



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:31 PM UTC

PDB ID : 4X06 / pdb_00004x06
Title : Crystal structure of P domain from norovirus strain Saga4 in complex with HBGA type B (triglycan)
Authors : Singh, B.K.; Hansman, G.S.
Deposited on : 2014-11-20
Resolution : 1.22 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

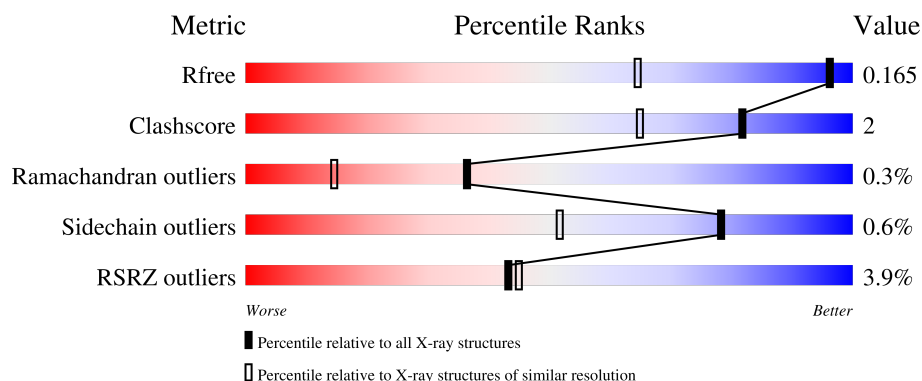
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.22 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

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	309	4% 66% 31% .
1	B	309	4% 65% 32% .
2	C	3	33% 33% 33%
2	D	3	33% 67%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10037 atoms, of which 4316 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.

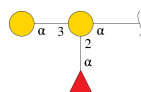
- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	H	N	O	S	0	8	0
			4605	1547	2168	417	463	10			
1	B	309	Total	C	H	N	O	S	0	9	0
			4576	1547	2148	409	462	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	THR	-	expression tag	UNP B5BTR7
A	223	GLY	-	expression tag	UNP B5BTR7
A	224	SER	-	expression tag	UNP B5BTR7
B	222	THR	-	expression tag	UNP B5BTR7
B	223	GLY	-	expression tag	UNP B5BTR7
B	224	SER	-	expression tag	UNP B5BTR7

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranoside-(1-3)]alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	3	0
			66	36	30			
2	D	3	Total	C	O	0	3	0
			66	36	30			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

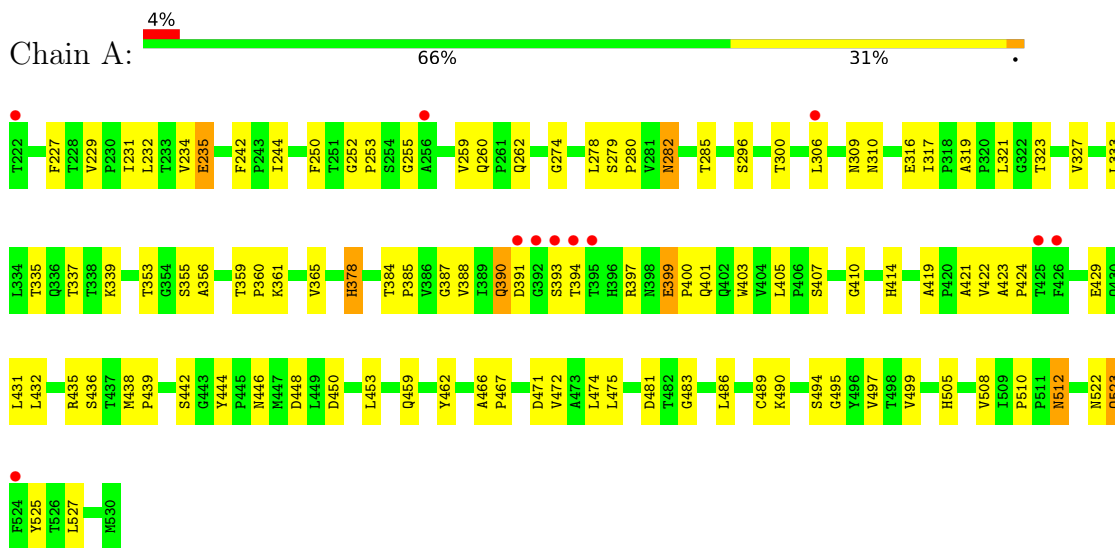
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	358	Total	O	0	0
			358	358		
4	B	358	Total	O	0	0
			358	358		

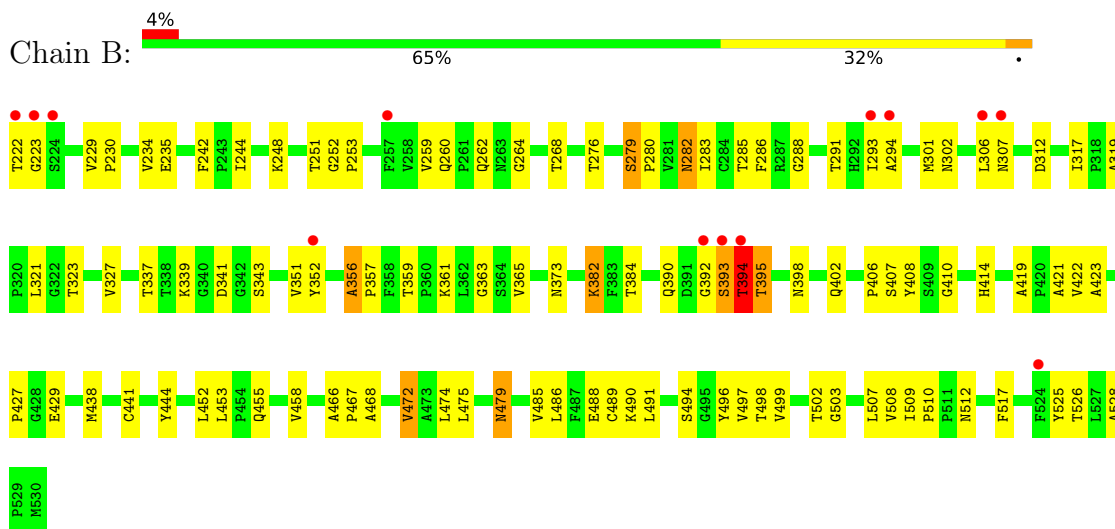
3 Residue-property plots

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.

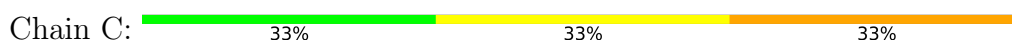
• Molecule 1: VP1



• Molecule 1: VP1



• Molecule 2: alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galactopyranose





- Molecule 2: alpha-L-fucopyranose-(1-2)-[alpha-D-galactopyranose-(1-3)]alpha-D-galactopyranoside

Chain D:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.83Å 58.65Å 97.31Å 90.00° 107.34° 90.00°	Depositor
Resolution (Å)	32.32 – 1.22 32.32 – 1.22	Depositor EDS
% Data completeness (in resolution range)	96.7 (32.32-1.22) 96.7 (32.32-1.22)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.22Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.134 , 0.161 0.146 , 0.165	Depositor DCC
R_{free} test set	8824 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10037	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 76.14 % 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 1.1028e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ACT, GLA, FUC

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	2.00	88/2515 (3.5%)	1.13	13/3442 (0.4%)
1	B	2.05	100/2510 (4.0%)	1.11	6/3438 (0.2%)
All	All	2.03	188/5025 (3.7%)	1.12	19/6880 (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	3
All	All	0	7

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	ILE	C-O	-15.43	1.13	1.24
1	A	356	ALA	C-O	-12.85	1.12	1.24
1	B	302[A]	ASN	CA-C	11.99	1.68	1.52
1	B	302[B]	ASN	CA-C	11.99	1.68	1.52
1	B	407[A]	SER	CA-C	11.84	1.67	1.52
1	B	407[B]	SER	CA-C	11.84	1.67	1.52
1	A	317	ILE	C-O	-11.47	1.15	1.24
1	B	244	ILE	C-O	-11.31	1.16	1.24
1	B	356	ALA	C-O	-10.91	1.14	1.24
1	B	422	VAL	C-O	-10.15	1.14	1.24
1	B	229	VAL	C-O	-9.81	1.12	1.24
1	B	352[A]	TYR	CA-C	9.37	1.65	1.53
1	B	352[B]	TYR	CA-C	9.37	1.65	1.53
1	B	242	PHE	C-O	-9.29	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	SER	C-O	-9.19	1.12	1.24
1	A	467	PRO	C-O	-9.17	1.13	1.23
1	A	384	THR	C-O	-9.14	1.14	1.24
1	B	497	VAL	C-O	-9.09	1.14	1.24
1	A	229	VAL	C-O	-8.89	1.13	1.24
1	B	419	ALA	C-O	-8.62	1.13	1.24
1	A	497	VAL	C-O	-8.53	1.15	1.24
1	A	235[A]	GLU	CA-C	8.42	1.64	1.52
1	A	235[B]	GLU	CA-C	8.42	1.64	1.52
1	B	317	ILE	C-O	-8.30	1.15	1.24
1	B	466	ALA	C-O	-8.25	1.13	1.24
1	B	359	THR	C-O	-8.18	1.14	1.23
1	A	424	PRO	C-O	-8.16	1.14	1.23
1	A	419	ALA	C-O	-8.07	1.13	1.24
1	B	510	PRO	C-O	-8.05	1.18	1.24
1	B	384	THR	C-O	-8.04	1.15	1.24
1	A	353	THR	C-O	-7.99	1.13	1.24
1	B	512	ASN	C-O	-7.77	1.13	1.24
1	A	323	THR	C-O	-7.73	1.14	1.24
1	A	390	GLN	CA-C	7.46	1.61	1.52
1	B	444	TYR	C-O	-7.44	1.15	1.24
1	B	260	GLN	C-O	-7.43	1.14	1.24
1	A	423	ALA	C-O	-7.42	1.14	1.24
1	A	260	GLN	C-O	-7.40	1.14	1.24
1	B	253	PRO	C-O	-7.40	1.15	1.23
1	B	499	VAL	C-O	-7.33	1.15	1.23
1	B	453	LEU	C-O	-7.29	1.15	1.24
1	B	234	VAL	C-O	-7.28	1.15	1.24
1	A	444	TYR	C-O	-7.25	1.15	1.24
1	B	438	MET	C-O	-7.19	1.14	1.24
1	B	264	GLY	C-O	-7.15	1.16	1.24
1	A	242	PHE	C-O	-7.13	1.15	1.24
1	A	438	MET	C-O	-7.05	1.14	1.24
1	B	474	LEU	C-O	-7.02	1.15	1.24
1	A	359	THR	C-O	-6.97	1.15	1.23
1	A	327	VAL	C-O	-6.94	1.16	1.24
1	B	339	LYS	C-O	-6.88	1.16	1.24
1	B	323	THR	C-O	-6.87	1.15	1.24
1	B	312	ASP	C-O	-6.85	1.16	1.24
1	B	408	TYR	C-O	-6.85	1.15	1.24
1	A	252	GLY	C-O	-6.83	1.14	1.24
1	B	279	SER	C-O	-6.83	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	GLY	C-O	-6.79	1.15	1.23
1	A	259	VAL	C-O	-6.78	1.14	1.23
1	A	410	GLY	C-O	-6.77	1.16	1.24
1	A	510	PRO	C-O	-6.77	1.17	1.24
1	B	525	TYR	C-O	-6.76	1.15	1.23
1	B	319	ALA	C-O	-6.73	1.15	1.24
1	B	365	VAL	C-O	-6.68	1.16	1.23
1	B	406	PRO	C-O	-6.60	1.16	1.23
1	A	453	LEU	C-O	-6.57	1.16	1.24
1	B	285	THR	C-O	-6.53	1.15	1.23
1	A	525	TYR	C-O	-6.52	1.16	1.23
1	A	459	GLN	C-O	-6.48	1.16	1.24
1	A	296	SER	C-O	-6.47	1.16	1.23
1	A	499	VAL	C-O	-6.47	1.16	1.23
1	A	319	ALA	C-O	-6.47	1.16	1.24
1	B	475	LEU	C-O	-6.45	1.16	1.24
1	B	455	GLN	C-O	-6.44	1.16	1.24
1	B	363	GLY	C-O	-6.42	1.15	1.24
1	B	423	ALA	C-O	-6.38	1.16	1.24
1	B	321	LEU	C-O	-6.36	1.16	1.23
1	B	526	THR	C-O	-6.35	1.16	1.24
1	B	489	CYS	C-O	-6.34	1.16	1.23
1	A	407	SER	C-O	-6.30	1.15	1.23
1	A	401	GLN	C-O	-6.29	1.16	1.23
1	A	512[A]	ASN	CA-C	6.28	1.61	1.52
1	A	512[B]	ASN	CA-C	6.28	1.61	1.52
1	A	300	THR	C-O	-6.25	1.16	1.24
1	A	522	ASN	C-O	-6.25	1.15	1.23
1	A	255	GLY	C-O	-6.23	1.15	1.24
1	A	361	LYS	C-O	-6.20	1.16	1.24
1	A	431	LEU	C-O	-6.20	1.16	1.23
1	B	429	GLU	C-O	-6.17	1.16	1.23
1	B	337	THR	C-O	-6.17	1.16	1.24
1	B	458	VAL	C-O	-6.15	1.17	1.24
1	A	339	LYS	C-O	-6.15	1.17	1.24
1	B	502	THR	C-O	-6.15	1.17	1.24
1	B	509	ILE	C-O	-6.14	1.16	1.24
1	A	232	LEU	C-O	-6.13	1.16	1.23
1	A	475	LEU	C-O	-6.13	1.16	1.23
1	A	227	PHE	C-O	-6.11	1.16	1.23
1	B	286	PHE	C-O	-6.09	1.16	1.23
1	A	422	VAL	C-O	-6.08	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	PHE	C-O	-6.07	1.16	1.23
1	A	446	ASN	C-O	-6.05	1.16	1.24
1	B	479	ASN	C-O	-6.03	1.16	1.24
1	B	283	ILE	C-O	-6.02	1.17	1.24
1	B	498	THR	C-O	-6.01	1.16	1.23
1	A	466	ALA	C-O	-6.01	1.16	1.24
1	A	489	CYS	C-O	-5.99	1.16	1.23
1	A	421	ALA	C-O	-5.96	1.16	1.23
1	A	231	ILE	C-O	-5.95	1.17	1.24
1	A	321	LEU	C-O	-5.95	1.16	1.23
1	B	276	THR	C-O	-5.94	1.16	1.23
1	B	488	GLU	C-O	-5.92	1.16	1.23
1	A	399	GLU	C-O	-5.92	1.16	1.24
1	B	252	GLY	C-O	-5.87	1.16	1.24
1	B	517	PHE	C-O	-5.84	1.17	1.23
1	B	398	ASN	C-O	-5.84	1.16	1.24
1	A	378	HIS	C-O	-5.78	1.16	1.23
1	A	474	LEU	C-O	-5.75	1.17	1.24
1	B	343	SER	C-O	-5.72	1.16	1.23
1	B	291	THR	C-O	-5.70	1.17	1.24
1	B	507	LEU	C-O	-5.67	1.17	1.23
1	A	486	LEU	C-O	-5.65	1.17	1.24
1	A	405	LEU	C-O	-5.64	1.16	1.24
1	B	288	GLY	C-O	-5.63	1.16	1.24
1	A	387	GLY	C-O	-5.59	1.17	1.23
1	B	268	THR	C-O	-5.58	1.16	1.24
1	A	385	PRO	C-O	-5.58	1.17	1.23
1	A	435	ARG	C-O	-5.57	1.17	1.24
1	B	494	SER	C-O	-5.57	1.16	1.24
1	A	429	GLU	C-O	-5.57	1.17	1.23
1	A	360	PRO	C-O	-5.55	1.17	1.24
1	A	439	PRO	C-O	-5.55	1.17	1.23
1	A	335	THR	C-O	-5.55	1.16	1.23
1	A	253	PRO	C-O	-5.54	1.17	1.23
1	A	508	VAL	C-O	-5.53	1.18	1.24
1	A	448	ASP	C-O	-5.52	1.17	1.23
1	B	230	PRO	C-O	-5.51	1.17	1.23
1	B	486	LEU	C-O	-5.51	1.17	1.24
1	A	365	VAL	C-O	-5.50	1.17	1.23
1	B	307	ASN	C-O	-5.50	1.16	1.24
1	A	450	ASP	C-O	-5.46	1.17	1.24
1	B	293	ILE	C-O	-5.46	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	421	ALA	C-O	-5.45	1.17	1.23
1	B	467	PRO	C-O	-5.43	1.17	1.23
1	B	441	CYS	C-O	-5.42	1.16	1.24
1	A	309	ASN	C-O	-5.42	1.16	1.23
1	B	373	ASN	C-O	-5.41	1.17	1.23
1	B	327	VAL	C-O	-5.40	1.18	1.24
1	A	442	SER	C-O	-5.37	1.17	1.24
1	A	316	GLU	C-O	-5.37	1.17	1.23
1	B	361	LYS	C-O	-5.36	1.17	1.24
1	B	235	GLU	C-O	-5.34	1.17	1.24
1	B	496	TYR	C-O	-5.34	1.17	1.23
1	B	414	HIS	C-O	-5.33	1.17	1.23
1	A	527	LEU	C-O	-5.32	1.17	1.23
1	A	414	HIS	C-O	-5.32	1.17	1.23
1	B	351	VAL	CA-C	-5.31	1.46	1.52
1	B	472	VAL	C-O	-5.30	1.18	1.24
1	A	432	LEU	C-O	-5.26	1.17	1.24
1	B	395	THR	C-O	-5.25	1.17	1.23
1	B	508	VAL	C-O	-5.25	1.18	1.24
1	B	427	PRO	C-O	-5.24	1.17	1.23
1	B	259	VAL	C-O	-5.24	1.16	1.23
1	A	436	SER	C-O	-5.23	1.17	1.23
1	A	337	THR	C-O	-5.22	1.17	1.24
1	B	262	GLN	C-O	-5.21	1.17	1.23
1	A	388	VAL	C-O	-5.21	1.18	1.24
1	B	390	GLN	CA-C	5.20	1.59	1.52
1	B	468	ALA	C-O	-5.19	1.17	1.23
1	A	523	GLN	C-O	-5.19	1.17	1.24
1	B	294	ALA	C-O	-5.18	1.17	1.23
1	B	407[A]	SER	N-CA	5.18	1.53	1.46
1	B	407[B]	SER	N-CA	5.18	1.53	1.46
1	B	251	THR	C-O	-5.18	1.17	1.23
1	B	491	LEU	C-O	-5.17	1.17	1.23
1	B	341	ASP	C-O	-5.14	1.17	1.24
1	A	355	SER	C-O	-5.14	1.17	1.23
1	A	262	GLN	C-O	-5.13	1.17	1.23
1	A	495	GLY	C-O	-5.12	1.17	1.23
1	A	274	GLY	C-O	-5.10	1.17	1.24
1	B	452	LEU	C-O	-5.10	1.17	1.24
1	A	483	GLY	C-O	-5.10	1.17	1.24
1	A	505	HIS	C-O	-5.10	1.18	1.23
1	A	403	TRP	C-O	-5.07	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	VAL	C-O	-5.07	1.18	1.24
1	B	503	GLY	C-O	-5.04	1.18	1.23
1	A	494	SER	C-O	-5.04	1.17	1.24
1	B	402	GLN	C-O	-5.01	1.17	1.24
1	B	528	ALA	C-O	-5.01	1.17	1.24
1	B	382	LYS	C-O	-5.01	1.17	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512[A]	ASN	CA-C-O	9.74	131.06	119.28
1	A	512[B]	ASN	CA-C-O	9.74	131.06	119.28
1	A	235[A]	GLU	CA-C-O	8.95	130.32	119.49
1	A	235[B]	GLU	CA-C-O	8.95	130.32	119.49
1	A	512[A]	ASN	N-CA-C	8.58	123.80	113.16
1	A	512[B]	ASN	N-CA-C	8.58	123.80	113.16
1	A	235[A]	GLU	N-CA-C	7.98	122.12	112.38
1	A	235[B]	GLU	N-CA-C	7.98	122.12	112.38
1	B	301	MET	CA-C-O	7.63	128.71	120.32
1	A	280	PRO	N-CA-C	-7.31	104.72	113.86
1	B	280	PRO	N-CA-C	-7.29	104.74	113.86
1	A	279	SER	CA-C-O	6.83	124.72	119.46
1	B	351	VAL	CA-C-O	6.12	126.81	120.39
1	B	302[A]	ASN	CA-C-O	6.00	127.46	120.98
1	B	302[B]	ASN	CA-C-O	6.00	127.46	120.98
1	A	397	ARG	NE-CZ-NH2	-5.97	113.82	119.20
1	A	234	VAL	CA-C-O	5.29	126.77	121.17
1	B	406	PRO	CA-C-O	5.24	128.79	122.08
1	A	397	ARG	NE-CZ-NH1	5.15	126.65	121.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282[B]	ASN	Mainchain
1	A	390	GLN	Peptide
1	A	393[A]	SER	Peptide
1	A	394[A]	THR	Mainchain
1	B	282[A]	ASN	Mainchain
1	B	282[B]	ASN	Mainchain
1	B	394[A]	THR	Mainchain

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	2437	2168	2327	12	1
1	B	2428	2148	2312	11	1
2	C	66	0	60	1	0
2	D	66	0	60	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	358	0	0	3	0
4	B	358	0	0	4	1
All	All	5721	4316	4765	24	2

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 2.

All (24) 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:282[B]:ASN:OD1	4:A:1028:HOH:O	1.89	0.90
1:A:310:ASN:ND2	4:A:701:HOH:O	2.17	0.73
1:A:282[B]:ASN:HD21	1:A:306:LEU:HD13	1.56	0.71
4:A:713:HOH:O	2:C:3[B]:GLA:H2	1.91	0.69
1:B:223:GLY:HA2	4:B:771:HOH:O	2.01	0.60
1:B:248:LYS:NZ	4:B:1024:HOH:O	2.36	0.59
1:A:481:ASP:OD1	1:A:512[B]:ASN:ND2	2.37	0.56
1:A:282[B]:ASN:HD21	1:A:306:LEU:CD1	2.19	0.56
1:A:282[B]:ASN:ND2	1:A:306:LEU:HD13	2.23	0.53
1:A:278:LEU:HD11	1:A:462:TYR:CE2	2.46	0.51
1:A:471:ASP:OD2	1:A:523:GLN:OE1	2.30	0.49
1:B:279:SER:HB3	1:B:282[B]:ASN:HB2	1.93	0.49
1:B:356:ALA:HB3	1:B:357:PRO:HD3	1.95	0.48
1:B:282[B]:ASN:HD21	1:B:306:LEU:HD13	1.80	0.47
1:A:235[B]:GLU:H	1:A:235[B]:GLU:CD	2.22	0.47
1:B:392[B]:GLY:O	1:B:393[B]:SER:C	2.59	0.46
1:B:222:THR:N	4:B:702:HOH:O	2.50	0.44
1:A:282[B]:ASN:O	1:A:285:THR:OG1	2.35	0.43
1:B:382:LYS:HD2	4:B:1023:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:HA	1:A:400:PRO:C	2.44	0.43
1:B:356:ALA:N	1:B:357:PRO:CD	2.82	0.42
1:B:472:VAL:HG11	1:B:490:LYS:HG2	2.02	0.41
1:A:472:VAL:HG11	1:A:490:LYS:HG2	2.02	0.41
1:B:393[B]:SER:O	1:B:394[B]:THR:CB	2.70	0.40

All (2) 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)
1:A:378:HIS:HB3	1:B:479:ASN:HD21[4_955]	1.31	0.29
4:B:749:HOH:O	4:B:755:HOH:O[2_1056]	2.15	0.05

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	315/309 (102%)	309 (98%)	6 (2%)	0	100	100
1	B	316/309 (102%)	307 (97%)	5 (2%)	4 (1%)	9	1
All	All	631/618 (102%)	616 (98%)	11 (2%)	4 (1%)	36	4

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	393[A]	SER
1	B	393[B]	SER
1	B	394[A]	THR
1	B	394[B]	THR

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	270/268 (101%)	267 (99%)	3 (1%)	65	32
1	B	268/268 (100%)	267 (100%)	1 (0%)	84	63
All	All	538/536 (100%)	534 (99%)	4 (1%)	78	47

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

Mol	Chain	Res	Type
1	A	333	LEU
1	A	391[A]	ASP
1	A	391[B]	ASP
1	B	395	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	263	ASN

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](#)

12 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	GLA	C	1[A]	2	12,12,12	0.46	0	17,17,17	0.87	1 (5%)
2	GLA	C	1[B]	2	12,12,12	0.53	0	17,17,17	0.94	1 (5%)
2	FUC	C	2[A]	2	10,10,11	0.75	0	14,14,16	0.73	0
2	FUC	C	2[B]	2	10,10,11	0.29	0	14,14,16	0.58	0
2	GLA	C	3[A]	2	11,11,12	0.70	0	15,15,17	0.89	1 (6%)
2	GLA	C	3[B]	2	11,11,12	0.77	0	15,15,17	1.08	1 (6%)
2	GLA	D	1[A]	2	12,12,12	0.52	0	17,17,17	0.96	1 (5%)
2	GLA	D	1[B]	2	12,12,12	0.53	0	17,17,17	0.96	1 (5%)
2	FUC	D	2[A]	2	10,10,11	0.74	0	14,14,16	0.71	0
2	FUC	D	2[B]	2	10,10,11	0.29	0	14,14,16	0.58	0
2	GLA	D	3[A]	2	11,11,12	0.69	0	15,15,17	1.07	1 (6%)
2	GLA	D	3[B]	2	11,11,12	0.79	0	15,15,17	1.12	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	GLA	C	1[A]	2	-	2/2/22/22	0/1/1/1
2	GLA	C	1[B]	2	-	1/2/22/22	0/1/1/1
2	FUC	C	2[A]	2	-	-	0/1/1/1
2	FUC	C	2[B]	2	-	-	0/1/1/1
2	GLA	C	3[A]	2	-	0/2/19/22	0/1/1/1
2	GLA	C	3[B]	2	-	1/2/19/22	0/1/1/1
2	GLA	D	1[A]	2	-	1/2/22/22	0/1/1/1
2	GLA	D	1[B]	2	-	0/2/22/22	0/1/1/1
2	FUC	D	2[A]	2	-	-	0/1/1/1
2	FUC	D	2[B]	2	-	-	0/1/1/1
2	GLA	D	3[A]	2	-	0/2/19/22	0/1/1/1
2	GLA	D	3[B]	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3[B]	GLA	C1-O5-C5	-3.58	107.39	112.19
2	C	3[B]	GLA	C1-O5-C5	-3.22	107.88	112.19
2	D	3[A]	GLA	C1-O5-C5	-3.12	108.00	112.19
2	C	1[B]	GLA	C1-O5-C5	-3.10	107.65	113.65
2	D	1[B]	GLA	C1-O5-C5	-3.08	107.68	113.65
2	C	3[A]	GLA	C2-C3-C4	-2.34	106.74	110.86
2	D	1[A]	GLA	C6-C5-C4	-2.10	107.85	113.02
2	C	1[A]	GLA	O3-C3-C2	-2.02	105.62	110.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

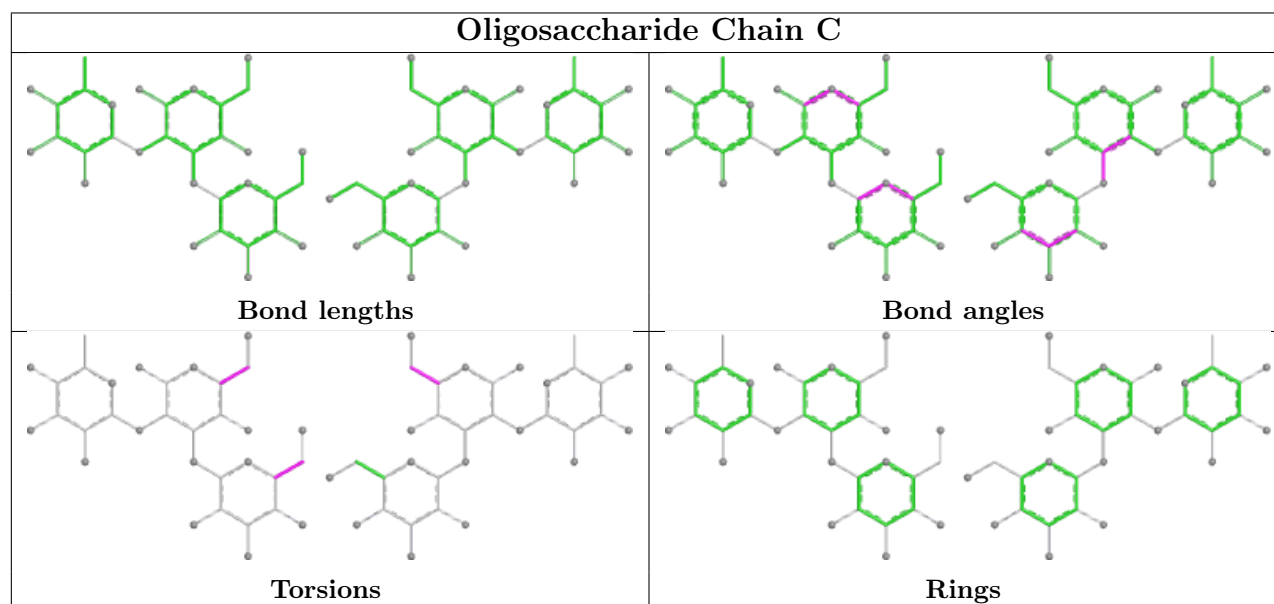
Mol	Chain	Res	Type	Atoms
2	C	1[A]	GLA	O5-C5-C6-O6
2	C	1[A]	GLA	C4-C5-C6-O6
2	C	1[B]	GLA	O5-C5-C6-O6
2	D	1[A]	GLA	C4-C5-C6-O6
2	C	3[B]	GLA	C4-C5-C6-O6

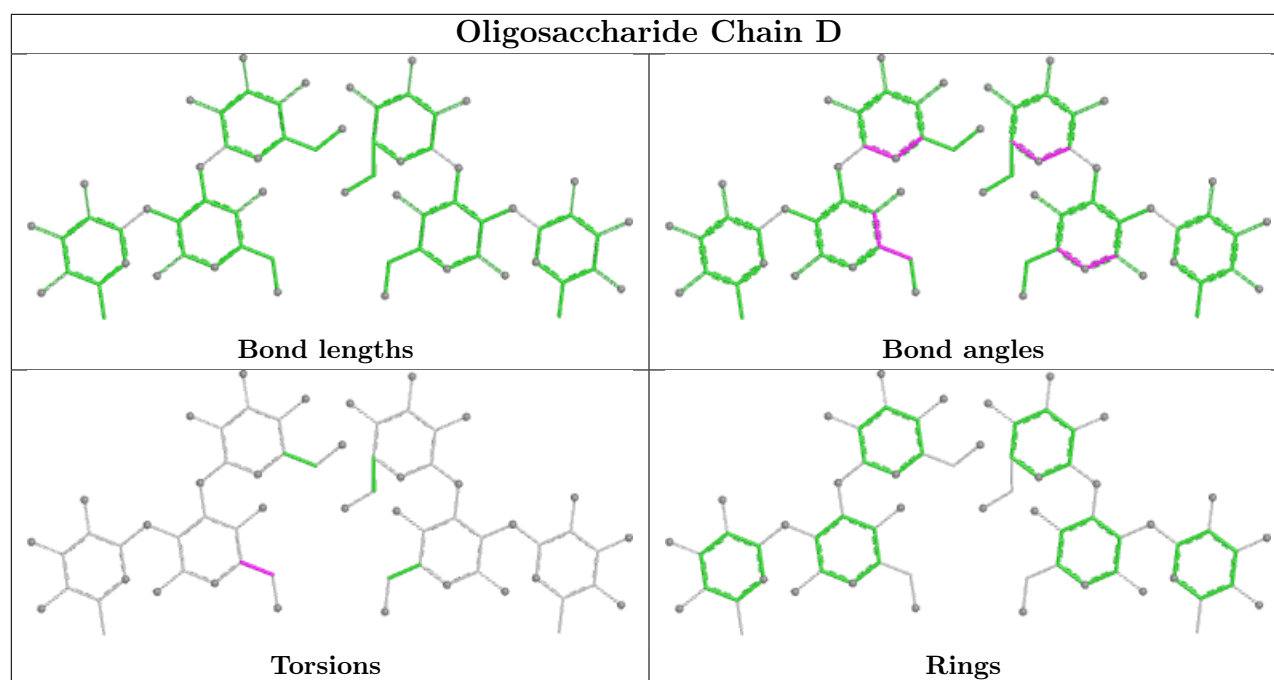
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3[B]	GLA	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](#)

2 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	$\# Z > 2$
3	ACT	B	604	-	3,3,3	1.08	0	3,3,3	0.78	0
3	ACT	A	604	-	3,3,3	0.70	0	3,3,3	1.53	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	ACT	OXT-C-CH3	2.03	123.58	115.05

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

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	309/309 (100%)	-0.14	11 (3%)	46	47	6, 16, 28, 38	8 (2%)
1	B	309/309 (100%)	-0.15	13 (4%)	40	42	5, 15, 29, 44	9 (2%)
All	All	618/618 (100%)	-0.15	24 (3%)	43	45	5, 16, 29, 44	17 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394[A]	THR	6.7
1	A	392[A]	GLY	6.2
1	A	393[A]	SER	6.2
1	B	306	LEU	5.4
1	A	394[A]	THR	5.3
1	B	393[A]	SER	5.0
1	A	391[A]	ASP	4.7
1	A	306	LEU	4.6
1	B	222	THR	4.5
1	B	392[A]	GLY	4.4
1	B	524	PHE	2.8
1	A	425	THR	2.7
1	B	352[A]	TYR	2.5
1	B	307	ASN	2.3
1	B	223	GLY	2.3
1	A	426	PHE	2.2
1	A	395	THR	2.2
1	B	224	SER	2.2
1	B	294	ALA	2.2
1	A	524	PHE	2.1
1	A	256	ALA	2.1
1	B	257	PHE	2.1
1	B	293	ILE	2.1
1	A	222	THR	2.0

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

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

6.3 Carbohydrates ⓘ

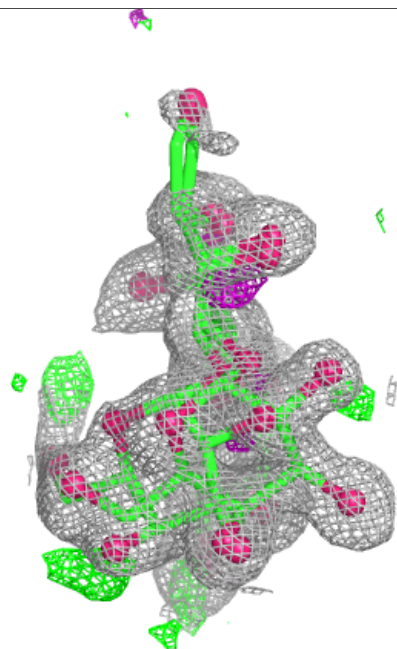
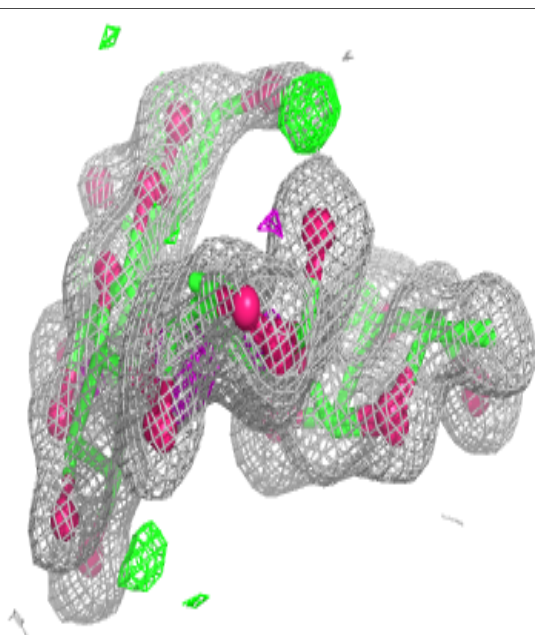
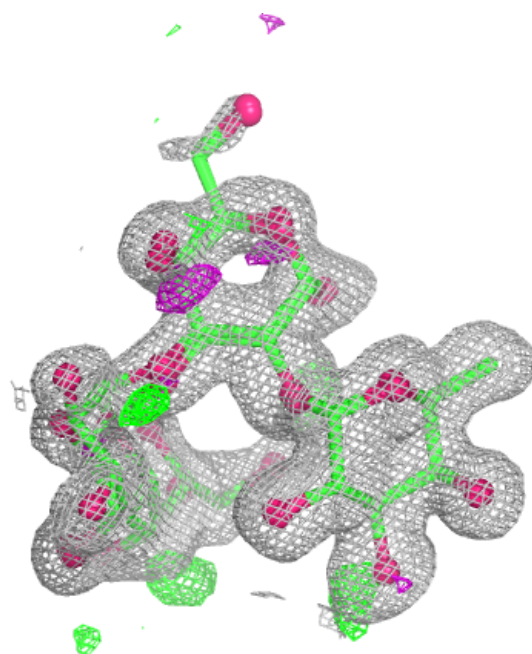
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

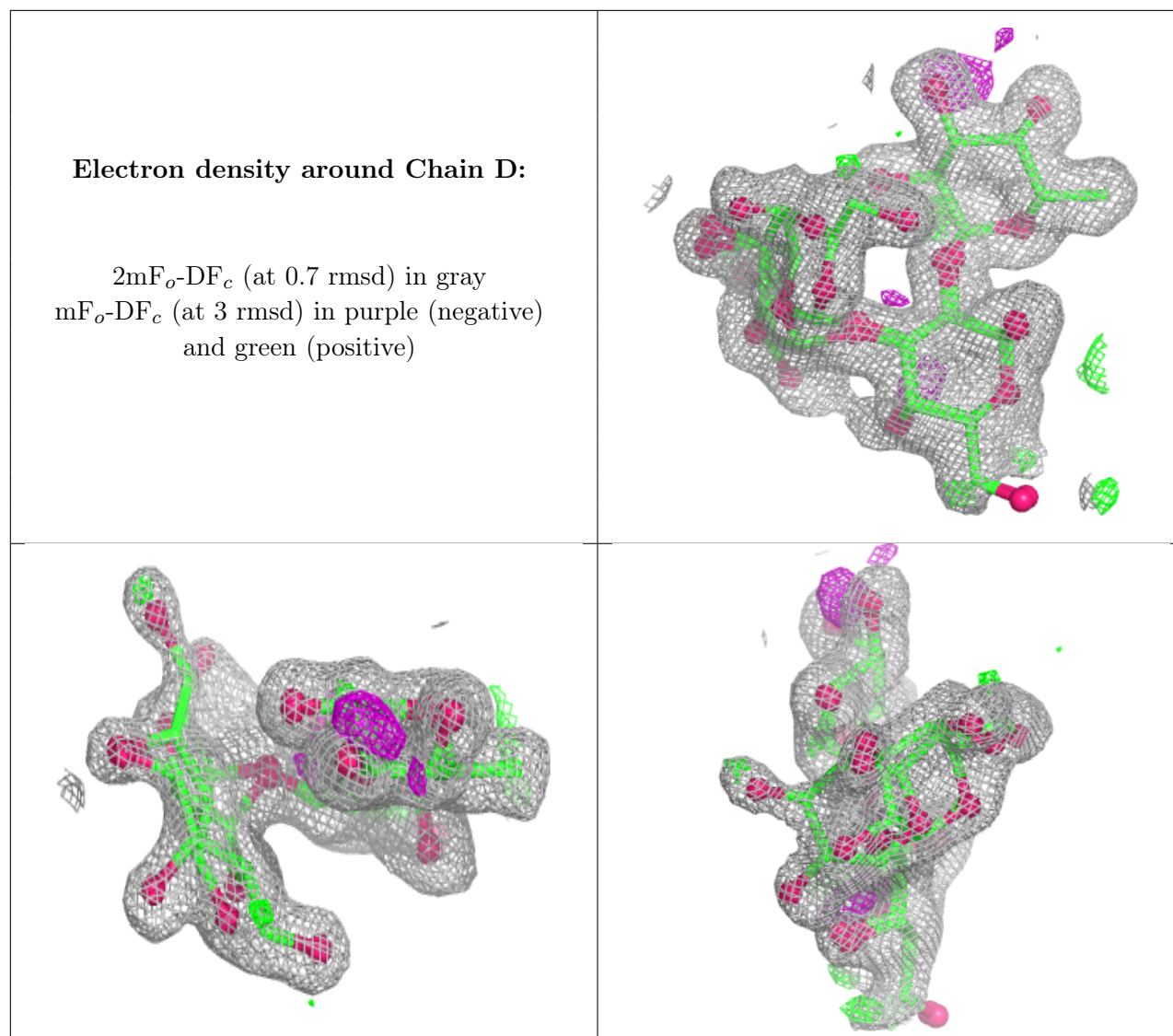
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLA	D	3[A]	11/12	0.79	0.17	20,34,38,41	11
2	GLA	D	3[B]	11/12	0.79	0.17	28,33,40,41	11
2	GLA	D	1[A]	12/12	0.84	0.14	23,39,44,50	12
2	GLA	D	1[B]	12/12	0.84	0.14	35,39,44,47	12
2	FUC	D	2[A]	10/11	0.90	0.11	20,23,26,29	10
2	FUC	D	2[B]	10/11	0.90	0.11	17,18,20,23	10
2	GLA	C	3[A]	11/12	0.91	0.10	17,21,28,33	11
2	GLA	C	3[B]	11/12	0.91	0.10	23,25,29,33	11
2	GLA	C	1[A]	12/12	0.92	0.11	17,26,39,46	12
2	GLA	C	1[B]	12/12	0.92	0.11	22,26,38,44	12
2	FUC	C	2[A]	10/11	0.96	0.07	14,16,17,28	10
2	FUC	C	2[B]	10/11	0.96	0.07	13,14,15,16	10

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](#)

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
3	ACT	A	604	4/4	0.88	0.12	23,27,28,31	0
3	ACT	B	604	4/4	0.90	0.12	24,26,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.