	ASN	2.1
1	B	123	PRO	2.1
1	B	53	THR	2.1
1	B	218	ASN	2.1
1	A	1369	ASN	2.1
1	B	58	ASP	2.0
1	B	10	TRP	2.0
1	B	51	ALA	2.0
1	B	28	GLU	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)

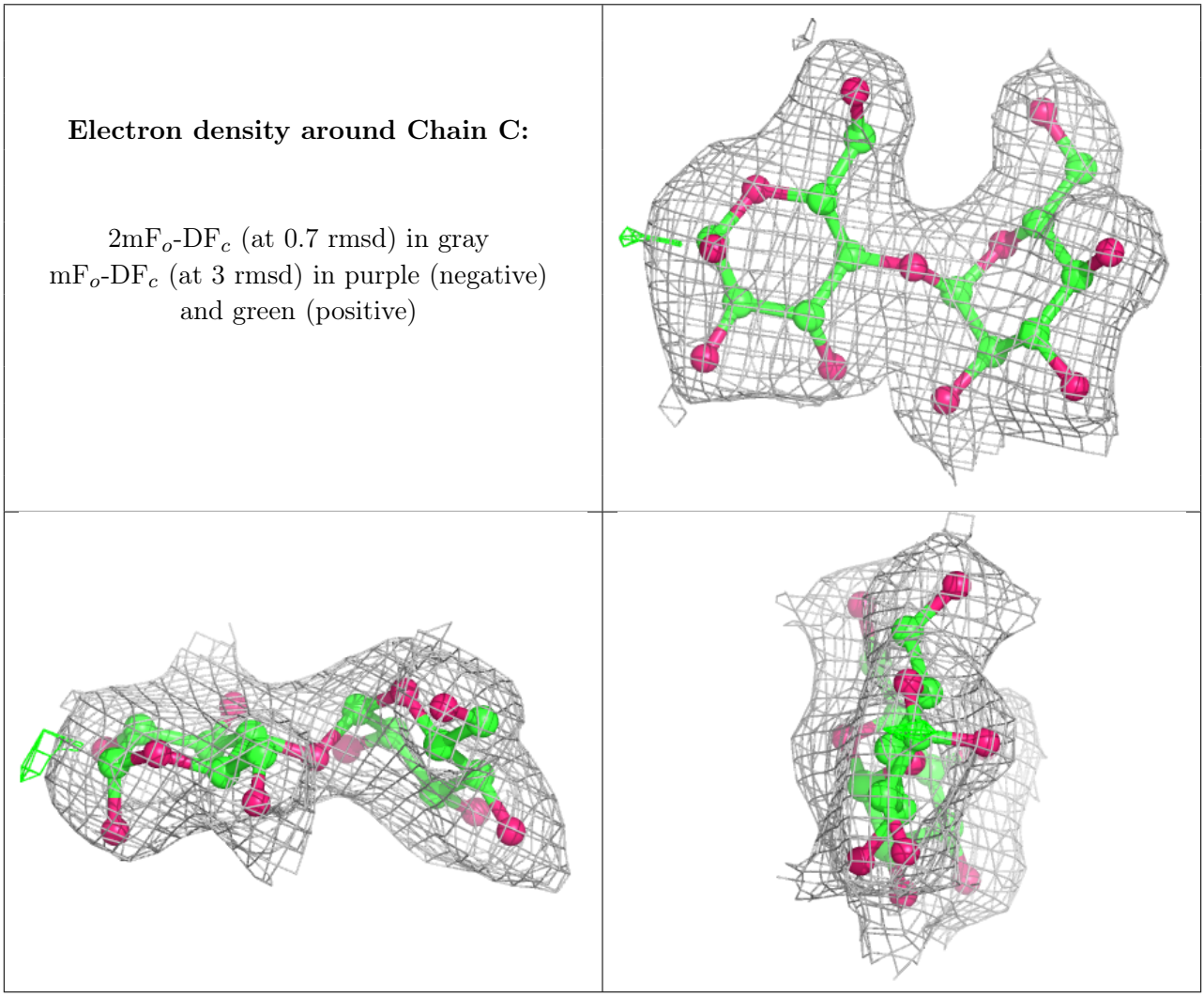
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GLC	D	1	12/12	0.94	0.17	46,53,58,58	0
2	GLC	D	2	11/12	0.94	0.22	42,51,53,54	0
2	GLC	C	1	12/12	0.97	0.25	20,25,27,33	0
2	GLC	C	2	11/12	0.99	0.23	16,17,18,18	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.

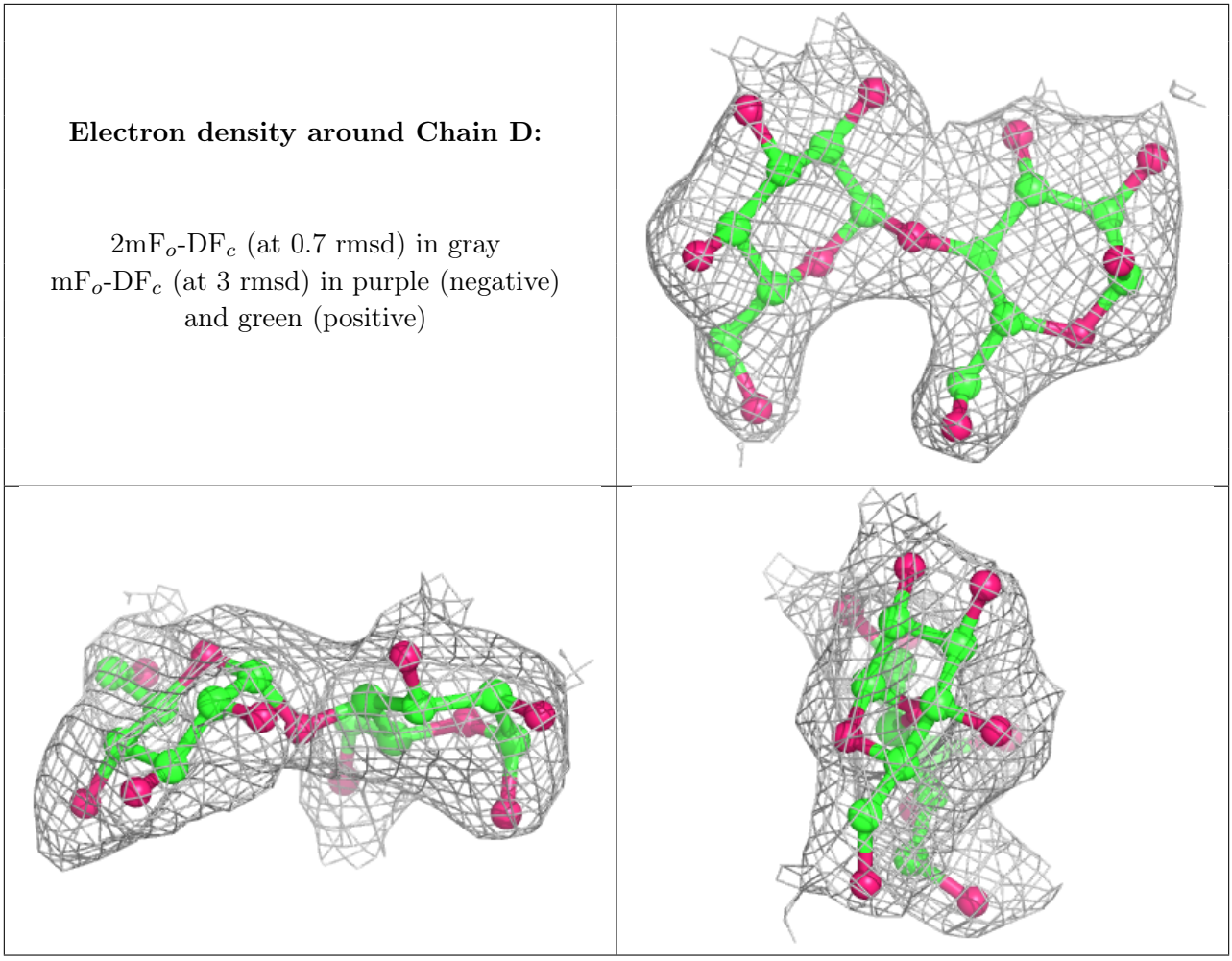
Electron density around Chain C:

$2mF_o$-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)



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, 95^{th} 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
3	ACT	A	1502	4/4	0.81	0.27	47,48,49,58	0
4	NA	A	1503	1/1	0.95	0.10	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.