



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 02:41 PM EDT

PDB ID : 5V8L  
EMDB ID: : EMD-8643  
Title : BG505 SOSIP.664 trimer in complex with broadly neutralizing HIV antibodies  
3BNC117 and PGT145  
Authors : Lee, J.H.; Ward, A.B.  
Deposited on : unknown  
Resolution : 4.30 Å(reported)

This is a wwPDB/EMDatabank EM Map/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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

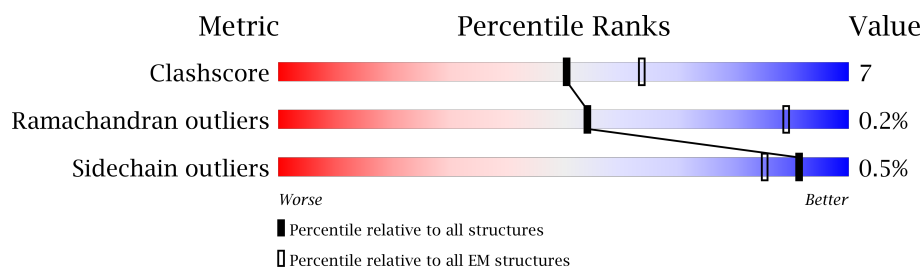
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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.



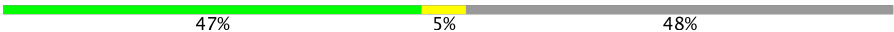




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. 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. 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	481	86% 6% • 6%
1	C	481	89% 5% 6%
1	D	481	88% 6% 6%
2	B	153	78% • • 18%
2	E	153	79% • 19%
2	F	153	73% 7% • 20%
3	G	226	50% • 46%
3	H	226	49% 5% 46%
3	I	226	50% • 46%

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Mol	Chain	Length	Quality of chain
4	J	267	
5	K	206	
5	L	206	
5	M	206	
6	N	219	

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
7	NAG	A	605	-	-	X	-
7	NAG	C	627	-	-	X	-
7	NAG	C	631	-	-	X	-
7	NAG	C	640	X	-	-	-
7	NAG	D	606	-	-	X	-
7	NAG	D	607	-	-	X	-
7	NAG	D	632	-	-	X	-
7	NAG	D	636	-	-	X	-
7	NAG	D	639	X	-	-	-
9	MAN	D	612	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22934 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 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3545	2227	625	665	28		
1	C	451	Total	C	N	O	S	0	0
			3553	2231	627	667	28		
1	D	452	Total	C	N	O	S	0	0
			3562	2236	628	670	28		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
D	332	ASN	THR	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6
D	509	ARG	-	expression tag	UNP Q2N0S6
D	510	ARG	-	expression tag	UNP Q2N0S6
D	511	ARG	-	expression tag	UNP Q2N0S6
D	512	ARG	-	expression tag	UNP Q2N0S6
D	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			1004	635	173	190	6		
2	E	124	Total	C	N	O	S	0	0
			987	623	170	188	6		
2	F	123	Total	C	N	O	S	0	0
			981	620	169	186	6		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called 3BNC117 antibody, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	H	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	I	121	Total	C	N	O	S	0	0
			985	626	177	179	3		

- Molecule 4 is a protein called PGT145 antibody, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	140	Total	C	N	O	S	0	0
			1094	685	191	213	5		

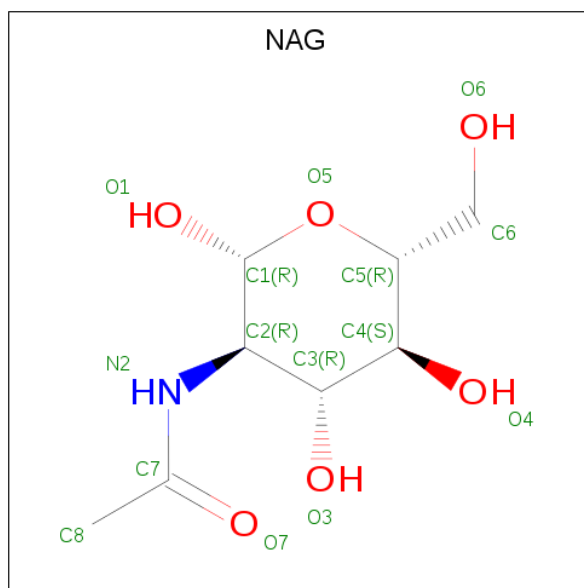
- Molecule 5 is a protein called 3BNC117 antibody, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
5	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
5	M	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

- Molecule 6 is a protein called PGT145 antibody, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	112	Total	C	N	O	S	0	0
			859	542	153	160	4		

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	
7	A	1	Total	C	N	O	0
			420	240	30	150	

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Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	A	1	Total 420	C 240	N 30	O 150	0
7	B	1	Total 42	C 24	N 3	O 15	0

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Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	C	1	Total 420	C 240	N 30	O 150	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0
7	D	1	Total 406	C 232	N 29	O 145	0

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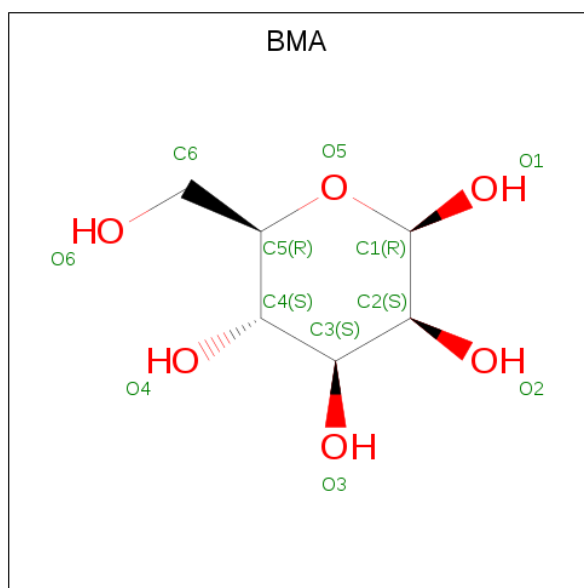
Mol	Chain	Residues	Atoms				AltConf
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	D	1	Total	C	N	O	0
			406	232	29	145	
7	E	1	Total	C	N	O	0
			56	32	4	20	
7	E	1	Total	C	N	O	0
			56	32	4	20	

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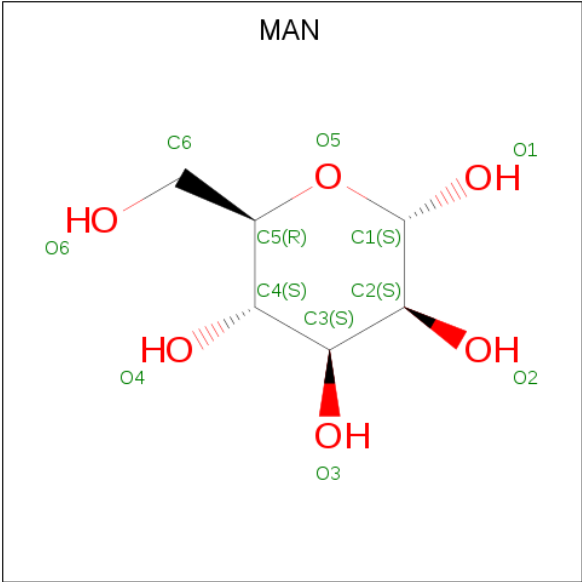
Mol	Chain	Residues	Atoms				AltConf
7	E	1	Total	C	N	O	0
			56	32	4	20	
7	E	1	Total	C	N	O	0
			56	32	4	20	
7	F	1	Total	C	N	O	0
			56	32	4	20	
7	F	1	Total	C	N	O	0
			56	32	4	20	
7	F	1	Total	C	N	O	0
			56	32	4	20	
7	F	1	Total	C	N	O	0
			56	32	4	20	
7	K	1	Total	C	N	O	0
			28	16	2	10	
7	K	1	Total	C	N	O	0
			28	16	2	10	
7	L	1	Total	C	N	O	0
			28	16	2	10	
7	L	1	Total	C	N	O	0
			28	16	2	10	
7	M	1	Total	C	N	O	0
			28	16	2	10	
7	M	1	Total	C	N	O	0
			28	16	2	10	

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			55	30	25	
8	A	1	Total	C	O	0
			55	30	25	
8	A	1	Total	C	O	0
			55	30	25	
8	A	1	Total	C	O	0
			55	30	25	
8	A	1	Total	C	O	0
			55	30	25	
8	C	1	Total	C	O	0
			55	30	25	
8	C	1	Total	C	O	0
			55	30	25	
8	C	1	Total	C	O	0
			55	30	25	
8	C	1	Total	C	O	0
			55	30	25	
8	C	1	Total	C	O	0
			55	30	25	
8	D	1	Total	C	O	0
			55	30	25	
8	D	1	Total	C	O	0
			55	30	25	
8	D	1	Total	C	O	0
			55	30	25	
8	D	1	Total	C	O	0
			55	30	25	
8	D	1	Total	C	O	0
			55	30	25	

- Molecule 9 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
9	A	1	Total	C	O	0
			99	54	45	
9	A	1	Total	C	O	0
			99	54	45	
9	A	1	Total	C	O	0
			99	54	45	
9	A	1	Total	C	O	0
			99	54	45	
9	A	1	Total	C	O	0
			99	54	45	
9	A	1	Total	C	O	0
			99	54	45	
9	A	1	Total	C	O	0
			99	54	45	
9	A	1	Total	C	O	0
			99	54	45	
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	

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Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	
9	C	1	Total	C	O	0
			121	66	55	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	
9	D	1	Total	C	O	0
			176	96	80	

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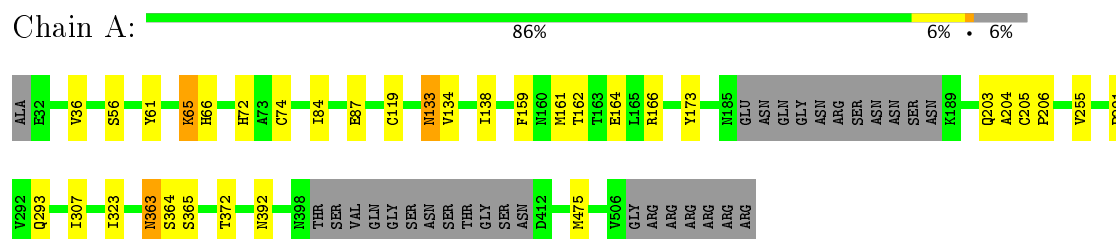
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	D	1	176	96	80	0

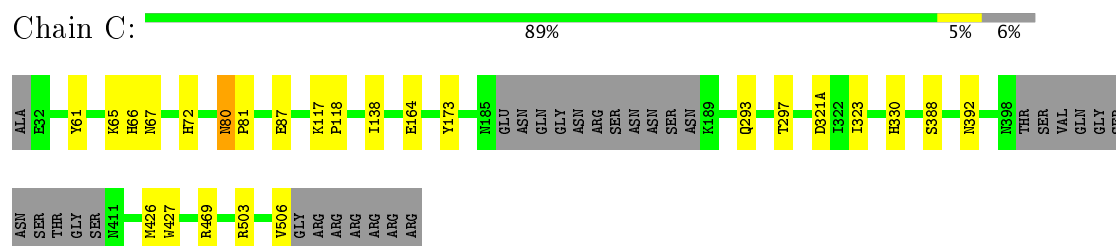
### 3 Residue-property plots

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.

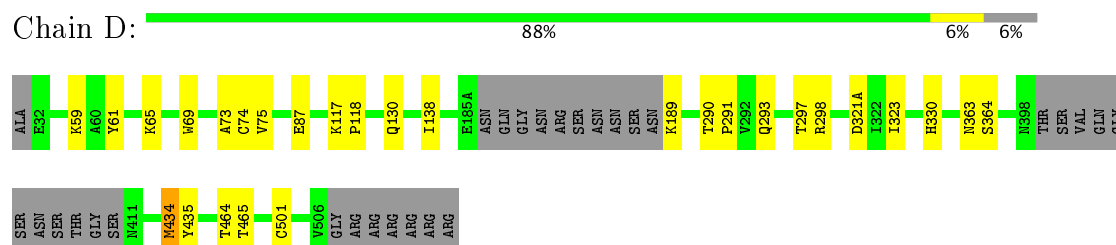
- Molecule 1: gp120



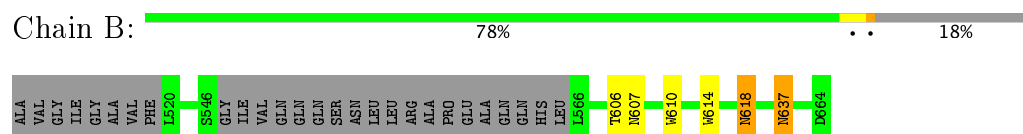
- Molecule 1: gp120



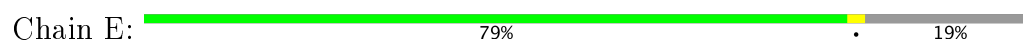
- Molecule 1: gp120



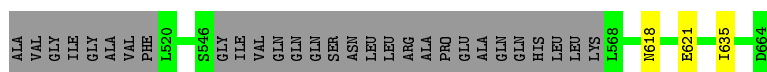
- Molecule 2: gp41



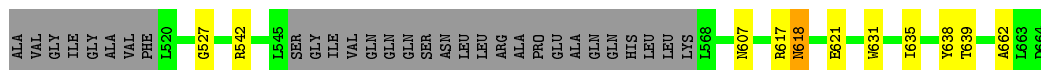
- Molecule 2: gp41



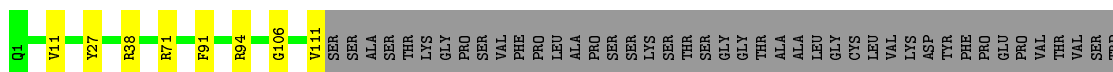




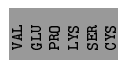
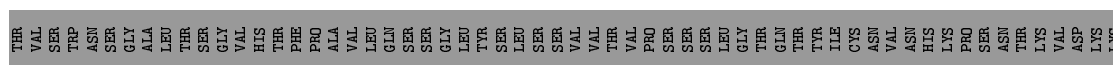
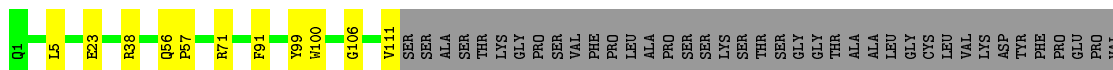
- Molecule 2: gp41



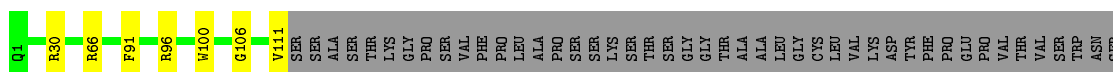
- Molecule 3: 3BNC117 antibody, heavy chain



- Molecule 3: 3BNC117 antibody, heavy chain



- Molecule 3: 3BNC117 antibody, heavy chain



- Molecule 4: PGT145 antibody, heavy chain



PRO LEU ALA ALA PRO SER SER LYS SER SER THR THR GLY GLY GLY THR ALA ALA ALA LEU LEU GLY CYS LEU VAL VAL ASP LYS TYR PHE PRO PRO PRO VAL THR VAL VAL VAL SER SER TRP TRP ASN SER SER SER GLY GLY ALA LEU LEU THR THR SER GLY GLY VAL HIS PHE PHE THR PRO PRO VAL VAL LEU GLN SER SER SER GLY GLY TYR SER LEU SER SER SER VAL VAL

THR	VAL	PRO	SER	SER	SER	LEU	GLY	THR	GLN	THR	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	SER	ASN	THR	LYS	VAL	ASP	LYS	LYS	VAL	GLU	PRO	LYS	SER	CYS	ASP
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- Molecule 5: 3BNC117 antibody, light chain

Chain K:  44% 0% 52%

D1	S7	P8	T22	R66	w67	M72	Y91	L106	LYS	ARG	THR	VAL	ALA	ALA	PRO	SER	SER	VAL	PHE	PHE	ILE	PRO	PRO	SER	ASP	GLU	GLN	LEU	LYS	SER	GLY	THR	ALA	ALA	SER	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	THR	PRO	ARG	GLU	GLU	LYS	VAL	GLN	TRP	LYS	VAL	ASP
----	----	----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	ALA	LEU	GLN	SER	GLY	ASN	SER	GLU	GLN	SER	VAL	THR	GLU	GLN	ASP	ASP	LYS	ASP	SER	THR	TYR	SER	LEU	SER	SER	THR	THR	LEU	LEU	SER	LYS	LYS	LYS	VAL	VAL	TYR	ALA	ALA	CYS	GLU	VAL	VAL	THR	THR	HIS	GLN	GLY	LEU	SER	SER	SER	PRO	VAL	THR	LYS	LYS	SER	PHE	ASN	ASN	ASP	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY  
GLU  
CYS

- Molecule 5: 3BNC117 antibody, light chain

Chain L:  42% 5% 52%

D1	S7	P8	L11	T22	Y32	S52	R33	E54	R66	N72	D105	L106	LYS	ARG	THR	THR	VAL	ALA	ALA	PRO	SER	SER	VAL	PHE	ILE	PHE	PRO	PRO	SER	SER	ASP	GLU	GLN	LEU	LYS	SER	GLY	THR	ALA	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA
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LYS VAL GLN TRP LYS VAL ASP ASN ALU LEU GLN SER GLY ASN SER GLN SER VAL THR GLU GLN ASP SER LYS SER SER SER TYR SER LEU THR LYS HIS LYS ASP TYR GLU LYS VAL ALA CYS VAL THR HIS GLN GLY LEU SER SER DEO

VAL  
THR  
LYS  
SER  
PHE  
ASN  
ARG  
GLY  
GLU  
CYS

- Molecule 5: 3BNC117 antibody, light chain

Chain M:  43% 0% 52%

[illegible]

LYS VAL ASP ASN ALA LEU GLN SER SER GLY ASP LYS LYS THR THR TYR TYR LEU LEU LEU LYS ASP ASP TYR TYR CYS VAL HIS HIS GLY LEU SER SER PRO VAL VAL THR THR LYS

PHE  
ASN  
ARG  
GLY  
GLU  
CYS

- Molecule 6: PGT145 antibody, light chain

Chain N:  50% . 49%

GLU	V2	T28	H63	R108	THR	VAL	ALA	ALA	PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO	SER	ASP	GLY	GLN	LEU	LYS	SER	SER	THR	ALA	SER	VAL	VAL	CYS	LEU	ARG	ASN	ASP	PHE	TYR	PRO	ARG	GLY	ALA	ALA	LYS	VAL	GLN	TRP	LYS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	CTR
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GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	TYR	SER	LEU	SER	SER	THR	LEU	THR	LEU	SER	LYS	ALA	ASP	THR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65060	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 ( $e^-/\text{\AA}^2$ )	32	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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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  >2	RMSZ	# Z  >2
1	A	0.80	0/3619	0.80	0/4914
1	C	0.81	0/3627	0.81	1/4925 (0.0%)
1	D	0.82	0/3636	0.81	1/4937 (0.0%)
2	B	0.85	0/1021	0.78	0/1384
2	E	0.84	0/1004	0.79	0/1362
2	F	0.86	0/998	0.77	1/1354 (0.1%)
3	G	0.82	0/1017	0.86	1/1386 (0.1%)
3	H	0.80	0/1017	0.88	2/1386 (0.1%)
3	I	0.83	0/1017	0.88	3/1386 (0.2%)
4	J	0.77	0/1121	0.84	0/1519
5	K	0.76	0/800	0.83	0/1086
5	L	0.77	0/800	0.89	0/1086
5	M	0.76	0/800	0.85	0/1086
6	N	0.68	0/882	0.78	0/1199
All	All	0.80	0/21359	0.82	9/29010 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	38	ARG	NE-CZ-NH2	-8.52	116.04	120.30
3	H	99	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	C	469	ARG	NE-CZ-NH1	-6.17	117.21	120.30
2	F	542	ARG	NE-CZ-NH2	-6.13	117.24	120.30
3	G	38	ARG	NE-CZ-NH2	-6.08	117.26	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	3545	0	3481	64	0
1	C	3553	0	3488	55	0
1	D	3562	0	3494	53	0
2	B	1004	0	989	6	0
2	E	987	0	965	2	0
2	F	981	0	960	19	0
3	G	985	0	919	4	0
3	H	985	0	919	7	0
3	I	985	0	919	5	0
4	J	1094	0	1033	30	0
5	K	783	0	763	6	0
5	L	783	0	763	13	0
5	M	783	0	763	10	0
6	N	859	0	841	8	0
7	A	420	0	372	42	0
7	B	42	0	39	0	0
7	C	420	0	372	44	0
7	D	406	0	360	63	0
7	E	56	0	51	0	0
7	F	56	0	51	0	0
7	K	28	0	25	0	0
7	L	28	0	25	0	0
7	M	28	0	25	0	0
8	A	55	0	44	0	0
8	C	55	0	44	0	0
8	D	55	0	42	5	0
9	A	99	0	87	0	0
9	C	121	0	105	0	0
9	D	176	0	152	11	0
All	All	22934	0	22091	295	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 7.

The worst 5 of 295 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:134:VAL:HG11	7:A:605:NAG:O7	1.16	1.28
1:C:330:HIS:HE1	7:C:631:NAG:N2	1.29	1.28
1:C:330:HIS:CE1	7:C:631:NAG:HN2	1.56	1.23
1:A:173:TYR:OH	7:A:605:NAG:H3	1.38	1.20
1:C:87:GLU:CG	7:C:601:NAG:H82	1.72	1.19

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	444/481 (92%)	433 (98%)	11 (2%)	0	100	100
1	C	445/481 (92%)	434 (98%)	10 (2%)	1 (0%)	51	85
1	D	446/481 (93%)	439 (98%)	7 (2%)	0	100	100
2	B	122/153 (80%)	122 (100%)	0	0	100	100
2	E	120/153 (78%)	118 (98%)	2 (2%)	0	100	100
2	F	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
3	G	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	H	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	I	119/226 (53%)	119 (100%)	0	0	100	100
4	J	138/267 (52%)	137 (99%)	1 (1%)	0	100	100
5	K	96/206 (47%)	93 (97%)	2 (2%)	1 (1%)	18	61
5	L	96/206 (47%)	92 (96%)	2 (2%)	2 (2%)	8	47
5	M	96/206 (47%)	93 (97%)	2 (2%)	1 (1%)	18	61
6	N	110/219 (50%)	108 (98%)	2 (2%)	0	100	100
All	All	2589/3684 (70%)	2539 (98%)	45 (2%)	5 (0%)	54	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	52	SER
1	C	80	ASN
5	M	52	SER
5	K	7	SER
5	L	7	SER

### 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 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	402/428 (94%)	399 (99%)	3 (1%)	87	93
1	C	403/428 (94%)	403 (100%)	0	100	100
1	D	404/428 (94%)	402 (100%)	2 (0%)	91	95
2	B	109/129 (84%)	107 (98%)	2 (2%)	64	84
2	E	107/129 (83%)	106 (99%)	1 (1%)	82	91
2	F	106/129 (82%)	105 (99%)	1 (1%)	82	91
3	G	102/193 (53%)	101 (99%)	1 (1%)	80	90
3	H	102/193 (53%)	101 (99%)	1 (1%)	80	90
3	I	102/193 (53%)	102 (100%)	0	100	100
4	J	115/223 (52%)	114 (99%)	1 (1%)	82	91
5	K	86/183 (47%)	86 (100%)	0	100	100
5	L	86/183 (47%)	86 (100%)	0	100	100
5	M	86/183 (47%)	86 (100%)	0	100	100
6	N	95/191 (50%)	95 (100%)	0	100	100
All	All	2305/3213 (72%)	2293 (100%)	12 (0%)	91	95

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	65	LYS
1	D	434	MET
3	G	71	ARG

*Continued on next page...*



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Mol	Chain	Res	Type
2	B	637	ASN
2	F	618	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	293	GLN
6	N	53	HIS
4	J	52(A)	HIS
1	C	330	HIS
3	H	56	GLN

### 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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

157 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$
7	NAG	A	601	1,7	14,14,15	0.80	1 (7%)	15,19,21	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	602	7	14,14,15	0.44	0	15,19,21	1.55	3 (20%)
7	NAG	A	603	1,7	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
7	NAG	A	604	7	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
7	NAG	A	605	1,7	14,14,15	0.25	0	15,19,21	0.63	0
7	NAG	A	606	7	14,14,15	0.30	0	15,19,21	0.68	0
7	NAG	A	607	1,7	14,14,15	0.47	0	15,19,21	2.60	3 (20%)
7	NAG	A	608	7	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
7	NAG	A	609	1,7	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	A	610	8,7	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
8	BMA	A	611	7	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
7	NAG	A	612	1	14,14,15	0.49	0	15,19,21	0.54	0
7	NAG	A	613	1,7	14,14,15	0.49	0	15,19,21	2.62	3 (20%)
7	NAG	A	614	8,7	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
8	BMA	A	615	9,7	11,11,12	0.66	0	13,15,17	1.52	3 (23%)
9	MAN	A	616	9,8	11,11,12	0.55	0	13,15,17	1.59	3 (23%)
9	MAN	A	617	9	11,11,12	0.60	0	13,15,17	2.58	5 (38%)
9	MAN	A	618	8	11,11,12	0.60	0	13,15,17	2.60	3 (23%)
7	NAG	A	619	1,7	14,14,15	0.77	1 (7%)	15,19,21	0.72	0
7	NAG	A	620	8,7	14,14,15	0.40	0	15,19,21	0.53	0
8	BMA	A	621	9,7	11,11,12	1.67	3 (27%)	13,15,17	1.89	2 (15%)
9	MAN	A	622	8	11,11,12	1.62	3 (27%)	13,15,17	1.39	2 (15%)
9	MAN	A	623	9,8	11,11,12	0.61	0	13,15,17	2.58	3 (23%)
9	MAN	A	624	9	11,11,12	0.57	0	13,15,17	2.03	5 (38%)
9	MAN	A	625	9	11,11,12	0.59	0	13,15,17	2.40	6 (46%)
7	NAG	A	626	1,7	14,14,15	0.30	0	15,19,21	0.77	0
7	NAG	A	627	7	14,14,15	0.65	0	15,19,21	0.56	0
7	NAG	A	628	1,7	14,14,15	0.44	0	15,19,21	0.49	0
7	NAG	A	629	7	14,14,15	0.60	0	15,19,21	0.61	0
7	NAG	A	630	1,7	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
7	NAG	A	631	8,7	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
8	BMA	A	632	7	11,11,12	0.63	0	13,15,17	1.51	3 (23%)
7	NAG	A	633	1	14,14,15	0.29	0	15,19,21	0.46	0
7	NAG	A	634	1	14,14,15	0.50	0	15,19,21	0.43	0
7	NAG	A	635	1,7	14,14,15	0.31	0	15,19,21	0.65	0
7	NAG	A	636	8,7	14,14,15	0.34	0	15,19,21	0.88	1 (6%)
8	BMA	A	637	9,7	11,11,12	0.64	0	13,15,17	1.51	3 (23%)
9	MAN	A	638	8	11,11,12	0.53	0	13,15,17	1.58	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	A	639	8	11,11,12	0.63	0	13,15,17	2.56	3 (23%)
7	NAG	A	640	1,7	14,14,15	1.00	1 (7%)	15,19,21	1.13	1 (6%)
7	NAG	A	641	7	14,14,15	0.49	0	15,19,21	0.63	0
7	NAG	A	642	1	14,14,15	0.46	0	15,19,21	0.60	0
7	NAG	A	643	1,7	14,14,15	0.50	0	15,19,21	0.59	0
7	NAG	A	644	7	14,14,15	0.39	0	15,19,21	0.45	0
7	NAG	B	701	2	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
7	NAG	B	702	2	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	B	703	2	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	C	601	1	14,14,15	0.80	1 (7%)	15,19,21	0.94	1 (6%)
7	NAG	C	602	1,7	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	C	603	7	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
7	NAG	C	604	1,7	14,14,15	0.26	0	15,19,21	0.62	0
7	NAG	C	605	7	14,14,15	0.30	0	15,19,21	0.68	0
7	NAG	C	606	1,7	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
7	NAG	C	607	8,7	14,14,15	0.51	0	15,19,21	1.20	2 (13%)
8	BMA	C	608	7	11,11,12	0.64	0	13,15,17	1.50	3 (23%)
7	NAG	C	609	1,7	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	C	610	7	14,14,15	0.52	0	15,19,21	1.19	2 (13%)
7	NAG	C	611	1	14,14,15	0.49	0	15,19,21	0.55	0
7	NAG	C	612	1,7	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
7	NAG	C	613	8,7	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
8	BMA	C	614	9,7	11,11,12	0.67	0	13,15,17	1.51	3 (23%)
9	MAN	C	615	9,8	11,11,12	0.57	0	13,15,17	1.61	3 (23%)
9	MAN	C	616	9	11,11,12	0.60	0	13,15,17	2.59	5 (38%)
9	MAN	C	617	9,8	11,11,12	0.59	0	13,15,17	2.58	3 (23%)
9	MAN	C	618	9	11,11,12	0.55	0	13,15,17	2.03	5 (38%)
7	NAG	C	619	1,7	14,14,15	0.76	1 (7%)	15,19,21	0.71	0
7	NAG	C	620	8,7	14,14,15	0.39	0	15,19,21	0.51	0
8	BMA	C	621	9,7	11,11,12	1.68	3 (27%)	13,15,17	1.92	2 (15%)
9	MAN	C	622	9,8	11,11,12	1.63	3 (27%)	13,15,17	1.38	2 (15%)
9	MAN	C	623	9	11,11,12	2.31	4 (36%)	13,15,17	1.98	5 (38%)
9	MAN	C	624	9,8	11,11,12	0.58	0	13,15,17	2.59	3 (23%)
9	MAN	C	625	9	11,11,12	0.58	0	13,15,17	2.04	5 (38%)
9	MAN	C	626	9	11,11,12	0.62	0	13,15,17	2.40	6 (46%)
7	NAG	C	627	1,7	14,14,15	0.31	0	15,19,21	0.77	0
7	NAG	C	628	7	14,14,15	0.65	0	15,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	C	629	1,7	14,14,15	0.42	0	15,19,21	0.48	0
7	NAG	C	630	7	14,14,15	0.60	0	15,19,21	0.62	0
7	NAG	C	631	1,7	14,14,15	0.41	0	15,19,21	0.83	1 (6%)
7	NAG	C	632	7	14,14,15	0.52	0	15,19,21	0.55	0
7	NAG	C	633	1	14,14,15	0.32	0	15,19,21	0.46	0
7	NAG	C	634	1	14,14,15	0.49	0	15,19,21	0.44	0
7	NAG	C	635	1,7	14,14,15	0.32	0	15,19,21	0.65	0
7	NAG	C	636	8,7	14,14,15	0.34	0	15,19,21	0.89	1 (6%)
8	BMA	C	637	9,7	11,11,12	0.65	0	13,15,17	1.54	3 (23%)
9	MAN	C	638	8	11,11,12	0.55	0	13,15,17	1.59	3 (23%)
9	MAN	C	639	8	11,11,12	0.64	0	13,15,17	2.57	3 (23%)
7	NAG	C	640	1,7	14,14,15	0.97	1 (7%)	15,19,21	1.13	1 (6%)
7	NAG	C	641	8,7	14,14,15	0.50	0	15,19,21	0.63	0
8	BMA	C	642	7	11,11,12	0.61	0	13,15,17	1.50	3 (23%)
7	NAG	C	643	1,7	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
7	NAG	C	644	7	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
7	NAG	C	645	1,7	14,14,15	0.50	0	15,19,21	0.61	0
7	NAG	C	646	7	14,14,15	0.38	0	15,19,21	0.44	0
7	NAG	D	601	1,7	14,14,15	0.80	1 (7%)	15,19,21	0.93	1 (6%)
7	NAG	D	602	7	14,14,15	0.44	0	15,19,21	1.55	3 (20%)
7	NAG	D	603	1	14,14,15	0.40	0	15,19,21	0.71	1 (6%)
7	NAG	D	604	1,7	14,14,15	0.26	0	15,19,21	0.61	0
7	NAG	D	605	7	14,14,15	0.30	0	15,19,21	0.68	0
7	NAG	D	606	1,7	14,14,15	1.47	3 (21%)	15,19,21	1.06	1 (6%)
7	NAG	D	607	8,7	14,14,15	1.33	1 (7%)	15,19,21	1.22	1 (6%)
8	BMA	D	608	9,7	11,11,12	1.40	2 (18%)	13,15,17	1.03	1 (7%)
9	MAN	D	609	9,8	11,11,12	1.65	3 (27%)	13,15,17	1.52	2 (15%)
9	MAN	D	610	9	11,11,12	1.43	2 (18%)	13,15,17	1.49	1 (7%)
9	MAN	D	611	9	11,11,12	1.53	3 (27%)	13,15,17	1.44	1 (7%)
9	MAN	D	612	9,8	11,11,12	1.48	3 (27%)	13,15,17	1.73	3 (23%)
9	MAN	D	613	9	11,11,12	1.52	3 (27%)	13,15,17	1.74	2 (15%)
7	NAG	D	614	1,7	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
7	NAG	D	615	7	14,14,15	0.49	0	15,19,21	1.20	2 (13%)
7	NAG	D	616	1	14,14,15	0.50	0	15,19,21	0.54	0
7	NAG	D	617	1,7	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	D	618	8,7	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
8	BMA	D	619	9,7	11,11,12	0.66	0	13,15,17	1.52	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	D	620	9,8	11,11,12	0.58	0	13,15,17	1.61	3 (23%)
9	MAN	D	621	9	11,11,12	0.59	0	13,15,17	2.57	5 (38%)
9	MAN	D	622	9,8	11,11,12	0.59	0	13,15,17	2.60	3 (23%)
9	MAN	D	623	9	11,11,12	0.56	0	13,15,17	2.04	5 (38%)
7	NAG	D	624	1,7	14,14,15	0.77	1 (7%)	15,19,21	0.72	0
7	NAG	D	625	8,7	14,14,15	0.40	0	15,19,21	0.53	0
8	BMA	D	626	9,7	11,11,12	1.68	3 (27%)	13,15,17	1.90	2 (15%)
9	MAN	D	627	9,8	11,11,12	1.63	3 (27%)	13,15,17	1.38	2 (15%)
9	MAN	D	628	9	11,11,12	2.32	4 (36%)	13,15,17	1.98	5 (38%)
9	MAN	D	629	9,8	11,11,12	0.58	0	13,15,17	2.59	3 (23%)
9	MAN	D	630	9	11,11,12	0.58	0	13,15,17	2.05	5 (38%)
9	MAN	D	631	9	11,11,12	0.59	0	13,15,17	2.40	6 (46%)
7	NAG	D	632	1,7	14,14,15	0.30	0	15,19,21	0.77	0
7	NAG	D	633	7	14,14,15	0.64	0	15,19,21	0.56	0
7	NAG	D	634	1,7	14,14,15	0.42	0	15,19,21	0.47	0
7	NAG	D	635	7	14,14,15	0.59	0	15,19,21	0.62	0
7	NAG	D	636	1,7	14,14,15	0.40	0	15,19,21	0.83	1 (6%)
7	NAG	D	637	7	14,14,15	0.53	0	15,19,21	0.55	0
7	NAG	D	638	1	14,14,15	0.32	0	15,19,21	0.45	0
7	NAG	D	639	1	14,14,15	0.49	0	15,19,21	0.44	0
7	NAG	D	640	1,7	14,14,15	0.32	0	15,19,21	0.65	0
7	NAG	D	641	8,7	14,14,15	0.35	0	15,19,21	0.88	1 (6%)
8	BMA	D	642	9,7	11,11,12	0.64	0	13,15,17	1.52	3 (23%)
9	MAN	D	643	8	11,11,12	0.53	0	13,15,17	1.59	3 (23%)
9	MAN	D	644	8	11,11,12	0.60	0	13,15,17	2.56	3 (23%)
7	NAG	D	645	1,7	14,14,15	0.98	1 (7%)	15,19,21	1.14	1 (6%)
7	NAG	D	646	8,7	14,14,15	0.49	0	15,19,21	0.63	0
8	BMA	D	647	7	11,11,12	0.63	0	13,15,17	1.49	3 (23%)
7	NAG	D	648	1	14,14,15	0.47	0	15,19,21	0.60	0
7	NAG	D	649	1,7	14,14,15	0.52	0	15,19,21	0.61	0
7	NAG	D	650	7	14,14,15	0.38	0	15,19,21	0.47	0
7	NAG	E	701	2	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
7	NAG	E	702	2	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
7	NAG	E	703	2,7	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
7	NAG	E	704	7	14,14,15	0.50	0	15,19,21	1.19	2 (13%)
7	NAG	F	701	2,7	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
7	NAG	F	702	7	14,14,15	0.50	0	15,19,21	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	F	703	2	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	F	704	2	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
7	NAG	K	301	5,7	14,14,15	0.50	0	15,19,21	2.61	3 (20%)
7	NAG	K	302	7	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
7	NAG	L	301	5,7	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
7	NAG	L	302	7	14,14,15	0.51	0	15,19,21	1.18	2 (13%)
7	NAG	M	301	5,7	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
7	NAG	M	302	7	14,14,15	0.51	0	15,19,21	1.19	2 (13%)

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
7	NAG	A	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	602	7	-	0/6/23/26	0/1/1/1
7	NAG	A	603	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	604	7	-	0/6/23/26	0/1/1/1
7	NAG	A	605	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	606	7	-	0/6/23/26	0/1/1/1
7	NAG	A	607	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	608	7	-	0/6/23/26	0/1/1/1
7	NAG	A	609	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	610	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	611	7	-	0/2/19/22	0/1/1/1
7	NAG	A	612	1	-	0/6/23/26	0/1/1/1
7	NAG	A	613	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	614	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	615	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	616	9,8	-	0/2/19/22	0/1/1/1
9	MAN	A	617	9	-	0/2/19/22	0/1/1/1
9	MAN	A	618	8	-	0/2/19/22	0/1/1/1
7	NAG	A	619	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	620	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	621	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	622	8	-	0/2/19/22	0/1/1/1
9	MAN	A	623	9,8	-	0/2/19/22	0/1/1/1
9	MAN	A	624	9	-	0/2/19/22	0/1/1/1
9	MAN	A	625	9	-	0/2/19/22	0/1/1/1
7	NAG	A	626	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	627	7	-	0/6/23/26	0/1/1/1
7	NAG	A	628	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	629	7	-	0/6/23/26	0/1/1/1
7	NAG	A	630	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	631	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	632	7	-	0/2/19/22	0/1/1/1
7	NAG	A	633	1	-	0/6/23/26	0/1/1/1
7	NAG	A	634	1	-	0/6/23/26	0/1/1/1
7	NAG	A	635	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	636	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	637	9,7	-	0/2/19/22	0/1/1/1
9	MAN	A	638	8	-	0/2/19/22	0/1/1/1
9	MAN	A	639	8	-	0/2/19/22	0/1/1/1
7	NAG	A	640	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	641	7	-	0/6/23/26	0/1/1/1
7	NAG	A	642	1	-	0/6/23/26	0/1/1/1
7	NAG	A	643	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	644	7	-	0/6/23/26	0/1/1/1
7	NAG	B	701	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	0/6/23/26	0/1/1/1
7	NAG	B	703	2	-	0/6/23/26	0/1/1/1
7	NAG	C	601	1	-	0/6/23/26	0/1/1/1
7	NAG	C	602	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	603	7	-	0/6/23/26	0/1/1/1
7	NAG	C	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	605	7	-	0/6/23/26	0/1/1/1
7	NAG	C	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	607	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	608	7	-	0/2/19/22	0/1/1/1
7	NAG	C	609	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	610	7	-	0/6/23/26	0/1/1/1
7	NAG	C	611	1	-	0/6/23/26	0/1/1/1
7	NAG	C	612	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	613	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	614	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	615	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	616	9	-	0/2/19/22	0/1/1/1
9	MAN	C	617	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	618	9	-	0/2/19/22	0/1/1/1
7	NAG	C	619	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	620	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	621	9,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	C	622	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	623	9	-	0/2/19/22	0/1/1/1
9	MAN	C	624	9,8	-	0/2/19/22	0/1/1/1
9	MAN	C	625	9	-	0/2/19/22	0/1/1/1
9	MAN	C	626	9	-	0/2/19/22	0/1/1/1
7	NAG	C	627	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	628	7	-	0/6/23/26	0/1/1/1
7	NAG	C	629	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	630	7	-	0/6/23/26	0/1/1/1
7	NAG	C	631	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	632	7	-	0/6/23/26	0/1/1/1
7	NAG	C	633	1	-	0/6/23/26	0/1/1/1
7	NAG	C	634	1	-	0/6/23/26	0/1/1/1
7	NAG	C	635	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	636	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	637	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	638	8	-	0/2/19/22	0/1/1/1
9	MAN	C	639	8	-	0/2/19/22	0/1/1/1
7	NAG	C	640	1,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	C	641	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	642	7	-	0/2/19/22	0/1/1/1
7	NAG	C	643	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	644	7	-	0/6/23/26	0/1/1/1
7	NAG	C	645	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	646	7	-	0/6/23/26	0/1/1/1
7	NAG	D	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	602	7	-	0/6/23/26	0/1/1/1
7	NAG	D	603	1	-	0/6/23/26	0/1/1/1
7	NAG	D	604	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	605	7	-	0/6/23/26	0/1/1/1
7	NAG	D	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	607	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	608	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	609	9,8	-	0/2/19/22	0/1/1/1
9	MAN	D	610	9	-	0/2/19/22	0/1/1/1
9	MAN	D	611	9	-	0/2/19/22	0/1/1/1
9	MAN	D	612	9,8	-	0/2/19/22	0/1/1/1
9	MAN	D	613	9	-	0/2/19/22	0/1/1/1
7	NAG	D	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	615	7	-	0/6/23/26	0/1/1/1
7	NAG	D	616	1	-	0/6/23/26	0/1/1/1
7	NAG	D	617	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	618	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	619	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	620	9,8	-	0/2/19/22	0/1/1/1
9	MAN	D	621	9	-	0/2/19/22	0/1/1/1
9	MAN	D	622	9,8	-	0/2/19/22	0/1/1/1
9	MAN	D	623	9	-	0/2/19/22	0/1/1/1
7	NAG	D	624	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	625	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	626	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	627	9,8	-	0/2/19/22	0/1/1/1
9	MAN	D	628	9	-	0/2/19/22	0/1/1/1
9	MAN	D	629	9,8	-	0/2/19/22	0/1/1/1
9	MAN	D	630	9	-	0/2/19/22	0/1/1/1
9	MAN	D	631	9	-	0/2/19/22	0/1/1/1
7	NAG	D	632	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	633	7	-	0/6/23/26	0/1/1/1
7	NAG	D	634	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	635	7	-	0/6/23/26	0/1/1/1
7	NAG	D	636	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	637	7	-	0/6/23/26	0/1/1/1
7	NAG	D	638	1	-	0/6/23/26	0/1/1/1
7	NAG	D	639	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	D	640	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	641	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	642	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	643	8	-	0/2/19/22	0/1/1/1
9	MAN	D	644	8	-	0/2/19/22	0/1/1/1
7	NAG	D	645	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	646	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	647	7	-	0/2/19/22	0/1/1/1
7	NAG	D	648	1	-	0/6/23/26	0/1/1/1
7	NAG	D	649	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	650	7	-	0/6/23/26	0/1/1/1
7	NAG	E	701	2	-	0/6/23/26	0/1/1/1
7	NAG	E	702	2	-	0/6/23/26	0/1/1/1
7	NAG	E	703	2,7	-	0/6/23/26	0/1/1/1
7	NAG	E	704	7	-	0/6/23/26	0/1/1/1
7	NAG	F	701	2,7	-	0/6/23/26	0/1/1/1
7	NAG	F	702	7	-	0/6/23/26	0/1/1/1
7	NAG	F	703	2	-	0/6/23/26	0/1/1/1
7	NAG	F	704	2	-	0/6/23/26	0/1/1/1
7	NAG	K	301	5,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	302	7	-	0/6/23/26	0/1/1/1
7	NAG	L	301	5,7	-	0/6/23/26	0/1/1/1
7	NAG	L	302	7	-	0/6/23/26	0/1/1/1
7	NAG	M	301	5,7	-	0/6/23/26	0/1/1/1
7	NAG	M	302	7	-	0/6/23/26	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	619	NAG	O5-C1	-2.36	1.39	1.43
7	D	624	NAG	O5-C1	-2.35	1.39	1.43
7	C	619	NAG	O5-C1	-2.32	1.39	1.43
7	D	601	NAG	O5-C1	-2.26	1.40	1.43
7	C	601	NAG	O5-C1	-2.26	1.40	1.43

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	613	NAG	O5-C1-C2	-8.51	99.63	111.47
7	M	301	NAG	O5-C1-C2	-8.51	99.63	111.47
7	C	602	NAG	O5-C1-C2	-8.51	99.63	111.47
7	C	643	NAG	O5-C1-C2	-8.51	99.63	111.47
7	D	617	NAG	O5-C1-C2	-8.51	99.64	111.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	640	NAG	C1
7	D	639	NAG	C1

There are no torsion outliers.

There are no ring outliers.

42 monomers are involved in 165 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	601	NAG	2	0
7	A	602	NAG	1	0
7	A	605	NAG	15	0
7	A	619	NAG	5	0
7	A	620	NAG	1	0
7	A	626	NAG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	628	NAG	3	0
7	A	629	NAG	1	0
7	A	635	NAG	6	0
7	A	643	NAG	4	0
7	C	601	NAG	5	0
7	C	604	NAG	4	0
7	C	620	NAG	2	0
7	C	627	NAG	12	0
7	C	629	NAG	2	0
7	C	630	NAG	1	0
7	C	631	NAG	12	0
7	C	635	NAG	2	0
7	C	640	NAG	5	0
7	C	645	NAG	2	0
7	C	646	NAG	2	0
7	D	601	NAG	4	0
7	D	602	NAG	1	0
7	D	604	NAG	5	0
7	D	606	NAG	7	0
7	D	607	NAG	11	0
8	D	608	BMA	5	0
9	D	610	MAN	2	0
9	D	612	MAN	9	0
7	D	624	NAG	4	0
7	D	625	NAG	2	0
7	D	632	NAG	9	0
7	D	634	NAG	4	0
7	D	635	NAG	1	0
7	D	636	NAG	9	0
7	D	640	NAG	2	0
7	D	641	NAG	1	0
7	D	645	NAG	1	0
7	D	646	NAG	3	0
7	D	648	NAG	3	0
7	D	649	NAG	2	0
7	D	650	NAG	2	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.