



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:51 PM GMT

PDB ID : 4GDI  
Title : A subtype N10 neuraminidase-like protein of A/little yellow-shouldered bat/  
Guatemala/164/2009  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2012-07-31  
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

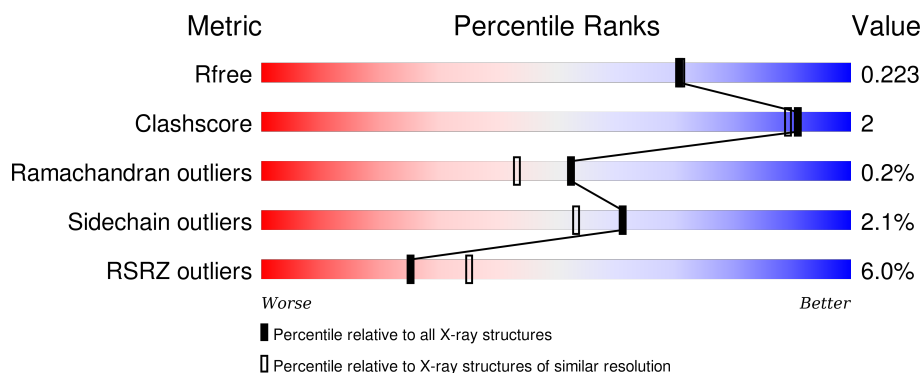
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	373	<div> <div>3%</div> <div>93%</div> <div>5%</div> </div>
1	B	373	<div> <div>7%</div> <div>92%</div> <div>6%</div> </div>
1	C	373	<div> <div>10%</div> <div>87%</div> <div>11%</div> </div>
1	D	373	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>
1	E	373	<div> <div>6%</div> <div>89%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	373	

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	NAG	F	505	-	-	-	X
5	GOL	A	512	-	-	-	X
5	GOL	B	511	-	-	-	X
5	GOL	D	508	-	-	-	X
5	GOL	E	511	-	-	-	X
5	GOL	E	512	-	-	-	X
5	GOL	F	512	-	-	-	X
5	GOL	F	515	-	-	-	X
6	NO3	A	513	-	X	-	X
6	NO3	A	514	-	X	-	X
6	NO3	B	513	-	X	-	-
6	NO3	B	514	-	X	-	-
6	NO3	B	515	-	X	-	-
6	NO3	B	516	-	X	-	X
6	NO3	B	517	-	X	-	X
6	NO3	C	510	-	X	-	X
6	NO3	C	511	-	X	-	X
6	NO3	D	509	-	X	-	-
6	NO3	D	510	-	X	-	X
6	NO3	F	516	-	X	-	-
6	NO3	F	517	-	X	-	-
6	NO3	F	518	-	X	-	X
9	FUC	D	503	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 36150 atoms, of which 16780 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 Neuraminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	B	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	C	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	D	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	E	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	F	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	EXPRESSION TAG	UNP H6QM85
A	78	SER	-	EXPRESSION TAG	UNP H6QM85
A	79	PRO	-	EXPRESSION TAG	UNP H6QM85
A	80	SER	-	EXPRESSION TAG	UNP H6QM85
A	81	ARG	-	EXPRESSION TAG	UNP H6QM85
B	77	GLY	-	EXPRESSION TAG	UNP H6QM85
B	78	SER	-	EXPRESSION TAG	UNP H6QM85
B	79	PRO	-	EXPRESSION TAG	UNP H6QM85
B	80	SER	-	EXPRESSION TAG	UNP H6QM85
B	81	ARG	-	EXPRESSION TAG	UNP H6QM85
C	77	GLY	-	EXPRESSION TAG	UNP H6QM85
C	78	SER	-	EXPRESSION TAG	UNP H6QM85
C	79	PRO	-	EXPRESSION TAG	UNP H6QM85
C	80	SER	-	EXPRESSION TAG	UNP H6QM85
C	81	ARG	-	EXPRESSION TAG	UNP H6QM85
D	77	GLY	-	EXPRESSION TAG	UNP H6QM85
D	78	SER	-	EXPRESSION TAG	UNP H6QM85

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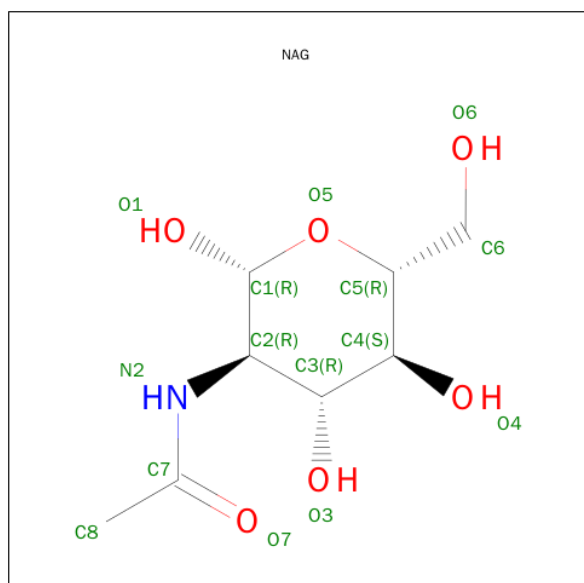
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Chain	Residue	Modelled	Actual	Comment	Reference
D	79	PRO	-	EXPRESSION TAG	UNP H6QM85
D	80	SER	-	EXPRESSION TAG	UNP H6QM85
D	81	ARG	-	EXPRESSION TAG	UNP H6QM85
E	77	GLY	-	EXPRESSION TAG	UNP H6QM85
E	78	SER	-	EXPRESSION TAG	UNP H6QM85
E	79	PRO	-	EXPRESSION TAG	UNP H6QM85
E	80	SER	-	EXPRESSION TAG	UNP H6QM85
E	81	ARG	-	EXPRESSION TAG	UNP H6QM85
F	77	GLY	-	EXPRESSION TAG	UNP H6QM85
F	78	SER	-	EXPRESSION TAG	UNP H6QM85
F	79	PRO	-	EXPRESSION TAG	UNP H6QM85
F	80	SER	-	EXPRESSION TAG	UNP H6QM85
F	81	ARG	-	EXPRESSION TAG	UNP H6QM85

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			59	34	2	23		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

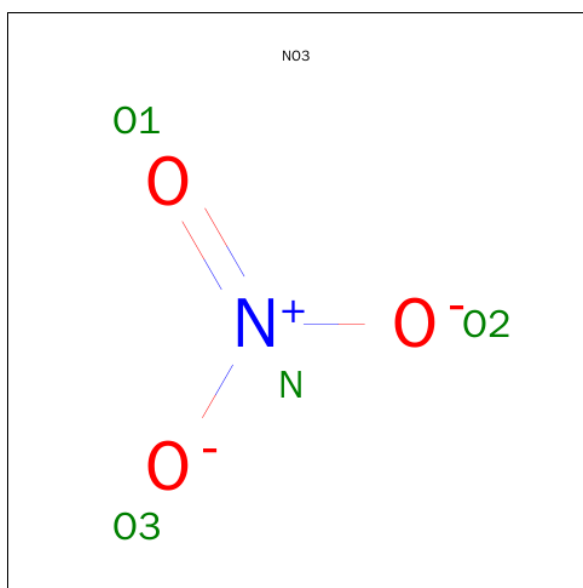
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Ca	0	0
			2	2		
4	E	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	A	1	Total	Ca	0	0
			1	1		
4	F	2	Total	Ca	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		
6	F	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	6	Total	C	N	O	0	0
			70	40	2	28		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	4	Total	C	N	O	0	0
			48	28	2	18		
8	E	4	Total	C	N	O	0	0
			48	28	2	18		
8	F	4	Total	C	N	O	0	0
			48	28	2	18		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	E	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	F	3	Total	C	N	O	0	0
			38	22	2	14		

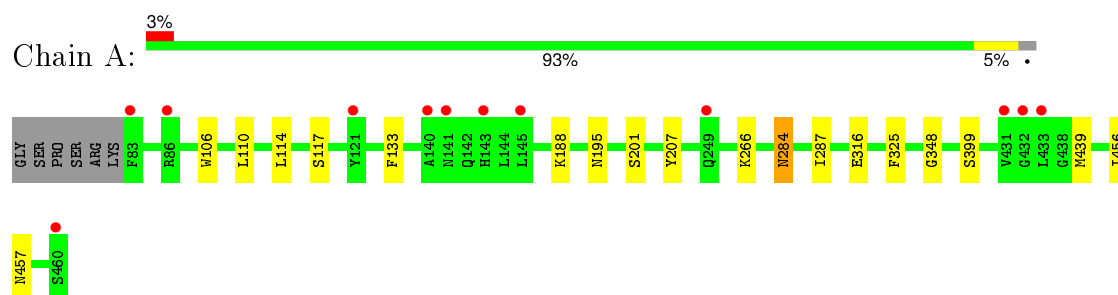
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	247	Total 247	O 247	0	0
12	B	246	Total 246	O 246	0	0
12	C	176	Total 176	O 176	0	0
12	D	213	Total 213	O 213	0	0
12	E	207	Total 207	O 207	0	0
12	F	319	Total 319	O 319	0	0

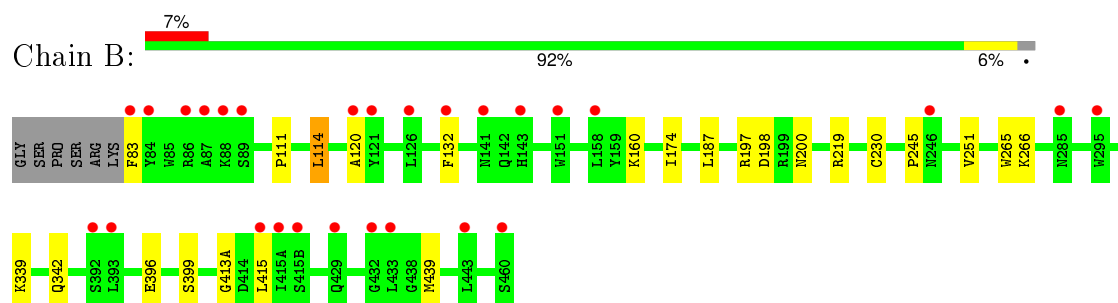
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

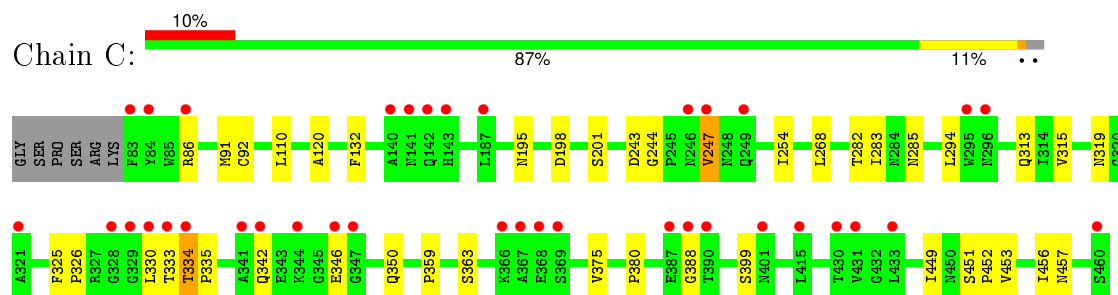
- Molecule 1: Neuraminidase



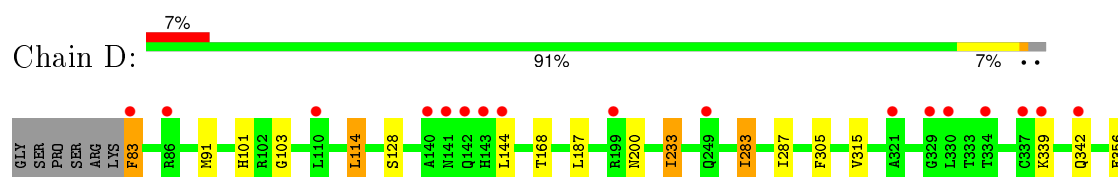
- Molecule 1: Neuraminidase

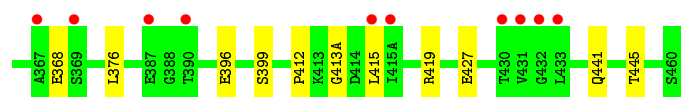


- Molecule 1: Neuraminidase

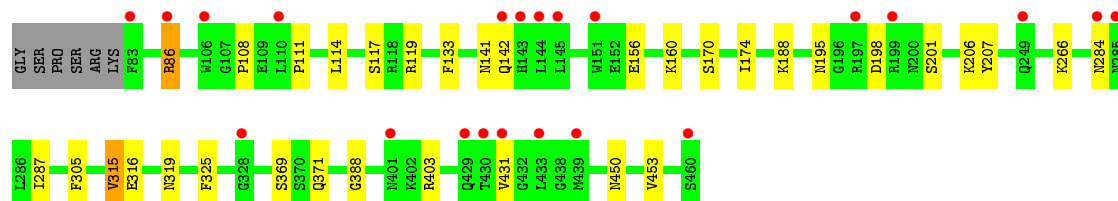
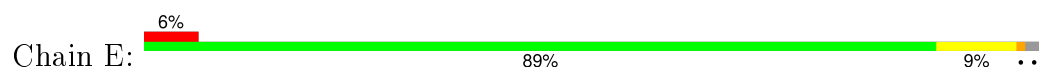


- Molecule 1: Neuraminidase

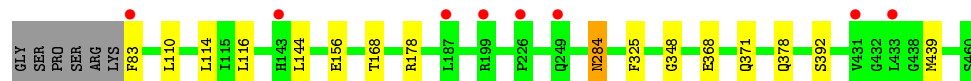
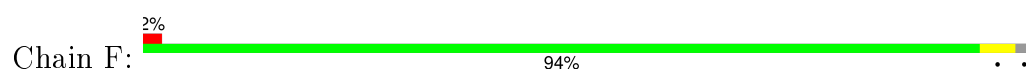




• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.32Å 176.32Å 193.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.11 – 1.95 40.11 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.11-1.95) 98.6 (40.11-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.2_869)	Depositor
R, $R_{free}$	0.180 , 0.223 0.181 , 0.223	Depositor DCC
$R_{free}$ test set	10572 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 52.9	EDS
Estimated twinning fraction	0.018 for -h,k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 210682 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	36150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, BMA, NAG, CA, FUC, FUL, NO3, MAN

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	0.39	0/2945	0.58	0/3990
1	B	0.40	0/2945	0.58	0/3990
1	C	0.35	0/2945	0.55	0/3990
1	D	0.37	0/2945	0.55	0/3990
1	E	0.37	0/2945	0.56	0/3990
1	F	0.42	0/2945	0.59	0/3990
All	All	0.39	0/17670	0.57	0/23940

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	2876	2778	2775	9	0
1	B	2876	2778	2776	12	0
1	C	2876	2778	2776	19	0
1	D	2876	2778	2776	15	0
1	E	2876	2778	2775	14	0
1	F	2876	2778	2775	8	0
2	A	59	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	42	0	39	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
3	E	28	0	26	1	0
3	F	28	0	26	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	18	24	24	2	0
5	B	12	16	16	0	0
5	C	6	8	8	0	0
5	D	6	8	8	1	0
5	E	18	24	24	1	0
5	F	24	32	32	0	0
6	A	8	0	0	1	0
6	B	20	0	0	1	0
6	C	8	0	0	1	0
6	D	8	0	0	0	0
6	F	12	0	0	0	0
7	B	70	0	61	1	0
8	C	48	0	43	0	0
8	E	48	0	43	0	0
8	F	48	0	43	0	0
9	D	38	0	34	0	0
10	E	24	0	22	0	0
11	F	38	0	34	0	0
12	A	247	0	0	0	0
12	B	246	0	0	1	0
12	C	176	0	0	0	0
12	D	213	0	0	1	0
12	E	207	0	0	1	0
12	F	319	0	0	1	0
All	All	19370	16780	17266	78	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.

The worst 5 of 78 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:C:451:SER:HB2	1:C:452:PRO:CD	2.29	0.63
1:E:108:PRO:HB2	1:E:431:VAL:HG13	1.82	0.60
1:D:91:MET:HE1	1:D:356:GLU:HG3	1.84	0.59
1:B:396:GLU:OE2	1:B:399:SER:OG	2.19	0.58
1:D:103:GLY:O	5:D:508:GOL:O3	2.21	0.57

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	365/373 (98%)	354 (97%)	10 (3%)	1 (0%)	46	35
1	B	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	C	365/373 (98%)	349 (96%)	13 (4%)	3 (1%)	24	11
1	D	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	E	365/373 (98%)	351 (96%)	13 (4%)	1 (0%)	46	35
1	F	365/373 (98%)	352 (96%)	13 (4%)	0	100	100
All	All	2190/2238 (98%)	2112 (96%)	73 (3%)	5 (0%)	52	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ASN
1	C	198	ASP
1	C	285	ASN
1	E	198	ASP
1	C	335	PRO



### 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	320/325 (98%)	316 (99%)	4 (1%)	76	72
1	B	320/325 (98%)	314 (98%)	6 (2%)	65	58
1	C	320/325 (98%)	313 (98%)	7 (2%)	60	51
1	D	320/325 (98%)	310 (97%)	10 (3%)	47	34
1	E	320/325 (98%)	311 (97%)	9 (3%)	51	39
1	F	320/325 (98%)	316 (99%)	4 (1%)	76	72
All	All	1920/1950 (98%)	1880 (98%)	40 (2%)	61	53

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	114	LEU
1	D	283	ILE
1	F	83	PHE
1	D	144	LEU
1	D	315	VAL

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

Mol	Chain	Res	Type
1	C	143	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

31 carbohydrates 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	NAG	A	501	1,2	14,14,15	0.53	0	15,19,21	1.23	2 (13%)
2	NAG	A	502	2	14,14,15	0.43	0	15,19,21	0.69	0
2	BMA	A	503	2	11,11,12	0.59	0	14,15,17	0.69	0
2	FUC	A	504	2	10,10,11	0.63	0	14,14,16	1.01	1 (7%)
2	FUL	A	505	2	10,10,11	0.69	0	14,14,16	2.25	4 (28%)
7	NAG	B	501	1,7	14,14,15	0.60	0	15,19,21	1.43	2 (13%)
7	NAG	B	502	7	14,14,15	0.44	0	15,19,21	0.59	0
7	BMA	B	503	7	11,11,12	0.62	0	14,15,17	0.60	0
7	MAN	B	504	7	11,11,12	0.53	0	14,15,17	1.04	2 (14%)
7	FUC	B	505	7	10,10,11	0.66	0	14,14,16	1.21	2 (14%)
7	FUL	B	506	7	10,10,11	0.78	0	14,14,16	2.80	5 (35%)
8	NAG	C	501	1,8	14,14,15	0.63	0	15,19,21	1.25	2 (13%)
8	NAG	C	502	8	14,14,15	0.42	0	15,19,21	0.95	0
8	FUC	C	503	8	10,10,11	0.57	0	14,14,16	1.05	1 (7%)
8	FUL	C	504	8	10,10,11	0.59	0	14,14,16	0.77	0
9	NAG	D	501	9,1	14,14,15	0.58	0	15,19,21	1.12	1 (6%)
9	NAG	D	502	9	14,14,15	0.42	0	15,19,21	0.78	0
9	FUC	D	503	9	10,10,11	0.55	0	14,14,16	0.85	0
8	NAG	E	501	1,8	14,14,15	0.53	0	15,19,21	1.14	2 (13%)
8	NAG	E	502	8	14,14,15	0.47	0	15,19,21	0.62	0
8	FUC	E	503	8	10,10,11	0.62	0	14,14,16	1.02	2 (14%)
8	FUL	E	504	8	10,10,11	0.68	0	14,14,16	2.41	4 (28%)
10	NAG	E	506	1,10	14,14,15	0.51	0	15,19,21	1.14	2 (13%)
10	FUC	E	507	10	10,10,11	0.71	0	14,14,16	1.20	1 (7%)
8	NAG	F	501	1,8	14,14,15	0.48	0	15,19,21	1.24	1 (6%)
8	NAG	F	502	8	14,14,15	0.49	0	15,19,21	0.86	0
8	FUC	F	503	8	10,10,11	0.68	0	14,14,16	1.23	1 (7%)
8	FUL	F	504	8	10,10,11	0.64	0	14,14,16	2.19	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	F	507	11,1	14,14,15	0.57	0	15,19,21	1.18	2 (13%)
11	NAG	F	508	11	14,14,15	0.47	0	15,19,21	0.81	0
11	FUL	F	509	11	10,10,11	0.60	0	14,14,16	0.74	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
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	BMA	A	503	2	-	0/2/19/22	0/1/1/1
2	FUC	A	504	2	-	0/0/17/20	0/1/1/1
2	FUL	A	505	2	-	0/0/17/20	0/1/1/1
7	NAG	B	501	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	502	7	-	0/6/23/26	0/1/1/1
7	BMA	B	503	7	-	0/2/19/22	1/1/1/1
7	MAN	B	504	7	-	0/2/19/22	1/1/1/1
7	FUC	B	505	7	-	0/0/17/20	0/1/1/1
7	FUL	B	506	7	-	0/0/17/20	0/1/1/1
8	NAG	C	501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	502	8	-	0/6/23/26	0/1/1/1
8	FUC	C	503	8	-	0/0/17/20	0/1/1/1
8	FUL	C	504	8	-	0/0/17/20	0/1/1/1
9	NAG	D	501	9,1	-	0/6/23/26	0/1/1/1
9	NAG	D	502	9	-	0/6/23/26	0/1/1/1
9	FUC	D	503	9	-	0/0/17/20	0/1/1/1
8	NAG	E	501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	502	8	-	0/6/23/26	0/1/1/1
8	FUC	E	503	8	-	0/0/17/20	0/1/1/1
8	FUL	E	504	8	-	0/0/17/20	0/1/1/1
10	NAG	E	506	1,10	-	0/6/23/26	0/1/1/1
10	FUC	E	507	10	-	0/0/17/20	0/1/1/1
8	NAG	F	501	1,8	-	0/6/23/26	0/1/1/1
8	NAG	F	502	8	-	0/6/23/26	0/1/1/1
8	FUC	F	503	8	-	0/0/17/20	0/1/1/1
8	FUL	F	504	8	-	0/0/17/20	0/1/1/1
11	NAG	F	507	11,1	-	0/6/23/26	0/1/1/1
11	NAG	F	508	11	-	0/6/23/26	0/1/1/1
11	FUL	F	509	11	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	506	FUL	C1-C2-C3	-7.39	100.80	109.54
8	E	504	FUL	C1-C2-C3	-6.30	102.09	109.54
2	A	505	FUL	C1-C2-C3	-5.63	102.88	109.54
8	F	504	FUL	C1-O5-C5	-5.08	104.53	112.38
8	F	504	FUL	C1-C2-C3	-4.65	104.03	109.54

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	503	BMA	C1-C2-C3-C4-C5-O5
7	B	504	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	503	BMA	1	0
7	B	504	MAN	1	0

## 5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 11 are monoatomic - leaving 41 for Mogul analysis.

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	A	506	1	14,14,15	0.49	0	15,19,21	0.87	0
3	NAG	A	507	1	14,14,15	0.40	0	15,19,21	1.32	2 (13%)
3	NAG	A	508	1	14,14,15	0.55	0	15,19,21	0.95	0
5	GOL	A	510	-	5,5,5	0.29	0	5,5,5	0.45	0
5	GOL	A	511	-	5,5,5	0.43	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	A	512	-	5,5,5	0.41	0	5,5,5	0.21	0
6	NO3	A	513	-	3,3,3	3.21	3 (100%)	3,3,3	0.08	0
6	NO3	A	514	-	3,3,3	3.34	3 (100%)	3,3,3	0.17	0
3	NAG	B	507	1	14,14,15	0.60	0	15,19,21	0.92	0
3	NAG	B	508	1	14,14,15	0.52	0	15,19,21	0.82	0
5	GOL	B	511	-	5,5,5	0.28	0	5,5,5	0.40	0
5	GOL	B	512	-	5,5,5	0.29	0	5,5,5	0.27	0
6	NO3	B	513	-	3,3,3	3.33	3 (100%)	3,3,3	0.11	0
6	NO3	B	514	-	3,3,3	3.19	3 (100%)	3,3,3	0.17	0
6	NO3	B	515	-	3,3,3	3.30	3 (100%)	3,3,3	0.12	0
6	NO3	B	516	-	3,3,3	3.10	3 (100%)	3,3,3	0.16	0
6	NO3	B	517	-	3,3,3	3.27	3 (100%)	3,3,3	0.18	0
3	NAG	C	505	1	14,14,15	0.54	0	15,19,21	0.75	0
3	NAG	C	506	1	14,14,15	0.63	0	15,19,21	1.11	2 (13%)
5	GOL	C	509	-	5,5,5	0.30	0	5,5,5	0.49	0
6	NO3	C	510	-	3,3,3	3.23	3 (100%)	3,3,3	0.24	0
6	NO3	C	511	-	3,3,3	3.20	3 (100%)	3,3,3	0.22	0
3	NAG	D	504	1	14,14,15	0.52	0	15,19,21	1.47	1 (6%)
3	NAG	D	505	1	14,14,15	0.56	0	15,19,21	1.09	1 (6%)
5	GOL	D	508	-	5,5,5	0.37	0	5,5,5	0.36	0
6	NO3	D	509	-	3,3,3	3.27	3 (100%)	3,3,3	0.22	0
6	NO3	D	510	-	3,3,3	3.26	3 (100%)	3,3,3	0.11	0
3	NAG	E	505	1	14,14,15	0.60	0	15,19,21	0.88	0
3	NAG	E	508	1	14,14,15	0.65	0	15,19,21	1.28	2 (13%)
5	GOL	E	511	-	5,5,5	0.29	0	5,5,5	0.42	0
5	GOL	E	512	-	5,5,5	0.45	0	5,5,5	0.28	0
5	GOL	E	513	-	5,5,5	0.32	0	5,5,5	0.27	0
3	NAG	F	505	1	14,14,15	0.56	0	15,19,21	0.75	0
3	NAG	F	506	1	14,14,15	0.49	0	15,19,21	0.96	1 (6%)
5	GOL	F	512	-	5,5,5	0.51	0	5,5,5	0.63	0
5	GOL	F	513	-	5,5,5	0.30	0	5,5,5	0.46	0
5	GOL	F	514	-	5,5,5	0.31	0	5,5,5	0.32	0
5	GOL	F	515	-	5,5,5	0.34	0	5,5,5	0.48	0
6	NO3	F	516	-	3,3,3	3.27	3 (100%)	3,3,3	0.16	0
6	NO3	F	517	-	3,3,3	3.40	3 (100%)	3,3,3	0.05	0
6	NO3	F	518	-	3,3,3	3.18	3 (100%)	3,3,3	0.13	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
3	NAG	A	506	1	-	0/6/23/26	0/1/1/1
3	NAG	A	507	1	-	0/6/23/26	0/1/1/1
3	NAG	A	508	1	-	0/6/23/26	0/1/1/1
5	GOL	A	510	-	-	0/4/4/4	0/0/0/0
5	GOL	A	511	-	-	0/4/4/4	0/0/0/0
5	GOL	A	512	-	-	0/4/4/4	0/0/0/0
6	NO3	A	513	-	-	0/0/0/0	0/0/0/0
6	NO3	A	514	-	-	0/0/0/0	0/0/0/0
3	NAG	B	507	1	-	0/6/23/26	0/1/1/1
3	NAG	B	508	1	-	0/6/23/26	0/1/1/1
5	GOL	B	511	-	-	0/4/4/4	0/0/0/0
5	GOL	B	512	-	-	0/4/4/4	0/0/0/0
6	NO3	B	513	-	-	0/0/0/0	0/0/0/0
6	NO3	B	514	-	-	0/0/0/0	0/0/0/0
6	NO3	B	515	-	-	0/0/0/0	0/0/0/0
6	NO3	B	516	-	-	0/0/0/0	0/0/0/0
6	NO3	B	517	-	-	0/0/0/0	0/0/0/0
3	NAG	C	505	1	-	0/6/23/26	0/1/1/1
3	NAG	C	506	1	-	0/6/23/26	0/1/1/1
5	GOL	C	509	-	-	0/4/4/4	0/0/0/0
6	NO3	C	510	-	-	0/0/0/0	0/0/0/0
6	NO3	C	511	-	-	0/0/0/0	0/0/0/0
3	NAG	D	504	1	-	0/6/23/26	0/1/1/1
3	NAG	D	505	1	-	0/6/23/26	0/1/1/1
5	GOL	D	508	-	-	0/4/4/4	0/0/0/0
6	NO3	D	509	-	-	0/0/0/0	0/0/0/0
6	NO3	D	510	-	-	0/0/0/0	0/0/0/0
3	NAG	E	505	1	-	0/6/23/26	0/1/1/1
3	NAG	E	508	1	-	0/6/23/26	0/1/1/1
5	GOL	E	511	-	-	0/4/4/4	0/0/0/0
5	GOL	E	512	-	-	0/4/4/4	0/0/0/0
5	GOL	E	513	-	-	0/4/4/4	0/0/0/0
3	NAG	F	505	1	-	0/6/23/26	0/1/1/1
3	NAG	F	506	1	-	0/6/23/26	0/1/1/1
5	GOL	F	512	-	-	0/4/4/4	0/0/0/0
5	GOL	F	513	-	-	0/4/4/4	0/0/0/0
5	GOL	F	514	-	-	0/4/4/4	0/0/0/0
5	GOL	F	515	-	-	0/4/4/4	0/0/0/0
6	NO3	F	516	-	-	0/0/0/0	0/0/0/0
6	NO3	F	517	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NO3	F	518	-	-	0/0/0/0	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	513	NO3	O3-N	2.67	1.39	1.25
6	C	511	NO3	O2-N	2.76	1.39	1.25
6	B	516	NO3	O2-N	2.77	1.39	1.25
6	B	515	NO3	O2-N	2.81	1.39	1.25
6	B	517	NO3	O2-N	2.82	1.39	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	508	NAG	C2-N2-C7	-3.46	118.59	123.04
3	A	507	NAG	C4-C3-C2	-3.02	106.53	111.23
3	E	508	NAG	C1-O5-C5	-2.74	108.77	112.25
3	F	506	NAG	C2-N2-C7	-2.47	119.86	123.04
3	C	506	NAG	C2-N2-C7	-2.22	120.19	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	511	GOL	1	0
5	A	512	GOL	1	0
6	A	513	NO3	1	0
6	B	517	NO3	1	0
6	C	510	NO3	1	0
5	D	508	GOL	1	0
3	E	505	NAG	1	0
5	E	511	GOL	1	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	367/373 (98%)	0.36	12 (3%)	50	61	19, 30, 52, 77	0
1	B	367/373 (98%)	0.45	27 (7%)	17	27	20, 32, 61, 93	0
1	C	367/373 (98%)	0.62	37 (10%)	9	14	23, 39, 66, 85	0
1	D	367/373 (98%)	0.51	27 (7%)	17	27	23, 36, 62, 88	0
1	E	367/373 (98%)	0.48	22 (5%)	25	35	22, 36, 60, 92	0
1	F	367/373 (98%)	0.23	8 (2%)	65	74	18, 28, 49, 76	0
All	All	2202/2238 (98%)	0.44	133 (6%)	25	35	18, 33, 60, 93	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	7.6
1	C	83	PHE	7.0
1	E	83	PHE	6.5
1	F	83	PHE	6.4
1	B	83	PHE	6.3

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	FUC	D	503	10/11	0.92	0.21	3.43	49,55,64,70	0
2	FUC	A	504	10/11	0.90	0.15	1.45	23,39,45,49	0
8	FUC	E	503	10/11	0.93	0.16	0.81	35,41,50,56	0
8	FUC	C	503	10/11	0.87	0.16	0.09	47,64,80,86	0
7	FUC	B	505	10/11	0.94	0.10	-0.02	30,45,49,51	0
7	NAG	B	501	14/15	0.92	0.13	-0.22	40,43,55,59	0
8	FUC	F	503	10/11	0.96	0.10	-0.59	27,35,40,47	0
8	NAG	E	502	14/15	0.92	0.23	-	53,64,80,89	0
8	FUL	F	504	10/11	0.82	0.19	-	66,72,76,90	0
8	FUL	C	504	10/11	0.75	0.30	-	100,113,123,132	0
7	FUL	B	506	10/11	0.78	0.30	-	63,76,83,83	0
8	FUL	E	504	10/11	0.75	0.30	-	73,80,87,88	0
2	NAG	A	501	14/15	0.93	0.16	-	38,47,53,63	0
7	MAN	B	504	11/12	0.54	0.46	-	106,118,121,124	0
7	BMA	B	503	11/12	0.77	0.38	-	98,112,119,120	0
8	NAG	C	501	14/15	0.83	0.19	-	64,72,87,101	0
8	NAG	C	502	14/15	0.78	0.28	-	72,83,94,98	0
2	FUL	A	505	10/11	0.79	0.23	-	59,70,83,96	0
8	NAG	F	501	14/15	0.93	0.10	-	28,35,51,57	0
2	BMA	A	503	11/12	0.66	0.28	-	102,115,122,126	0
7	NAG	B	502	14/15	0.89	0.17	-	46,54,72,83	0
8	NAG	F	502	14/15	0.91	0.18	-	41,58,67,89	0
2	NAG	A	502	14/15	0.93	0.14	-	48,62,76,87	0
9	NAG	D	502	14/15	0.83	0.37	-	71,78,90,96	0
11	NAG	F	507	14/15	0.79	0.25	-	53,72,95,97	0
11	FUL	F	509	10/11	0.68	0.45	-	103,113,123,131	0
11	NAG	F	508	14/15	0.69	0.43	-	90,105,113,114	0
10	FUC	E	507	10/11	0.87	0.24	-	87,96,100,100	0
8	NAG	E	501	14/15	0.89	0.16	-	39,45,68,70	0
10	NAG	E	506	14/15	0.87	0.19	-	48,55,72,75	0
9	NAG	D	501	14/15	0.79	0.23	-	50,64,73,92	0

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	E	511	6/6	0.67	0.26	13.53	62,74,80,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NO3	B	517	4/4	0.92	0.22	9.42	53,57,58,72	0
5	GOL	F	512	6/6	0.88	0.25	7.64	33,58,76,92	0
5	GOL	B	511	6/6	0.53	0.22	5.04	37,64,76,77	0
6	NO3	A	514	4/4	0.90	0.25	4.72	26,46,53,69	0
6	NO3	C	511	4/4	0.97	0.15	3.98	42,45,49,52	0
5	GOL	D	508	6/6	0.77	0.20	3.82	54,73,85,87	0
6	NO3	F	518	4/4	0.97	0.20	3.67	36,48,50,62	0
6	NO3	B	516	4/4	0.98	0.15	3.59	32,35,37,42	0
6	NO3	D	510	4/4	0.97	0.19	3.11	50,57,61,64	0
5	GOL	A	512	6/6	0.93	0.23	2.97	42,58,69,69	0
6	NO3	C	510	4/4	0.92	0.21	2.93	37,54,59,70	0
5	GOL	F	515	6/6	0.89	0.16	2.62	47,56,58,58	0
3	NAG	F	505	14/15	0.85	0.22	2.46	50,67,74,92	0
6	NO3	A	513	4/4	0.93	0.18	2.35	37,46,49,50	0
5	GOL	E	512	6/6	0.92	0.15	2.11	33,43,74,88	0
6	NO3	F	517	4/4	0.81	0.16	1.95	62,66,73,74	0
5	GOL	B	512	6/6	0.86	0.17	1.83	43,60,74,75	0
3	NAG	E	505	14/15	0.85	0.20	1.81	35,55,63,68	0
6	NO3	D	509	4/4	0.92	0.19	1.76	46,48,54,61	0
3	NAG	A	506	14/15	0.73	0.29	1.71	47,82,97,105	0
6	NO3	F	516	4/4	0.94	0.12	1.62	55,66,66,76	0
6	NO3	B	514	4/4	0.98	0.16	1.34	36,41,47,50	0
5	GOL	A	511	6/6	0.96	0.16	1.06	32,61,82,89	0
5	GOL	E	513	6/6	0.81	0.16	1.05	73,88,97,97	0
3	NAG	C	505	14/15	0.73	0.29	0.99	62,73,80,87	0
5	GOL	F	513	6/6	0.91	0.12	0.97	31,52,68,70	0
3	NAG	D	504	14/15	0.86	0.18	0.95	37,54,69,73	0
5	GOL	C	509	6/6	0.95	0.13	0.58	36,49,58,66	0
5	GOL	F	514	6/6	0.93	0.11	0.58	28,40,70,84	0
5	GOL	A	510	6/6	0.96	0.12	0.54	26,39,55,66	0
6	NO3	B	515	4/4	0.97	0.19	0.33	37,38,43,61	0
4	CA	E	510	1/1	0.91	0.10	0.09	69,69,69,69	0
4	CA	A	509	1/1	1.00	0.11	-0.07	25,25,25,25	0
6	NO3	B	513	4/4	0.97	0.15	-0.25	27,50,51,69	0
4	CA	F	510	1/1	0.99	0.09	-0.72	22,22,22,22	0
4	CA	B	509	1/1	0.99	0.08	-0.96	25,25,25,25	0
4	CA	E	509	1/1	0.97	0.07	-1.18	32,32,32,32	0
4	CA	C	507	1/1	0.94	0.07	-1.20	48,48,48,48	0
4	CA	D	506	1/1	0.98	0.06	-1.45	33,33,33,33	0
4	CA	D	507	1/1	0.89	0.05	-2.93	55,55,55,55	0
4	CA	F	511	1/1	0.97	0.05	-3.90	45,45,45,45	0
4	CA	C	508	1/1	0.76	0.06	-4.69	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	B	510	1/1	0.95	0.04	-9.41	59,59,59,59	0
3	NAG	B	508	14/15	0.77	0.32	-	68,73,90,92	0
3	NAG	C	506	14/15	0.74	0.31	-	65,74,98,101	0
3	NAG	A	508	14/15	0.73	0.27	-	65,82,93,98	0
3	NAG	F	506	14/15	0.74	0.36	-	66,80,88,95	0
3	NAG	D	505	14/15	0.68	0.33	-	56,75,86,92	0
3	NAG	B	507	14/15	0.84	0.22	-	65,86,92,100	0
3	NAG	A	507	14/15	0.81	0.26	-	67,79,88,89	0
3	NAG	E	508	14/15	0.68	0.29	-	68,87,102,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.