



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:31 AM UTC

PDB ID : 5F7Y / pdb_00005f7y
Title : Blood group antigen binding adhesin BabA of Helicobacter pylori strain 17875
in complex with blood group A type-1 hexasaccharide
Authors : Moonens, K.; Gideonsson, P.; Subedi, S.; Romao, E.; Oscarson, S.; Muylder-
mans, S.; Boren, T.; Remaut, H.
Deposited on : 2015-12-08
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

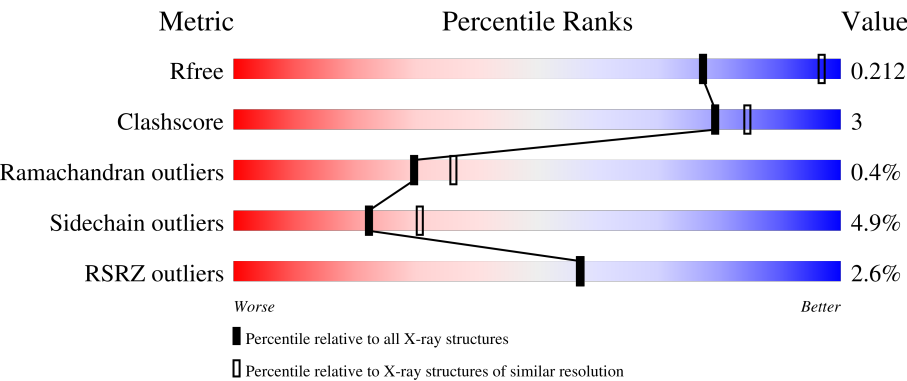
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	466	2% 81%8%11%
2	B	466	3% 82%8%10%
3	C	120	2% 82%13%5%
3	D	120	2% 88%7%5%
4	E	6	17%83%

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Mol	Chain	Length	Quality of chain
4	F	6	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8260 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 Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	1	0
			3109	1917	537	642	13			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP O52269
A	4	SER	-	expression tag	UNP O52269
A	5	TRP	-	expression tag	UNP O52269
A	6	SER	-	expression tag	UNP O52269
A	7	HIS	-	expression tag	UNP O52269
A	8	PRO	-	expression tag	UNP O52269
A	9	GLN	-	expression tag	UNP O52269
A	10	PHE	-	expression tag	UNP O52269
A	11	GLU	-	expression tag	UNP O52269
A	12	LYS	-	expression tag	UNP O52269
A	13	SER	-	expression tag	UNP O52269
A	14	GLY	-	expression tag	UNP O52269
A	15	GLY	-	expression tag	UNP O52269
A	16	GLY	-	expression tag	UNP O52269
A	17	GLY	-	expression tag	UNP O52269
A	18	GLY	-	expression tag	UNP O52269
A	19	LEU	-	expression tag	UNP O52269
A	20	VAL	-	expression tag	UNP O52269
A	21	PRO	-	expression tag	UNP O52269
A	22	ARG	-	expression tag	UNP O52269
A	23	GLY	-	expression tag	UNP O52269
A	24	SER	-	expression tag	UNP O52269
A	226	LYS	THR	conflict	UNP O52269
A	461	GLY	-	expression tag	UNP O52269
A	462	SER	-	expression tag	UNP O52269
A	463	HIS	-	expression tag	UNP O52269
A	464	HIS	-	expression tag	UNP O52269

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Chain	Residue	Modelled	Actual	Comment	Reference
A	465	HIS	-	expression tag	UNP O52269
A	466	HIS	-	expression tag	UNP O52269
A	467	HIS	-	expression tag	UNP O52269
A	468	HIS	-	expression tag	UNP O52269

- Molecule 2 is a protein called Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3124	1926	540	645	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	-	expression tag	UNP O52269
B	4	SER	-	expression tag	UNP O52269
B	5	TRP	-	expression tag	UNP O52269
B	6	SER	-	expression tag	UNP O52269
B	7	HIS	-	expression tag	UNP O52269
B	8	PRO	-	expression tag	UNP O52269
B	9	GLN	-	expression tag	UNP O52269
B	10	PHE	-	expression tag	UNP O52269
B	11	GLU	-	expression tag	UNP O52269
B	12	LYS	-	expression tag	UNP O52269
B	13	SER	-	expression tag	UNP O52269
B	14	GLY	-	expression tag	UNP O52269
B	15	GLY	-	expression tag	UNP O52269
B	16	GLY	-	expression tag	UNP O52269
B	17	GLY	-	expression tag	UNP O52269
B	18	GLY	-	expression tag	UNP O52269
B	19	LEU	-	expression tag	UNP O52269
B	20	VAL	-	expression tag	UNP O52269
B	21	PRO	-	expression tag	UNP O52269
B	22	ARG	-	expression tag	UNP O52269
B	23	GLY	-	expression tag	UNP O52269
B	24	SER	-	expression tag	UNP O52269
B	461	GLY	-	expression tag	UNP O52269
B	462	SER	-	expression tag	UNP O52269
B	463	HIS	-	expression tag	UNP O52269
B	464	HIS	-	expression tag	UNP O52269
B	465	HIS	-	expression tag	UNP O52269
B	466	HIS	-	expression tag	UNP O52269

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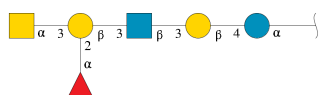
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Chain	Residue	Modelled	Actual	Comment	Reference
B	467	HIS	-	expression tag	UNP O52269
B	468	HIS	-	expression tag	UNP O52269

- Molecule 3 is a protein called Nanobody Nb-ER19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	114	Total	C	N	O	S	0	0	0
			873	546	158	164	5			
3	D	114	Total	C	N	O	S	0	0	0
			873	546	158	164	5			

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O	0	0	0
			72	40	2	30			
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

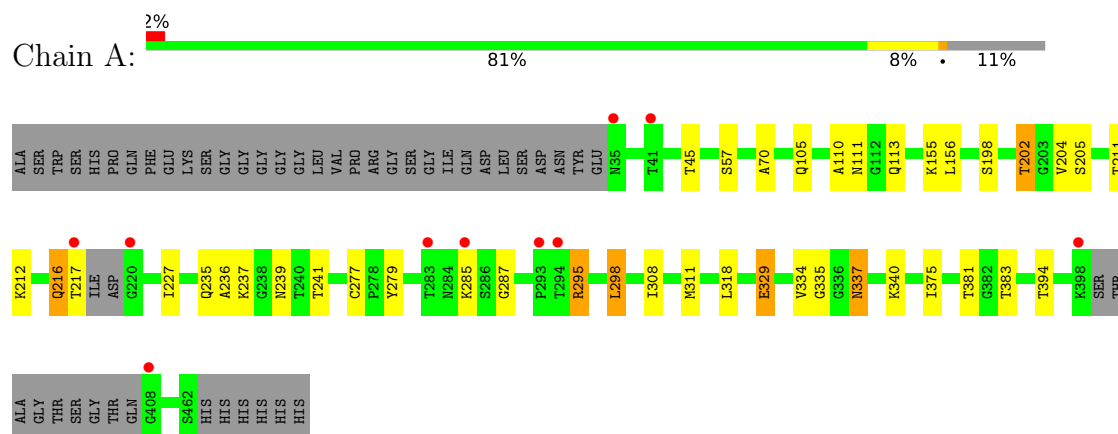
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total	O	0	0
			52	52		
5	B	37	Total	O	0	0
			37	37		
5	C	15	Total	O	0	0
			15	15		
5	D	33	Total	O	0	0
			33	33		

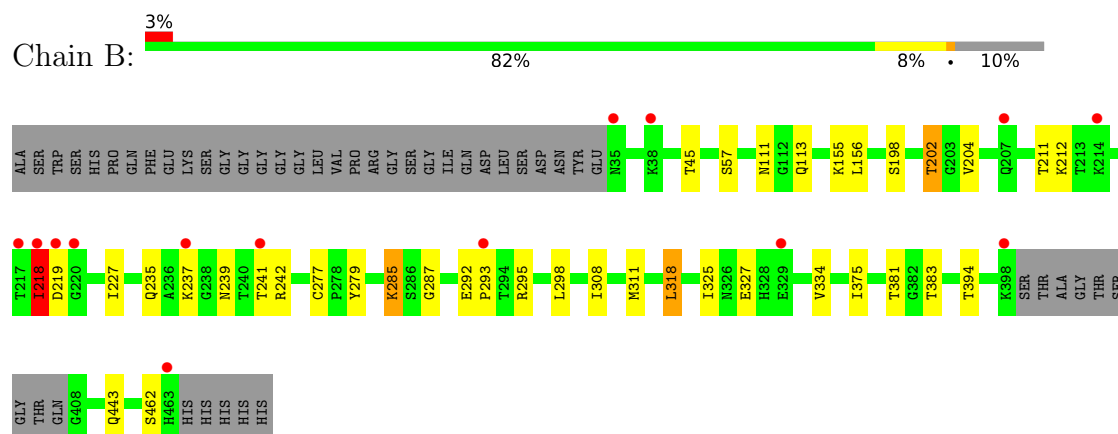
3 Residue-property plots [i](#)

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.

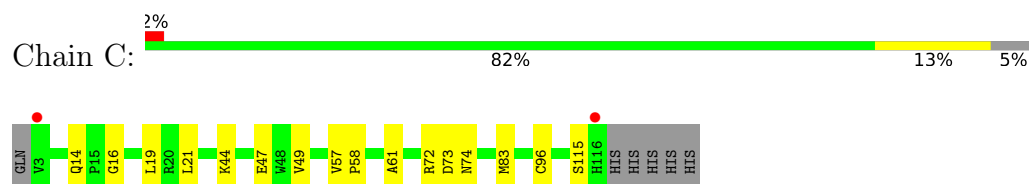
- Molecule 1: Adhesin binding fucosylated histo-blood group antigen



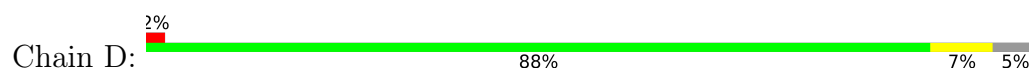
- Molecule 2: Adhesin binding fucosylated histo-blood group antigen



- Molecule 3: Nanobody Nb-ER19



- Molecule 3: Nanobody Nb-ER19



- Molecule 4: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 4: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.87Å 131.71Å 123.61Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	34.90 – 2.44 34.90 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.90-2.44) 99.6 (34.90-2.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.176 , 0.205 0.183 , 0.212	Depositor DCC
R_{free} test set	3012 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8260	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: GLC, GAL, A2G, FUC, NAG

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	1.15	2/3154 (0.1%)	1.06	5/4283 (0.1%)
2	B	1.13	2/3171 (0.1%)	1.02	2/4310 (0.0%)
3	C	1.17	0/893	1.05	3/1210 (0.2%)
3	D	1.26	1/893 (0.1%)	1.07	0/1210
All	All	1.15	5/8111 (0.1%)	1.05	10/11013 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	CYS	C-O	-6.48	1.20	1.23
3	D	97	ASN	N-CA	-5.93	1.39	1.46
2	B	277	CYS	C-O	-5.75	1.21	1.23
2	B	443	GLN	CA-C	-5.40	1.45	1.52
1	A	70	ALA	C-O	-5.06	1.18	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ALA	CA-C-N	-7.25	111.67	122.83
1	A	110	ALA	C-N-CA	-7.25	111.67	122.83
2	B	462	SER	N-CA-C	7.06	119.31	109.15
2	B	325	ILE	N-CA-C	6.41	117.16	110.62
3	C	61	ALA	N-CA-C	-5.52	102.31	110.48
1	A	295	ARG	N-CA-C	-5.42	100.94	109.50
1	A	205	SER	N-CA-C	5.31	116.76	110.97
3	C	16	GLY	N-CA-C	-5.24	108.45	114.69
1	A	111	ASN	CB-CA-C	5.19	119.11	111.06
3	C	49	VAL	N-CA-CB	-5.07	107.48	111.64

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	3109	0	3039	19	0
2	B	3124	0	3051	17	0
3	C	873	0	852	5	0
3	D	873	0	852	2	0
4	E	72	0	62	0	0
4	F	72	0	62	0	0
5	A	52	0	0	0	0
5	B	37	0	0	1	0
5	C	15	0	0	0	0
5	D	33	0	0	0	0
All	All	8260	0	7918	43	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 3.

All (43) 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)
2:B:292:GLU:OE2	2:B:293:PRO:HA	1.93	0.68
1:A:198:SER:O	1:A:202:THR:HB	1.98	0.64
2:B:198:SER:O	2:B:202:THR:HB	1.99	0.62
2:B:311:MET:HE1	2:B:375:ILE:HD13	1.83	0.61
1:A:216:GLN:HG3	1:A:217:THR:N	2.15	0.60
1:A:311:MET:HE1	1:A:375:ILE:HD13	1.82	0.59
2:B:241:THR:O	2:B:242:ARG:HB2	2.03	0.59
1:A:279:TYR:OH	1:A:295:ARG:HD2	2.06	0.55
1:A:318:LEU:C	1:A:318:LEU:HD23	2.32	0.55
2:B:218:ILE:HG22	2:B:219:ASP:N	2.23	0.53
3:C:72:ARG:HD3	3:C:74:ASN:OD1	2.10	0.51
2:B:318:LEU:C	2:B:318:LEU:HD23	2.35	0.51
1:A:308:ILE:HA	1:A:311:MET:HE3	1.93	0.50
2:B:308:ILE:HA	2:B:311:MET:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:72:ARG:HD3	3:D:74:ASN:OD1	2.12	0.49
2:B:285:LYS:HG3	5:B:637:HOH:O	2.13	0.47
1:A:156:LEU:C	1:A:156:LEU:HD23	2.41	0.46
2:B:156:LEU:C	2:B:156:LEU:HD23	2.40	0.46
1:A:279:TYR:OH	1:A:295:ARG:HG2	2.16	0.46
2:B:204:VAL:O	2:B:204:VAL:HG13	2.15	0.46
2:B:279:TYR:OH	2:B:295:ARG:HG2	2.16	0.45
1:A:155:LYS:HE3	1:A:155:LYS:HB2	1.78	0.44
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.87	0.44
1:A:329:GLU:O	1:A:329:GLU:HG2	2.11	0.44
3:C:19:LEU:HB2	3:C:83:MET:HE3	2.00	0.44
1:A:202:THR:HG22	1:A:204:VAL:H	1.82	0.44
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.90	0.44
2:B:155:LYS:HE3	2:B:155:LYS:HB2	1.77	0.43
1:A:235:GLN:O	1:A:236:ALA:C	2.61	0.43
2:B:292:GLU:HA	2:B:293:PRO:C	2.42	0.42
1:A:202:THR:HG22	1:A:204:VAL:HG23	2.01	0.42
3:D:19:LEU:HB2	3:D:83:MET:HE3	2.02	0.42
1:A:105:GLN:CD	1:A:279:TYR:CD2	2.98	0.42
1:A:202:THR:CG2	1:A:204:VAL:HG23	2.50	0.41
3:C:57:VAL:HA	3:C:58:PRO:HD3	1.94	0.41
1:A:279:TYR:OH	1:A:295:ARG:CG	2.69	0.41
2:B:239:ASN:OD1	2:B:241:THR:CG2	2.67	0.41
1:A:239:ASN:OD1	1:A:241:THR:CG2	2.69	0.41
3:C:73:ASP:C	3:C:73:ASP:OD1	2.64	0.41
1:A:337:ASN:O	1:A:340:LYS:HB3	2.21	0.40
2:B:204:VAL:O	2:B:204:VAL:CG1	2.69	0.40
2:B:239:ASN:OD1	2:B:241:THR:HG23	2.21	0.40
3:C:21:LEU:HG	3:C:83:MET:HE2	2.03	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	412/466 (88%)	397 (96%)	13 (3%)	2 (0%)	24	29
2	B	416/466 (89%)	398 (96%)	16 (4%)	2 (0%)	24	29
3	C	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
3	D	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
All	All	1052/1172 (90%)	1017 (97%)	31 (3%)	4 (0%)	30	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	218	ILE
1	A	335	GLY
2	B	287	GLY
1	A	287	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/381 (90%)	327 (95%)	17 (5%)	22	31
2	B	346/381 (91%)	328 (95%)	18 (5%)	21	28
3	C	93/99 (94%)	88 (95%)	5 (5%)	20	27
3	D	93/99 (94%)	90 (97%)	3 (3%)	34	46
All	All	876/960 (91%)	833 (95%)	43 (5%)	22	31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	57	SER
1	A	113	GLN
1	A	202	THR
1	A	211	THR
1	A	212	LYS
1	A	216	GLN

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Mol	Chain	Res	Type
1	A	227	ILE
1	A	237	LYS
1	A	285	LYS
1	A	298	LEU
1	A	329	GLU
1	A	334	VAL
1	A	337	ASN
1	A	381	THR
1	A	383	THR
1	A	394	THR
2	B	45	THR
2	B	57	SER
2	B	111	ASN
2	B	113	GLN
2	B	202	THR
2	B	211	THR
2	B	212	LYS
2	B	218	ILE
2	B	227	ILE
2	B	235	GLN
2	B	237	LYS
2	B	285	LYS
2	B	318	LEU
2	B	327	GLU
2	B	334	VAL
2	B	381	THR
2	B	383	THR
2	B	394	THR
3	C	14	GLN
3	C	44	LYS
3	C	47	GLU
3	C	96	CYS
3	C	115	SER
3	D	44	LYS
3	D	47	GLU
3	D	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	274	ASN

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Mol	Chain	Res	Type
1	A	316	GLN
1	A	459	ASN
2	B	260	GLN
2	B	274	ASN
2	B	316	GLN
2	B	379	ASN
3	C	40	GLN
3	C	55	GLN
3	C	82	GLN
3	C	110	GLN
3	D	40	GLN
3	D	77	ASN
3	D	82	GLN
3	D	110	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 ⓘ

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	$\# Z > 2$
4	GLC	E	1	4	12,12,12	0.47	0	17,17,17	0.52	0
4	GAL	E	2	4	11,11,12	0.81	0	15,15,17	1.41	2 (13%)
4	NAG	E	3	4	14,14,15	0.84	1 (7%)	17,19,21	2.08	3 (17%)
4	GAL	E	4	4	11,11,12	0.74	0	15,15,17	1.46	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	E	5	4	10,10,11	0.87	0	14,14,16	1.31	3 (21%)
4	A2G	E	6	4	14,14,15	0.37	0	17,19,21	1.54	2 (11%)
4	GLC	F	1	4	12,12,12	0.59	0	17,17,17	1.24	3 (17%)
4	GAL	F	2	4	11,11,12	0.62	0	15,15,17	1.62	4 (26%)
4	NAG	F	3	4	14,14,15	0.72	0	17,19,21	1.22	2 (11%)
4	GAL	F	4	4	11,11,12	0.91	1 (9%)	15,15,17	1.26	2 (13%)
4	FUC	F	5	4	10,10,11	0.74	0	14,14,16	1.09	1 (7%)
4	A2G	F	6	4	14,14,15	0.46	0	17,19,21	0.95	1 (5%)

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
4	GLC	E	1	4	-	2/2/22/22	0/1/1/1
4	GAL	E	2	4	-	2/2/19/22	0/1/1/1
4	NAG	E	3	4	-	0/6/23/26	0/1/1/1
4	GAL	E	4	4	-	0/2/19/22	0/1/1/1
4	FUC	E	5	4	-	-	0/1/1/1
4	A2G	E	6	4	-	0/6/23/26	0/1/1/1
4	GLC	F	1	4	-	0/2/22/22	0/1/1/1
4	GAL	F	2	4	-	2/2/19/22	0/1/1/1
4	NAG	F	3	4	-	0/6/23/26	0/1/1/1
4	GAL	F	4	4	-	2/2/19/22	0/1/1/1
4	FUC	F	5	4	-	-	0/1/1/1
4	A2G	F	6	4	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	NAG	O5-C1	-2.27	1.39	1.43
4	F	4	GAL	O5-C1	-2.16	1.40	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	NAG	C1-O5-C5	6.36	120.71	112.19
4	E	6	A2G	C1-O5-C5	5.11	119.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	GAL	C1-O5-C5	3.45	116.81	112.19
4	F	2	GAL	C1-C2-C3	3.25	114.37	109.64
4	F	4	GAL	C1-C2-C3	3.05	114.08	109.64
4	F	5	FUC	O2-C2-C3	-3.02	103.91	110.15
4	E	3	NAG	O7-C7-C8	-2.80	117.06	122.05
4	F	2	GAL	O2-C2-C3	-2.80	104.35	110.15
4	E	2	GAL	C2-C3-C4	-2.62	106.25	110.86
4	E	2	GAL	C1-C2-C3	2.55	113.36	109.64
4	F	3	NAG	O7-C7-N2	2.50	126.41	121.98
4	E	3	NAG	C1-C2-N2	2.40	114.22	110.43
4	F	2	GAL	C1-O5-C5	2.40	115.40	112.19
4	F	4	GAL	O4-C4-C5	2.38	115.19	109.32
4	F	1	GLC	O5-C1-C2	2.20	114.16	110.30
4	E	5	FUC	C2-C3-C4	-2.19	107.01	110.86
4	F	1	GLC	C4-C3-C2	-2.18	107.01	110.83
4	F	1	GLC	O4-C4-C5	2.13	114.58	109.32
4	E	5	FUC	O2-C2-C3	-2.13	105.73	110.15
4	E	5	FUC	O2-C2-C1	2.08	113.99	109.22
4	F	6	A2G	O3-C3-C4	2.07	115.25	110.38
4	F	3	NAG	O7-C7-C8	-2.06	118.39	122.05
4	E	6	A2G	O6-C6-C5	-2.02	104.44	111.33
4	F	2	GAL	O3-C3-C2	-2.01	105.96	110.05

There are no chirality outliers.

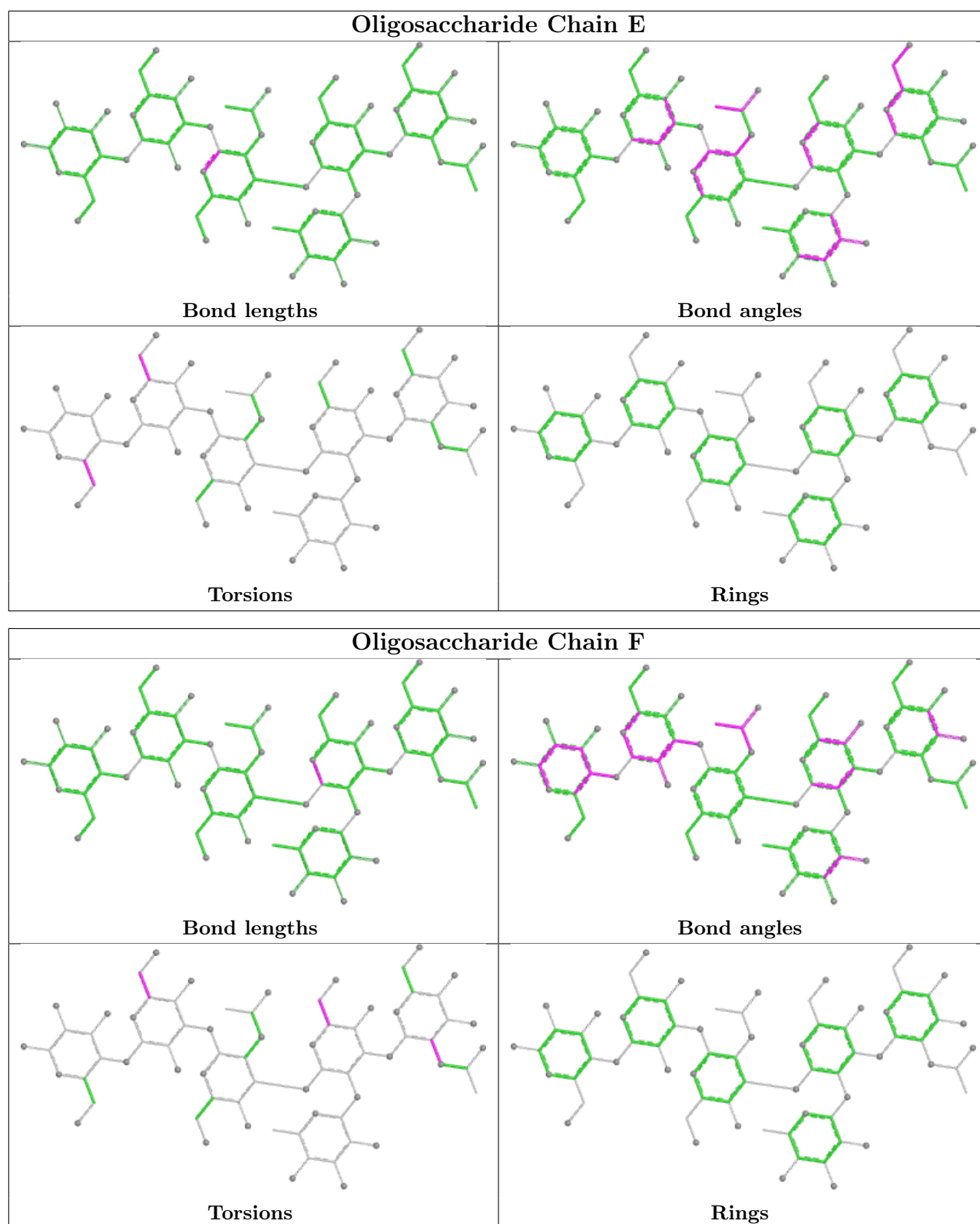
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	GLC	O5-C5-C6-O6
4	E	2	GAL	O5-C5-C6-O6
4	E	1	GLC	C4-C5-C6-O6
4	E	2	GAL	C4-C5-C6-O6
4	F	4	GAL	O5-C5-C6-O6
4	F	2	GAL	C4-C5-C6-O6
4	F	2	GAL	O5-C5-C6-O6
4	F	4	GAL	C4-C5-C6-O6
4	F	6	A2G	C1-C2-N2-C7

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.



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	417/466 (89%)	-0.16	10 (2%) 59 60	24, 52, 101, 124	1 (0%)
2	B	420/466 (90%)	-0.01	14 (3%) 49 48	35, 56, 112, 141	0
3	C	114/120 (95%)	-0.27	2 (1%) 67 68	38, 52, 74, 120	0
3	D	114/120 (95%)	-0.42	2 (1%) 67 68	31, 44, 66, 93	0
All	All	1065/1172 (90%)	-0.14	28 (2%) 57 57	24, 53, 103, 141	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	3	VAL	7.1
3	C	3	VAL	6.5
3	C	116	HIS	4.9
2	B	207	GLN	4.6
2	B	218	ILE	4.3
2	B	463	HIS	3.8
1	A	217	THR	3.7
1	A	398	LYS	3.5
1	A	285	LYS	3.1
1	A	35	ASN	2.9
2	B	293	PRO	2.8
1	A	220	GLY	2.8
1	A	41	THR	2.8
1	A	294	THR	2.6
2	B	35	ASN	2.5
2	B	237	LYS	2.4
2	B	398	LYS	2.4
2	B	38	LYS	2.4
2	B	217	THR	2.3
1	A	408	GLY	2.3
2	B	220	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	329	GLU	2.2
1	A	293	PRO	2.2
2	B	241	THR	2.1
2	B	214	LYS	2.1
1	A	283	THR	2.1
2	B	219	ASP	2.0
3	D	116	HIS	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](#)

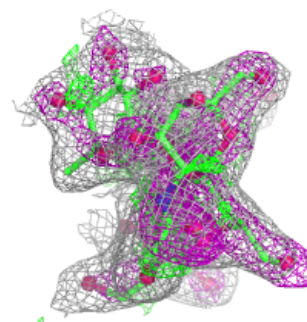
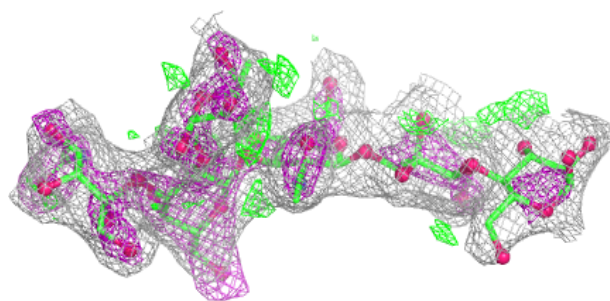
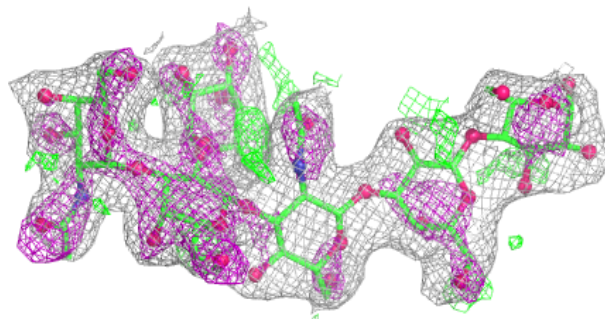
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	E	1	12/12	0.51	0.17	74,86,93,95	0
4	GLC	F	1	12/12	0.59	0.16	70,77,83,84	0
4	GAL	F	4	11/12	0.71	0.16	35,39,41,41	0
4	GAL	F	2	11/12	0.74	0.13	48,56,61,62	0
4	A2G	F	6	14/15	0.75	0.15	43,47,53,56	0
4	GAL	E	2	11/12	0.81	0.11	43,54,59,60	0
4	NAG	F	3	14/15	0.83	0.13	39,43,45,45	0
4	FUC	F	5	10/11	0.84	0.12	32,36,39,40	0
4	A2G	E	6	14/15	0.88	0.12	32,37,45,46	0
4	GAL	E	4	11/12	0.89	0.11	30,35,38,43	0
4	NAG	E	3	14/15	0.89	0.11	38,43,47,52	0
4	FUC	E	5	10/11	0.90	0.09	27,30,31,31	0

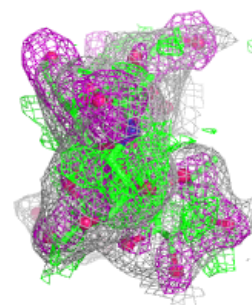
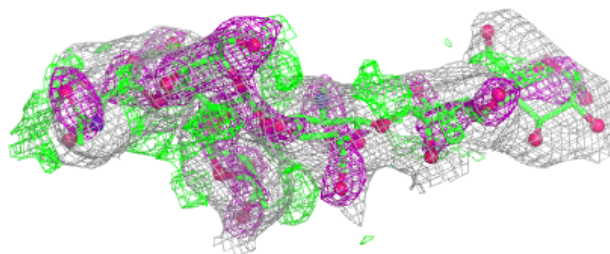
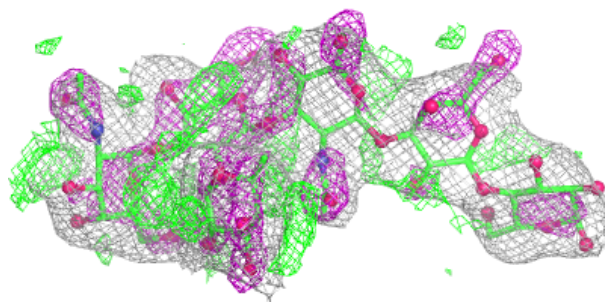
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.