



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 25, 2019 – 11:16 AM EST

PDB ID : 6NQD
EMDB ID: : EMD-0485
Title : Cryo-EM structure of T/F100 SOSIP.664 HIV-1 Env trimer in complex with 8ANC195 Fab
Authors : Fang, Q.; Rossmann, M.G.
Deposited on : 2019-01-21
Resolution : 3.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
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) : rb-20031633

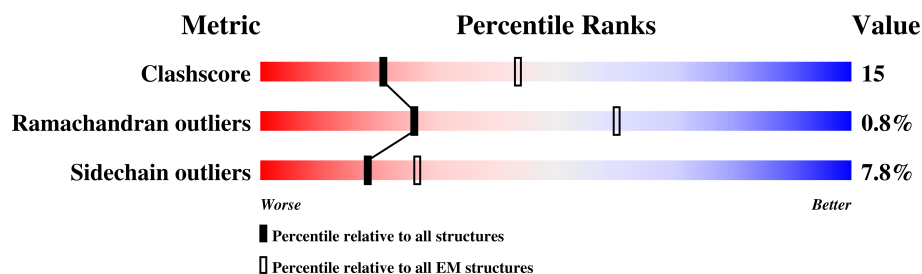
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	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. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	486	58% 30% • 10%
1	E	486	59% 28% • 10%
1	I	486	59% 29% • 10%
2	B	184	51% 16% • 33%
2	F	184	52% 15% • 33%
2	J	184	49% 18% • 33%
3	C	244	35% 16% • 47%
3	G	244	36% 16% • 47%
3	K	244	35% 16% • 47%

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Mol	Chain	Length	Quality of chain
4	D	215	 38% 12% • 50%
4	H	215	 37% 13% • 50%
4	L	215	 37% 12% • 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20175 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 T/F100 Env gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3399	2151	595	626	27		
1	E	439	Total	C	N	O	S	0	0
			3399	2151	595	626	27		
1	I	439	Total	C	N	O	S	0	0
			3399	2151	595	626	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	conflict	UNP A0A140EMT3
A	508	ARG	-	expression tag	UNP A0A140EMT3
A	509	ARG	-	expression tag	UNP A0A140EMT3
A	510	ARG	-	expression tag	UNP A0A140EMT3
A	511	ARG	-	expression tag	UNP A0A140EMT3
A	512	ARG	-	expression tag	UNP A0A140EMT3
A	513	ARG	-	expression tag	UNP A0A140EMT3
E	501	CYS	ALA	conflict	UNP A0A140EMT3
E	508	ARG	-	expression tag	UNP A0A140EMT3
E	509	ARG	-	expression tag	UNP A0A140EMT3
E	510	ARG	-	expression tag	UNP A0A140EMT3
E	511	ARG	-	expression tag	UNP A0A140EMT3
E	512	ARG	-	expression tag	UNP A0A140EMT3
E	513	ARG	-	expression tag	UNP A0A140EMT3
I	501	CYS	ALA	conflict	UNP A0A140EMT3
I	508	ARG	-	expression tag	UNP A0A140EMT3
I	509	ARG	-	expression tag	UNP A0A140EMT3
I	510	ARG	-	expression tag	UNP A0A140EMT3
I	511	ARG	-	expression tag	UNP A0A140EMT3
I	512	ARG	-	expression tag	UNP A0A140EMT3
I	513	ARG	-	expression tag	UNP A0A140EMT3

- Molecule 2 is a protein called T/F100 Env gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	124	Total 944	C 599	N 158	O 182	S 5	0	0
2	F	124	Total 944	C 599	N 158	O 182	S 5	0	0
2	J	124	Total 944	C 599	N 158	O 182	S 5	0	0

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP A0A140EMT3
B	605	CYS	THR	conflict	UNP A0A140EMT3
B	665	ALA	-	expression tag	UNP A0A140EMT3
B	666	ALA	-	expression tag	UNP A0A140EMT3
B	667	ALA	-	expression tag	UNP A0A140EMT3
B	668	TRP	-	expression tag	UNP A0A140EMT3
B	669	SER	-	expression tag	UNP A0A140EMT3
B	670	HIS	-	expression tag	UNP A0A140EMT3
B	671	PRO	-	expression tag	UNP A0A140EMT3
B	672	GLN	-	expression tag	UNP A0A140EMT3
B	673	PHE	-	expression tag	UNP A0A140EMT3
B	674	GLU	-	expression tag	UNP A0A140EMT3
B	675	LYS	-	expression tag	UNP A0A140EMT3
B	676	GLY	-	expression tag	UNP A0A140EMT3
B	677	GLY	-	expression tag	UNP A0A140EMT3
B	678	GLY	-	expression tag	UNP A0A140EMT3
B	679	SER	-	expression tag	UNP A0A140EMT3
B	680	GLY	-	expression tag	UNP A0A140EMT3
B	681	GLY	-	expression tag	UNP A0A140EMT3
B	682	GLY	-	expression tag	UNP A0A140EMT3
B	683	SER	-	expression tag	UNP A0A140EMT3
B	684	GLY	-	expression tag	UNP A0A140EMT3
B	685	GLY	-	expression tag	UNP A0A140EMT3
B	686	SER	-	expression tag	UNP A0A140EMT3
B	687	ALA	-	expression tag	UNP A0A140EMT3
B	688	TRP	-	expression tag	UNP A0A140EMT3
B	689	SER	-	expression tag	UNP A0A140EMT3
B	690	HIS	-	expression tag	UNP A0A140EMT3
B	691	PRO	-	expression tag	UNP A0A140EMT3
B	692	GLN	-	expression tag	UNP A0A140EMT3
B	693	PHE	-	expression tag	UNP A0A140EMT3
B	694	GLU	-	expression tag	UNP A0A140EMT3
B	695	LYS	-	expression tag	UNP A0A140EMT3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	559	PRO	ILE	conflict	UNP A0A140EMT3
F	605	CYS	THR	conflict	UNP A0A140EMT3
F	665	ALA	-	expression tag	UNP A0A140EMT3
F	666	ALA	-	expression tag	UNP A0A140EMT3
F	667	ALA	-	expression tag	UNP A0A140EMT3
F	668	TRP	-	expression tag	UNP A0A140EMT3
F	669	SER	-	expression tag	UNP A0A140EMT3
F	670	HIS	-	expression tag	UNP A0A140EMT3
F	671	PRO	-	expression tag	UNP A0A140EMT3
F	672	GLN	-	expression tag	UNP A0A140EMT3
F	673	PHE	-	expression tag	UNP A0A140EMT3
F	674	GLU	-	expression tag	UNP A0A140EMT3
F	675	LYS	-	expression tag	UNP A0A140EMT3
F	676	GLY	-	expression tag	UNP A0A140EMT3
F	677	GLY	-	expression tag	UNP A0A140EMT3
F	678	GLY	-	expression tag	UNP A0A140EMT3
F	679	SER	-	expression tag	UNP A0A140EMT3
F	680	GLY	-	expression tag	UNP A0A140EMT3
F	681	GLY	-	expression tag	UNP A0A140EMT3
F	682	GLY	-	expression tag	UNP A0A140EMT3
F	683	SER	-	expression tag	UNP A0A140EMT3
F	684	GLY	-	expression tag	UNP A0A140EMT3
F	685	GLY	-	expression tag	UNP A0A140EMT3
F	686	SER	-	expression tag	UNP A0A140EMT3
F	687	ALA	-	expression tag	UNP A0A140EMT3
F	688	TRP	-	expression tag	UNP A0A140EMT3
F	689	SER	-	expression tag	UNP A0A140EMT3
F	690	HIS	-	expression tag	UNP A0A140EMT3
F	691	PRO	-	expression tag	UNP A0A140EMT3
F	692	GLN	-	expression tag	UNP A0A140EMT3
F	693	PHE	-	expression tag	UNP A0A140EMT3
F	694	GLU	-	expression tag	UNP A0A140EMT3
F	695	LYS	-	expression tag	UNP A0A140EMT3
J	559	PRO	ILE	conflict	UNP A0A140EMT3
J	605	CYS	THR	conflict	UNP A0A140EMT3
J	665	ALA	-	expression tag	UNP A0A140EMT3
J	666	ALA	-	expression tag	UNP A0A140EMT3
J	667	ALA	-	expression tag	UNP A0A140EMT3
J	668	TRP	-	expression tag	UNP A0A140EMT3
J	669	SER	-	expression tag	UNP A0A140EMT3
J	670	HIS	-	expression tag	UNP A0A140EMT3
J	671	PRO	-	expression tag	UNP A0A140EMT3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	672	GLN	-	expression tag	UNP A0A140EMT3
J	673	PHE	-	expression tag	UNP A0A140EMT3
J	674	GLU	-	expression tag	UNP A0A140EMT3
J	675	LYS	-	expression tag	UNP A0A140EMT3
J	676	GLY	-	expression tag	UNP A0A140EMT3
J	677	GLY	-	expression tag	UNP A0A140EMT3
J	678	GLY	-	expression tag	UNP A0A140EMT3
J	679	SER	-	expression tag	UNP A0A140EMT3
J	680	GLY	-	expression tag	UNP A0A140EMT3
J	681	GLY	-	expression tag	UNP A0A140EMT3
J	682	GLY	-	expression tag	UNP A0A140EMT3
J	683	SER	-	expression tag	UNP A0A140EMT3
J	684	GLY	-	expression tag	UNP A0A140EMT3
J	685	GLY	-	expression tag	UNP A0A140EMT3
J	686	SER	-	expression tag	UNP A0A140EMT3
J	687	ALA	-	expression tag	UNP A0A140EMT3
J	688	TRP	-	expression tag	UNP A0A140EMT3
J	689	SER	-	expression tag	UNP A0A140EMT3
J	690	HIS	-	expression tag	UNP A0A140EMT3
J	691	PRO	-	expression tag	UNP A0A140EMT3
J	692	GLN	-	expression tag	UNP A0A140EMT3
J	693	PHE	-	expression tag	UNP A0A140EMT3
J	694	GLU	-	expression tag	UNP A0A140EMT3
J	695	LYS	-	expression tag	UNP A0A140EMT3

- Molecule 3 is a protein called 8ANC195 G52K5 heavy chain, IG gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	130	Total	C	N	O	S	0	0
			976	619	167	187	3		
3	G	130	Total	C	N	O	S	0	0
			976	619	167	187	3		
3	K	130	Total	C	N	O	S	0	0
			976	619	167	187	3		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	221	HIS	-	expression tag	UNP S6B2A6
C	222	HIS	-	expression tag	UNP S6B2A6
C	223	HIS	-	expression tag	UNP S6B2A6
C	224	HIS	-	expression tag	UNP S6B2A6

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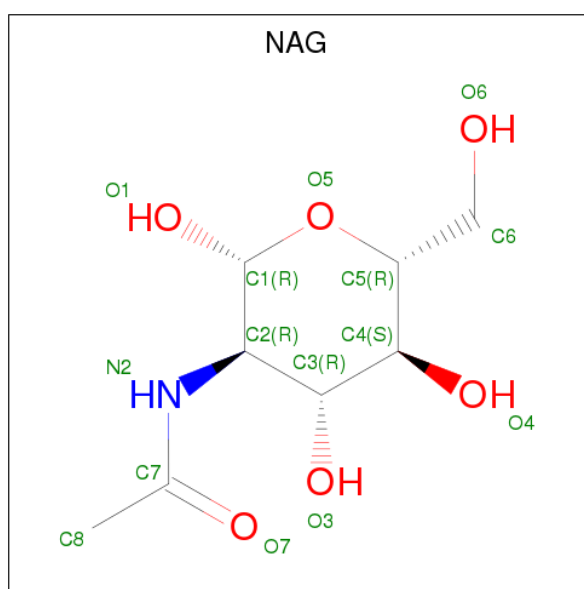
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Chain	Residue	Modelled	Actual	Comment	Reference
C	225	HIS	-	expression tag	UNP S6B2A6
G	221	HIS	-	expression tag	UNP S6B2A6
G	222	HIS	-	expression tag	UNP S6B2A6
G	223	HIS	-	expression tag	UNP S6B2A6
G	224	HIS	-	expression tag	UNP S6B2A6
G	225	HIS	-	expression tag	UNP S6B2A6
K	221	HIS	-	expression tag	UNP S6B2A6
K	222	HIS	-	expression tag	UNP S6B2A6
K	223	HIS	-	expression tag	UNP S6B2A6
K	224	HIS	-	expression tag	UNP S6B2A6
K	225	HIS	-	expression tag	UNP S6B2A6

- Molecule 4 is a protein called 8ANC195 G52K5 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	108	Total	C	N	O	S	0	0
			793	500	139	151	3		
4	H	108	Total	C	N	O	S	0	0
			793	500	139	151	3		
4	L	108	Total	C	N	O	S	0	0
			793	500	139	151	3		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	
5	A	1	Total	C	N	O	0
			364	208	26	130	

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 364	C 208	N 26	O 130	0
5	A	1	Total 364	C 208	N 26	O 130	0
5	A	1	Total 364	C 208	N 26	O 130	0
5	A	1	Total 364	C 208	N 26	O 130	0
5	B	1	Total 70	C 40	N 5	O 25	0
5	B	1	Total 70	C 40	N 5	O 25	0
5	B	1	Total 70	C 40	N 5	O 25	0
5	B	1	Total 70	C 40	N 5	O 25	0
5	B	1	Total 70	C 40	N 5	O 25	0
5	B	1	Total 70	C 40	N 5	O 25	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0
5	E	1	Total 364	C 208	N 26	O 130	0

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Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	E	1	Total	C	N	O	0
			364	208	26	130	
5	F	1	Total	C	N	O	0
			70	40	5	25	
5	F	1	Total	C	N	O	0
			70	40	5	25	
5	F	1	Total	C	N	O	0
			70	40	5	25	
5	F	1	Total	C	N	O	0
			70	40	5	25	
5	F	1	Total	C	N	O	0
			70	40	5	25	
5	G	1	Total	C	N	O	0
			14	8	1	5	

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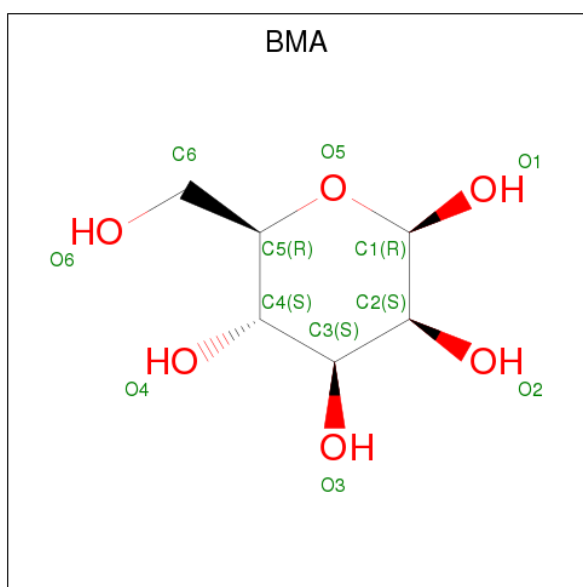
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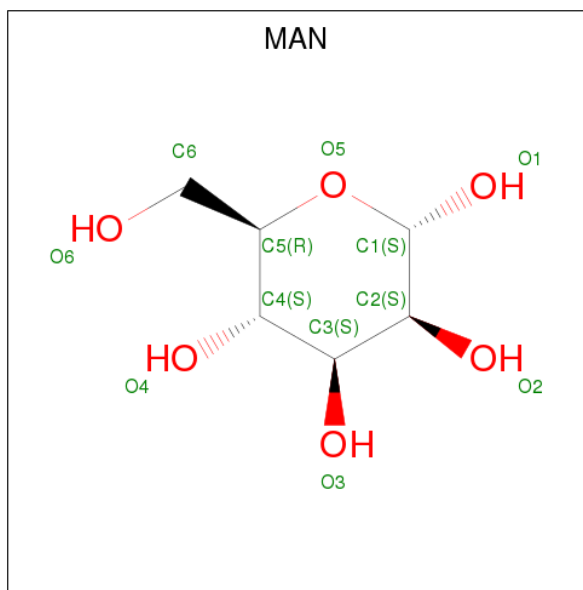
Mol	Chain	Residues	Atoms				AltConf
5	I	1	Total	C	N	O	0
			364	208	26	130	
5	I	1	Total	C	N	O	0
			364	208	26	130	
5	I	1	Total	C	N	O	0
			364	208	26	130	
5	I	1	Total	C	N	O	0
			364	208	26	130	
5	I	1	Total	C	N	O	0
			364	208	26	130	
5	J	1	Total	C	N	O	0
			70	40	5	25	
5	J	1	Total	C	N	O	0
			70	40	5	25	
5	J	1	Total	C	N	O	0
			70	40	5	25	
5	J	1	Total	C	N	O	0
			70	40	5	25	
5	J	1	Total	C	N	O	0
			70	40	5	25	
5	K	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			33	18	15	
6	A	1	Total	C	O	0
			33	18	15	
6	A	1	Total	C	O	0
			33	18	15	
6	B	1	Total	C	O	0
			11	6	5	
6	E	1	Total	C	O	0
			33	18	15	
6	E	1	Total	C	O	0
			33	18	15	
6	E	1	Total	C	O	0
			33	18	15	
6	F	1	Total	C	O	0
			11	6	5	
6	I	1	Total	C	O	0
			33	18	15	
6	I	1	Total	C	O	0
			33	18	15	
6	I	1	Total	C	O	0
			33	18	15	
6	J	1	Total	C	O	0
			11	6	5	

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			110	60	50	
7	B	1	Total	C	O	0
			11	6	5	
7	E	1	Total	C	O	0
			110	60	50	
7	E	1	Total	C	O	0
			110	60	50	
7	E	1	Total	C	O	0
			110	60	50	
7	E	1	Total	C	O	0
			110	60	50	
7	E	1	Total	C	O	0
			110	60	50	
7	E	1	Total	C	O	0
			110	60	50	
7	E	1	Total	C	O	0
			110	60	50	
7	E	1	Total	C	O	0
			110	60	50	
7	F	1	Total	C	O	0
			11	6	5	

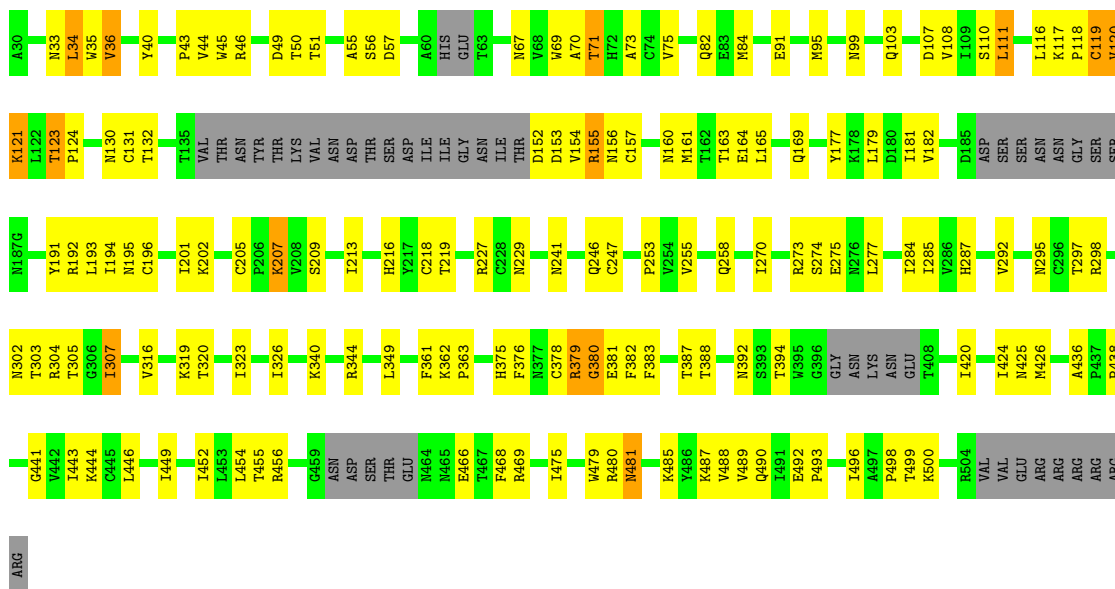
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Mol	Chain	Residues	Atoms			AltConf
7	I	1	Total	C	O	0
			110	60	50	
7	I	1	Total	C	O	0
			110	60	50	
7	I	1	Total	C	O	0
			110	60	50	
7	I	1	Total	C	O	0
			110	60	50	
7	I	1	Total	C	O	0
			110	60	50	
7	I	1	Total	C	O	0
			110	60	50	
7	I	1	Total	C	O	0
			110	60	50	
7	I	1	Total	C	O	0
			110	60	50	
7	J	1	Total	C	O	0
			11	6	5	

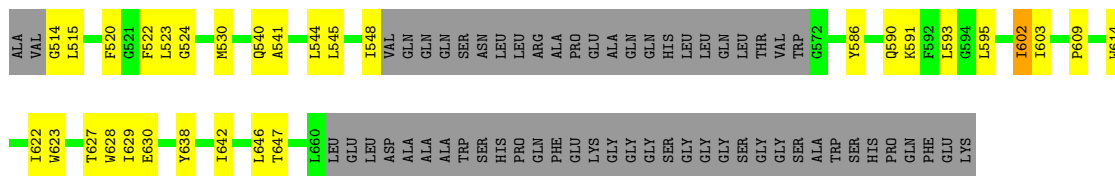
- Molecule 1: T/F100 Env gp120

Chain I: 59% 29% • 10%



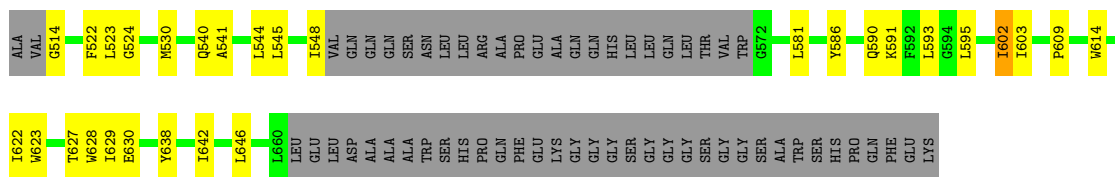
- Molecule 2: T/F100 Env gp41

Chain B: 51% 16% . 33%



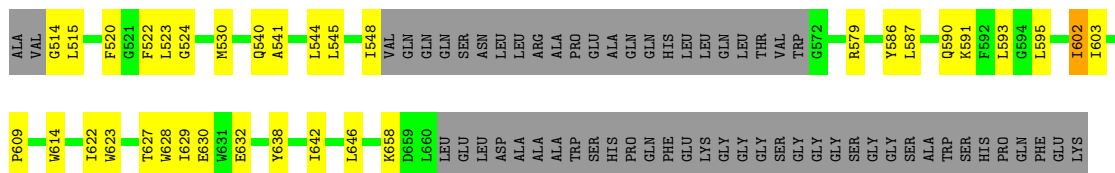
- Molecule 2: T/F100 Env gp41

Chain F: 52% 15% . 33%

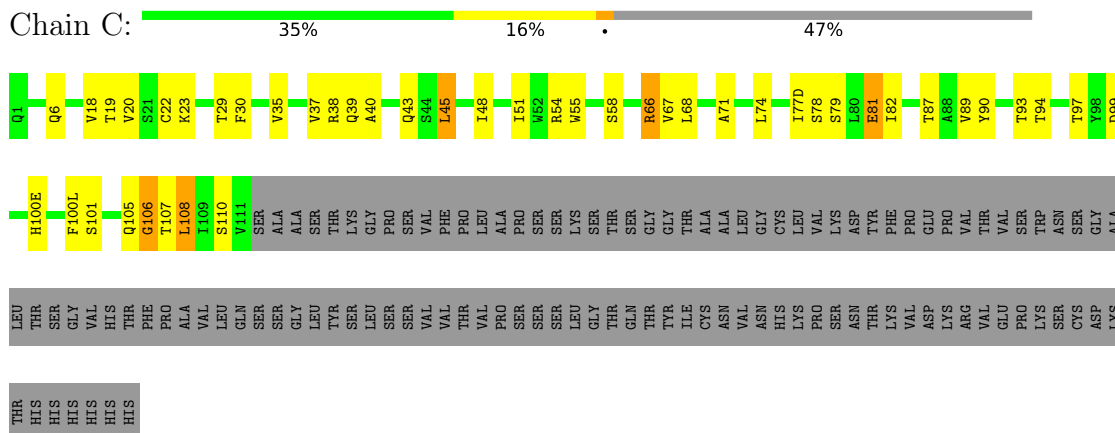


- Molecule 2: T/F100 Env gp41

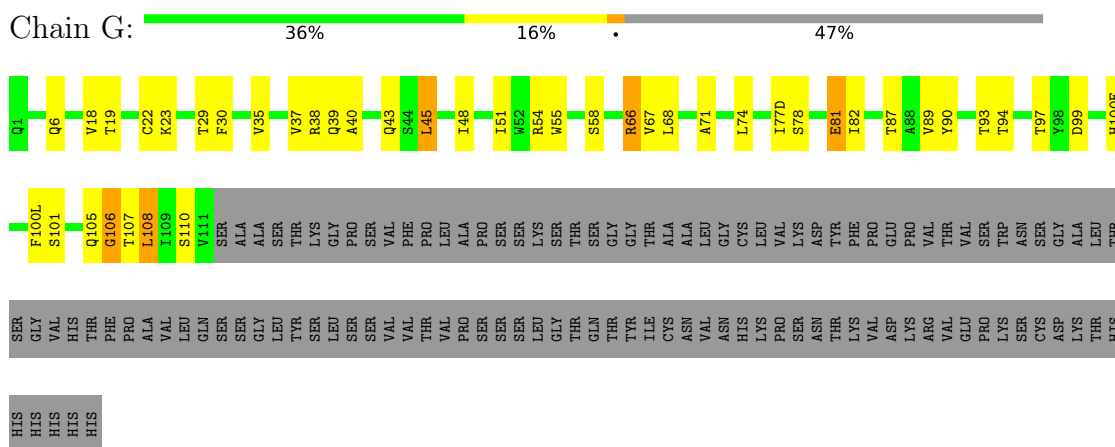
Chain J: 49% 18% • 33%



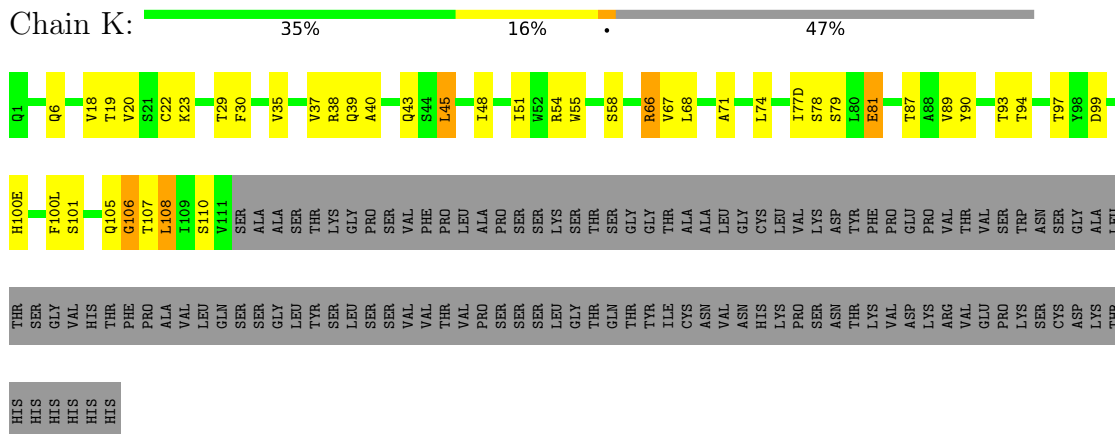
- Molecule 3: 8ANC195 G52K5 heavy chain, IG gamma-1 chain



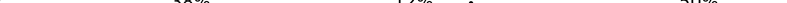
- Molecule 3: 8ANC195 G52K5 heavy chain, IG gamma-1 chain

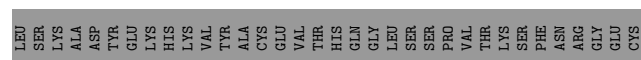
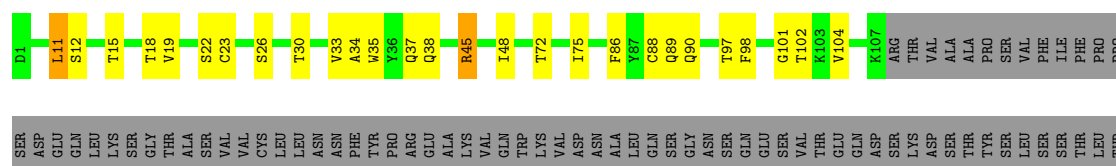


- Molecule 3: 8ANC195 G52K5 heavy chain, IG gamma-1 chain



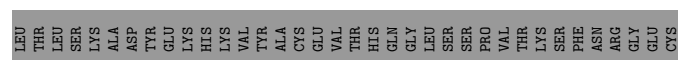
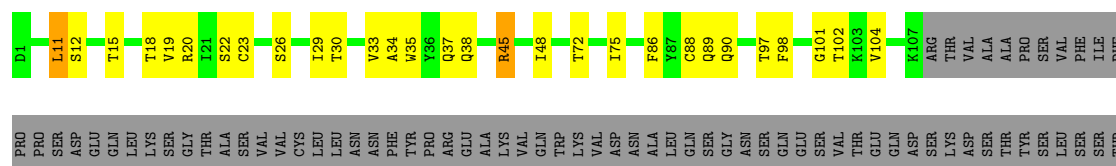
- Molecule 4: 8ANC195 G52K5 light chain

Chain D:  38% 12% . 50%



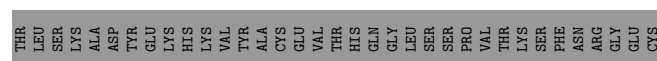
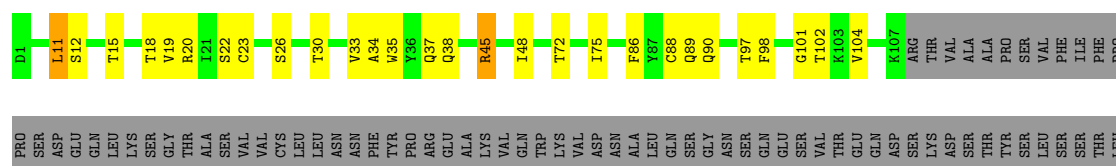
- Molecule 4: 8ANC195 G52K5 light chain

Chain H: 37% 13% 50%



- Molecule 4: 8ANC195 G52K5 light chain

Chain L: 37% 12% 50%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	170716	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 ($e^-/\text{\AA}^2$)	64	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	0.57	0/3473	0.71	2/4720 (0.0%)
1	E	0.57	0/3473	0.71	2/4720 (0.0%)
1	I	0.57	0/3473	0.71	1/4720 (0.0%)
2	B	0.62	0/961	0.80	0/1304
2	F	0.62	0/961	0.80	0/1304
2	J	0.62	0/961	0.80	0/1304
3	C	0.54	0/1003	0.67	0/1372
3	G	0.54	0/1003	0.67	0/1372
3	K	0.54	0/1003	0.67	0/1372
4	D	0.49	0/811	0.70	0/1106
4	H	0.48	0/811	0.70	0/1106
4	L	0.48	0/811	0.70	0/1106
All	All	0.56	0/18744	0.72	5/25506 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	CYS	CA-CB-SG	5.97	124.74	114.00
1	E	205	CYS	CA-CB-SG	5.97	124.74	114.00
1	I	205	CYS	CA-CB-SG	5.97	124.74	114.00
1	A	131	CYS	CA-CB-SG	5.01	123.03	114.00
1	E	131	CYS	CA-CB-SG	5.01	123.02	114.00

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	3399	0	3303	113	0
1	E	3399	0	3303	109	0
1	I	3399	0	3303	110	0
2	B	944	0	894	40	0
2	F	944	0	894	41	0
2	J	944	0	894	42	0
3	C	976	0	914	40	0
3	G	976	0	914	39	0
3	K	976	0	914	37	0
4	D	793	0	748	28	0
4	H	793	0	748	31	0
4	L	793	0	748	28	0
5	A	364	0	325	2	0
5	B	70	0	63	0	0
5	C	14	0	13	0	0
5	E	364	0	325	2	0
5	F	70	0	63	0	0
5	G	14	0	13	0	0
5	I	364	0	325	2	0
5	J	70	0	63	0	0
5	K	14	0	13	0	0
6	A	33	0	26	0	0
6	B	11	0	9	0	0
6	E	33	0	26	0	0
6	F	11	0	9	0	0
6	I	33	0	26	0	0
6	J	11	0	9	0	0
7	A	110	0	94	0	0
7	B	11	0	10	0	0
7	E	110	0	94	0	0
7	F	11	0	10	0	0
7	I	110	0	94	0	0
7	J	11	0	10	0	0
All	All	20175	0	19197	572	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 15.

The worst 5 of 572 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)
3:C:45:LEU:HD11	4:D:98:PHE:CE2	1.57	1.40
3:K:45:LEU:HD11	4:L:98:PHE:CE2	1.57	1.39
3:G:45:LEU:HD11	4:H:98:PHE:CE2	1.57	1.36
2:B:541:ALA:HA	2:B:544:LEU:CD2	1.83	1.09
2:F:541:ALA:HA	2:F:544:LEU:CD2	1.83	1.08

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	427/486 (88%)	368 (86%)	54 (13%)	5 (1%)	14	55
1	E	427/486 (88%)	368 (86%)	54 (13%)	5 (1%)	14	55
1	I	427/486 (88%)	368 (86%)	54 (13%)	5 (1%)	14	55
2	B	120/184 (65%)	112 (93%)	8 (7%)	0	100	100
2	F	120/184 (65%)	112 (93%)	8 (7%)	0	100	100
2	J	120/184 (65%)	112 (93%)	8 (7%)	0	100	100
3	C	128/244 (52%)	114 (89%)	13 (10%)	1 (1%)	21	62
3	G	128/244 (52%)	114 (89%)	13 (10%)	1 (1%)	21	62
3	K	128/244 (52%)	114 (89%)	13 (10%)	1 (1%)	21	62
4	D	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
4	H	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
4	L	106/215 (49%)	96 (91%)	10 (9%)	0	100	100
All	All	2343/3387 (69%)	2070 (88%)	255 (11%)	18 (1%)	26	62

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	155	ARG
1	A	380	GLY
1	E	121	LYS
1	E	155	ARG

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	376/434 (87%)	346 (92%)	30 (8%)	13	46
1	E	376/434 (87%)	346 (92%)	30 (8%)	13	46
1	I	376/434 (87%)	346 (92%)	30 (8%)	13	46
2	B	96/149 (64%)	93 (97%)	3 (3%)	43	71
2	F	96/149 (64%)	93 (97%)	3 (3%)	43	71
2	J	96/149 (64%)	93 (97%)	3 (3%)	43	71
3	C	104/210 (50%)	95 (91%)	9 (9%)	11	42
3	G	104/210 (50%)	95 (91%)	9 (9%)	11	42
3	K	104/210 (50%)	95 (91%)	9 (9%)	11	42
4	D	78/182 (43%)	69 (88%)	9 (12%)	6	31
4	H	78/182 (43%)	69 (88%)	9 (12%)	6	31
4	L	78/182 (43%)	69 (88%)	9 (12%)	6	31
All	All	1962/2925 (67%)	1809 (92%)	153 (8%)	18	47

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	307	ILE
3	G	45	LEU
3	K	81	GLU
1	E	362	LYS
1	E	481	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	249	HIS
1	E	478	ASN
2	J	590	GLN
1	E	375	HIS
1	E	481	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

141 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	601	1,5	14,14,15	0.22	0	17,19,21	0.56	0
5	NAG	A	602	5,6	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
6	BMA	A	603	5,7	11,11,12	1.07	1 (9%)	15,15,17	0.97	1 (6%)
7	MAN	A	604	7,6	11,11,12	0.86	0	15,15,17	0.94	0
7	MAN	A	605	7	11,11,12	0.77	0	15,15,17	1.61	2 (13%)
7	MAN	A	606	7	11,11,12	0.71	0	15,15,17	1.45	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	A	607	7,6	11,11,12	0.88	1 (9%)	15,15,17	1.39	2 (13%)
7	MAN	A	608	7	11,11,12	0.76	0	15,15,17	1.03	2 (13%)
7	MAN	A	609	7	11,11,12	1.13	1 (9%)	15,15,17	1.10	1 (6%)
7	MAN	A	610	7	11,11,12	0.56	0	15,15,17	1.25	2 (13%)
5	NAG	A	611	1,5	14,14,15	0.44	0	17,19,21	0.48	0
5	NAG	A	612	5,6	14,14,15	0.41	0	17,19,21	0.57	0
6	BMA	A	613	5,7	11,11,12	0.64	0	15,15,17	0.82	1 (6%)
7	MAN	A	614	7,6	11,11,12	1.07	1 (9%)	15,15,17	1.05	1 (6%)
7	MAN	A	615	6	11,11,12	0.78	0	15,15,17	1.03	2 (13%)
7	MAN	A	616	7	11,11,12	1.22	2 (18%)	15,15,17	1.37	2 (13%)
5	NAG	A	617	1,5	14,14,15	0.43	0	17,19,21	0.54	0
5	NAG	A	618	5	14,14,15	0.23	0	17,19,21	0.54	0
5	NAG	A	619	1	14,14,15	0.87	1 (7%)	17,19,21	0.56	0
5	NAG	A	620	1	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
5	NAG	A	621	1,5	14,14,15	0.76	1 (7%)	17,19,21	0.82	0
5	NAG	A	622	5	14,14,15	0.24	0	17,19,21	0.61	0
5	NAG	A	623	1	14,14,15	0.36	0	17,19,21	0.51	0
5	NAG	A	624	1	14,14,15	0.26	0	17,19,21	0.86	1 (5%)
5	NAG	A	625	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.74	0
5	NAG	A	626	5	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
5	NAG	A	627	1	14,14,15	0.49	0	17,19,21	1.29	1 (5%)
5	NAG	A	628	1,5	14,14,15	0.38	0	17,19,21	1.28	3 (17%)
5	NAG	A	629	5	14,14,15	0.26	0	17,19,21	0.56	0
5	NAG	A	630	1,5	14,14,15	1.16	1 (7%)	17,19,21	2.26	2 (11%)
5	NAG	A	631	5	14,14,15	0.42	0	17,19,21	1.02	1 (5%)
5	NAG	A	632	1	14,14,15	0.40	0	17,19,21	0.49	0
5	NAG	A	633	1,5	14,14,15	1.16	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	A	634	5	14,14,15	0.32	0	17,19,21	0.56	0
5	NAG	A	635	1,5	14,14,15	0.46	0	17,19,21	0.62	0
5	NAG	A	636	5	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	A	637	1,5	14,14,15	0.55	0	17,19,21	0.52	0
5	NAG	A	638	5,6	14,14,15	0.37	0	17,19,21	0.57	0
6	BMA	A	639	5	11,11,12	0.90	0	15,15,17	1.00	1 (6%)
5	NAG	B	701	2,5	14,14,15	0.63	0	17,19,21	0.84	1 (5%)
5	NAG	B	702	5,6	14,14,15	0.24	0	17,19,21	0.65	0
6	BMA	B	703	5,7	11,11,12	0.82	0	15,15,17	0.82	0
7	MAN	B	704	6	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
5	NAG	B	705	2	14,14,15	0.32	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	706	2	14,14,15	1.43	2 (14%)	17,19,21	1.38	1 (5%)
5	NAG	B	707	2	14,14,15	0.34	0	17,19,21	0.61	0
5	NAG	C	301	3	14,14,15	0.46	0	17,19,21	0.72	1 (5%)
5	NAG	E	601	1,5	14,14,15	0.22	0	17,19,21	0.56	0
5	NAG	E	602	5,6	14,14,15	0.32	0	17,19,21	1.03	1 (5%)
6	BMA	E	603	5,7	11,11,12	1.07	1 (9%)	15,15,17	0.97	1 (6%)
7	MAN	E	604	7,6	11,11,12	0.86	0	15,15,17	0.94	0
7	MAN	E	605	7	11,11,12	0.78	0	15,15,17	1.60	2 (13%)
7	MAN	E	606	7	11,11,12	0.71	0	15,15,17	1.44	1 (6%)
7	MAN	E	607	7,6	11,11,12	0.88	1 (9%)	15,15,17	1.40	2 (13%)
7	MAN	E	608	7	11,11,12	0.77	0	15,15,17	1.03	2 (13%)
7	MAN	E	609	7	11,11,12	1.13	1 (9%)	15,15,17	1.10	1 (6%)
7	MAN	E	610	7	11,11,12	0.57	0	15,15,17	1.26	2 (13%)
5	NAG	E	611	1,5	14,14,15	0.44	0	17,19,21	0.48	0
5	NAG	E	612	5,6	14,14,15	0.42	0	17,19,21	0.58	0
6	BMA	E	613	5,7	11,11,12	0.63	0	15,15,17	0.82	1 (6%)
7	MAN	E	614	7,6	11,11,12	1.08	1 (9%)	15,15,17	1.05	1 (6%)
7	MAN	E	615	6	11,11,12	0.78	0	15,15,17	1.02	2 (13%)
7	MAN	E	616	7	11,11,12	1.21	2 (18%)	15,15,17	1.37	2 (13%)
5	NAG	E	617	1,5	14,14,15	0.43	0	17,19,21	0.54	0
5	NAG	E	618	5	14,14,15	0.22	0	17,19,21	0.55	0
5	NAG	E	619	1	14,14,15	0.87	1 (7%)	17,19,21	0.56	0
5	NAG	E	620	1	14,14,15	0.35	0	17,19,21	0.64	1 (5%)
5	NAG	E	621	1,5	14,14,15	0.77	1 (7%)	17,19,21	0.82	0
5	NAG	E	622	5	14,14,15	0.24	0	17,19,21	0.61	0
5	NAG	E	623	1	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	E	624	1	14,14,15	0.25	0	17,19,21	0.86	1 (5%)
5	NAG	E	625	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.74	0
5	NAG	E	626	5	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
5	NAG	E	627	1	14,14,15	0.49	0	17,19,21	1.28	1 (5%)
5	NAG	E	628	1,5	14,14,15	0.38	0	17,19,21	1.28	3 (17%)
5	NAG	E	629	5	14,14,15	0.26	0	17,19,21	0.56	0
5	NAG	E	630	1,5	14,14,15	1.15	1 (7%)	17,19,21	2.27	2 (11%)
5	NAG	E	631	5	14,14,15	0.42	0	17,19,21	1.02	1 (5%)
5	NAG	E	632	1	14,14,15	0.39	0	17,19,21	0.50	0
5	NAG	E	633	1,5	14,14,15	1.17	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	E	634	5	14,14,15	0.33	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	635	1,5	14,14,15	0.46	0	17,19,21	0.62	0
5	NAG	E	636	5	14,14,15	0.32	0	17,19,21	0.49	0
5	NAG	E	637	1,5	14,14,15	0.54	0	17,19,21	0.52	0
5	NAG	E	638	5,6	14,14,15	0.37	0	17,19,21	0.57	0
6	BMA	E	639	5	11,11,12	0.91	0	15,15,17	0.99	1 (6%)
5	NAG	F	701	2,5	14,14,15	0.63	0	17,19,21	0.84	1 (5%)
5	NAG	F	702	5,6	14,14,15	0.25	0	17,19,21	0.65	0
6	BMA	F	703	5,7	11,11,12	0.82	0	15,15,17	0.82	0
7	MAN	F	704	6	11,11,12	0.67	0	15,15,17	1.08	2 (13%)
5	NAG	F	705	2	14,14,15	0.32	0	17,19,21	0.79	1 (5%)
5	NAG	F	706	2	14,14,15	1.43	2 (14%)	17,19,21	1.38	1 (5%)
5	NAG	F	707	2	14,14,15	0.35	0	17,19,21	0.61	0
5	NAG	G	301	3	14,14,15	0.46	0	17,19,21	0.71	1 (5%)
5	NAG	I	601	1,5	14,14,15	0.22	0	17,19,21	0.56	0
5	NAG	I	602	5,6	14,14,15	0.31	0	17,19,21	1.02	1 (5%)
6	BMA	I	603	5,7	11,11,12	1.07	1 (9%)	15,15,17	0.97	1 (6%)
7	MAN	I	604	7,6	11,11,12	0.86	0	15,15,17	0.93	0
7	MAN	I	605	7	11,11,12	0.78	0	15,15,17	1.60	2 (13%)
7	MAN	I	606	7	11,11,12	0.71	0	15,15,17	1.44	1 (6%)
7	MAN	I	607	7,6	11,11,12	0.88	1 (9%)	15,15,17	1.40	2 (13%)
7	MAN	I	608	7	11,11,12	0.75	0	15,15,17	1.04	2 (13%)
7	MAN	I	609	7	11,11,12	1.12	1 (9%)	15,15,17	1.10	1 (6%)
7	MAN	I	610	7	11,11,12	0.55	0	15,15,17	1.26	2 (13%)
5	NAG	I	611	1,5	14,14,15	0.45	0	17,19,21	0.48	0
5	NAG	I	612	5,6	14,14,15	0.42	0	17,19,21	0.58	0
6	BMA	I	613	5,7	11,11,12	0.64	0	15,15,17	0.82	1 (6%)
7	MAN	I	614	7,6	11,11,12	1.07	1 (9%)	15,15,17	1.05	1 (6%)
7	MAN	I	615	6	11,11,12	0.78	0	15,15,17	1.03	2 (13%)
7	MAN	I	616	7	11,11,12	1.22	2 (18%)	15,15,17	1.37	2 (13%)
5	NAG	I	617	1,5	14,14,15	0.43	0	17,19,21	0.54	0
5	NAG	I	618	5	14,14,15	0.23	0	17,19,21	0.54	0
5	NAG	I	619	1	14,14,15	0.88	1 (7%)	17,19,21	0.55	0
5	NAG	I	620	1	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
5	NAG	I	621	1,5	14,14,15	0.76	1 (7%)	17,19,21	0.82	0
5	NAG	I	622	5	14,14,15	0.24	0	17,19,21	0.60	0
5	NAG	I	623	1	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	I	624	1	14,14,15	0.25	0	17,19,21	0.87	1 (5%)
5	NAG	I	625	1,5	14,14,15	0.62	1 (7%)	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	I	626	5	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
5	NAG	I	627	1	14,14,15	0.49	0	17,19,21	1.29	1 (5%)
5	NAG	I	628	1,5	14,14,15	0.39	0	17,19,21	1.29	3 (17%)
5	NAG	I	629	5	14,14,15	0.26	0	17,19,21	0.57	0
5	NAG	I	630	1,5	14,14,15	1.17	1 (7%)	17,19,21	2.27	2 (11%)
5	NAG	I	631	5	14,14,15	0.42	0	17,19,21	1.02	1 (5%)
5	NAG	I	632	1	14,14,15	0.41	0	17,19,21	0.49	0
5	NAG	I	633	1,5	14,14,15	1.16	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	I	634	5	14,14,15	0.32	0	17,19,21	0.56	0
5	NAG	I	635	1,5	14,14,15	0.47	0	17,19,21	0.62	0
5	NAG	I	636	5	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	I	637	1,5	14,14,15	0.55	0	17,19,21	0.52	0
5	NAG	I	638	5,6	14,14,15	0.35	0	17,19,21	0.57	0
6	BMA	I	639	5	11,11,12	0.89	0	15,15,17	1.00	1 (6%)
5	NAG	J	701	2,5	14,14,15	0.63	0	17,19,21	0.84	1 (5%)
5	NAG	J	702	5,6	14,14,15	0.24	0	17,19,21	0.65	0
6	BMA	J	703	5,7	11,11,12	0.82	0	15,15,17	0.82	0
7	MAN	J	704	6	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
5	NAG	J	705	2	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
5	NAG	J	706	2	14,14,15	1.45	2 (14%)	17,19,21	1.38	1 (5%)
5	NAG	J	707	2	14,14,15	0.35	0	17,19,21	0.62	0
5	NAG	K	301	3	14,14,15	0.46	0	17,19,21	0.72	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
5	NAG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	603	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	604	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	605	7	-	0/2/19/22	0/1/1/1
7	MAN	A	606	7	-	0/2/19/22	0/1/1/1
7	MAN	A	607	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	608	7	-	0/2/19/22	0/1/1/1
7	MAN	A	609	7	-	0/2/19/22	0/1/1/1
7	MAN	A	610	7	-	0/2/19/22	0/1/1/1
5	NAG	A	611	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	612	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	613	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	614	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	615	6	-	0/2/19/22	0/1/1/1
7	MAN	A	616	7	-	0/2/19/22	0/1/1/1
5	NAG	A	617	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	618	5	-	0/6/23/26	0/1/1/1
5	NAG	A	619	1	-	0/6/23/26	0/1/1/1
5	NAG	A	620	1	-	0/6/23/26	0/1/1/1
5	NAG	A	621	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	622	5	-	0/6/23/26	0/1/1/1
5	NAG	A	623	1	-	0/6/23/26	0/1/1/1
5	NAG	A	624	1	-	0/6/23/26	0/1/1/1
5	NAG	A	625	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	626	5	-	0/6/23/26	0/1/1/1
5	NAG	A	627	1	-	0/6/23/26	0/1/1/1
5	NAG	A	628	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	629	5	-	0/6/23/26	0/1/1/1
5	NAG	A	630	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	631	5	-	0/6/23/26	0/1/1/1
5	NAG	A	632	1	-	0/6/23/26	0/1/1/1
5	NAG	A	633	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	634	5	-	0/6/23/26	0/1/1/1
5	NAG	A	635	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	636	5	-	0/6/23/26	0/1/1/1
5	NAG	A	637	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	638	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	639	5	-	0/2/19/22	0/1/1/1
5	NAG	B	701	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	B	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	B	704	6	-	0/2/19/22	0/1/1/1
5	NAG	B	705	2	-	0/6/23/26	0/1/1/1
5	NAG	B	706	2	-	0/6/23/26	0/1/1/1
5	NAG	B	707	2	-	0/6/23/26	0/1/1/1
5	NAG	C	301	3	-	0/6/23/26	0/1/1/1
5	NAG	E	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	602	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	603	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	604	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	605	7	-	0/2/19/22	0/1/1/1
7	MAN	E	606	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	E	607	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	608	7	-	0/2/19/22	0/1/1/1
7	MAN	E	609	7	-	0/2/19/22	0/1/1/1
7	MAN	E	610	7	-	0/2/19/22	0/1/1/1
5	NAG	E	611	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	612	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	613	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	614	7,6	-	0/2/19/22	0/1/1/1
7	MAN	E	615	6	-	0/2/19/22	0/1/1/1
7	MAN	E	616	7	-	0/2/19/22	0/1/1/1
5	NAG	E	617	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	618	5	-	0/6/23/26	0/1/1/1
5	NAG	E	619	1	-	0/6/23/26	0/1/1/1
5	NAG	E	620	1	-	0/6/23/26	0/1/1/1
5	NAG	E	621	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	622	5	-	0/6/23/26	0/1/1/1
5	NAG	E	623	1	-	0/6/23/26	0/1/1/1
5	NAG	E	624	1	-	0/6/23/26	0/1/1/1
5	NAG	E	625	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	626	5	-	0/6/23/26	0/1/1/1
5	NAG	E	627	1	-	0/6/23/26	0/1/1/1
5	NAG	E	628	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	629	5	-	0/6/23/26	0/1/1/1
5	NAG	E	630	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	631	5	-	0/6/23/26	0/1/1/1
5	NAG	E	632	1	-	0/6/23/26	0/1/1/1
5	NAG	E	633	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	634	5	-	0/6/23/26	0/1/1/1
5	NAG	E	635	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	636	5	-	0/6/23/26	0/1/1/1
5	NAG	E	637	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	638	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	639	5	-	0/2/19/22	0/1/1/1
5	NAG	F	701	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	704	6	-	0/2/19/22	0/1/1/1
5	NAG	F	705	2	-	0/6/23/26	0/1/1/1
5	NAG	F	706	2	-	0/6/23/26	0/1/1/1
5	NAG	F	707	2	-	0/6/23/26	0/1/1/1
5	NAG	G	301	3	-	0/6/23/26	0/1/1/1
5	NAG	I	601	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	602	5,6	-	0/6/23/26	0/1/1/1
6	BMA	I	603	5,7	-	0/2/19/22	0/1/1/1
7	MAN	I	604	7,6	-	0/2/19/22	0/1/1/1
7	MAN	I	605	7	-	0/2/19/22	0/1/1/1
7	MAN	I	606	7	-	0/2/19/22	0/1/1/1
7	MAN	I	607	7,6	-	0/2/19/22	0/1/1/1
7	MAN	I	608	7	-	0/2/19/22	0/1/1/1
7	MAN	I	609	7	-	0/2/19/22	0/1/1/1
7	MAN	I	610	7	-	0/2/19/22	0/1/1/1
5	NAG	I	611	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	612	5,6	-	0/6/23/26	0/1/1/1
6	BMA	I	613	5,7	-	0/2/19/22	0/1/1/1
7	MAN	I	614	7,6	-	0/2/19/22	0/1/1/1
7	MAN	I	615	6	-	0/2/19/22	0/1/1/1
7	MAN	I	616	7	-	0/2/19/22	0/1/1/1
5	NAG	I	617	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	618	5	-	0/6/23/26	0/1/1/1
5	NAG	I	619	1	-	0/6/23/26	0/1/1/1
5	NAG	I	620	1	-	0/6/23/26	0/1/1/1
5	NAG	I	621	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	622	5	-	0/6/23/26	0/1/1/1
5	NAG	I	623	1	-	0/6/23/26	0/1/1/1
5	NAG	I	624	1	-	0/6/23/26	0/1/1/1
5	NAG	I	625	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	626	5	-	0/6/23/26	0/1/1/1
5	NAG	I	627	1	-	0/6/23/26	0/1/1/1
5	NAG	I	628	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	629	5	-	0/6/23/26	0/1/1/1
5	NAG	I	630	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	631	5	-	0/6/23/26	0/1/1/1
5	NAG	I	632	1	-	0/6/23/26	0/1/1/1
5	NAG	I	633	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	634	5	-	0/6/23/26	0/1/1/1
5	NAG	I	635	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	636	5	-	0/6/23/26	0/1/1/1
5	NAG	I	637	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	638	5,6	-	0/6/23/26	0/1/1/1
6	BMA	I	639	5	-	0/2/19/22	0/1/1/1
5	NAG	J	701	2,5	-	0/6/23/26	0/1/1/1
5	NAG	J	702	5,6	-	0/6/23/26	0/1/1/1
6	BMA	J	703	5,7	-	0/2/19/22	0/1/1/1
7	MAN	J	704	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	705	2	-	0/6/23/26	0/1/1/1
5	NAG	J	706	2	-	0/6/23/26	0/1/1/1
5	NAG	J	707	2	-	0/6/23/26	0/1/1/1
5	NAG	K	301	3	-	0/6/23/26	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	633	NAG	O5-C1	-3.68	1.37	1.43
5	E	633	NAG	O5-C1	-3.67	1.37	1.43
5	I	633	NAG	O5-C1	-3.64	1.37	1.43
5	E	621	NAG	O5-C1	-2.72	1.39	1.43
5	I	621	NAG	O5-C1	-2.70	1.39	1.43

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	607	MAN	O2-C2-C3	-2.82	104.68	110.19
7	E	607	MAN	O2-C2-C3	-2.82	104.69	110.19
7	I	607	MAN	O2-C2-C3	-2.81	104.70	110.19
7	I	609	MAN	O2-C2-C3	-2.65	105.02	110.19
7	A	609	MAN	O2-C2-C3	-2.63	105.07	110.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	621	NAG	2	0
5	E	621	NAG	2	0
5	I	621	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.