



# wwPDB EM Model Validation Summary Report ⓘ

Mar 23, 2020 – 12:41 PM EDT

PDB ID : 6V0R  
EMDB ID : EMD-20396  
Title : BG505 SOSIP.664 Trimer  
Authors : Nogal, B.; Cottrell, C.A.; Ward, A.B.  
Deposited on : 2019-11-19  
Resolution : 3.87 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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 : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.8

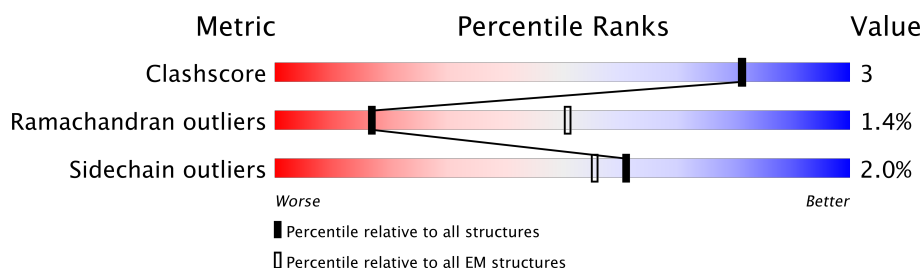
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.87 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	475	86% 5% • 8%
1	C	475	86% 5% • 8%
1	D	475	86% 6% • 8%
2	B	153	73% 8% •• 16%
2	E	153	73% 8% •• 16%
2	F	153	73% 8% •• 16%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 BG505 SOSIPv5.2 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3462	2177	610	646	29		
1	C	439	Total	C	N	O	S	0	0
			3462	2177	610	646	29		
1	D	439	Total	C	N	O	S	0	0
			3462	2177	610	646	29		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	CYS	ALA	conflict	UNP Q2N0S6
A	316	TRP	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	73	CYS	ALA	conflict	UNP Q2N0S6
C	316	TRP	ALA	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
D	73	CYS	ALA	conflict	UNP Q2N0S6
D	316	TRP	ALA	conflict	UNP Q2N0S6
D	332	ASN	THR	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIPv5.2 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	129	Total	C	N	O	S	0	0
			1030	650	180	193	7		
2	E	129	Total	C	N	O	S	0	0
			1030	650	180	193	7		
2	F	129	Total	C	N	O	S	0	0
			1030	650	180	193	7		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	CYS	ALA	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
E	559	PRO	ILE	conflict	UNP Q2N0S6
E	561	CYS	ALA	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	561	CYS	ALA	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			350	200	25	125	
3	A	1	Total	C	N	O	0
			350	200	25	125	
3	A	1	Total	C	N	O	0
			350	200	25	125	
3	A	1	Total	C	N	O	0
			350	200	25	125	
3	A	1	Total	C	N	O	0
			350	200	25	125	
3	A	1	Total	C	N	O	0
			350	200	25	125	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	A	1	Total 350	C 200	N 25	O 125	0
3	B	1	Total 42	C 24	N 3	O 15	0
3	B	1	Total 42	C 24	N 3	O 15	0

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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total 350	C 200	N 25	O 125	0
3	C	1	Total 350	C 200	N 25	O 125	0
3	C	1	Total 350	C 200	N 25	O 125	0
3	C	1	Total 350	C 200	N 25	O 125	0
3	C	1	Total 350	C 200	N 25	O 125	0
3	E	1	Total 42	C 24	N 3	O 15	0
3	E	1	Total 42	C 24	N 3	O 15	0
3	E	1	Total 42	C 24	N 3	O 15	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0
3	D	1	Total 350	C 200	N 25	O 125	0

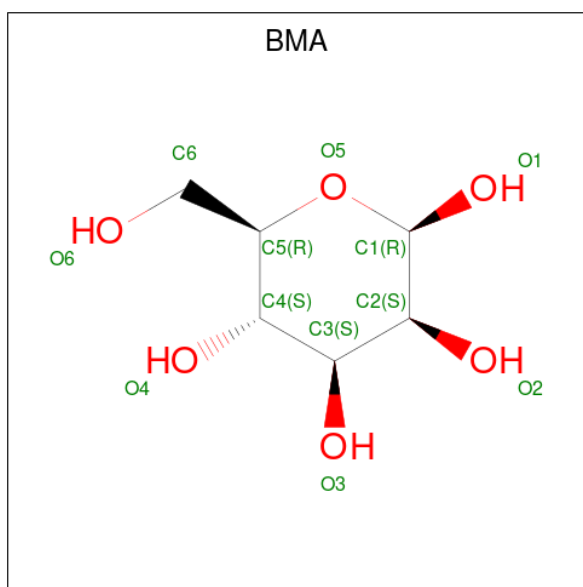
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Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	D	1	Total	C	N	O	0
			350	200	25	125	
3	F	1	Total	C	N	O	0
			42	24	3	15	
3	F	1	Total	C	N	O	0
			42	24	3	15	
3	F	1	Total	C	N	O	0
			42	24	3	15	

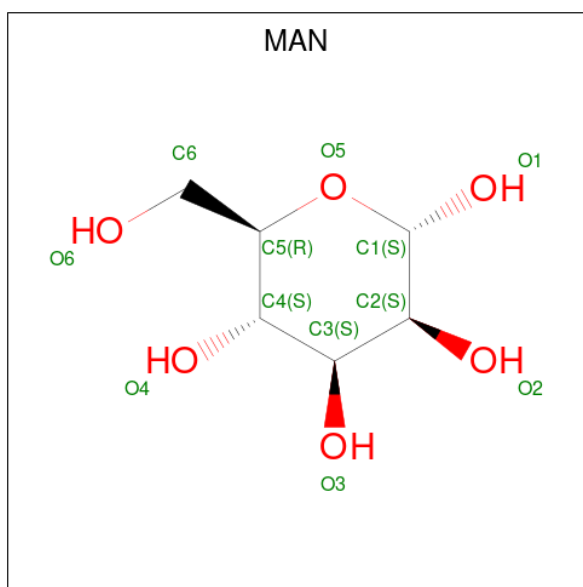
- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).





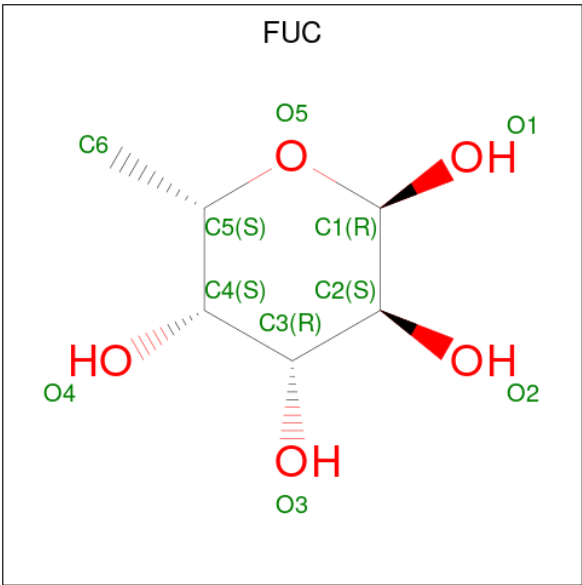
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			33	18	15	
4	A	1	Total	C	O	0
			33	18	15	
4	A	1	Total	C	O	0
			33	18	15	
4	C	1	Total	C	O	0
			33	18	15	
4	C	1	Total	C	O	0
			33	18	15	
4	C	1	Total	C	O	0
			33	18	15	
4	D	1	Total	C	O	0
			33	18	15	
4	D	1	Total	C	O	0
			33	18	15	
4	D	1	Total	C	O	0
			33	18	15	

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			33	18	15	
5	A	1	Total	C	O	0
			33	18	15	
5	A	1	Total	C	O	0
			33	18	15	
5	C	1	Total	C	O	0
			33	18	15	
5	C	1	Total	C	O	0
			33	18	15	
5	C	1	Total	C	O	0
			33	18	15	
5	D	1	Total	C	O	0
			33	18	15	
5	D	1	Total	C	O	0
			33	18	15	
5	D	1	Total	C	O	0
			33	18	15	

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).

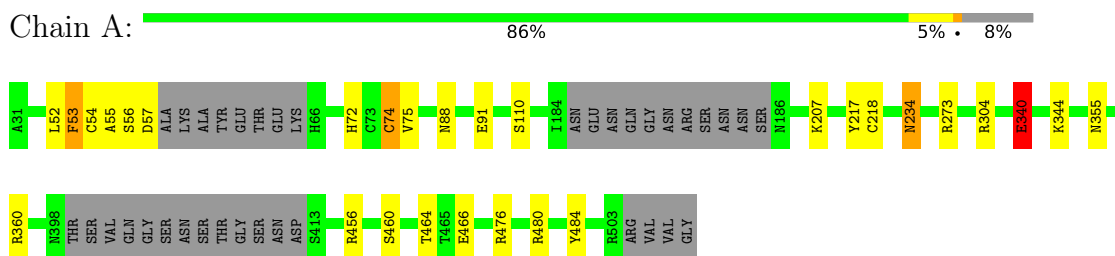


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			10	6	4	
6	B	1	Total	C	O	0
			10	6	4	
6	C	1	Total	C	O	0
			10	6	4	
6	E	1	Total	C	O	0
			10	6	4	
6	D	1	Total	C	O	0
			10	6	4	
6	F	1	Total	C	O	0
			10	6	4	

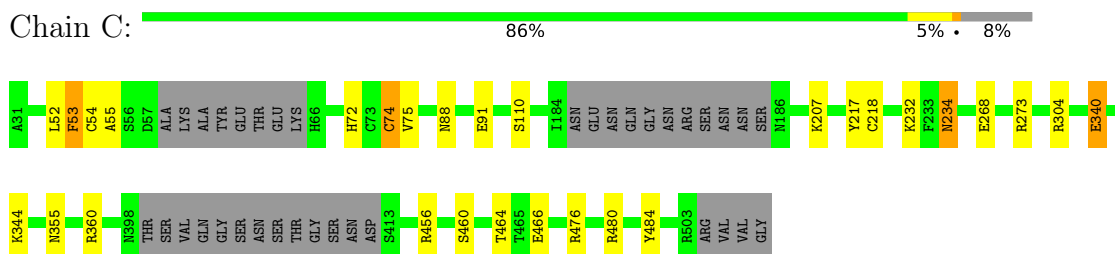
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

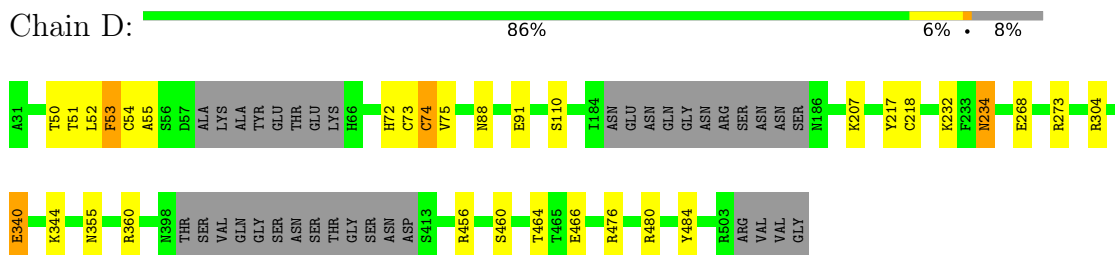
- Molecule 1: BG505 SOSIPv5.2 gp120



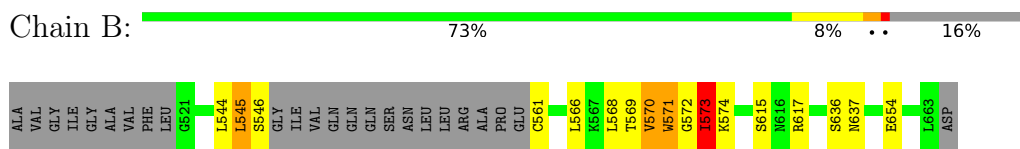
- Molecule 1: BG505 SOSIPv5.2 gp120



- Molecule 1: BG505 SOSIPv5.2 gp120



- Molecule 2: BG505 SOSIPv5.2 gp41



- Molecule 2: BG505 SOSIPv5.2 gp41

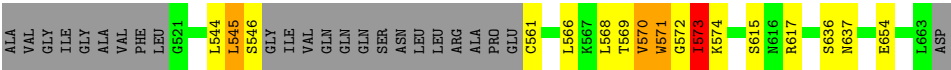
Chain E: 

73%

8%

••

16%



● Molecule 2: BG505 SOSIPv5.2 gp41

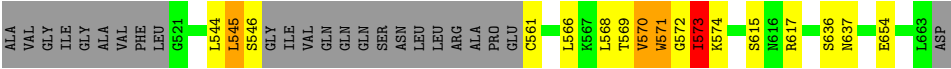
Chain F: 

73%

8%

••

16%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	155394	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 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: FUC, BMA, NAG, 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	1.03	8/3536 (0.2%)	0.91	7/4802 (0.1%)
1	C	1.03	7/3536 (0.2%)	0.91	7/4802 (0.1%)
1	D	1.03	7/3536 (0.2%)	0.91	7/4802 (0.1%)
2	B	1.00	1/1048 (0.1%)	0.83	2/1420 (0.1%)
2	E	1.00	1/1048 (0.1%)	0.83	2/1420 (0.1%)
2	F	1.00	1/1048 (0.1%)	0.83	2/1420 (0.1%)
All	All	1.02	25/13752 (0.2%)	0.89	27/18666 (0.1%)

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	TYR	CB-CG	-8.46	1.39	1.51
1	C	484	TYR	CB-CG	-8.44	1.39	1.51
1	D	484	TYR	CB-CG	-8.41	1.39	1.51
1	C	217	TYR	CB-CG	-6.81	1.41	1.51
1	A	217	TYR	CB-CG	-6.81	1.41	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	D	480	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	C	480	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	476	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	476	ARG	NE-CZ-NH2	-7.98	116.31	120.30

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	3462	0	3395	15	0
1	C	3462	0	3395	15	0
1	D	3462	0	3395	18	0
2	B	1030	0	1013	13	0
2	E	1030	0	1013	12	0
2	F	1030	0	1013	12	0
3	A	350	0	313	0	0
3	B	42	0	38	0	0
3	C	350	0	313	0	0
3	D	350	0	313	0	0
3	E	42	0	38	0	0
3	F	42	0	38	0	0
4	A	33	0	25	0	0
4	C	33	0	25	0	0
4	D	33	0	25	0	0
5	A	33	0	27	0	0
5	C	33	0	27	0	0
5	D	33	0	27	0	0
6	A	10	0	10	0	0
6	B	10	0	10	0	0
6	C	10	0	10	0	0
6	D	10	0	10	0	0
6	E	10	0	10	0	0
6	F	10	0	10	0	0
All	All	14910	0	14493	75	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.

The worst 5 of 75 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:D:54:CYS:HG	1:D:73:CYS:HG	0.84	0.69
2:B:568:LEU:HD21	2:B:571:TRP:CE3	2.33	0.64
2:E:568:LEU:HD21	2:E:571:TRP:CE3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:568:LEU:HD21	2:F:571:TRP:CE3	2.33	0.63
1:D:53:PHE:CE1	1:D:218:CYS:HB2	2.34	0.62

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 PDB entries followed by that with respect to all EM entries.

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	431/475 (91%)	405 (94%)	22 (5%)	4 (1%)	19	59
1	C	431/475 (91%)	405 (94%)	22 (5%)	4 (1%)	19	59
1	D	431/475 (91%)	405 (94%)	22 (5%)	4 (1%)	19	59
2	B	125/153 (82%)	119 (95%)	2 (2%)	4 (3%)	4	37
2	E	125/153 (82%)	119 (95%)	2 (2%)	4 (3%)	4	37
2	F	125/153 (82%)	119 (95%)	2 (2%)	4 (3%)	4	37
All	All	1668/1884 (88%)	1572 (94%)	72 (4%)	24 (1%)	17	52

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	569	THR
2	B	636	SER
2	E	569	THR
2	E	636	SER
2	F	569	THR

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	394/424 (93%)	389 (99%)	5 (1%)	71	86
1	C	394/424 (93%)	389 (99%)	5 (1%)	71	86
1	D	394/424 (93%)	389 (99%)	5 (1%)	71	86
2	B	112/130 (86%)	107 (96%)	5 (4%)	30	64
2	E	112/130 (86%)	107 (96%)	5 (4%)	30	64
2	F	112/130 (86%)	107 (96%)	5 (4%)	30	64
All	All	1518/1662 (91%)	1488 (98%)	30 (2%)	61	81

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	234	ASN
2	E	545	LEU
2	F	570	VAL
2	E	544	LEU
2	E	570	VAL

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

Mol	Chain	Res	Type
1	A	72	HIS
1	C	72	HIS
1	D	72	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

108 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	601	1,3	14,14,15	0.80	0	17,19,21	1.24	2 (11%)
3	NAG	A	602	3	14,14,15	0.78	0	17,19,21	0.97	1 (5%)
3	NAG	A	603	1	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
3	NAG	A	604	1,3	14,14,15	0.87	0	17,19,21	2.03	5 (29%)
3	NAG	A	605	3	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
3	NAG	A	606	1	14,14,15	0.77	0	17,19,21	0.90	1 (5%)
3	NAG	A	607	1,3	14,14,15	0.76	0	17,19,21	1.03	1 (5%)
3	NAG	A	608	3	14,14,15	0.77	0	17,19,21	1.21	2 (11%)
3	NAG	A	609	1	14,14,15	0.84	0	17,19,21	1.25	1 (5%)
3	NAG	A	610	1	14,14,15	0.82	0	17,19,21	0.98	1 (5%)
3	NAG	A	611	1	14,14,15	0.87	0	17,19,21	1.20	2 (11%)
3	NAG	A	612	1,3	14,14,15	0.74	0	17,19,21	1.15	1 (5%)
3	NAG	A	613	3,4	14,14,15	0.79	1 (7%)	17,19,21	1.18	2 (11%)
4	BMA	A	614	3,5	11,11,12	1.85	2 (18%)	15,15,17	1.13	1 (6%)
5	MAN	A	615	5,4	11,11,12	1.58	1 (9%)	15,15,17	1.09	2 (13%)
5	MAN	A	616	5	11,11,12	1.86	3 (27%)	15,15,17	1.18	2 (13%)
5	MAN	A	617	4	11,11,12	1.81	2 (18%)	15,15,17	1.14	2 (13%)
3	NAG	A	618	1	14,14,15	0.88	0	17,19,21	1.04	2 (11%)
3	NAG	A	619	1,3	14,14,15	0.77	0	17,19,21	1.19	2 (11%)
3	NAG	A	620	3,4	14,14,15	0.80	0	17,19,21	0.81	0
4	BMA	A	621	3	11,11,12	1.81	2 (18%)	15,15,17	0.89	1 (6%)
3	NAG	A	622	1	14,14,15	0.82	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	623	1	14,14,15	0.87	0	17,19,21	0.88	1 (5%)
3	NAG	A	624	1,3	14,14,15	0.80	1 (7%)	17,19,21	1.35	2 (11%)
3	NAG	A	625	3,4	14,14,15	0.80	0	17,19,21	1.00	2 (11%)
4	BMA	A	626	3	11,11,12	1.81	2 (18%)	15,15,17	1.00	1 (6%)
3	NAG	A	627	1,3,6	14,14,15	0.80	1 (7%)	17,19,21	1.03	0
3	NAG	A	628	3	14,14,15	0.79	0	17,19,21	1.17	1 (5%)
6	FUC	A	629	3	9,10,11	0.72	0	13,14,16	1.04	1 (7%)
3	NAG	A	630	1,3	14,14,15	0.79	0	17,19,21	0.94	0
3	NAG	A	631	3	14,14,15	0.78	0	17,19,21	1.23	2 (11%)
3	NAG	A	632	1	14,14,15	0.80	0	17,19,21	1.08	1 (5%)
3	NAG	B	701	2,6	14,14,15	0.74	0	17,19,21	1.09	1 (5%)
6	FUC	B	702	3	9,10,11	1.40	2 (22%)	13,14,16	4.26	5 (38%)
3	NAG	B	703	2	14,14,15	0.85	0	17,19,21	0.82	1 (5%)
3	NAG	B	704	2	14,14,15	0.90	0	17,19,21	0.96	1 (5%)
3	NAG	C	601	1,3	14,14,15	0.80	0	17,19,21	1.23	2 (11%)
3	NAG	C	602	3	14,14,15	0.79	0	17,19,21	0.97	1 (5%)
3	NAG	C	603	1	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
3	NAG	C	604	1,3	14,14,15	0.88	0	17,19,21	2.03	5 (29%)
3	NAG	C	605	3	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
3	NAG	C	606	1	14,14,15	0.78	0	17,19,21	0.90	1 (5%)
3	NAG	C	607	1,3	14,14,15	0.76	0	17,19,21	1.02	1 (5%)
3	NAG	C	608	3	14,14,15	0.76	0	17,19,21	1.20	2 (11%)
3	NAG	C	609	1	14,14,15	0.85	0	17,19,21	1.25	1 (5%)
3	NAG	C	610	1	14,14,15	0.82	0	17,19,21	0.99	1 (5%)
3	NAG	C	611	1	14,14,15	0.87	0	17,19,21	1.20	2 (11%)
3	NAG	C	612	1,3	14,14,15	0.75	0	17,19,21	1.15	1 (5%)
3	NAG	C	613	3,4	14,14,15	0.79	1 (7%)	17,19,21	1.18	2 (11%)
4	BMA	C	614	3,5	11,11,12	1.85	2 (18%)	15,15,17	1.13	1 (6%)
5	MAN	C	615	5,4	11,11,12	1.58	1 (9%)	15,15,17	1.09	2 (13%)
5	MAN	C	616	5	11,11,12	1.86	3 (27%)	15,15,17	1.18	2 (13%)
5	MAN	C	617	4	11,11,12	1.80	2 (18%)	15,15,17	1.14	3 (20%)
3	NAG	C	618	1	14,14,15	0.88	0	17,19,21	1.04	2 (11%)
3	NAG	C	619	1,3	14,14,15	0.76	0	17,19,21	1.19	2 (11%)
3	NAG	C	620	3,4	14,14,15	0.80	0	17,19,21	0.81	0
4	BMA	C	621	3	11,11,12	1.81	2 (18%)	15,15,17	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	622	1	14,14,15	0.82	0	17,19,21	0.76	0
3	NAG	C	623	1	14,14,15	0.88	0	17,19,21	0.88	2 (11%)
3	NAG	C	624	1,3	14,14,15	0.82	1 (7%)	17,19,21	1.36	2 (11%)
3	NAG	C	625	3,4	14,14,15	0.80	0	17,19,21	1.00	2 (11%)
4	BMA	C	626	3	11,11,12	1.81	2 (18%)	15,15,17	1.01	1 (6%)
3	NAG	C	627	1,3,6	14,14,15	0.80	1 (7%)	17,19,21	1.03	0
3	NAG	C	628	3	14,14,15	0.78	0	17,19,21	1.17	1 (5%)
6	FUC	C	629	3	9,10,11	0.72	0	13,14,16	1.04	1 (7%)
3	NAG	C	630	1,3	14,14,15	0.78	0	17,19,21	0.94	0
3	NAG	C	631	3	14,14,15	0.78	0	17,19,21	1.23	2 (11%)
3	NAG	C	632	1	14,14,15	0.80	0	17,19,21	1.08	1 (5%)
3	NAG	D	601	1,3	14,14,15	0.80	0	17,19,21	1.24	2 (11%)
3	NAG	D	602	3	14,14,15	0.79	0	17,19,21	0.96	1 (5%)
3	NAG	D	603	1	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
3	NAG	D	604	1,3	14,14,15	0.87	0	17,19,21	2.03	5 (29%)
3	NAG	D	605	3	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
3	NAG	D	606	1	14,14,15	0.77	0	17,19,21	0.90	1 (5%)
3	NAG	D	607	1,3	14,14,15	0.76	0	17,19,21	1.03	1 (5%)
3	NAG	D	608	3	14,14,15	0.77	0	17,19,21	1.21	2 (11%)
3	NAG	D	609	1	14,14,15	0.85	0	17,19,21	1.25	1 (5%)
3	NAG	D	610	1	14,14,15	0.81	0	17,19,21	0.98	1 (5%)
3	NAG	D	611	1	14,14,15	0.87	0	17,19,21	1.21	2 (11%)
3	NAG	D	612	1,3	14,14,15	0.75	0	17,19,21	1.16	1 (5%)
3	NAG	D	613	3,4	14,14,15	0.78	1 (7%)	17,19,21	1.19	2 (11%)
4	BMA	D	614	3,5	11,11,12	1.86	2 (18%)	15,15,17	1.14	1 (6%)
5	MAN	D	615	5,4	11,11,12	1.58	1 (9%)	15,15,17	1.09	2 (13%)
5	MAN	D	616	5	11,11,12	1.85	3 (27%)	15,15,17	1.18	2 (13%)
5	MAN	D	617	4	11,11,12	1.81	2 (18%)	15,15,17	1.14	3 (20%)
3	NAG	D	618	1	14,14,15	0.88	0	17,19,21	1.04	2 (11%)
3	NAG	D	619	1,3	14,14,15	0.77	0	17,19,21	1.19	2 (11%)
3	NAG	D	620	3,4	14,14,15	0.80	0	17,19,21	0.81	0
4	BMA	D	621	3	11,11,12	1.81	2 (18%)	15,15,17	0.89	1 (6%)
3	NAG	D	622	1	14,14,15	0.82	0	17,19,21	0.76	0
3	NAG	D	623	1	14,14,15	0.88	0	17,19,21	0.88	2 (11%)
3	NAG	D	624	1,3	14,14,15	0.81	1 (7%)	17,19,21	1.36	2 (11%)
3	NAG	D	625	3,4	14,14,15	0.79	0	17,19,21	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	D	626	3	11,11,12	1.81	2 (18%)	15,15,17	1.00	1 (6%)
3	NAG	D	627	1,3,6	14,14,15	0.80	1 (7%)	17,19,21	1.03	0
3	NAG	D	628	3	14,14,15	0.79	0	17,19,21	1.17	1 (5%)
6	FUC	D	629	3	9,10,11	0.72	0	13,14,16	1.04	1 (7%)
3	NAG	D	630	1,3	14,14,15	0.79	0	17,19,21	0.94	0
3	NAG	D	631	3	14,14,15	0.78	0	17,19,21	1.23	2 (11%)
3	NAG	D	632	1	14,14,15	0.80	0	17,19,21	1.08	1 (5%)
3	NAG	E	701	2,6	14,14,15	0.74	0	17,19,21	1.10	1 (5%)
6	FUC	E	702	3	9,10,11	1.41	2 (22%)	13,14,16	4.27	5 (38%)
3	NAG	E	703	2	14,14,15	0.85	0	17,19,21	0.83	1 (5%)
3	NAG	E	704	2	14,14,15	0.89	0	17,19,21	0.96	1 (5%)
3	NAG	F	701	2,6	14,14,15	0.73	0	17,19,21	1.09	1 (5%)
6	FUC	F	702	3	9,10,11	1.41	2 (22%)	13,14,16	4.27	5 (38%)
3	NAG	F	703	2	14,14,15	0.85	0	17,19,21	0.83	1 (5%)
3	NAG	F	704	2	14,14,15	0.89	0	17,19,21	0.96	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
3	NAG	A	601	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	602	3	-	2/6/23/26	0/1/1/1
3	NAG	A	603	1	-	1/6/23/26	0/1/1/1
3	NAG	A	604	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	605	3	-	1/6/23/26	0/1/1/1
3	NAG	A	606	1	-	2/6/23/26	0/1/1/1
3	NAG	A	607	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	608	3	-	2/6/23/26	0/1/1/1
3	NAG	A	609	1	-	1/6/23/26	0/1/1/1
3	NAG	A	610	1	-	1/6/23/26	0/1/1/1
3	NAG	A	611	1	-	2/6/23/26	0/1/1/1
3	NAG	A	612	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	613	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	614	3,5	-	2/2/19/22	0/1/1/1
5	MAN	A	615	5,4	-	1/2/19/22	0/1/1/1
5	MAN	A	616	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	617	4	-	1/2/19/22	0/1/1/1
3	NAG	A	618	1	-	1/6/23/26	0/1/1/1
3	NAG	A	619	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	620	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	621	3	-	1/2/19/22	0/1/1/1
3	NAG	A	622	1	-	2/6/23/26	0/1/1/1
3	NAG	A	623	1	-	2/6/23/26	0/1/1/1
3	NAG	A	624	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	625	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	626	3	-	1/2/19/22	0/1/1/1
3	NAG	A	627	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	A	628	3	-	2/6/23/26	0/1/1/1
6	FUC	A	629	3	-	-	0/1/1/1
3	NAG	A	630	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	631	3	-	2/6/23/26	0/1/1/1
3	NAG	A	632	1	-	2/6/23/26	0/1/1/1
3	NAG	B	701	2,6	-	2/6/23/26	0/1/1/1
6	FUC	B	702	3	-	-	0/1/1/1
3	NAG	B	703	2	-	1/6/23/26	0/1/1/1
3	NAG	B	704	2	-	1/6/23/26	0/1/1/1
3	NAG	C	601	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	602	3	-	2/6/23/26	0/1/1/1
3	NAG	C	603	1	-	1/6/23/26	0/1/1/1
3	NAG	C	604	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	605	3	-	1/6/23/26	0/1/1/1
3	NAG	C	606	1	-	2/6/23/26	0/1/1/1
3	NAG	C	607	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	608	3	-	2/6/23/26	0/1/1/1
3	NAG	C	609	1	-	1/6/23/26	0/1/1/1
3	NAG	C	610	1	-	1/6/23/26	0/1/1/1
3	NAG	C	611	1	-	2/6/23/26	0/1/1/1
3	NAG	C	612	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	613	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	614	3,5	-	2/2/19/22	0/1/1/1
5	MAN	C	615	5,4	-	1/2/19/22	0/1/1/1
5	MAN	C	616	5	-	2/2/19/22	0/1/1/1
5	MAN	C	617	4	-	1/2/19/22	0/1/1/1
3	NAG	C	618	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	619	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	620	3,4	-	2/6/23/26	0/1/1/1
4	BMA	C	621	3	-	1/2/19/22	0/1/1/1
3	NAG	C	622	1	-	2/6/23/26	0/1/1/1
3	NAG	C	623	1	-	2/6/23/26	0/1/1/1
3	NAG	C	624	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	625	3,4	-	2/6/23/26	0/1/1/1
4	BMA	C	626	3	-	1/2/19/22	0/1/1/1
3	NAG	C	627	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	C	628	3	-	2/6/23/26	0/1/1/1
6	FUC	C	629	3	-	-	0/1/1/1
3	NAG	C	630	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	631	3	-	2/6/23/26	0/1/1/1
3	NAG	C	632	1	-	2/6/23/26	0/1/1/1
3	NAG	D	601	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	602	3	-	2/6/23/26	0/1/1/1
3	NAG	D	603	1	-	1/6/23/26	0/1/1/1
3	NAG	D	604	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	605	3	-	1/6/23/26	0/1/1/1
3	NAG	D	606	1	-	2/6/23/26	0/1/1/1
3	NAG	D	607	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	608	3	-	2/6/23/26	0/1/1/1
3	NAG	D	609	1	-	1/6/23/26	0/1/1/1
3	NAG	D	610	1	-	1/6/23/26	0/1/1/1
3	NAG	D	611	1	-	2/6/23/26	0/1/1/1
3	NAG	D	612	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	613	3,4	-	0/6/23/26	0/1/1/1
4	BMA	D	614	3,5	-	2/2/19/22	0/1/1/1
5	MAN	D	615	5,4	-	1/2/19/22	0/1/1/1
5	MAN	D	616	5	-	2/2/19/22	0/1/1/1
5	MAN	D	617	4	-	1/2/19/22	0/1/1/1
3	NAG	D	618	1	-	1/6/23/26	0/1/1/1
3	NAG	D	619	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	620	3,4	-	2/6/23/26	0/1/1/1
4	BMA	D	621	3	-	1/2/19/22	0/1/1/1
3	NAG	D	622	1	-	2/6/23/26	0/1/1/1
3	NAG	D	623	1	-	2/6/23/26	0/1/1/1
3	NAG	D	624	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	625	3,4	-	2/6/23/26	0/1/1/1
4	BMA	D	626	3	-	1/2/19/22	0/1/1/1
3	NAG	D	627	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	D	628	3	-	2/6/23/26	0/1/1/1
6	FUC	D	629	3	-	-	0/1/1/1
3	NAG	D	630	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	631	3	-	2/6/23/26	0/1/1/1
3	NAG	D	632	1	-	2/6/23/26	0/1/1/1
3	NAG	E	701	2,6	-	2/6/23/26	0/1/1/1
6	FUC	E	702	3	-	-	0/1/1/1
3	NAG	E	703	2	-	1/6/23/26	0/1/1/1
3	NAG	E	704	2	-	1/6/23/26	0/1/1/1
3	NAG	F	701	2,6	-	2/6/23/26	0/1/1/1
6	FUC	F	702	3	-	-	0/1/1/1
3	NAG	F	703	2	-	1/6/23/26	0/1/1/1
3	NAG	F	704	2	-	1/6/23/26	0/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	616	MAN	O2-C2	-4.21	1.34	1.43
5	A	616	MAN	O2-C2	-4.20	1.34	1.43
5	D	616	MAN	O2-C2	-4.20	1.34	1.43
4	C	621	BMA	O2-C2	-4.12	1.34	1.43
4	D	621	BMA	O2-C2	-4.10	1.34	1.43

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FUC	C6-C5-C4	-12.35	91.79	113.08
6	B	702	FUC	C6-C5-C4	-12.35	91.80	113.08
6	F	702	FUC	C6-C5-C4	-12.35	91.80	113.08
6	F	702	FUC	C3-C4-C5	6.54	120.00	109.74
6	B	702	FUC	C3-C4-C5	6.54	120.00	109.74

There are no chirality outliers.

5 of 135 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	604	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	604	NAG	O5-C5-C6-O6
3	D	604	NAG	O5-C5-C6-O6
3	D	631	NAG	O5-C5-C6-O6
3	C	631	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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.