



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 03:32 PM BST

PDB ID : 7CDX
Title : Complex STRUCTURE OF A NOVEL VIRULENCE REGULATION FACTOR SghR with its effector sucrose
Authors : Ye, F.Z.; Wang, C.; Yan, X.F.; Zhang, L.H.; Gao, Y.G.
Deposited on : 2020-06-20
Resolution : 2.10 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 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 : 2.14.2
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) : 2.14.2

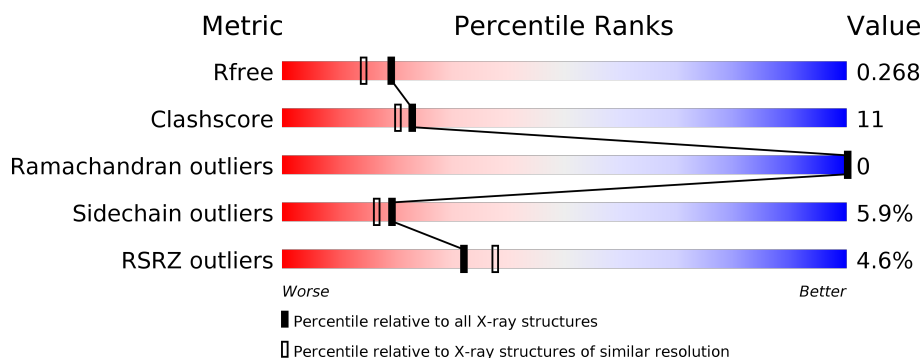
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	370	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>13%</div> <div>•</div> <div>26%</div> </div> </div>
1	B	370	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>15%</div> <div>•</div> <div>26%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	D	1	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4487 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 LacI-type transcription factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2123	1343	375	396	9			
1	B	272	Total	C	N	O	S	0	0	0
			2122	1343	374	396	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A0A2I4PGE9
A	-18	GLY	-	expression tag	UNP A0A2I4PGE9
A	-17	SER	-	expression tag	UNP A0A2I4PGE9
A	-16	SER	-	expression tag	UNP A0A2I4PGE9
A	-15	HIS	-	expression tag	UNP A0A2I4PGE9
A	-14	HIS	-	expression tag	UNP A0A2I4PGE9
A	-13	HIS	-	expression tag	UNP A0A2I4PGE9
A	-12	HIS	-	expression tag	UNP A0A2I4PGE9
A	-11	HIS	-	expression tag	UNP A0A2I4PGE9
A	-10	HIS	-	expression tag	UNP A0A2I4PGE9
A	-9	SER	-	expression tag	UNP A0A2I4PGE9
A	-8	SER	-	expression tag	UNP A0A2I4PGE9
A	-7	GLY	-	expression tag	UNP A0A2I4PGE9
A	-6	LEU	-	expression tag	UNP A0A2I4PGE9
A	-5	VAL	-	expression tag	UNP A0A2I4PGE9
A	-4	PRO	-	expression tag	UNP A0A2I4PGE9
A	-3	ARG	-	expression tag	UNP A0A2I4PGE9
A	-2	GLY	-	expression tag	UNP A0A2I4PGE9
A	-1	SER	-	expression tag	UNP A0A2I4PGE9
A	0	HIS	-	expression tag	UNP A0A2I4PGE9
B	-19	MET	-	expression tag	UNP A0A2I4PGE9
B	-18	GLY	-	expression tag	UNP A0A2I4PGE9
B	-17	SER	-	expression tag	UNP A0A2I4PGE9
B	-16	SER	-	expression tag	UNP A0A2I4PGE9
B	-15	HIS	-	expression tag	UNP A0A2I4PGE9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A0A2I4PGE9
B	-13	HIS	-	expression tag	UNP A0A2I4PGE9
B	-12	HIS	-	expression tag	UNP A0A2I4PGE9
B	-11	HIS	-	expression tag	UNP A0A2I4PGE9
B	-10	HIS	-	expression tag	UNP A0A2I4PGE9
B	-9	SER	-	expression tag	UNP A0A2I4PGE9
B	-8	SER	-	expression tag	UNP A0A2I4PGE9
B	-7	GLY	-	expression tag	UNP A0A2I4PGE9
B	-6	LEU	-	expression tag	UNP A0A2I4PGE9
B	-5	VAL	-	expression tag	UNP A0A2I4PGE9
B	-4	PRO	-	expression tag	UNP A0A2I4PGE9
B	-3	ARG	-	expression tag	UNP A0A2I4PGE9
B	-2	GLY	-	expression tag	UNP A0A2I4PGE9
B	-1	SER	-	expression tag	UNP A0A2I4PGE9
B	0	HIS	-	expression tag	UNP A0A2I4PGE9

- 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	89	Total	O	0	0
			89	89		
3	B	107	Total	O	0	0
			107	107		

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.

- Chain A:
-
- 4% 59% 13% 26%
- NET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL VAL PRO ARG ARG GLY SER HIS HIS ASN ASP THR GLY GLY SER SER GLY ASP GLY ALA LYS ALA THR THR GLY ARG ARG PRO THR LEU LYS THR THR ILE ALA TYR MET THR GLY LEU GLY ILE THR THR VAL SER ARG ALA LEU
- LYS ASP ALA PRO ASP ILE GLY ALA GLU THR LYS GLU ARG VAL ARG LEU ILE ALA GLN ILE GLY TYR GLN PRO ASN ARG ALA GLY VAL ARG LEU ARG THR G75 G76 T94 T97 P116 H119 A120 K121 L131 S135 S142 K143 D148 P149 R166 P177
- E181 A182 Y183 E189 R190 R196 V203 P204 P205 F208 R220 R225 A234 I235 T236 I237 E238 T239 P240 P241 L241 D242 R243 I244 R250 S254 D255 D256 R257 P258 D259 G260 I261 I264 S265 I270 A271 L272 E277 R282 I283 G284 K285 D286 I287 D288
- F297 L298 H299 W300 I301 Q302 P303 Q304 T307 R317 R340 S344 S345 R346 ALA PRO PRO LYS PRO

- Chain B:

Category	Count	Percentage
MET	3	3%
GLY	57	57%
ASP	1	1%
ALA	1	1%
SER	1	1%
PRO	1	1%
HIS	1	1%
LEU	1	1%
VAL	1	1%
ARG	1	1%
THR	1	1%
LYS	1	1%
ILE	1	1%
TYR	1	1%
MET	1	1%
GLY	1	1%
LEU	1	1%
GLY	1	1%
THR	1	1%
VAL	1	1%
SER	1	1%
ARG	1	1%
ALA	1	1%
LEU	1	1%

- Chain C:  100%

GLC1
FRU2

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

Chain D:



GLC1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	35.68Å 120.15Å 122.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.83 – 2.10 42.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.83-2.10) 99.5 (42.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.225 , 0.270 0.227 , 0.268	Depositor DCC
R_{free} test set	1567 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4487	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2976e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, 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	0.57	2/2167 (0.1%)	0.64	0/2934
1	B	0.54	0/2167	0.60	2/2937 (0.1%)
All	All	0.55	2/4334 (0.0%)	0.62	2/5871 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	TRP	CB-CG	-7.79	1.36	1.50
1	A	300	TRP	CE3-CZ3	-5.05	1.29	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	ILE	CB-CA-C	-5.83	99.93	111.60
1	B	166	ARG	NE-CZ-NH2	5.83	123.21	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2123	0	2126	53	0
1	B	2122	0	2122	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	23	0	21	4	0
2	D	23	0	21	2	0
3	A	89	0	0	2	0
3	B	107	0	0	7	0
All	All	4487	0	4290	98	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 11.

All (98) 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:203:VAL:O	1:A:236:THR:HG23	1.42	1.18
1:A:236:THR:HG22	1:A:237:ILE:H	1.16	1.09
1:A:283:ILE:HB	1:A:304:GLN:NE2	1.68	1.08
1:A:298:LEU:HA	1:A:301:ILE:HD13	1.33	1.08
1:A:282:ARG:HD3	1:A:285:LYS:HG3	1.41	0.99
1:A:236:THR:HG22	1:A:237:ILE:N	1.73	0.99
1:B:154:MET:SD	3:B:604:HOH:O	2.24	0.95
1:A:283:ILE:HB	1:A:304:GLN:HE21	1.29	0.95
1:A:236:THR:CG2	1:A:237:ILE:H	1.79	0.94
1:B:127:ILE:HG23	1:B:154:MET:HE3	1.52	0.91
1:B:244:ILE:HD11	3:B:501:HOH:O	1.76	0.83
1:A:297:PHE:O	1:A:301:ILE:HG23	1.80	0.81
1:A:283:ILE:CB	1:A:304:GLN:HE21	1.98	0.76
1:A:282:ARG:CD	1:A:285:LYS:HG3	2.16	0.75
1:A:283:ILE:HB	1:A:304:GLN:HG3	1.69	0.75
1:A:298:LEU:CA	1:A:301:ILE:HD13	2.15	0.74
1:A:237:ILE:HG13	1:A:265:SER:HB2	1.72	0.72
1:B:117:HIS:HE1	3:B:592:HOH:O	1.71	0.72
1:B:244:ILE:CD1	3:B:501:HOH:O	2.34	0.72
1:A:283:ILE:HB	1:A:304:GLN:CD	2.11	0.71
1:B:236:THR:HG23	1:B:238:GLU:H	1.54	0.70
1:A:283:ILE:CB	1:A:304:GLN:NE2	2.52	0.69
1:A:283:ILE:CG2	1:A:304:GLN:HG3	2.23	0.69
1:B:252:MET:O	1:B:257:ARG:CZ	2.40	0.68
1:B:211:HIS:NE2	3:B:504:HOH:O	2.25	0.68
1:A:297:PHE:O	1:A:301:ILE:CG2	2.42	0.68
1:A:283:ILE:HB	1:A:304:GLN:CG	2.23	0.67
1:B:77:THR:HG22	1:B:79:VAL:H	1.59	0.67
1:B:179:ASP:OD2	1:B:340:ARG:CZ	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:MET:O	1:B:257:ARG:NE	2.28	0.65
1:A:181:GLU:OE2	1:A:220:ARG:NH1	2.30	0.65
1:A:298:LEU:HA	1:A:301:ILE:CD1	2.21	0.64
1:A:283:ILE:CB	1:A:304:GLN:HG3	2.30	0.61
1:A:203:VAL:O	1:A:236:THR:CG2	2.34	0.60
3:A:525:HOH:O	2:C:1:GLC:H4	2.01	0.59
1:B:143:LYS:H	2:D:2:FRU:H62	1.68	0.59
3:A:504:HOH:O	2:C:1:GLC:H61	2.01	0.59
1:A:283:ILE:CG1	1:A:304:GLN:HE21	2.16	0.58
1:A:282:ARG:HD3	1:A:285:LYS:CG	2.26	0.58
1:A:301:ILE:HG13	1:B:301:ILE:HG23	1.84	0.58
1:A:166:ARG:NH1	1:A:177:ASP:HB3	2.19	0.57
1:B:235:ILE:HG22	1:B:239:THR:HG21	1.85	0.57
1:B:331:PRO:O	1:B:334:THR:HG22	2.04	0.56
1:A:236:THR:CG2	1:A:237:ILE:N	2.43	0.56
1:A:250:ARG:HB3	1:A:250:ARG:HH21	1.72	0.55
2:C:1:GLC:O5	2:C:2:FRU:H61	2.06	0.55
1:B:77:THR:N	3:B:512:HOH:O	2.40	0.54
1:B:179:ASP:OD2	1:B:340:ARG:NH2	2.41	0.54
1:B:261:ILE:HG12	1:B:287:ILE:HD11	1.90	0.53
1:B:77:THR:HG21	1:B:136:ALA:HA	1.90	0.53
1:A:240:PRO:O	1:A:244:ILE:HG12	2.10	0.51
1:B:93:PHE:HB3	1:B:96:GLN:HG3	1.92	0.51
1:B:77:THR:HB	1:B:137:ASP:OD1	2.10	0.51
1:A:270:ILE:HD11	1:A:301:ILE:HD12	1.94	0.50
1:B:308:VAL:HG23	1:B:343:TRP:CZ3	2.47	0.50
1:A:119:HIS:CE1	1:A:121:LYS:HB2	2.47	0.49
1:A:205:PRO:HD3	1:A:236:THR:HG21	1.94	0.49
1:A:196:ARG:NH1	1:A:288:ASP:OD2	2.35	0.48
1:A:237:ILE:HG13	1:A:265:SER:CB	2.41	0.48
1:B:317:ARG:O	1:B:321:LYS:HG3	2.13	0.48
1:B:179:ASP:OD2	1:B:340:ARG:NH1	2.46	0.48
1:B:175:TYR:CZ	1:B:336:GLN:HB3	2.49	0.47
1:B:148:ASP:H	1:B:169:MET:CE	2.28	0.47
1:B:236:THR:O	3:B:501:HOH:O	2.20	0.46
1:A:270:ILE:HD11	1:A:301:ILE:CD1	2.46	0.46
1:B:183:TYR:CE2	1:B:292:LYS:HG3	2.51	0.46
1:A:301:ILE:HB	1:B:301:ILE:HG21	1.98	0.46
1:B:307:THR:OG1	1:B:344:SER:HB3	2.16	0.46
1:B:196:ARG:NH1	1:B:288:ASP:OD2	2.44	0.46
1:A:237:ILE:HD12	1:A:237:ILE:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG11	1:B:302:GLN:HG3	1.99	0.45
1:B:143:LYS:N	2:D:2:FRU:H62	2.33	0.44
1:A:261:ILE:HG12	1:A:287:ILE:HD11	1.99	0.44
1:A:142:SER:HB2	2:C:2:FRU:O6	2.18	0.43
1:B:139:VAL:HG11	1:B:154:MET:HE1	2.00	0.43
1:B:164:HIS:HB2	1:B:319:LEU:HD11	2.00	0.43
1:A:239:THR:HB	1:A:244:ILE:HD11	2.00	0.43
1:A:282:ARG:HH11	1:A:282:ARG:HD3	1.63	0.43
1:A:116:PRO:HG3	1:B:102:THR:HB	2.01	0.42
1:A:283:ILE:HG22	1:A:304:GLN:HG3	1.98	0.42
1:A:148:ASP:HA	1:A:149:PRO:HD3	1.90	0.42
1:B:148:ASP:HA	1:B:149:PRO:HD3	1.86	0.42
1:B:131:LEU:HD21	1:B:159:MET:HB2	2.01	0.42
1:B:183:TYR:HE2	1:B:264:ILE:HD13	1.84	0.42
1:A:282:ARG:HH11	1:A:285:LYS:HG3	1.85	0.41
1:A:277:GLU:OE2	1:A:302:GLN:NE2	2.54	0.41
1:B:252:MET:HA	1:B:257:ARG:HD3	2.02	0.41
1:A:94:THR:HB	1:B:95:SER:HB3	2.02	0.41
1:B:167:SER:HB2	1:B:169:MET:HE2	2.01	0.41
1:B:277:GLU:OE2	1:B:302:GLN:NE2	2.53	0.41
1:A:189:GLU:HB2	1:A:225:PHE:CE2	2.55	0.41
1:A:183:TYR:HE2	1:A:264:ILE:HD13	1.85	0.40
1:B:301:ILE:H	1:B:301:ILE:HG13	1.42	0.40
1:A:205:PRO:CD	1:A:236:THR:HG21	2.50	0.40
1:B:290:VAL:CG1	1:B:343:TRP:HH2	2.35	0.40
1:A:143:LYS:HB3	1:A:208:PHE:CE1	2.57	0.40
1:A:307:THR:OG1	1:A:344:SER:HB3	2.22	0.40
1:B:307:THR:OG1	1:B:347:ALA:HB2	2.22	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	270/370 (73%)	261 (97%)	9 (3%)	0	100	100
1	B	270/370 (73%)	256 (95%)	14 (5%)	0	100	100
All	All	540/740 (73%)	517 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	230/308 (75%)	214 (93%)	16 (7%)	15	12
1	B	230/308 (75%)	219 (95%)	11 (5%)	25	24
All	All	460/616 (75%)	433 (94%)	27 (6%)	19	17

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LYS
1	A	97	MET
1	A	131	LEU
1	A	135	SER
1	A	190	ARG
1	A	196	ARG
1	A	237	ILE
1	A	242	ASP
1	A	250	ARG
1	A	257	ARG
1	A	259	ASP
1	A	272	LEU
1	A	282	ARG
1	A	301	ILE
1	A	317	ARG
1	A	340	ARG
1	B	77	THR
1	B	97	MET

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Mol	Chain	Res	Type
1	B	107	THR
1	B	131	LEU
1	B	196	ARG
1	B	242	ASP
1	B	245	ARG
1	B	272	LEU
1	B	301	ILE
1	B	312	ILE
1	B	334	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	GLN
1	B	117	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 ⓘ

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	0.66	0	15,15,17	2.32	5 (33%)
2	FRU	C	2	2	11,12,12	0.64	0	10,18,18	1.72	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	D	1	2	11,11,12	0.63	0	15,15,17	1.41	3 (20%)
2	FRU	D	2	2	11,12,12	0.72	0	10,18,18	1.43	1 (10%)

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	-	2/2/19/22	0/1/1/1
2	FRU	C	2	2	-	5/5/24/24	0/1/1/1
2	GLC	D	1	2	-	1/2/19/22	0/1/1/1
2	FRU	D	2	2	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C1-C2-C3	-6.36	101.85	109.67
2	C	2	FRU	C6-C5-C4	-3.04	107.76	115.09
2	C	1	GLC	O3-C3-C2	-2.94	104.36	109.99
2	C	1	GLC	O2-C2-C1	2.85	114.99	109.15
2	C	2	FRU	O2-C2-O5	-2.82	104.05	109.50
2	C	1	GLC	C3-C4-C5	2.79	115.21	110.24
2	D	2	FRU	O2-C2-O5	-2.55	104.57	109.50
2	D	1	GLC	O2-C2-C1	2.47	114.21	109.15
2	D	1	GLC	C3-C4-C5	2.45	114.60	110.24
2	C	1	GLC	O5-C5-C6	2.31	110.83	107.20
2	C	2	FRU	O4-C4-C3	2.13	118.54	112.15
2	D	1	GLC	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	FRU	O1-C1-C2-C3
2	C	2	FRU	O5-C5-C6-O6
2	C	2	FRU	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6

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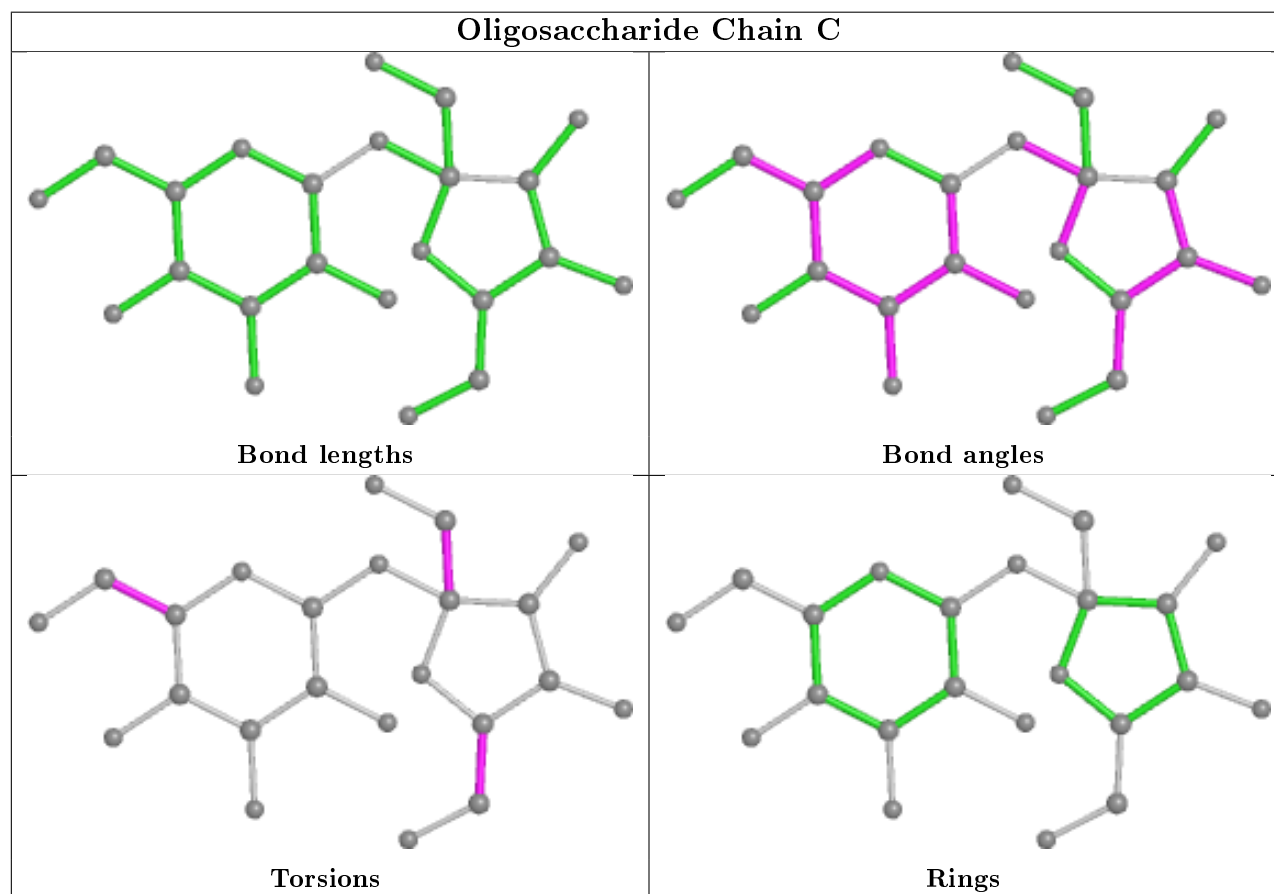
Mol	Chain	Res	Type	Atoms
2	C	2	FRU	O1-C1-C2-O5
2	D	1	GLC	O5-C5-C6-O6
2	D	2	FRU	O1-C1-C2-C3
2	D	2	FRU	O1-C1-C2-O5
2	C	2	FRU	O1-C1-C2-O2
2	D	2	FRU	O1-C1-C2-O2

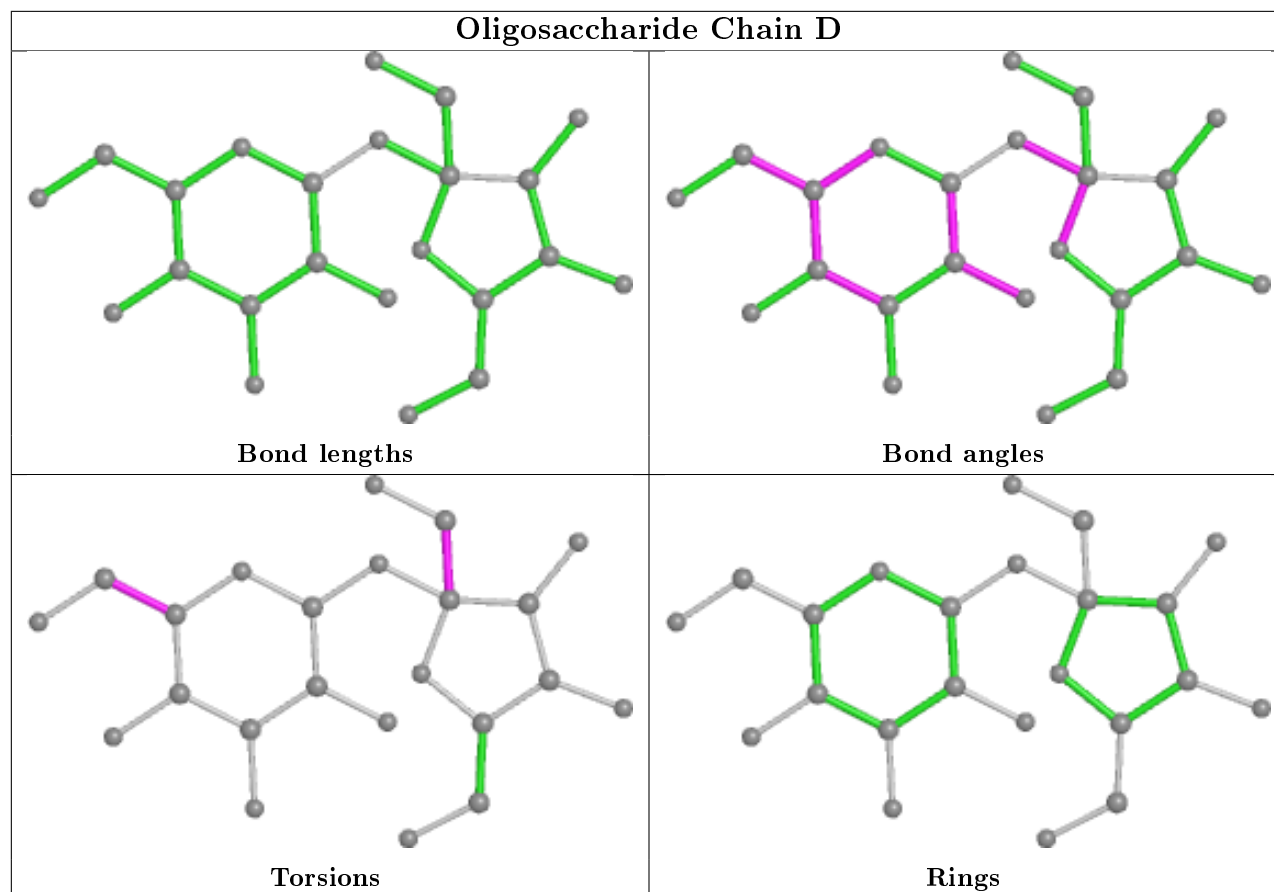
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	FRU	2	0
2	C	1	GLC	3	0
2	C	2	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.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 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	272/370 (73%)	0.10	13 (4%) 30 36	6, 20, 42, 54	0
1	B	272/370 (73%)	0.06	12 (4%) 34 40	6, 20, 39, 48	0
All	All	544/740 (73%)	0.08	25 (4%) 32 38	6, 20, 40, 54	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ASP	4.8
1	B	301	ILE	4.6
1	B	234	ALA	4.0
1	A	75	GLY	3.6
1	A	237	ILE	3.6
1	A	234	ALA	3.4
1	A	282	ARG	3.3
1	A	301	ILE	3.1
1	A	254	SER	3.0
1	B	233	ASP	2.9
1	A	250	ARG	2.7
1	B	282	ARG	2.7
1	B	257	ARG	2.6
1	B	242	ASP	2.5
1	B	204	PRO	2.5
1	B	237	ILE	2.5
1	A	304	GLN	2.5
1	A	76	LYS	2.5
1	B	256	ASP	2.4
1	B	250	ARG	2.3
1	A	204	PRO	2.2
1	B	255	ASP	2.1
1	A	285	LYS	2.1
1	A	345	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	345	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](#)

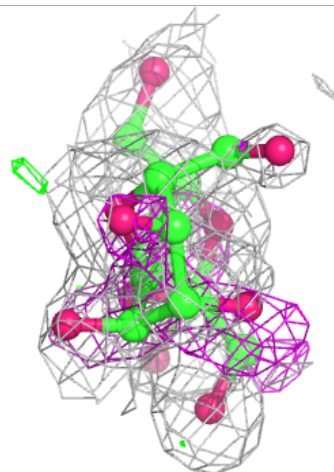
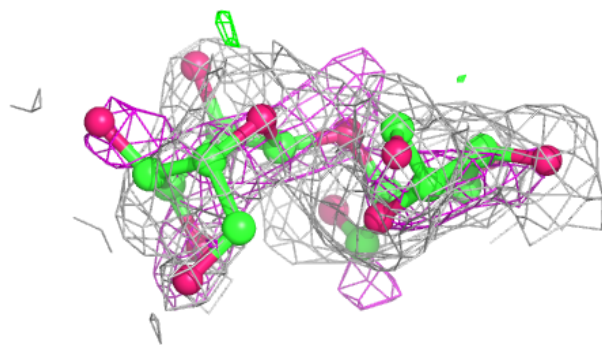
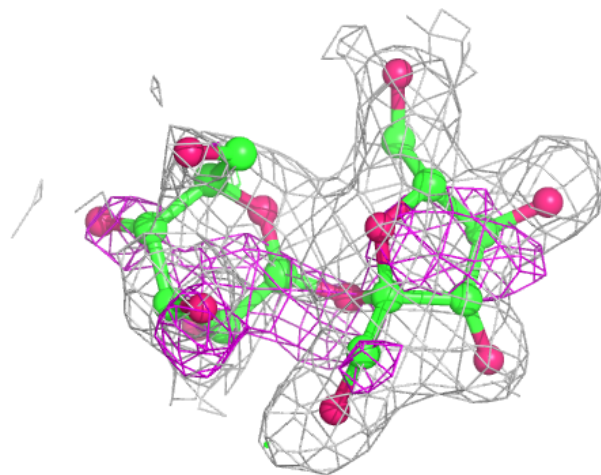
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

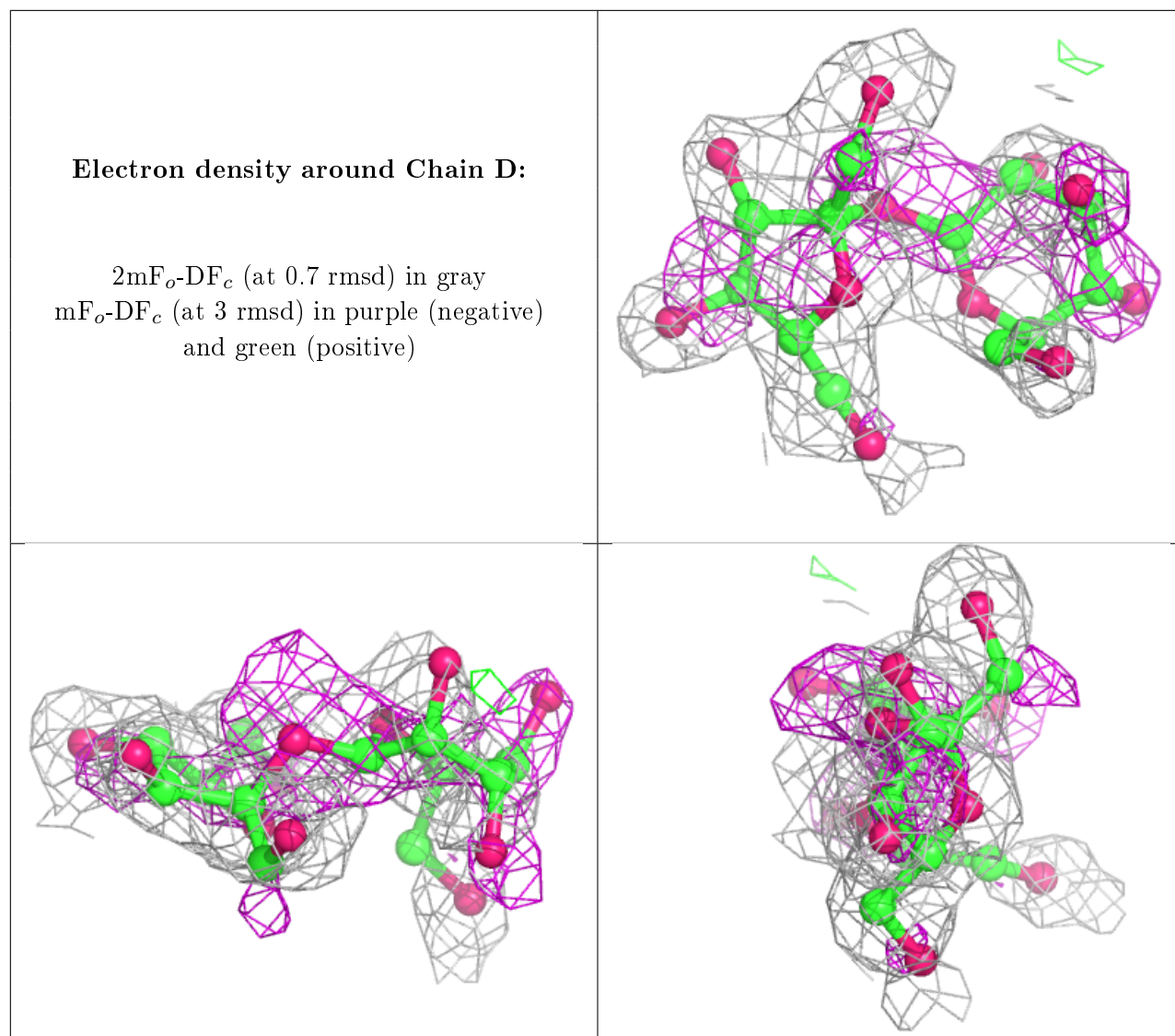
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	C	1	11/12	0.67	0.35	25,30,37,46	0
2	GLC	D	1	11/12	0.68	0.49	27,31,41,43	0
2	FRU	D	2	12/12	0.77	0.25	9,22,31,35	0
2	FRU	C	2	12/12	0.78	0.22	9,20,26,34	0

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.