



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 10:12 AM EDT

PDB ID : 9NNU / pdb_00009nnu
Title : Crystal Structure of Ebola Envelope glycoprotein GP in complex with compound LD4-189ZbR
Authors : Agrawal, S.; Wilson, I.A.
Deposited on : 2025-03-06
Resolution : 2.59 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

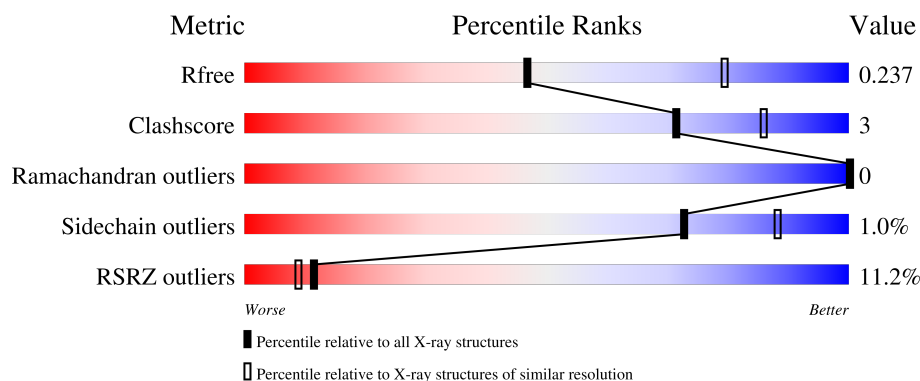
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	470	
2	B	168	
3	C	4	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3006 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	1	0
			1921	1230	324	362	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	THR	conflict	UNP Q05320

- Molecule 2 is a protein called GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			941	599	162	174	6			

There are 38 discrepancies between the modelled and reference sequences:

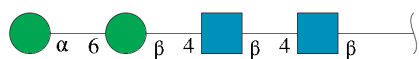
Chain	Residue	Modelled	Actual	Comment	Reference
B	613	ALA	HIS	conflict	UNP Q05320
B	633	GLY	-	expression tag	UNP Q05320
B	634	SER	-	expression tag	UNP Q05320
B	635	GLY	-	expression tag	UNP Q05320
B	636	TYR	-	expression tag	UNP Q05320
B	637	ILE	-	expression tag	UNP Q05320
B	638	PRO	-	expression tag	UNP Q05320
B	639	GLU	-	expression tag	UNP Q05320
B	640	ALA	-	expression tag	UNP Q05320
B	641	PRO	-	expression tag	UNP Q05320
B	642	ARG	-	expression tag	UNP Q05320
B	643	ASP	-	expression tag	UNP Q05320
B	644	GLY	-	expression tag	UNP Q05320
B	645	GLN	-	expression tag	UNP Q05320
B	646	ALA	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
B	647	TYR	-	expression tag	UNP Q05320
B	648	VAL	-	expression tag	UNP Q05320
B	649	ARG	-	expression tag	UNP Q05320
B	650	LYS	-	expression tag	UNP Q05320
B	651	ASP	-	expression tag	UNP Q05320
B	652	GLY	-	expression tag	UNP Q05320
B	653	GLU	-	expression tag	UNP Q05320
B	654	TRP	-	expression tag	UNP Q05320
B	655	VAL	-	expression tag	UNP Q05320
B	656	LEU	-	expression tag	UNP Q05320
B	657	LEU	-	expression tag	UNP Q05320
B	658	SER	-	expression tag	UNP Q05320
B	659	THR	-	expression tag	UNP Q05320
B	660	PHE	-	expression tag	UNP Q05320
B	661	LEU	-	expression tag	UNP Q05320
B	662	GLY	-	expression tag	UNP Q05320
B	663	THR	-	expression tag	UNP Q05320
B	664	HIS	-	expression tag	UNP Q05320
B	665	HIS	-	expression tag	UNP Q05320
B	666	HIS	-	expression tag	UNP Q05320
B	667	HIS	-	expression tag	UNP Q05320
B	668	HIS	-	expression tag	UNP Q05320
B	669	HIS	-	expression tag	UNP Q05320

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



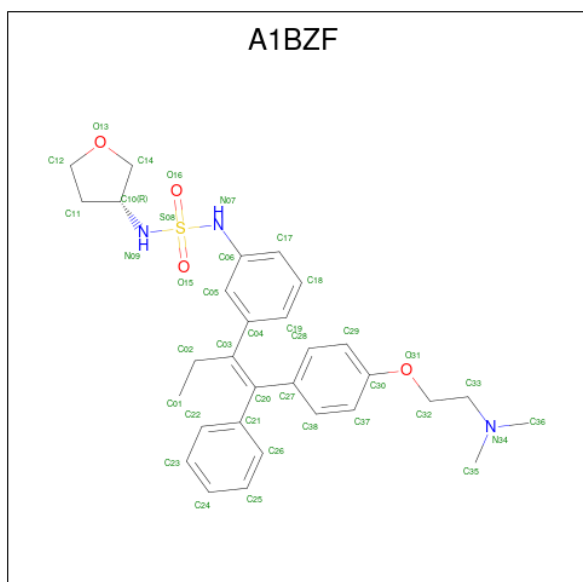
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

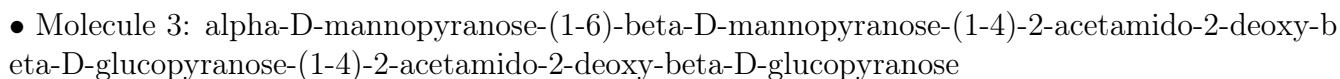
- Molecule 5 is N-{3-[(1Z)-1-{4-[2-(dimethylamino)ethoxy]phenyl}-1-phenylbut-1-en-2-yl]phenyl}-N'-[(3R)-oxolan-3-yl]sulfuric diamide (CCD ID: A1BZF) (formula: $C_{30}H_{37}N_3O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			38	30	3	4	1		

i

- Molecule 1: Envelope glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	114.22Å 114.22Å 306.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.27 – 2.59 29.27 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.27-2.59) 93.7 (29.27-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.70 (at 2.57Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.220 , 0.244 0.219 , 0.237	Depositor DCC
R_{free} test set	22189 reflections (8.31%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3006	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: BMA, MAN, NAG, A1BZF

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	0.15	0/1969	0.34	0/2674
2	B	0.21	0/964	0.37	0/1315
All	All	0.17	0/2933	0.35	0/3989

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1921	0	1852	16	0
2	B	941	0	910	5	0
3	C	50	0	43	2	0
4	A	56	0	52	0	0
5	A	38	0	0	1	0
All	All	3006	0	2857	19	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 (19) 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:46:SER:HA	1:A:50:LYS:HZ1	1.58	0.68
1:A:43:LEU:HD11	2:B:561:LEU:HD22	1.83	0.60
1:A:106:GLU:HG3	1:A:290:PHE:CD1	2.38	0.59
1:A:49:ASP:HA	2:B:595:GLN:HG3	1.88	0.55
1:A:156:GLU:HG2	3:C:2:NAG:H5	1.90	0.52
1:A:71:GLU:HB3	1:A:290:PHE:HE2	1.77	0.49
1:A:71:GLU:HG2	1:A:77:THR:HG21	1.95	0.48
1:A:88:PHE:HB3	1:A:149:GLY:HA3	1.96	0.47
1:A:188:GLN:H	1:A:188:GLN:CD	2.21	0.47
1:A:244:LEU:HD12	1:A:248:PHE:HD2	1.78	0.47
1:A:35:LEU:HD13	2:B:588:LYS:HD3	1.97	0.47
2:B:613:ALA:O	2:B:616:THR:HG22	2.17	0.45
3:C:3:BMA:H61	3:C:4:MAN:H2	1.46	0.45
1:A:64:ARG:HD2	5:A:605:A1BZF:C37	2.48	0.44
2:B:617:LYS:O	2:B:621:ASP:HB3	2.18	0.44
1:A:263:SER:CB	1:A:265:LYS:HZ1	2.31	0.43
1:A:267:SER:HB2	1:A:273:LEU:HB3	2.01	0.42
1:A:114:LYS:O	1:A:144:THR:HA	2.20	0.41
1:A:244:LEU:HD12	1:A:248:PHE:CD2	2.56	0.41

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	237/470 (50%)	233 (98%)	4 (2%)	0	100	100
2	B	118/168 (70%)	115 (98%)	3 (2%)	0	100	100
All	All	355/638 (56%)	348 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/399 (51%)	204 (100%)	1 (0%)	86	95
2	B	98/139 (70%)	96 (98%)	2 (2%)	50	74
All	All	303/538 (56%)	300 (99%)	3 (1%)	73	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	ASN
2	B	527	ILE
2	B	621	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	107	ASN
1	A	278	ASN
2	B	595	GLN
2	B	618	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](#)

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	$\# Z > 2$
3	NAG	C	1	2,3	14,14,15	0.73	0	17,19,21	0.91	0
3	NAG	C	2	3	14,14,15	0.73	0	17,19,21	1.03	1 (5%)
3	BMA	C	3	3	11,11,12	0.86	0	15,15,17	2.08	3 (20%)
3	MAN	C	4	3	11,11,12	0.67	0	15,15,17	1.39	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
3	NAG	C	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	5.99	120.22	112.19
3	C	4	MAN	C1-O5-C5	4.44	118.13	112.19
3	C	3	BMA	C2-C3-C4	2.77	115.73	110.86
3	C	3	BMA	C3-C4-C5	2.31	114.42	110.23
3	C	2	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	MAN	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O7-C7-N2-C2
3	C	4	MAN	C4-C5-C6-O6

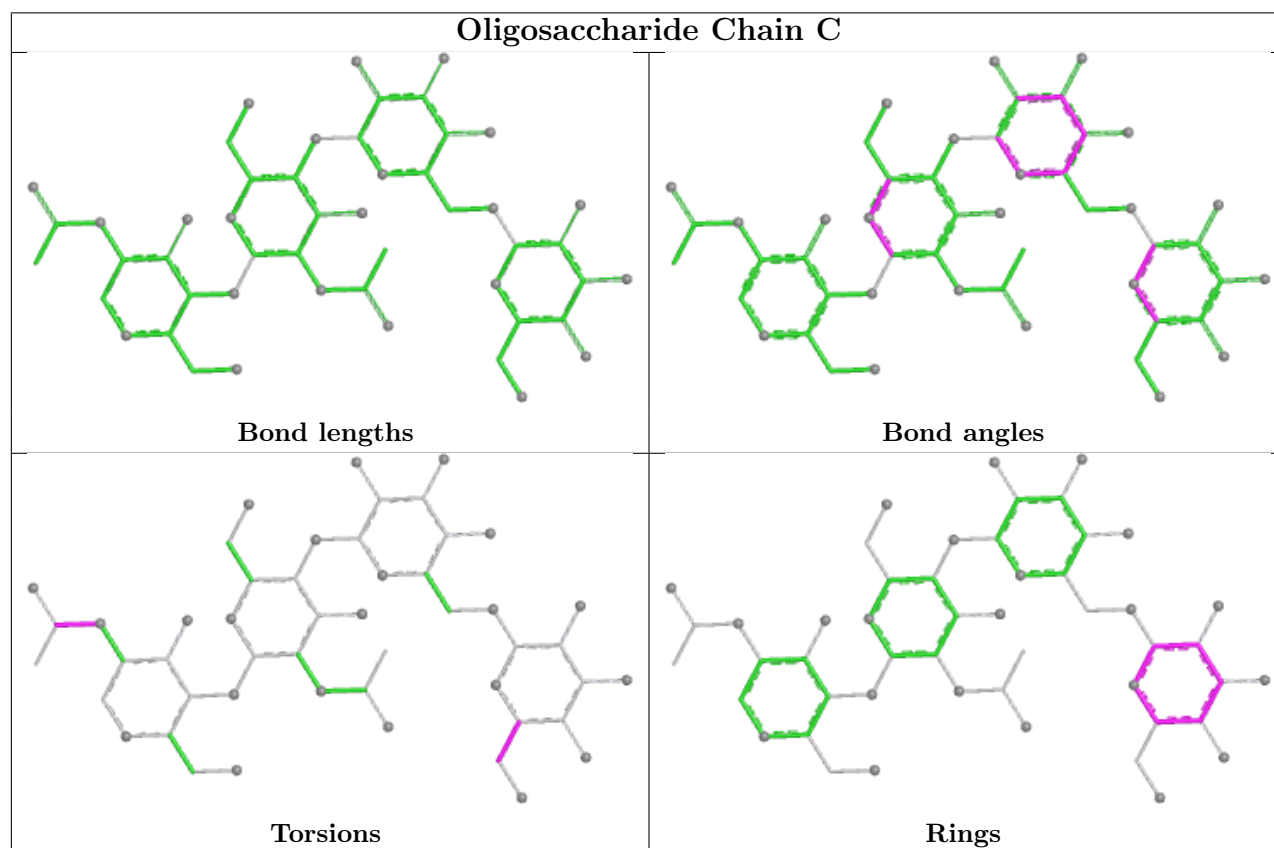
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	BMA	1	0
3	C	2	NAG	1	0
3	C	4	MAN	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

5 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	A1BZF	A	605	-	40,41,41	2.95	21 (52%)	53,56,56	3.38	17 (32%)
4	NAG	A	601	1	14,14,15	0.74	0	17,19,21	0.79	0
4	NAG	A	603	1	14,14,15	0.70	0	17,19,21	0.85	0
4	NAG	A	604	1	14,14,15	0.72	0	17,19,21	0.91	0
4	NAG	A	602	1	14,14,15	0.73	0	17,19,21	0.88	0

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	A1BZF	A	605	-	-	8/34/41/41	0/4/4/4
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1
4	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	602	1	-	1/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	A1BZF	S08-N09	10.67	1.75	1.62
5	A	605	A1BZF	C06-N07	5.23	1.51	1.43
5	A	605	A1BZF	C21-C20	4.57	1.57	1.49
5	A	605	A1BZF	C33-C32	3.86	1.62	1.50
5	A	605	A1BZF	C27-C20	3.73	1.55	1.49
5	A	605	A1BZF	C04-C03	3.52	1.55	1.49
5	A	605	A1BZF	C25-C26	3.51	1.44	1.38
5	A	605	A1BZF	C22-C21	3.36	1.44	1.39
5	A	605	A1BZF	C28-C27	3.32	1.44	1.39
5	A	605	A1BZF	C05-C06	3.20	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	A1BZF	C19-C04	3.08	1.44	1.39
5	A	605	A1BZF	C38-C37	2.93	1.43	1.38
5	A	605	A1BZF	C29-C28	2.86	1.43	1.38
5	A	605	A1BZF	C10-N09	2.50	1.51	1.47
5	A	605	A1BZF	C18-C17	2.50	1.43	1.38
5	A	605	A1BZF	C17-C06	2.40	1.43	1.39
5	A	605	A1BZF	C37-C30	2.35	1.43	1.38
5	A	605	A1BZF	C20-C03	2.28	1.39	1.35
5	A	605	A1BZF	C24-C23	2.23	1.43	1.38
5	A	605	A1BZF	O31-C30	2.21	1.42	1.37
5	A	605	A1BZF	C29-C30	2.19	1.42	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	A1BZF	C05-C04-C03	11.82	133.58	120.42
5	A	605	A1BZF	C19-C04-C03	-9.63	108.58	121.00
5	A	605	A1BZF	C01-C02-C03	9.39	126.31	112.87
5	A	605	A1BZF	C26-C21-C20	9.20	136.76	120.91
5	A	605	A1BZF	C22-C21-C20	-7.91	107.28	120.91
5	A	605	A1BZF	O16-S08-O15	-5.80	111.79	120.34
5	A	605	A1BZF	C23-C22-C21	2.98	123.29	120.36
5	A	605	A1BZF	C38-C27-C28	-2.80	115.01	118.57
5	A	605	A1BZF	C38-C27-C20	2.79	125.71	120.91
5	A	605	A1BZF	C29-C28-C27	2.61	123.58	120.80
5	A	605	A1BZF	C37-C30-C29	-2.50	116.51	120.16
5	A	605	A1BZF	C11-C10-N09	2.44	117.76	112.09
5	A	605	A1BZF	C38-C37-C30	2.35	122.41	119.73
5	A	605	A1BZF	C32-O31-C30	2.22	123.72	117.93
5	A	605	A1BZF	C17-C06-C05	-2.22	116.97	119.66
5	A	605	A1BZF	C26-C21-C22	-2.07	115.94	118.57
5	A	605	A1BZF	C14-C10-N09	2.03	114.90	112.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	A1BZF	C06-N07-S08-O15
5	A	605	A1BZF	C06-N07-S08-O16
5	A	605	A1BZF	C32-C33-N34-C35
4	A	602	NAG	O5-C5-C6-O6
5	A	605	A1BZF	C32-C33-N34-C36

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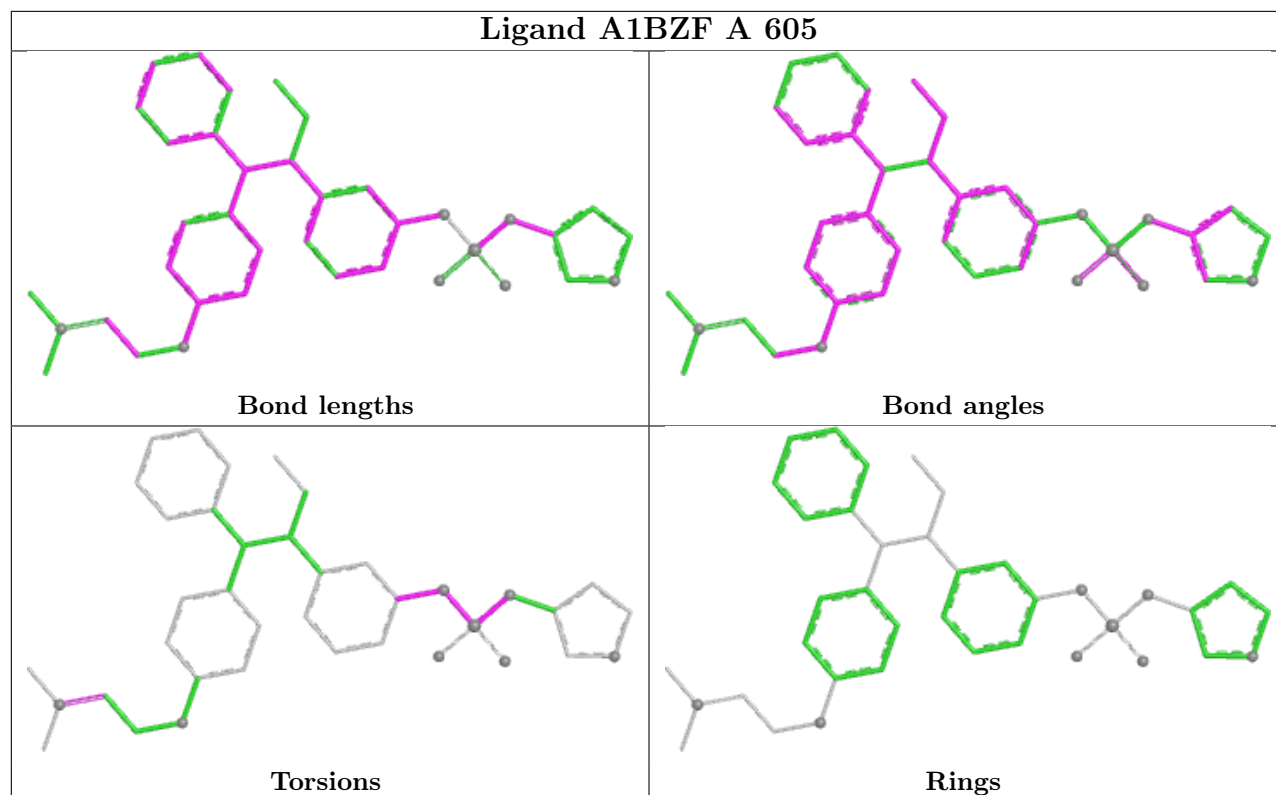
Mol	Chain	Res	Type	Atoms
5	A	605	A1BZF	C10-N09-S08-O15
5	A	605	A1BZF	C06-N07-S08-N09
5	A	605	A1BZF	C05-C06-N07-S08
5	A	605	A1BZF	C17-C06-N07-S08

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	A1BZF	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	246/470 (52%)	0.60	30 (12%) 10 7	43, 69, 128, 151	1 (0%)
2	B	120/168 (71%)	0.37	11 (9%) 16 13	47, 64, 128, 142	0
All	All	366/638 (57%)	0.52	41 (11%) 11 9	43, 67, 128, 151	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	VAL	6.9
1	A	309	THR	5.5
1	A	306	LEU	5.3
1	A	308	PHE	5.2
1	A	311	VAL	5.2
1	A	281	ILE	4.6
2	B	615	TRP	4.6
2	B	525	ALA	4.6
1	A	473	SER	4.4
2	B	522	ASP	4.3
1	A	477	GLY	4.2
1	A	472	GLU	4.0
1	A	288	TRP	3.8
1	A	277	VAL	3.7
1	A	188	GLN	3.6
2	B	527	ILE	3.5
1	A	476	SER	3.2
1	A	52	VAL	3.1
2	B	524	GLY	3.0
1	A	279	PRO	2.9
1	A	262	THR	2.8
1	A	54	ARG	2.7
1	A	214	TYR	2.6
1	A	290	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	307	SER	2.6
1	A	293	THR	2.6
2	B	620	THR	2.6
1	A	280	GLU	2.5
1	A	275	TRP	2.5
1	A	263	SER	2.5
2	B	619	ILE	2.4
1	A	212	GLY	2.4
1	A	46	SER	2.3
1	A	211	SER	2.3
2	B	526	ALA	2.3
1	A	475	SER	2.3
1	A	229	GLU	2.2
2	B	601	CYS	2.1
2	B	617	LYS	2.1
2	B	604	LEU	2.0
1	A	474	ALA	2.0

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

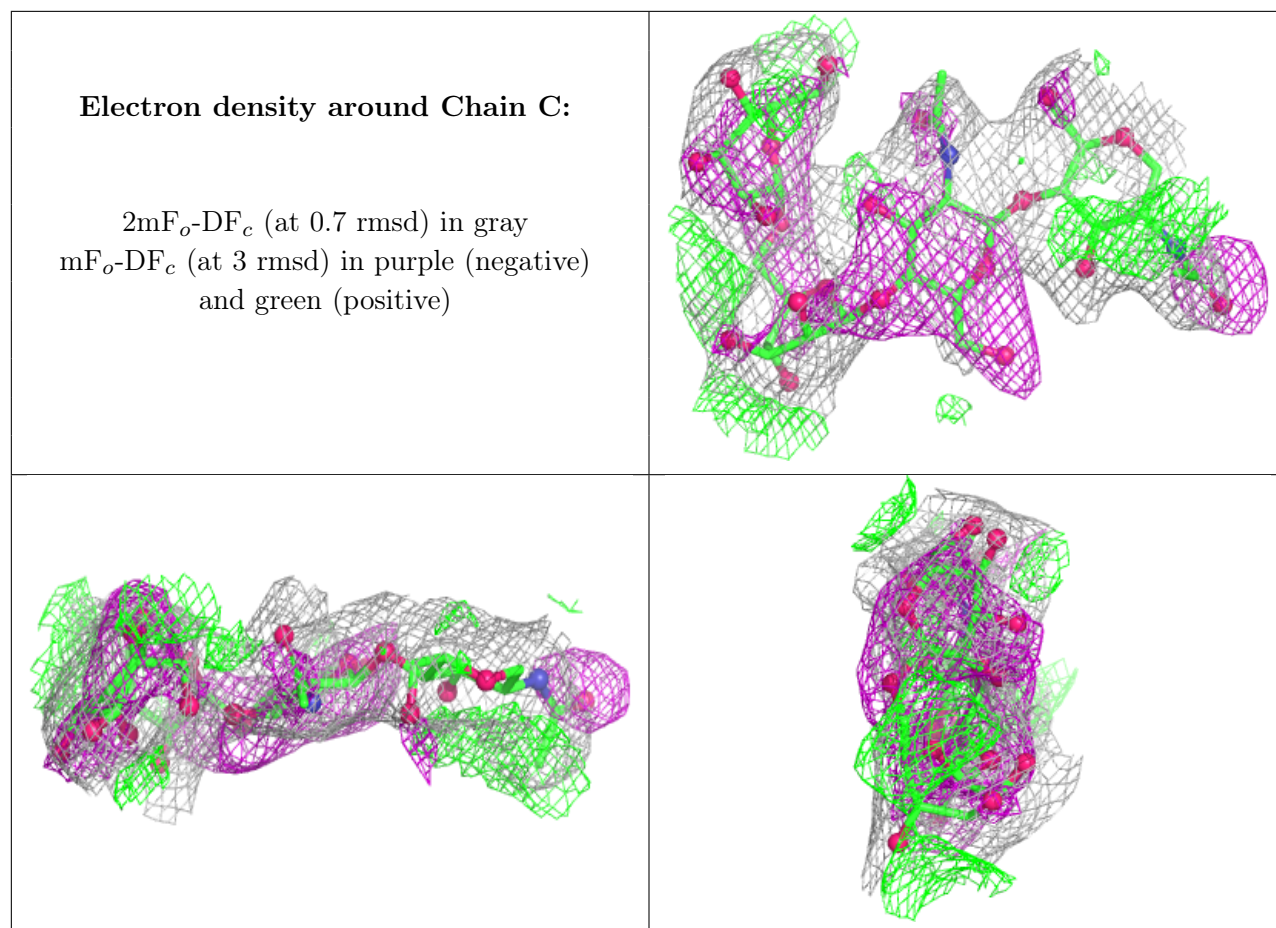
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	BMA	C	3	11/12	0.28	0.19	73,73,74,74	0
3	MAN	C	4	11/12	0.37	0.17	72,73,74,74	0
3	NAG	C	2	14/15	0.64	0.21	67,70,72,73	0
3	NAG	C	1	14/15	0.73	0.20	56,62,65,67	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.



6.4 Ligands [i](#)

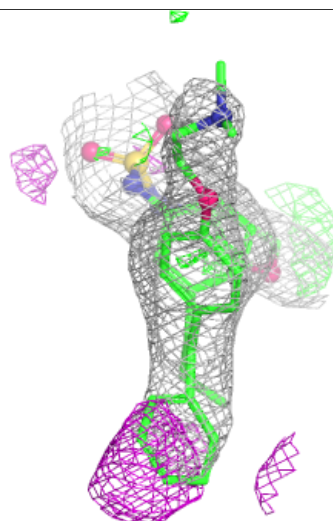
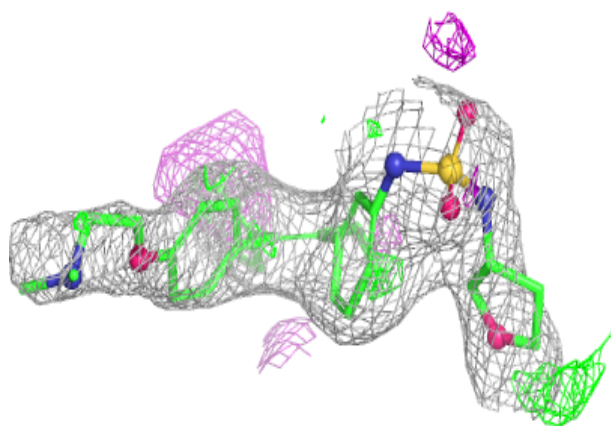
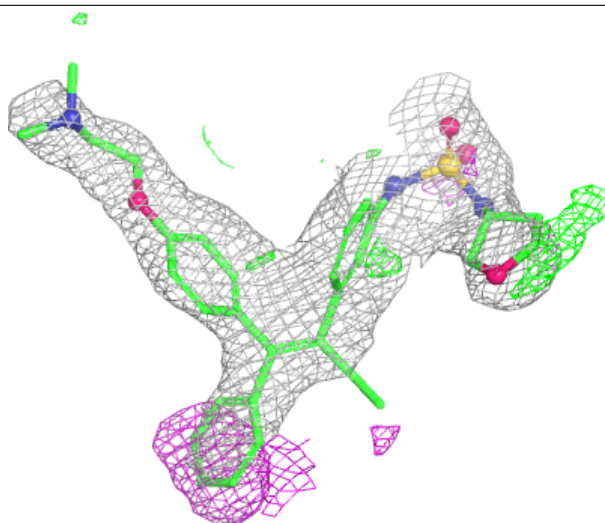
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	602	14/15	0.36	0.22	127,129,129,129	0
4	NAG	A	604	14/15	0.66	0.20	107,109,111,114	0
4	NAG	A	603	14/15	0.75	0.15	103,111,113,113	0
4	NAG	A	601	14/15	0.81	0.14	79,86,90,91	0
5	A1BZF	A	605	38/38	0.84	0.22	55,84,131,135	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1BZF A 605:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.