



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 11:37 pm GMT

PDB ID : 4BH4
Title : Haemagglutinin from a Transmissible Mutant H5 Influenza Virus in Complex with Avian Receptor Analogue 3'-SLN
Authors : Xiong, X.; Coombs, P.J.; Martin, S.R.; Liu, J.; Xiao, H.; McCauley, J.W.; Locher, K.; Walker, P.A.; Collins, P.J.; Kawaoka, Y.; Skehel, J.J.; Gamblin, S.J.
Deposited on : 2013-03-29
Resolution : 1.90 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

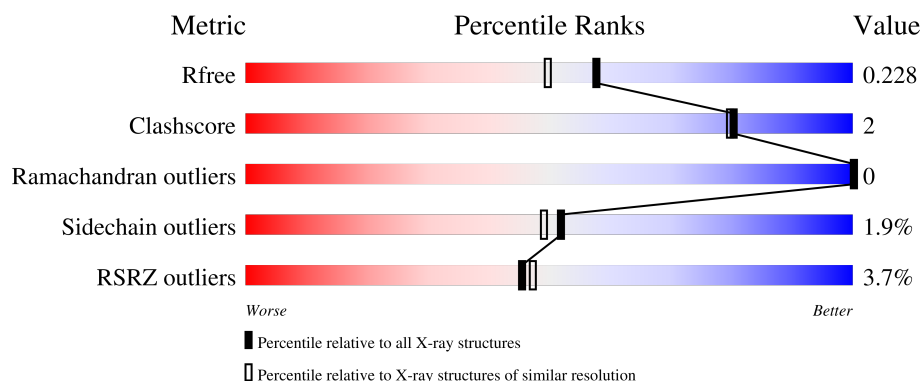
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	328	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>
2	B	167	<div> <div>%</div> <div> <div></div> <div>96%</div> <div></div> <div>.</div> </div> </div>
3	C	6	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
4	D	3	<div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	C	6	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4480 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 HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2578	1633	444	486	15	0	1	0

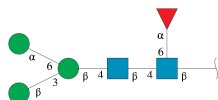
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP Q5EP31
A	0	PRO	-	expression tag	UNP Q5EP31
A	154	ASP	ASN	conflict	UNP Q5EP31
A	220	LYS	ASN	conflict	UNP Q5EP31
A	222	LEU	GLN	conflict	UNP Q5EP31
A	315	ILE	THR	conflict	UNP Q5EP31
A	325	THR	ARG	conflict	UNP Q5EP31

- Molecule 2 is a protein called HEMAGGLUTININ.

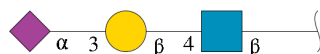
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	167	1345	837	231	269	8	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



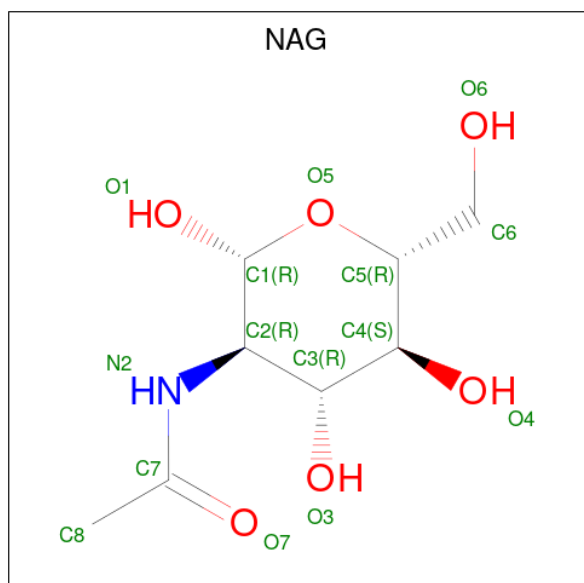
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	6	71	40	2	29	0	0	0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

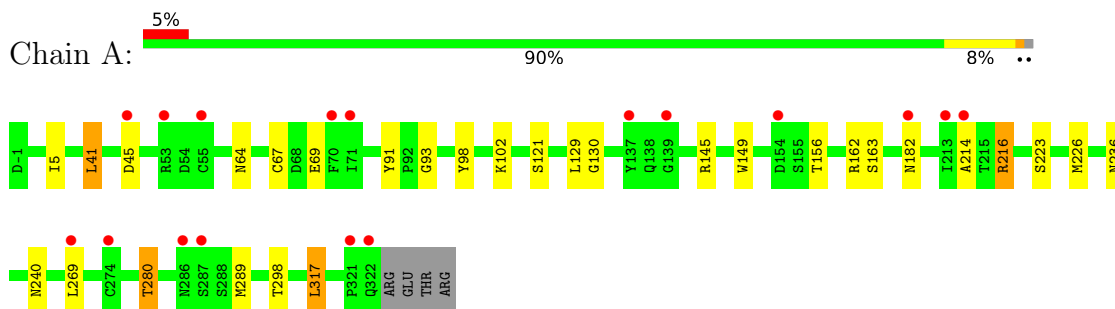
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	248	Total	O	0	0
			248	248		
7	B	149	Total	O	0	0
			149	149		

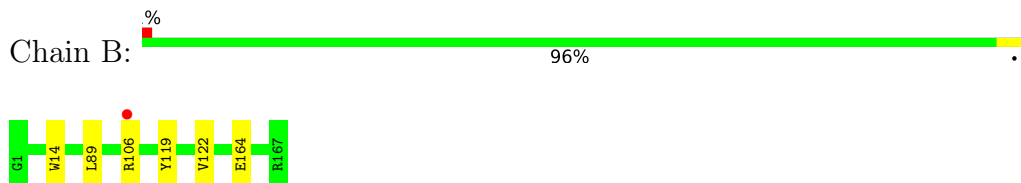
3 Residue-property plots [i](#)

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.

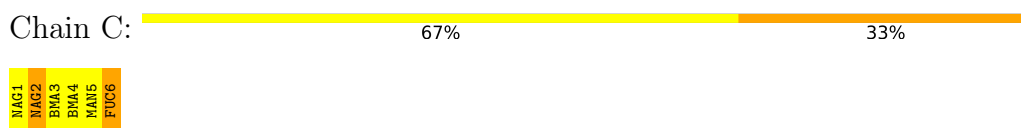
- Molecule 1: HEMAGGLUTININ



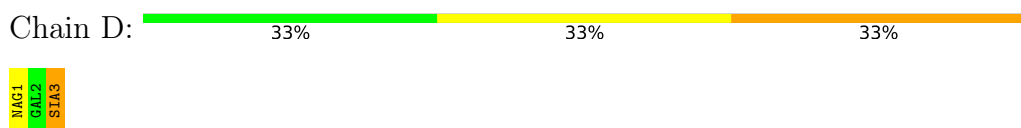
- Molecule 2: HEMAGGLUTININ



- Molecule 3: beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	101.74Å 101.74Å 329.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.84 – 1.90 77.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.84-1.90) 99.9 (77.84-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.223 0.194 , 0.228	Depositor DCC
R_{free} test set	2669 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.9	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	0.96	EDS
Total number of atoms	4480	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, GAL, SIA, NAG, EPE, 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	0.35	0/2644	0.60	0/3590
2	B	0.37	0/1372	0.56	0/1846
All	All	0.35	0/4016	0.59	0/5436

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	ASP	Peptide

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	2578	0	2533	17	0
2	B	1345	0	1242	4	0
3	C	71	0	61	1	0
4	D	46	0	40	1	0
5	A	28	0	26	0	0
6	B	15	0	18	1	0
7	A	248	0	0	1	0
7	B	149	0	0	1	0
All	All	4480	0	3920	20	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 2.

All (20) 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:289:MET:SD	7:A:2212:HOH:O	2.36	0.82
2:B:14:TRP:NE1	6:B:1168:EPE:O2S	2.29	0.65
1:A:98:TYR:CZ	1:A:102:LYS:HD2	2.39	0.58
1:A:5:ILE:HD11	2:B:122:VAL:HG21	1.86	0.56
2:B:106:ARG:NH2	7:B:2122:HOH:O	2.39	0.56
1:A:317:LEU:N	1:A:317:LEU:HD23	2.21	0.55
1:A:41:LEU:HD22	1:A:269:LEU:HB2	1.93	0.50
1:A:93:GLY:HA3	1:A:226:MET:O	2.12	0.49
3:C:2:NAG:H5	3:C:6:FUC:H61	1.95	0.49
1:A:129:LEU:O	4:D:3:SIA:H113	2.15	0.47
1:A:163:SER:OG	1:A:240:ASN:ND2	2.44	0.47
1:A:280:THR:HG22	1:A:298:THR:HG22	1.99	0.44
1:A:130:GLY:HA3	1:A:149:TRP:HB3	1.99	0.44
1:A:69:GLU:OE1	1:A:145:ARG:NH2	2.51	0.43
1:A:214:ALA:HB3	1:A:216:ARG:HD3	2.01	0.43
1:A:91:TYR:CD1	1:A:226:MET:HG2	2.55	0.42
1:A:5:ILE:HG13	2:B:119:TYR:HA	2.03	0.41
1:A:121:SER:O	1:A:162:ARG:NH2	2.54	0.41
1:A:64:ASN:O	1:A:67:CYS:HB2	2.22	0.40
1:A:182:ASN:OD1	1:A:223:SER:C	2.60	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	323/328 (98%)	312 (97%)	11 (3%)	0	100	100
2	B	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
All	All	488/495 (99%)	473 (97%)	15 (3%)	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	292/296 (99%)	286 (98%)	6 (2%)	48	45
2	B	141/142 (99%)	139 (99%)	2 (1%)	62	62
All	All	433/438 (99%)	425 (98%)	8 (2%)	52	52

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	156	THR
1	A	216	ARG
1	A	236	ASN
1	A	280	THR
1	A	317	LEU
2	B	89	LEU
2	B	164	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	240	ASN
2	B	42	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 ⓘ

9 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	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.58	0	17,19,21	1.47	3 (17%)
3	NAG	C	2	3	14,14,15	0.44	0	17,19,21	1.33	1 (5%)
3	BMA	C	3	3	11,11,12	0.57	0	15,15,17	1.97	3 (20%)
3	BMA	C	4	3	11,11,12	0.51	0	15,15,17	1.43	3 (20%)
3	MAN	C	5	3	11,11,12	0.53	0	15,15,17	1.17	1 (6%)
3	FUC	C	6	3	10,10,11	0.59	0	14,14,16	1.32	2 (14%)
4	NAG	D	1	4	15,15,15	0.44	0	21,21,21	1.48	3 (14%)
4	GAL	D	2	4	11,11,12	0.20	0	15,15,17	0.69	0
4	SIA	D	3	4	20,20,21	0.53	0	24,28,31	1.24	4 (16%)

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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	BMA	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	FUC	C	6	3	1/1/4/5	-	0/1/1/1
4	NAG	D	1	4	-	2/6/26/26	0/1/1/1
4	GAL	D	2	4	-	0/2/19/22	0/1/1/1
4	SIA	D	3	4	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	O3-C3-C2	5.82	121.14	109.99
4	D	1	NAG	C1-C2-N2	-3.91	106.20	110.73
3	C	5	MAN	C1-O5-C5	3.54	116.98	112.19
3	C	6	FUC	C1-O5-C5	3.20	120.02	112.78
3	C	1	NAG	C8-C7-N2	2.94	121.07	116.10
3	C	4	BMA	C3-C4-C5	2.85	115.33	110.24
3	C	1	NAG	C2-N2-C7	2.84	126.94	122.90
4	D	1	NAG	C3-C2-N2	-2.62	105.66	110.62
4	D	1	NAG	C4-C3-C2	2.47	113.95	110.34
4	D	3	SIA	O1B-C1-C2	2.45	120.01	113.03
3	C	2	NAG	C2-N2-C7	2.43	126.37	122.90
3	C	1	NAG	C1-O5-C5	2.35	115.37	112.19
3	C	4	BMA	O5-C1-C2	-2.30	107.22	110.77
4	D	3	SIA	C6-O6-C2	2.21	116.07	111.34
3	C	3	BMA	O3-C3-C4	-2.20	105.26	110.35
3	C	3	BMA	C2-C3-C4	-2.16	107.16	110.89
4	D	3	SIA	C4-C5-N5	-2.14	106.14	110.38
3	C	4	BMA	C1-O5-C5	-2.12	109.32	112.19
4	D	3	SIA	C6-C5-N5	-2.10	107.43	110.91
3	C	6	FUC	O5-C5-C6	2.00	111.63	107.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	6	FUC	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	4	BMA	O5-C5-C6-O6

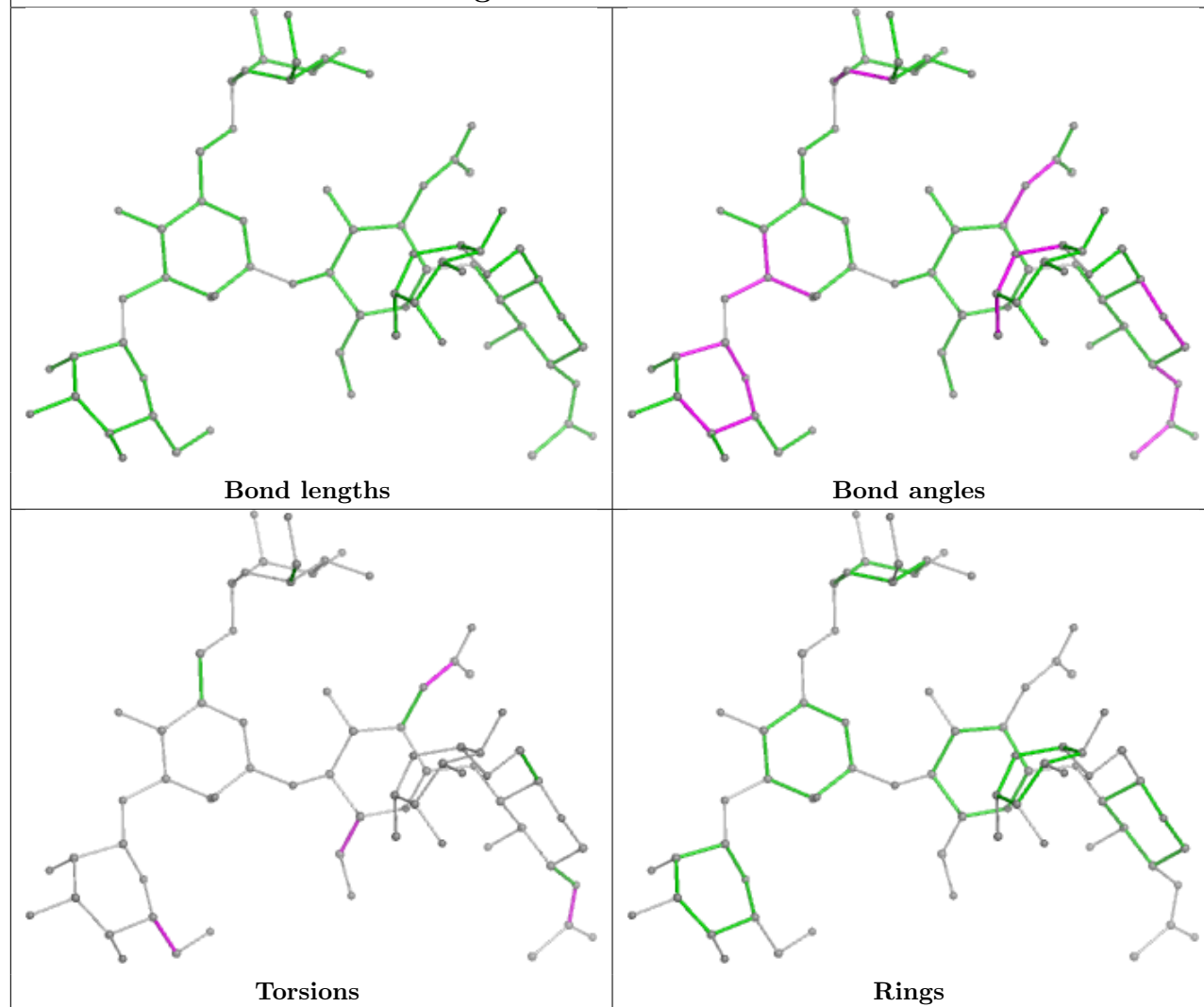
There are no ring outliers.

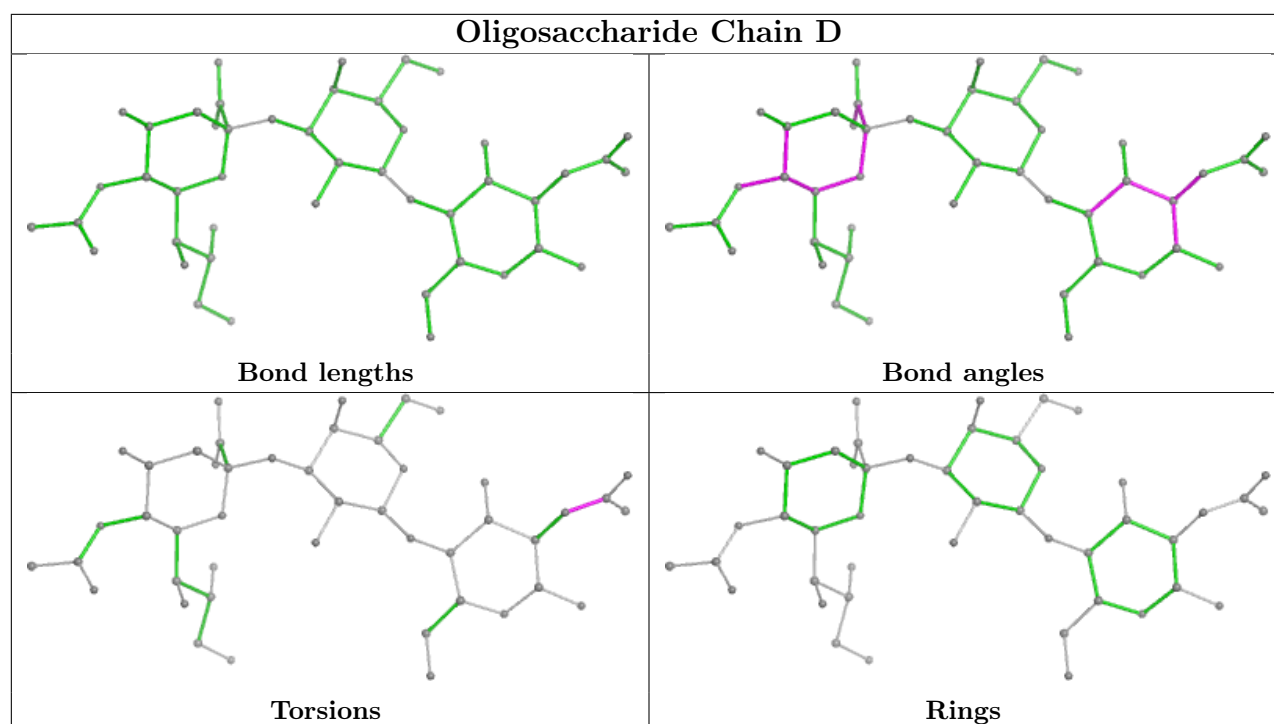
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	SIA	1	0
3	C	6	FUC	1	0
3	C	2	NAG	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.

Oligosaccharide Chain C





5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
5	NAG	A	1324	1	14,14,15	0.42	0	17,19,21	1.98	3 (17%)
6	EPE	B	1168	-	15,15,15	2.21	1 (6%)	18,20,20	2.73	9 (50%)
5	NAG	A	1323	1	14,14,15	0.38	0	17,19,21	1.16	2 (11%)

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
5	NAG	A	1324	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	B	1168	-	-	3/9/19/19	0/1/1/1
5	NAG	A	1323	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1168	EPE	C10-S	-8.28	1.65	1.77

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1324	NAG	C1-O5-C5	6.81	121.42	112.19
6	B	1168	EPE	C6-N1-C2	4.92	119.90	108.83
6	B	1168	EPE	C7-N4-C5	4.62	123.06	111.23
6	B	1168	EPE	C6-C5-N4	-4.26	101.89	110.64
6	B	1168	EPE	C7-N4-C3	3.79	120.93	111.23
6	B	1168	EPE	C9-N1-C2	3.56	120.34	111.23
6	B	1168	EPE	O1S-S-C10	3.43	111.04	106.92
6	B	1168	EPE	C9-N1-C6	3.33	119.75	111.23
6	B	1168	EPE	C5-N4-C3	3.19	116.00	108.83
5	A	1324	NAG	C6-C5-C4	-2.31	107.59	113.00
5	A	1324	NAG	C4-C3-C2	-2.30	107.65	111.02
5	A	1323	NAG	C8-C7-N2	2.21	119.84	116.10
6	B	1168	EPE	C5-C6-N1	-2.13	106.27	110.64
5	A	1323	NAG	O5-C5-C6	2.08	110.46	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1168	EPE	C8-C7-N4-C5
6	B	1168	EPE	N4-C7-C8-O8
5	A	1323	NAG	C8-C7-N2-C2
5	A	1323	NAG	O7-C7-N2-C2
5	A	1324	NAG	C4-C5-C6-O6
6	B	1168	EPE	C10-C9-N1-C2
5	A	1324	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1168	EPE	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	324/328 (98%)	0.25	17 (5%) 34 35	22, 38, 58, 78	1 (0%)
2	B	167/167 (100%)	-0.05	1 (0%) 85 87	21, 32, 55, 80	0
All	All	491/495 (99%)	0.15	18 (3%) 45 47	21, 36, 58, 80	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	CYS	4.6
1	A	213	ILE	3.6
1	A	71	ILE	3.3
1	A	55	CYS	3.0
1	A	287	SER	3.0
1	A	137	TYR	2.9
1	A	214	ALA	2.9
1	A	322	GLN	2.9
1	A	139	GLY	2.8
1	A	286	ASN	2.6
1	A	45	ASP	2.5
1	A	321	PRO	2.4
2	B	106	ARG	2.3
1	A	70	PHE	2.3
1	A	269	LEU	2.2
1	A	53	ARG	2.1
1	A	182	ASN	2.1
1	A	154	ASP	2.1

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

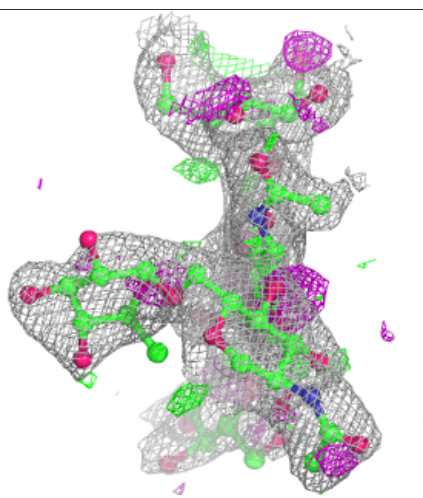
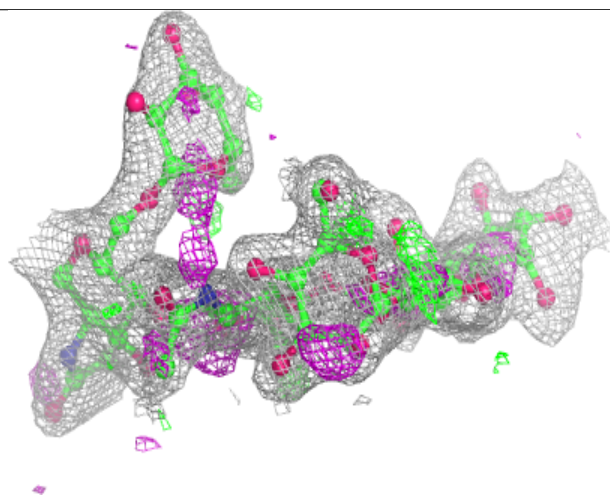
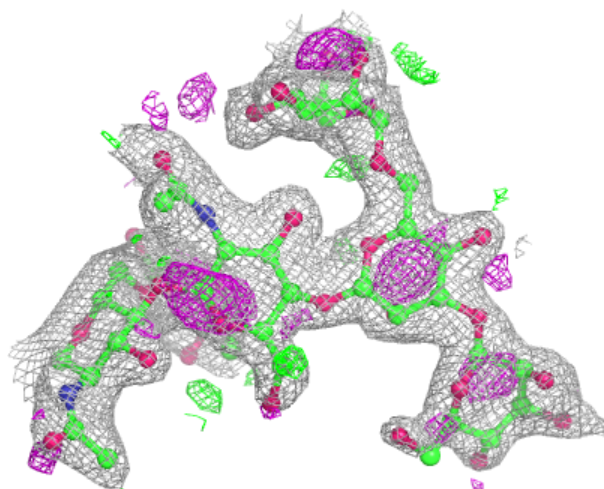
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

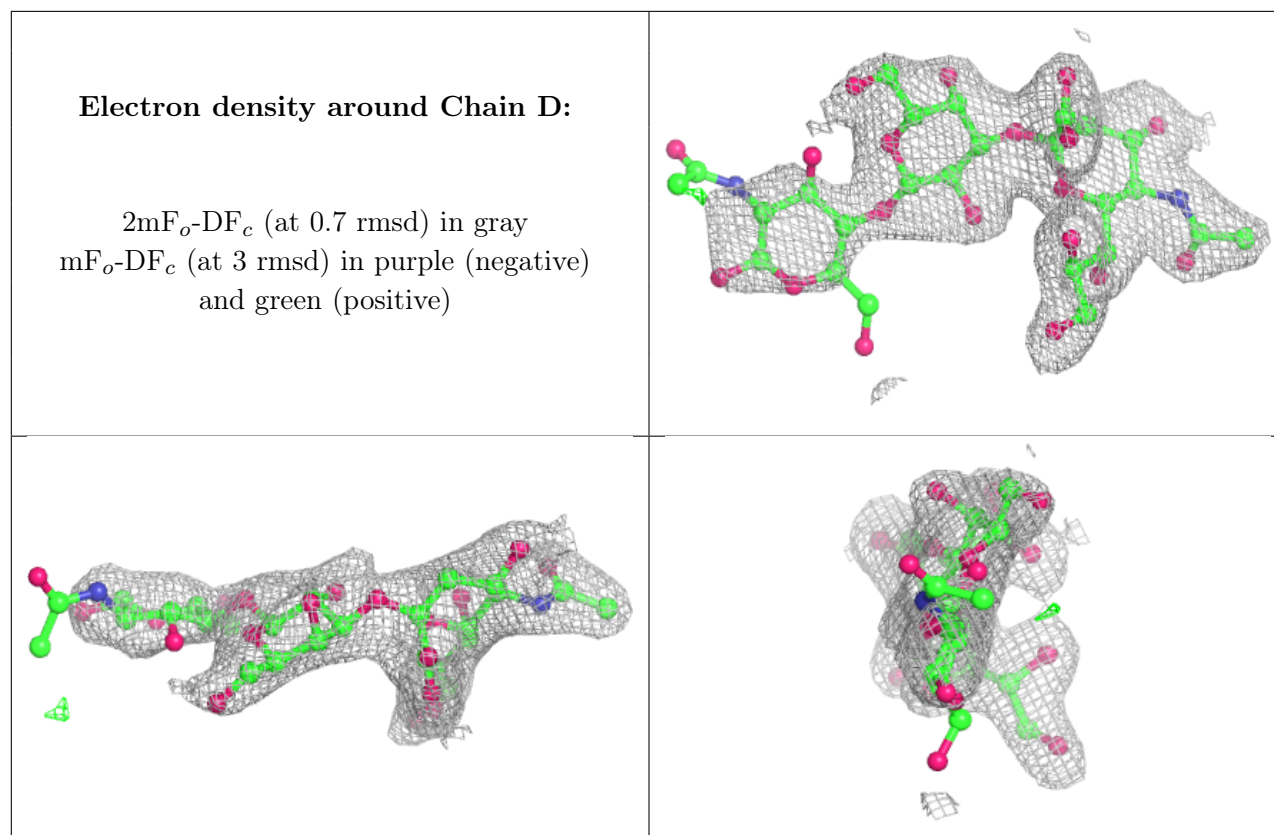
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	1	15/15	0.63	0.17	73,84,89,89	0
3	FUC	C	6	10/11	0.74	0.15	59,62,63,64	0
3	NAG	C	2	14/15	0.82	0.12	37,39,42,48	0
3	BMA	C	4	11/12	0.82	0.12	49,52,54,55	0
3	NAG	C	1	14/15	0.85	0.12	37,41,47,53	0
3	MAN	C	5	11/12	0.87	0.10	33,37,39,40	0
3	BMA	C	3	11/12	0.90	0.09	36,39,40,44	0
4	GAL	D	2	11/12	0.90	0.09	54,62,65,65	0
4	SIA	D	3	20/21	0.92	0.09	42,45,48,48	0

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

Electron density around Chain C:

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





6.4 Ligands [i](#)

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
5	NAG	A	1323	14/15	0.62	0.16	50,61,67,68	0
6	EPE	B	1168	15/15	0.68	0.25	64,66,73,78	0
5	NAG	A	1324	14/15	0.77	0.12	45,52,56,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.