



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 17, 2017 – 10:43 PM EDT

PDB ID : 5V8M
EMDB ID: : EMD-8644
Title : BG505 SOSIP.664 trimer in complex with broadly neutralizing HIV antibody 3BNC117
Authors : Lee, J.H.; Cottrell, C.A.; Ward, A.B.
Deposited on : unknown
Resolution : 4.40 Å(reported)

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

We welcome your comments at 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.

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

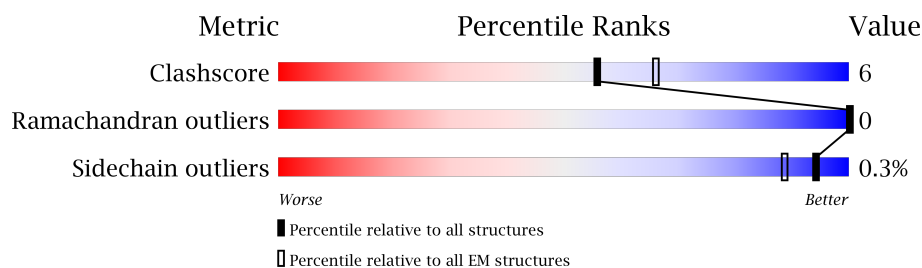
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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 ≥ 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	88% 5% 8%
1	F	481	88% • 8%
1	G	481	88% • 8%
2	B	153	79% 5% 16%
2	I	153	79% 5% 16%
2	J	153	78% 7% 16%
3	H	226	50% • 46%
3	R	226	50% • 46%
3	S	226	50% • 46%

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Mol	Chain	Length	Quality of chain
4	L	206	
4	T	206	
4	U	206	

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
5	NAG	A	627	-	-	X	-
5	NAG	F	627	-	-	X	-
5	NAG	G	627	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20835 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	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		
1	F	444	Total	C	N	O	S	0	0
			3493	2192	617	656	28		
1	G	444	Total	C	N	O	S	0	0
			3493	2192	617	656	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
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
2	I	129	Total	C	N	O	S	0	0
			1024	646	177	195	6		
2	J	129	Total	C	N	O	S	0	0
			1024	646	177	195	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
I	559	PRO	ILE	conflict	UNP Q2N0S6
I	605	CYS	THR	conflict	UNP Q2N0S6
J	559	PRO	ILE	conflict	UNP Q2N0S6
J	605	CYS	THR	conflict	UNP Q2N0S6

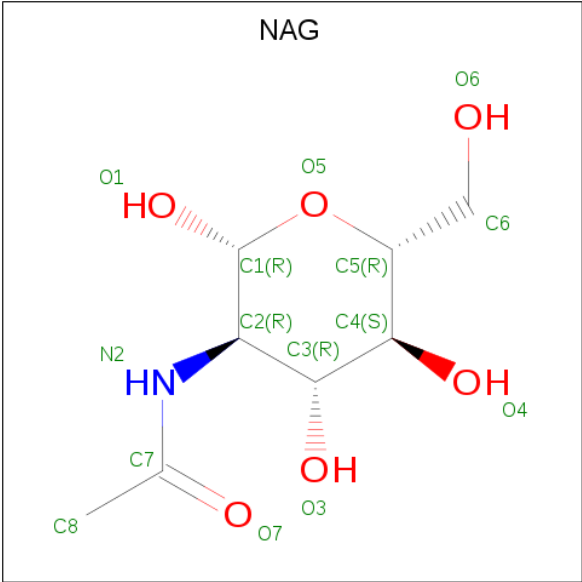
- Molecule 3 is a protein called antibody 3BNC117, heavy chain.

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

- Molecule 4 is a protein called antibody 3BNC117, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	T	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	U	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	
5	A	1	Total	C	N	O	0
			406	232	29	145	

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	A	1	Total 406	C 232	N 29	O 145	0
5	B	1	Total 28	C 16	N 2	O 10	0
5	B	1	Total 28	C 16	N 2	O 10	0
5	L	1	Total 28	C 16	N 2	O 10	0
5	L	1	Total 28	C 16	N 2	O 10	0
5	F	1	Total 406	C 232	N 29	O 145	0
5	F	1	Total 406	C 232	N 29	O 145	0

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Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total 406	C 232	N 29	O 145	0
5	F	1	Total 406	C 232	N 29	O 145	0
5	F	1	Total 406	C 232	N 29	O 145	0
5	F	1	Total 406	C 232	N 29	O 145	0
5	F	1	Total 406	C 232	N 29	O 145	0
5	F	1	Total 406	C 232	N 29	O 145	0
5	I	1	Total 28	C 16	N 2	O 10	0
5	I	1	Total 28	C 16	N 2	O 10	0
5	T	1	Total 28	C 16	N 2	O 10	0
5	T	1	Total 28	C 16	N 2	O 10	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0

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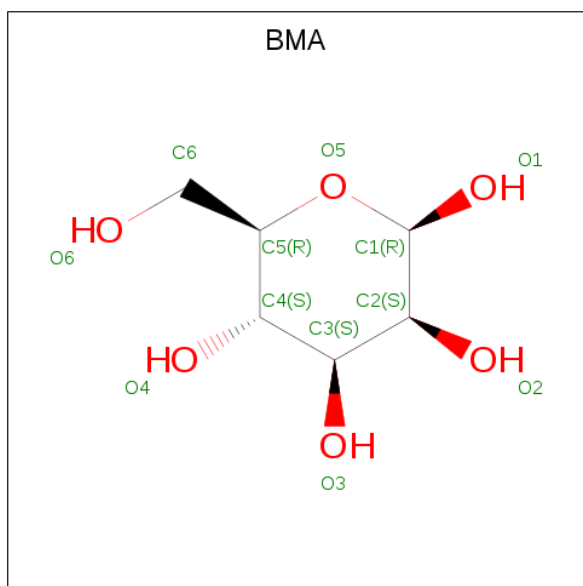
Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	G	1	Total 406	C 232	N 29	O 145	0
5	J	1	Total 28	C 16	N 2	O 10	0
5	J	1	Total 28	C 16	N 2	O 10	0
5	U	1	Total 28	C 16	N 2	O 10	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	U	1	28	16	2	10	0

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



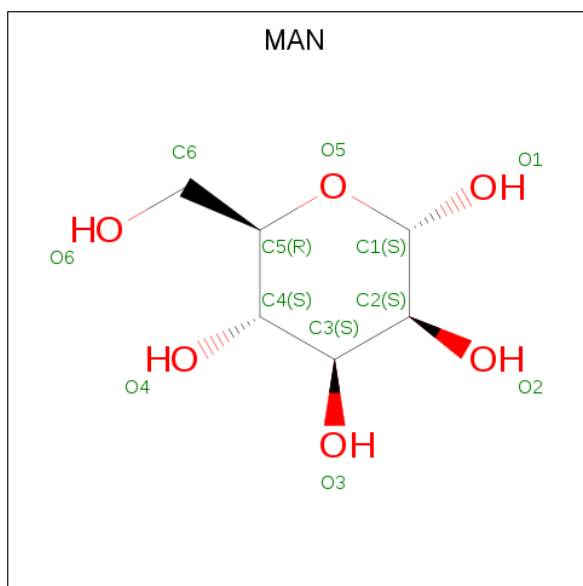
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	55	30	25	0
6	A	1	55	30	25	0
6	A	1	55	30	25	0
6	A	1	55	30	25	0
6	A	1	55	30	25	0
6	F	1	55	30	25	0
6	F	1	55	30	25	0
6	F	1	55	30	25	0
6	F	1	55	30	25	0
6	F	1	55	30	25	0

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Mol	Chain	Residues	Atoms			AltConf
6	G	1	Total	C	O	0
			55	30	25	
6	G	1	Total	C	O	0
			55	30	25	
6	G	1	Total	C	O	0
			55	30	25	
6	G	1	Total	C	O	0
			55	30	25	
6	G	1	Total	C	O	0
			55	30	25	

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



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			143	78	65	
7	A	1	Total	C	O	0
			143	78	65	
7	A	1	Total	C	O	0
			143	78	65	
7	A	1	Total	C	O	0
			143	78	65	
7	A	1	Total	C	O	0
			143	78	65	
7	A	1	Total	C	O	0
			143	78	65	

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Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total 143	C 78	O 65	0
7	A	1	Total 143	C 78	O 65	0
7	A	1	Total 143	C 78	O 65	0
7	A	1	Total 143	C 78	O 65	0
7	A	1	Total 143	C 78	O 65	0
7	A	1	Total 143	C 78	O 65	0
7	A	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	F	1	Total 143	C 78	O 65	0
7	G	1	Total 143	C 78	O 65	0

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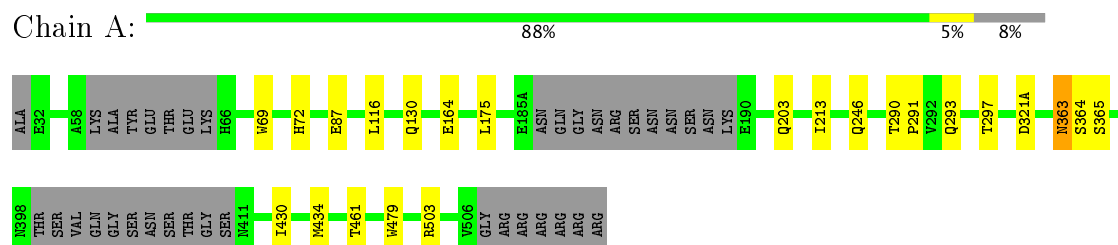
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Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	
7	G	1	Total	C	O	0
			143	78	65	

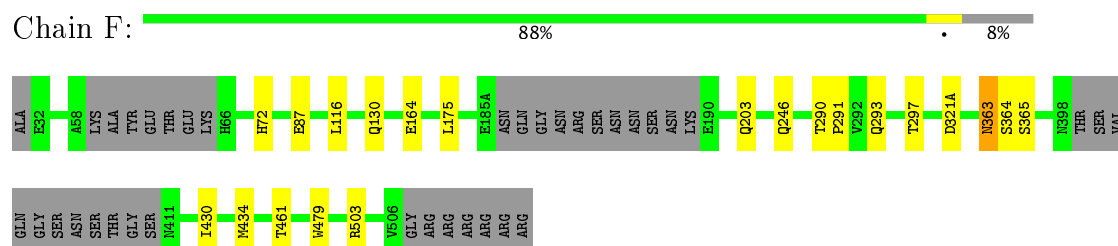
3 Residue-property plots

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.

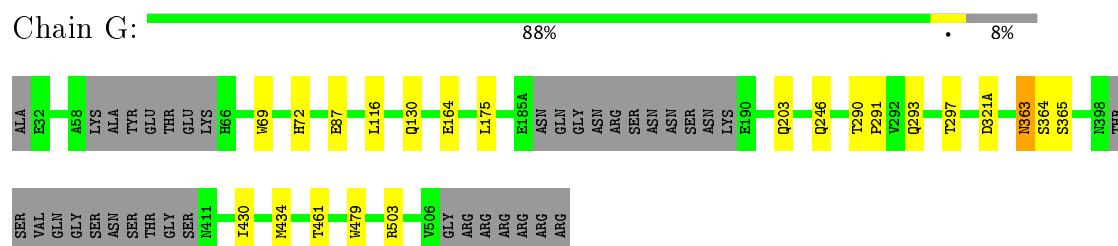
- Molecule 1: gp120



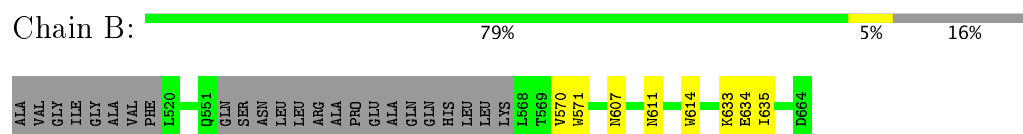
- Molecule 1: gp120



- Molecule 1: gp120



- Molecule 2: gp41



- Molecule 2: gp41

ALA	VAL	ILE	GLY	VAL	PHE	L520	Q551	GIN	SER	ASN	LEU	LEU	ARG	PRO	GLU	ALA	GIN	GIN	HIS	LEU	LEU	LYS	L568	T569	V570	W571	M607	M611	W614	K633	E634	I635	D664
-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------

- | |
|-------|
| ALA |
| VAl |
| Gly |
| Ile |
| Gly |
| AlA |
| VAl |
| PHE |
| L520 |
| M530 |
| Q55-1 |
| GLN |
| SER |
| ASN |
| LEU |
| LEU |
| ARG |
| ALA |
| PRO |
| GLU |
| ALA |
| GLN |
| GLN |
| HIS |
| LEU |
| LEU |
| LYS |
| T568 |
| T569 |
| V570 |
| W57-1 |
| N607 |
| N611 |
| W61-4 |
| W628 |
| K633 |
| E634 |
| I635 |
| D66-4 |

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|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | LEU | THR | SER | GLY | VAL | HIS | THR | PHE | PRO | ALA | LEU | GLN | SER | SER | GLY | LEU | TYR | SER | LEU | SER | SER | SER | VAL | VAL | THR | THR | VAL | PRO | SER | SER | SER | GLY | THR | GLN | THR | THR | CYS | ASN | VAL | VAL | ASN | HIS | LYS | PRO | SER | SER | THR | THR | VAL | ASP | GLU | PHE | CYS | LEU | LEU | VAL | LYS | ASP | LYS | VAL | PRO | GLU | THR | SER | THR | TRP | ASN | SER | CYS |
| Q1 | R38 | Q56 | R61 | R71 | F91 | G106 | V111 | SER | SER | ALA | SER | THR | THR | LYS | GLY | PRO | SER | VAL | PHE | PRO | LEU | ALA | PRO | SER | SER | SER | LYS | THR | SER | GLY | GLY | THR | THR | ALA | LEU | GLY | CYS | LEU | VAL | VAL | LYS | ASP | THR | PHE | PRO | GLU | PRO | VAL | THR | SER | THR | TRP | ASN | SER | CYS | | | | | | | | | | | | | | |

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|----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Q1 | R38 | Q66 | P57 | R61 | R71 | F91 | G106 | V111 | SER | SER | ALA | SER | SER | THR | LYS | GLY | PRO | SER | SER | VAL | PHE | PRO | LEU | ALA | ALA | PRO | SER | SER | LYS | SER | THR | SER | GLY | GLY | THR | ALA | ALA | LEU | GLY | CYS | LEU | VAL | VAL | LYS | ASP | THR | PHE | PRO | PRO | VAL | THR | GLU | PRO | THR | SER | TRP | ASN |
|----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

Q1 **R38** **Q66** **R61** **R71** **F91** **G106** **V111**

SER SER ALA SER SER THR LYS GLY PRO SER VAL VAL PHE PRO LEU LEU ALA PRO SER SER SER SER THR SER GLY GLY CYS VAL LEU VAL ASP LN S TRR PHE PRO PRO VAL THR VAL SER SER ASN

D1	S7	P8	L11	T22	Y32	W35	I46	R65	R66	K67	G68	Q69	N72	Y91	D105	L106	LNS	ARG	THR	VAL	ALA	ALA	ALA	PRO	PRO	PRO	PRO	PRO	PRO	ASP	GLU	GLN	LEU	LEU	LNS	LNS	SER	GLY	THR	VAL	VAL	CYS	LEU	LEU	ASN	ASP	THR
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GLY
LEU
SER
SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

- Chain T:  41% 7% 52%

Tyr	Pro	Arg	Glu	Ala	Lys	Val	Gln	Trp	Lys	Val	Asn	Leu	Ser	Gly	Asn	Ser	Glu	Glu	Ser	Val	Thr	Glu	Glu	Asp	Ser	Lys	Asp	Ser	Thr	Ser	Ser	Ser	Thr	Thr	Leu	Leu	Lys	His	Lys	Val	Val	Val	Thr	His
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY
LEU
SER
SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

- Chain U: 41% 7% 52%

Tyr	Pro	Arg	Glu	Ala	Lys	Val	Gln	Trp	Lys	Val	Asn	Leu	Ala	Gln	Ser	Gly	Asn	Ser	Glu	Glu	Ser	Thr	Lys	Asp	Ser	Thr	Ser	Ser	Thr	Thr	Leu	Leu	Ser	Lys	Lys	Lys	Val	Val	Val	Val	His	His
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GLY
LEU
SER
SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	22625	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	0.84	0/3565	0.82	0/4842
1	F	0.84	0/3565	0.82	0/4842
1	G	0.84	0/3565	0.82	0/4842
2	B	0.88	0/1041	0.80	0/1412
2	I	0.87	0/1041	0.80	0/1412
2	J	0.88	0/1041	0.80	0/1412
3	H	0.81	0/1017	0.88	3/1386 (0.2%)
3	R	0.81	0/1017	0.88	2/1386 (0.1%)
3	S	0.81	0/1017	0.88	2/1386 (0.1%)
4	L	0.77	0/800	0.88	1/1086 (0.1%)
4	T	0.77	0/800	0.88	1/1086 (0.1%)
4	U	0.77	0/800	0.88	1/1086 (0.1%)
All	All	0.83	0/19269	0.84	10/26178 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	38	ARG	NE-CZ-NH2	-8.48	116.06	120.30
3	H	38	ARG	NE-CZ-NH2	-8.41	116.09	120.30
3	R	38	ARG	NE-CZ-NH2	-8.39	116.10	120.30
4	U	91	TYR	CB-CG-CD2	-6.80	116.92	121.00
4	L	91	TYR	CB-CG-CD2	-6.77	116.94	121.00
4	T	91	TYR	CB-CG-CD2	-6.76	116.94	121.00
3	S	38	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	R	38	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	H	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	H	91	PHE	CB-CG-CD1	5.03	124.32	120.80

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	3493	0	3420	51	0
1	F	3493	0	3420	49	0
1	G	3493	0	3420	49	0
2	B	1024	0	1005	10	0
2	I	1024	0	1005	10	0
2	J	1024	0	1005	11	0
3	H	985	0	919	4	0
3	R	985	0	919	5	0
3	S	985	0	919	4	0
4	L	783	0	763	13	0
4	T	783	0	763	13	0
4	U	783	0	763	13	0
5	A	406	0	360	41	0
5	B	28	0	26	6	0
5	F	406	0	360	41	0
5	G	406	0	360	40	0
5	I	28	0	26	6	0
5	J	28	0	26	6	0
5	L	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
6	A	55	0	43	0	0
6	F	55	0	43	0	0
6	G	55	0	43	0	0
7	A	143	0	124	0	0
7	F	143	0	124	0	0
7	G	143	0	124	0	0
All	All	20835	0	20055	238	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 6.

All (238) 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:F:130:GLN:HG2	5:F:607:NAG:C8	1.79	1.12
1:A:130:GLN:HG2	5:A:607:NAG:C8	1.79	1.11
1:G:130:GLN:HG2	5:G:607:NAG:C8	1.79	1.11
1:A:130:GLN:HG2	5:A:607:NAG:H81	1.05	1.04
1:F:130:GLN:CG	5:F:607:NAG:H81	1.88	1.04
1:F:87:GLU:OE1	5:F:601:NAG:H81	1.59	1.03
1:A:130:GLN:CG	5:A:607:NAG:H81	1.88	1.03
1:G:87:GLU:OE1	5:G:601:NAG:H81	1.59	1.03
1:F:130:GLN:HG2	5:F:607:NAG:H81	1.04	1.02
1:A:87:GLU:OE1	5:A:601:NAG:H81	1.59	1.02
1:G:130:GLN:CG	5:G:607:NAG:H81	1.89	1.02
1:G:130:GLN:HG2	5:G:607:NAG:H81	1.05	1.01
1:A:293:GLN:HE22	5:A:627:NAG:H3	1.26	1.00
1:F:293:GLN:HE22	5:F:627:NAG:H3	1.26	0.99
1:G:293:GLN:HE22	5:G:627:NAG:H3	1.26	0.98
1:A:293:GLN:CD	5:A:627:NAG:HN2	1.67	0.97
1:F:130:GLN:CG	5:F:607:NAG:C8	2.43	0.97
1:G:293:GLN:CD	5:G:627:NAG:HN2	1.67	0.97
1:A:130:GLN:CG	5:A:607:NAG:C8	2.43	0.96
1:F:293:GLN:CD	5:F:627:NAG:HN2	1.68	0.96
1:G:130:GLN:CG	5:G:607:NAG:C8	2.43	0.94
4:T:66:ARG:O	4:T:67:TRP:CD1	2.21	0.93
4:L:66:ARG:O	4:L:67:TRP:CD1	2.21	0.93
4:T:66:ARG:O	4:T:67:TRP:HD1	1.51	0.93
4:U:66:ARG:O	4:U:67:TRP:HD1	1.51	0.93
4:U:66:ARG:O	4:U:67:TRP:CD1	2.21	0.92
4:L:66:ARG:O	4:L:67:TRP:HD1	1.51	0.92
5:G:646:NAG:H61	5:G:647:NAG:HN2	1.43	0.83
2:I:633:LYS:O	5:I:702:NAG:H82	1.79	0.83
5:F:646:NAG:H61	5:F:647:NAG:HN2	1.43	0.83
2:J:633:LYS:O	5:J:702:NAG:H82	1.79	0.82
2:B:633:LYS:O	5:B:702:NAG:H82	1.79	0.82
5:A:646:NAG:H61	5:A:647:NAG:HN2	1.43	0.82
1:F:130:GLN:HG3	5:F:607:NAG:H83	1.65	0.79
1:G:130:GLN:HG3	5:G:607:NAG:H83	1.65	0.79
1:A:130:GLN:HG3	5:A:607:NAG:H83	1.65	0.78
1:G:321(A):ASP:CG	5:G:605:NAG:H83	2.05	0.77
1:A:321(A):ASP:CG	5:A:605:NAG:H83	2.05	0.77
1:F:321(A):ASP:CG	5:F:605:NAG:H83	2.05	0.76
1:F:130:GLN:CG	5:F:607:NAG:H83	2.19	0.73
1:A:293:GLN:NE2	5:A:627:NAG:H3	2.04	0.72
3:S:111:VAL:HG12	3:S:111:VAL:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:GLN:CG	5:G:607:NAG:H83	2.19	0.72
3:H:111:VAL:O	3:H:111:VAL:HG12	1.90	0.72
3:R:111:VAL:HG12	3:R:111:VAL:O	1.90	0.71
1:A:130:GLN:CG	5:A:607:NAG:H83	2.19	0.71
1:F:293:GLN:NE2	5:F:627:NAG:H3	2.04	0.71
1:G:293:GLN:NE2	5:G:627:NAG:H3	2.04	0.70
1:F:203:GLN:OE1	1:F:434:MET:CE	2.40	0.69
1:G:203:GLN:OE1	1:G:434:MET:CE	2.40	0.69
1:A:293:GLN:NE2	5:A:627:NAG:HN2	1.91	0.69
1:A:203:GLN:OE1	1:A:434:MET:CE	2.41	0.68
5:A:619:NAG:H4	4:L:32:TYR:OH	1.94	0.68
5:G:619:NAG:H4	4:U:32:TYR:OH	1.94	0.68
1:F:293:GLN:NE2	5:F:627:NAG:HN2	1.92	0.67
5:F:619:NAG:H4	4:T:32:TYR:OH	1.94	0.67
1:F:363:ASN:OD1	1:F:364:SER:O	2.12	0.67
1:G:293:GLN:NE2	5:G:627:NAG:HN2	1.91	0.67
1:A:363:ASN:OD1	1:A:364:SER:O	2.12	0.67
1:G:363:ASN:OD1	1:G:364:SER:O	2.12	0.66
5:F:620:NAG:O7	4:T:66:ARG:NH1	2.30	0.65
1:G:293:GLN:HE22	5:G:627:NAG:C3	2.06	0.65
5:G:620:NAG:O7	4:U:66:ARG:NH1	2.30	0.65
1:G:203:GLN:OE1	1:G:434:MET:HE3	1.97	0.65
5:A:619:NAG:H4	4:L:32:TYR:CZ	2.33	0.64
5:F:619:NAG:H4	4:T:32:TYR:CZ	2.33	0.64
5:A:620:NAG:O7	4:L:66:ARG:NH1	2.30	0.64
5:G:619:NAG:H4	4:U:32:TYR:CZ	2.33	0.63
1:F:72:HIS:CD2	1:F:72:HIS:N	2.67	0.62
1:A:293:GLN:HE22	5:A:627:NAG:C3	2.06	0.62
1:F:293:GLN:HE22	5:F:627:NAG:C3	2.06	0.62
1:F:293:GLN:NE2	5:F:627:NAG:N2	2.48	0.62
1:A:72:HIS:N	1:A:72:HIS:CD2	2.67	0.61
1:A:293:GLN:NE2	5:A:627:NAG:N2	2.48	0.61
1:G:321(A):ASP:OD1	5:G:605:NAG:H82	2.01	0.61
4:L:65:ARG:NH2	4:L:67:TRP:HZ2	1.99	0.61
1:G:293:GLN:NE2	5:G:627:NAG:N2	2.48	0.61
1:F:321(A):ASP:OD1	5:F:605:NAG:H82	2.01	0.60
1:G:321(A):ASP:OD1	5:G:605:NAG:C8	2.50	0.60
1:F:203:GLN:OE1	1:F:434:MET:HE3	2.00	0.60
1:A:321(A):ASP:OD1	5:A:605:NAG:H82	2.01	0.60
1:F:321(A):ASP:OD1	5:F:605:NAG:C8	2.50	0.60
4:U:65:ARG:NH2	4:U:67:TRP:CZ2	2.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:65:ARG:NH2	4:U:67:TRP:HZ2	1.99	0.60
4:T:65:ARG:NH2	4:T:67:TRP:HZ2	1.99	0.59
1:A:203:GLN:OE1	1:A:434:MET:HE2	2.02	0.59
4:T:65:ARG:NH2	4:T:67:TRP:CZ2	2.70	0.59
1:G:72:HIS:N	1:G:72:HIS:CD2	2.67	0.59
1:A:293:GLN:HB3	5:A:627:NAG:C8	2.33	0.59
1:A:321(A):ASP:OD1	5:A:605:NAG:C8	2.50	0.59
1:A:175:LEU:HD21	5:A:605:NAG:H82	1.85	0.59
1:G:175:LEU:HD21	5:G:605:NAG:H82	1.85	0.59
1:G:293:GLN:HB3	5:G:627:NAG:C8	2.33	0.58
1:F:293:GLN:HB3	5:F:627:NAG:C8	2.33	0.58
1:G:293:GLN:NE2	5:G:627:NAG:C2	2.66	0.58
4:L:65:ARG:NH2	4:L:67:TRP:CZ2	2.70	0.58
1:F:203:GLN:OE1	1:F:434:MET:HE2	2.04	0.58
1:A:293:GLN:NE2	5:A:627:NAG:C2	2.66	0.58
1:F:175:LEU:HD21	5:F:605:NAG:H82	1.85	0.58
1:F:293:GLN:NE2	5:F:627:NAG:C2	2.66	0.58
4:L:69:GLN:N	4:L:69:GLN:OE1	2.31	0.57
4:U:69:GLN:N	4:U:69:GLN:OE1	2.31	0.57
2:B:633:LYS:O	5:B:702:NAG:C8	2.53	0.57
2:J:634:GLU:O	5:J:702:NAG:H81	2.05	0.57
1:G:461:THR:OG1	3:S:61:ARG:NH2	2.38	0.57
1:A:203:GLN:OE1	1:A:434:MET:HE3	2.02	0.56
2:I:634:GLU:O	5:I:702:NAG:H81	2.05	0.56
1:F:461:THR:OG1	3:R:61:ARG:NH2	2.38	0.56
1:A:461:THR:OG1	3:H:61:ARG:NH2	2.38	0.56
2:J:634:GLU:HA	5:J:702:NAG:H81	1.87	0.56
2:J:633:LYS:O	5:J:702:NAG:C8	2.53	0.56
2:I:634:GLU:HA	5:I:702:NAG:H81	1.87	0.56
2:B:634:GLU:O	5:B:702:NAG:H81	2.05	0.56
1:F:297:THR:CG2	5:F:632:NAG:H83	2.36	0.56
1:F:293:GLN:NE2	5:F:627:NAG:C1	2.69	0.56
1:G:293:GLN:NE2	5:G:627:NAG:C1	2.69	0.56
2:B:634:GLU:HA	5:B:702:NAG:H81	1.87	0.55
1:A:293:GLN:NE2	5:A:627:NAG:C1	2.69	0.55
1:G:297:THR:CG2	5:G:631:NAG:H83	2.36	0.55
1:G:203:GLN:OE1	1:G:434:MET:HE2	2.07	0.55
2:I:633:LYS:O	5:I:702:NAG:C8	2.53	0.55
1:A:297:THR:CG2	5:A:631:NAG:H83	2.36	0.54
1:F:87:GLU:CD	5:F:601:NAG:H81	2.27	0.54
4:T:69:GLN:N	4:T:69:GLN:OE1	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:GLN:HB3	5:F:627:NAG:H82	1.90	0.54
1:A:321(A):ASP:CG	5:A:605:NAG:C8	2.75	0.54
1:G:293:GLN:HB3	5:G:627:NAG:H82	1.90	0.54
1:G:87:GLU:CD	5:G:601:NAG:H81	2.27	0.54
1:F:321(A):ASP:CG	5:F:605:NAG:C8	2.75	0.54
1:A:87:GLU:CD	5:A:601:NAG:H81	2.27	0.53
2:I:611:ASN:ND2	5:I:701:NAG:O7	2.42	0.53
1:A:293:GLN:HB3	5:A:627:NAG:H82	1.90	0.53
1:G:321(A):ASP:CG	5:G:605:NAG:C8	2.75	0.53
1:G:297:THR:CG2	5:G:631:NAG:C8	2.87	0.52
2:B:611:ASN:ND2	5:B:701:NAG:O7	2.42	0.52
4:L:7:SER:N	4:L:8:PRO:CD	2.73	0.52
2:J:611:ASN:ND2	5:J:701:NAG:O7	2.42	0.52
2:I:634:GLU:HA	5:I:702:NAG:C8	2.40	0.52
2:J:634:GLU:HA	5:J:702:NAG:C8	2.40	0.52
1:A:297:THR:CG2	5:A:631:NAG:C8	2.87	0.52
4:T:7:SER:N	4:T:8:PRO:CD	2.73	0.52
1:F:297:THR:CG2	5:F:632:NAG:C8	2.88	0.51
4:U:7:SER:N	4:U:8:PRO:CD	2.73	0.51
2:B:634:GLU:HA	5:B:702:NAG:C8	2.40	0.51
5:A:602:NAG:H3	5:A:602:NAG:H83	1.92	0.51
5:F:602:NAG:H3	5:F:602:NAG:H83	1.92	0.50
1:F:365:SER:OG	3:R:56:GLN:NE2	2.44	0.50
1:G:365:SER:OG	3:S:56:GLN:NE2	2.44	0.50
1:A:297:THR:HG22	5:A:631:NAG:H82	1.94	0.50
1:F:246:GLN:N	1:F:246:GLN:OE1	2.36	0.50
5:G:602:NAG:H3	5:G:602:NAG:H83	1.92	0.50
1:A:365:SER:OG	3:H:56:GLN:NE2	2.44	0.49
1:A:293:GLN:NE2	5:A:627:NAG:C3	2.71	0.49
1:F:297:THR:HG22	5:F:632:NAG:H82	1.94	0.49
1:G:164:GLU:OE1	1:G:164:GLU:N	2.36	0.48
1:G:297:THR:HG22	5:G:631:NAG:C8	2.43	0.48
1:G:297:THR:HG22	5:G:631:NAG:H82	1.94	0.48
1:F:293:GLN:CD	5:F:627:NAG:N2	2.51	0.48
1:F:293:GLN:NE2	5:F:627:NAG:C3	2.71	0.48
1:G:246:GLN:N	1:G:246:GLN:OE1	2.36	0.48
1:F:297:THR:HG22	5:F:632:NAG:C8	2.43	0.47
1:A:293:GLN:CD	5:A:627:NAG:N2	2.51	0.47
1:A:479:TRP:HA	1:A:479:TRP:CE3	2.49	0.47
1:F:164:GLU:OE1	1:F:164:GLU:N	2.36	0.47
1:G:479:TRP:HA	1:G:479:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:GLN:NE2	5:G:627:NAG:C3	2.71	0.47
1:F:479:TRP:HE3	1:F:479:TRP:HA	1.80	0.47
1:G:479:TRP:HA	1:G:479:TRP:HE3	1.80	0.47
2:I:635:ILE:HG13	2:I:635:ILE:O	2.15	0.47
2:J:635:ILE:HG13	2:J:635:ILE:O	2.15	0.47
1:A:297:THR:HG22	5:A:631:NAG:C8	2.43	0.46
1:F:479:TRP:CE3	1:F:479:TRP:HA	2.49	0.46
1:A:479:TRP:HA	1:A:479:TRP:HE3	1.80	0.46
1:A:321(A):ASP:OD2	5:A:605:NAG:H83	2.16	0.46
2:B:635:ILE:HG13	2:B:635:ILE:O	2.15	0.46
1:A:246:GLN:N	1:A:246:GLN:OE1	2.36	0.46
1:A:293:GLN:HB3	5:A:627:NAG:H83	1.98	0.45
1:G:293:GLN:HB3	5:G:627:NAG:H83	1.98	0.45
1:A:297:THR:HG21	5:A:631:NAG:H83	1.97	0.45
4:L:11:LEU:O	4:L:105:ASP:N	2.50	0.45
1:G:321(A):ASP:OD2	5:G:605:NAG:H83	2.16	0.45
5:F:635:NAG:H2	5:F:641:NAG:H5	1.99	0.45
1:G:297:THR:HG21	5:G:631:NAG:H83	1.97	0.45
4:T:11:LEU:O	4:T:105:ASP:N	2.50	0.45
5:A:629:NAG:H61	5:A:630:NAG:N2	2.32	0.45
1:F:297:THR:HG21	5:F:632:NAG:H83	1.97	0.45
1:F:363:ASN:OD1	1:F:363:ASN:C	2.55	0.45
5:G:629:NAG:H61	5:G:630:NAG:N2	2.32	0.45
1:F:293:GLN:HB3	5:F:627:NAG:H83	1.98	0.44
5:G:646:NAG:H61	5:G:647:NAG:N2	2.22	0.44
4:L:22:THR:HG22	4:L:72:ASN:OD1	2.17	0.44
5:A:635:NAG:H2	5:A:641:NAG:H5	1.99	0.44
4:T:22:THR:HG22	4:T:72:ASN:OD1	2.17	0.44
5:F:629:NAG:H61	5:F:630:NAG:N2	2.32	0.44
3:H:91:PHE:HB3	3:H:106:GLY:HA2	1.99	0.44
1:F:321(A):ASP:OD2	5:F:605:NAG:H83	2.16	0.44
5:A:646:NAG:H61	5:A:647:NAG:N2	2.22	0.44
1:G:363:ASN:C	1:G:363:ASN:OD1	2.56	0.44
4:U:22:THR:HG22	4:U:72:ASN:OD1	2.17	0.43
5:G:635:NAG:H2	5:G:641:NAG:H5	1.99	0.43
3:R:91:PHE:HB3	3:R:106:GLY:HA2	1.99	0.43
4:U:11:LEU:O	4:U:105:ASP:N	2.50	0.43
1:A:363:ASN:OD1	1:A:363:ASN:C	2.56	0.43
2:B:614:TRP:CD1	2:B:614:TRP:N	2.85	0.43
3:S:91:PHE:HB3	3:S:106:GLY:HA2	1.99	0.43
2:I:614:TRP:CD1	2:I:614:TRP:N	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:614:TRP:N	2:J:614:TRP:CD1	2.85	0.42
1:F:290:THR:HB	1:F:291:PRO:HD2	2.02	0.42
1:G:290:THR:HB	1:G:291:PRO:HD2	2.02	0.42
1:F:479:TRP:CE3	1:F:479:TRP:CA	3.03	0.42
1:A:290:THR:HB	1:A:291:PRO:HD2	2.02	0.42
1:A:164:GLU:OE1	1:A:164:GLU:N	2.36	0.42
1:F:430:ILE:C	1:F:430:ILE:HD12	2.41	0.41
5:F:620:NAG:H81	4:T:66:ARG:CZ	2.50	0.41
1:F:503:ARG:HB3	2:I:607:ASN:HB2	2.02	0.41
1:A:69:TRP:CE3	1:A:69:TRP:HA	2.56	0.41
1:G:116:LEU:HD11	1:G:434:MET:SD	2.60	0.41
5:G:620:NAG:H81	4:U:66:ARG:CZ	2.50	0.41
1:A:116:LEU:HD11	1:A:434:MET:SD	2.60	0.41
1:A:479:TRP:CA	1:A:479:TRP:CE3	3.03	0.41
1:F:116:LEU:HD11	1:F:434:MET:SD	2.60	0.41
5:A:620:NAG:H81	4:L:66:ARG:CZ	2.50	0.41
1:G:479:TRP:CA	1:G:479:TRP:CE3	3.03	0.41
1:G:503:ARG:HB3	2:J:607:ASN:HB2	2.02	0.41
4:L:35:TRP:HB2	4:L:48:ILE:HG22	2.03	0.41
1:A:430:ILE:C	1:A:430:ILE:HD12	2.41	0.41
2:B:570:VAL:O	2:B:571:TRP:HB2	2.21	0.41
1:G:430:ILE:C	1:G:430:ILE:HD12	2.41	0.41
2:I:570:VAL:O	2:I:571:TRP:HB2	2.21	0.41
1:A:213:ILE:O	1:A:213:ILE:HG23	2.21	0.41
4:T:35:TRP:HB2	4:T:48:ILE:HG22	2.03	0.41
1:A:503:ARG:HB3	2:B:607:ASN:HB2	2.02	0.40
2:J:530:MET:HG2	2:J:628:TRP:HA	2.04	0.40
2:J:570:VAL:O	2:J:571:TRP:HB2	2.21	0.40
5:F:646:NAG:H61	5:F:647:NAG:N2	2.22	0.40
4:U:35:TRP:HB2	4:U:48:ILE:HG22	2.03	0.40
1:G:69:TRP:CE3	1:G:69:TRP:HA	2.56	0.40
3:R:56:GLN:HA	3:R:57:PRO:HD2	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	F	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	G	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
2	B	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
2	I	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
2	J	125/153 (82%)	122 (98%)	3 (2%)	0	100	100
3	H	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	R	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	S	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
4	L	96/206 (47%)	91 (95%)	5 (5%)	0	100	100
4	T	96/206 (47%)	91 (95%)	5 (5%)	0	100	100
4	U	96/206 (47%)	91 (95%)	5 (5%)	0	100	100
All	All	2328/3198 (73%)	2273 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	397/428 (93%)	396 (100%)	1 (0%)	94	96
1	F	397/428 (93%)	396 (100%)	1 (0%)	94	96
1	G	397/428 (93%)	396 (100%)	1 (0%)	94	96
2	B	111/129 (86%)	111 (100%)	0	100	100
2	I	111/129 (86%)	111 (100%)	0	100	100
2	J	111/129 (86%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	102/193 (53%)	101 (99%)	1 (1%)	80	90
3	R	102/193 (53%)	101 (99%)	1 (1%)	80	90
3	S	102/193 (53%)	101 (99%)	1 (1%)	80	90
4	L	86/183 (47%)	86 (100%)	0	100	100
4	T	86/183 (47%)	86 (100%)	0	100	100
4	U	86/183 (47%)	86 (100%)	0	100	100
All	All	2088/2799 (75%)	2082 (100%)	6 (0%)	94	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
3	H	71	ARG
1	F	363	ASN
3	R	71	ARG
1	G	363	ASN
3	S	71	ARG

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	293	GLN
1	F	293	GLN
1	G	293	GLN

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 ⓘ

153 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	0.80	1 (7%)	15,19,21	0.93	1 (6%)
5	NAG	A	602	5,6	14,14,15	0.44	0	15,19,21	1.56	3 (20%)
6	BMA	A	603	5	11,11,12	1.19	2 (18%)	13,15,17	1.57	2 (15%)
5	NAG	A	604	1	14,14,15	0.40	0	15,19,21	0.70	1 (6%)
5	NAG	A	605	1,5	14,14,15	0.25	0	15,19,21	0.62	0
5	NAG	A	606	5	14,14,15	0.30	0	15,19,21	0.69	1 (6%)
5	NAG	A	607	1,5	14,14,15	0.41	0	15,19,21	0.49	0
5	NAG	A	608	5	14,14,15	0.29	0	15,19,21	0.57	0
5	NAG	A	609	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	A	610	5	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
5	NAG	A	611	1	14,14,15	0.50	0	15,19,21	0.54	0
5	NAG	A	612	1,5	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	A	613	5,6	14,14,15	0.49	0	15,19,21	1.19	2 (13%)
6	BMA	A	614	5,7	11,11,12	0.66	0	13,15,17	1.51	3 (23%)
7	MAN	A	615	7,6	11,11,12	0.57	0	13,15,17	1.61	3 (23%)
7	MAN	A	616	7	11,11,12	0.59	0	13,15,17	2.58	5 (38%)
7	MAN	A	617	7,6	11,11,12	0.59	0	13,15,17	2.59	3 (23%)
7	MAN	A	618	7	11,11,12	0.56	0	13,15,17	2.04	5 (38%)
5	NAG	A	619	1,5	14,14,15	0.77	1 (7%)	15,19,21	0.71	0
5	NAG	A	620	5,6	14,14,15	0.40	0	15,19,21	0.53	0
6	BMA	A	621	5,7	11,11,12	1.68	3 (27%)	13,15,17	1.90	2 (15%)
7	MAN	A	622	7,6	11,11,12	1.63	3 (27%)	13,15,17	1.38	2 (15%)
7	MAN	A	623	7	11,11,12	2.31	4 (36%)	13,15,17	1.97	5 (38%)
7	MAN	A	624	7,6	11,11,12	0.60	0	13,15,17	2.59	3 (23%)
7	MAN	A	625	7	11,11,12	0.58	0	13,15,17	2.04	5 (38%)
7	MAN	A	626	7	11,11,12	0.61	0	13,15,17	2.40	6 (46%)
5	NAG	A	627	1,5	14,14,15	0.31	0	15,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	628	5	14,14,15	0.65	0	15,19,21	0.57	0
5	NAG	A	629	1,5	14,14,15	0.42	0	15,19,21	0.48	0
5	NAG	A	630	5	14,14,15	0.60	0	15,19,21	0.60	0
5	NAG	A	631	1,5	14,14,15	0.41	0	15,19,21	0.83	1 (6%)
5	NAG	A	632	5	14,14,15	0.53	0	15,19,21	0.55	0
5	NAG	A	633	1	14,14,15	0.31	0	15,19,21	0.45	0
5	NAG	A	634	1	14,14,15	0.49	0	15,19,21	0.44	0
5	NAG	A	635	1,5	14,14,15	0.32	0	15,19,21	0.64	0
5	NAG	A	636	5,6	14,14,15	0.34	0	15,19,21	0.88	1 (6%)
6	BMA	A	637	5,7	11,11,12	0.65	0	13,15,17	1.52	3 (23%)
7	MAN	A	638	6	11,11,12	0.54	0	13,15,17	1.58	3 (23%)
7	MAN	A	639	7,6	11,11,12	0.61	0	13,15,17	2.57	3 (23%)
7	MAN	A	640	7	11,11,12	0.55	0	13,15,17	2.06	5 (38%)
5	NAG	A	641	1,5	14,14,15	0.98	1 (7%)	15,19,21	1.13	1 (6%)
5	NAG	A	642	5,6	14,14,15	0.48	0	15,19,21	0.63	0
6	BMA	A	643	5,7	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
7	MAN	A	644	6	11,11,12	0.60	0	13,15,17	2.59	3 (23%)
5	NAG	A	645	1	14,14,15	0.45	0	15,19,21	0.61	0
5	NAG	A	646	1,5	14,14,15	0.51	0	15,19,21	0.61	0
5	NAG	A	647	5	14,14,15	0.37	0	15,19,21	0.45	0
5	NAG	B	701	2	14,14,15	0.33	0	15,19,21	0.64	0
5	NAG	B	702	2	14,14,15	0.51	0	15,19,21	0.56	0
5	NAG	F	601	1,5	14,14,15	0.81	1 (7%)	15,19,21	0.94	1 (6%)
5	NAG	F	602	5,6	14,14,15	0.43	0	15,19,21	1.56	3 (20%)
6	BMA	F	603	5	11,11,12	1.20	2 (18%)	13,15,17	1.57	2 (15%)
5	NAG	F	604	1	14,14,15	0.40	0	15,19,21	0.70	1 (6%)
5	NAG	F	605	1,5	14,14,15	0.26	0	15,19,21	0.62	0
5	NAG	F	606	5	14,14,15	0.30	0	15,19,21	0.69	1 (6%)
5	NAG	F	607	1,5	14,14,15	0.42	0	15,19,21	0.50	0
5	NAG	F	608	5	14,14,15	0.28	0	15,19,21	0.57	0
5	NAG	F	609	1,5	14,14,15	0.48	0	15,19,21	2.60	3 (20%)
5	NAG	F	610	5	14,14,15	0.51	0	15,19,21	1.20	2 (13%)
5	NAG	F	611	1	14,14,15	0.50	0	15,19,21	0.54	0
5	NAG	F	612	1,5	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	F	613	5,6	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
6	BMA	F	614	5,7	11,11,12	0.66	0	13,15,17	1.52	3 (23%)
7	MAN	F	615	7,6	11,11,12	0.58	0	13,15,17	1.60	3 (23%)
7	MAN	F	616	7	11,11,12	0.59	0	13,15,17	2.58	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	F	617	7,6	11,11,12	0.59	0	13,15,17	2.60	3 (23%)
7	MAN	F	618	7	11,11,12	0.57	0	13,15,17	2.04	5 (38%)
5	NAG	F	619	1,5	14,14,15	0.77	1 (7%)	15,19,21	0.71	0
5	NAG	F	620	5,6	14,14,15	0.40	0	15,19,21	0.53	0
6	BMA	F	621	5,7	11,11,12	1.68	3 (27%)	13,15,17	1.90	2 (15%)
7	MAN	F	622	7,6	11,11,12	1.63	3 (27%)	13,15,17	1.39	2 (15%)
7	MAN	F	623	7	11,11,12	2.31	4 (36%)	13,15,17	1.98	5 (38%)
7	MAN	F	624	7,6	11,11,12	0.59	0	13,15,17	2.59	3 (23%)
7	MAN	F	625	7	11,11,12	0.58	0	13,15,17	2.04	5 (38%)
7	MAN	F	626	7	11,11,12	0.61	0	13,15,17	2.40	6 (46%)
5	NAG	F	627	1,5	14,14,15	0.30	0	15,19,21	0.78	0
5	NAG	F	628	5	14,14,15	0.66	0	15,19,21	0.57	0
5	NAG	F	629	1,5	14,14,15	0.43	0	15,19,21	0.49	0
5	NAG	F	630	5	14,14,15	0.61	0	15,19,21	0.61	0
5	NAG	F	631	1	14,14,15	0.49	0	15,19,21	0.43	0
5	NAG	F	632	1,5	14,14,15	0.41	0	15,19,21	0.82	1 (6%)
5	NAG	F	633	5	14,14,15	0.55	0	15,19,21	0.55	0
5	NAG	F	634	1	14,14,15	0.31	0	15,19,21	0.45	0
5	NAG	F	635	1,5	14,14,15	0.32	0	15,19,21	0.64	0
5	NAG	F	636	5,6	14,14,15	0.33	0	15,19,21	0.87	1 (6%)
6	BMA	F	637	5,7	11,11,12	0.65	0	13,15,17	1.53	3 (23%)
7	MAN	F	638	6	11,11,12	0.54	0	13,15,17	1.59	3 (23%)
7	MAN	F	639	7,6	11,11,12	0.62	0	13,15,17	2.57	3 (23%)
7	MAN	F	640	7	11,11,12	0.54	0	13,15,17	2.06	5 (38%)
5	NAG	F	641	1,5	14,14,15	0.98	1 (7%)	15,19,21	1.13	1 (6%)
5	NAG	F	642	5,6	14,14,15	0.47	0	15,19,21	0.63	0
6	BMA	F	643	5,7	11,11,12	0.63	0	13,15,17	1.50	3 (23%)
7	MAN	F	644	6	11,11,12	0.60	0	13,15,17	2.58	3 (23%)
5	NAG	F	645	1	14,14,15	0.46	0	15,19,21	0.60	0
5	NAG	F	646	1,5	14,14,15	0.50	0	15,19,21	0.61	0
5	NAG	F	647	5	14,14,15	0.38	0	15,19,21	0.45	0
5	NAG	G	601	1,5	14,14,15	0.81	1 (7%)	15,19,21	0.93	1 (6%)
5	NAG	G	602	5,6	14,14,15	0.44	0	15,19,21	1.55	3 (20%)
6	BMA	G	603	5	11,11,12	1.19	2 (18%)	13,15,17	1.57	2 (15%)
5	NAG	G	604	1	14,14,15	0.41	0	15,19,21	0.70	1 (6%)
5	NAG	G	605	1,5	14,14,15	0.25	0	15,19,21	0.63	0
5	NAG	G	606	5	14,14,15	0.30	0	15,19,21	0.68	0
5	NAG	G	607	1,5	14,14,15	0.41	0	15,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	608	5	14,14,15	0.28	0	15,19,21	0.57	0
5	NAG	G	609	1,5	14,14,15	0.49	0	15,19,21	2.60	3 (20%)
5	NAG	G	610	5	14,14,15	0.51	0	15,19,21	1.19	2 (13%)
5	NAG	G	611	1	14,14,15	0.51	0	15,19,21	0.54	0
5	NAG	G	612	1,5	14,14,15	0.50	0	15,19,21	2.60	3 (20%)
5	NAG	G	613	5,6	14,14,15	0.48	0	15,19,21	1.19	2 (13%)
6	BMA	G	614	5,7	11,11,12	0.65	0	13,15,17	1.51	3 (23%)
7	MAN	G	615	7,6	11,11,12	0.57	0	13,15,17	1.61	3 (23%)
7	MAN	G	616	7	11,11,12	0.60	0	13,15,17	2.57	5 (38%)
7	MAN	G	617	7,6	11,11,12	0.59	0	13,15,17	2.59	3 (23%)
7	MAN	G	618	7	11,11,12	0.55	0	13,15,17	2.04	5 (38%)
5	NAG	G	619	1,5	14,14,15	0.78	1 (7%)	15,19,21	0.72	0
5	NAG	G	620	5,6	14,14,15	0.40	0	15,19,21	0.53	0
6	BMA	G	621	5,7	11,11,12	1.67	3 (27%)	13,15,17	1.89	2 (15%)
7	MAN	G	622	7,6	11,11,12	1.63	3 (27%)	13,15,17	1.38	2 (15%)
7	MAN	G	623	7	11,11,12	2.31	4 (36%)	13,15,17	1.98	5 (38%)
7	MAN	G	624	7,6	11,11,12	0.61	0	13,15,17	2.59	3 (23%)
7	MAN	G	625	7	11,11,12	0.58	0	13,15,17	2.05	5 (38%)
7	MAN	G	626	7	11,11,12	0.61	0	13,15,17	2.40	6 (46%)
5	NAG	G	627	1,5	14,14,15	0.31	0	15,19,21	0.77	0
5	NAG	G	628	5	14,14,15	0.65	0	15,19,21	0.56	0
5	NAG	G	629	1,5	14,14,15	0.43	0	15,19,21	0.48	0
5	NAG	G	630	5	14,14,15	0.61	0	15,19,21	0.61	0
5	NAG	G	631	1,5	14,14,15	0.41	0	15,19,21	0.83	1 (6%)
5	NAG	G	632	5	14,14,15	0.55	0	15,19,21	0.55	0
5	NAG	G	633	1	14,14,15	0.32	0	15,19,21	0.45	0
5	NAG	G	634	1	14,14,15	0.48	0	15,19,21	0.44	0
5	NAG	G	635	1,5	14,14,15	0.32	0	15,19,21	0.64	0
5	NAG	G	636	5,6	14,14,15	0.34	0	15,19,21	0.88	1 (6%)
6	BMA	G	637	5,7	11,11,12	0.64	0	13,15,17	1.53	3 (23%)
7	MAN	G	638	6	11,11,12	0.54	0	13,15,17	1.58	3 (23%)
7	MAN	G	639	7,6	11,11,12	0.61	0	13,15,17	2.57	3 (23%)
7	MAN	G	640	7	11,11,12	0.56	0	13,15,17	2.05	5 (38%)
5	NAG	G	641	1,5	14,14,15	0.97	1 (7%)	15,19,21	1.14	1 (6%)
5	NAG	G	642	5,6	14,14,15	0.48	0	15,19,21	0.63	0
6	BMA	G	643	5,7	11,11,12	0.64	0	13,15,17	1.49	3 (23%)
7	MAN	G	644	6	11,11,12	0.62	0	13,15,17	2.59	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	645	1	14,14,15	0.46	0	15,19,21	0.61	0
5	NAG	G	646	1,5	14,14,15	0.51	0	15,19,21	0.60	0
5	NAG	G	647	5	14,14,15	0.38	0	15,19,21	0.45	0
5	NAG	I	701	2	14,14,15	0.33	0	15,19,21	0.64	0
5	NAG	I	702	2	14,14,15	0.51	0	15,19,21	0.56	0
5	NAG	J	701	2	14,14,15	0.33	0	15,19,21	0.63	0
5	NAG	J	702	2	14,14,15	0.51	0	15,19,21	0.56	0
5	NAG	L	301	5,4	14,14,15	0.49	0	15,19,21	2.61	3 (20%)
5	NAG	L	302	5	14,14,15	0.50	0	15,19,21	1.18	2 (13%)
5	NAG	T	301	5,4	14,14,15	0.48	0	15,19,21	2.61	3 (20%)
5	NAG	T	302	5	14,14,15	0.51	0	15,19,21	1.18	2 (13%)
5	NAG	U	301	5,4	14,14,15	0.49	0	15,19,21	2.62	3 (20%)
5	NAG	U	302	5	14,14,15	0.50	0	15,19,21	1.18	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
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	-	0/2/19/22	0/1/1/1
5	NAG	A	604	1	-	0/6/23/26	0/1/1/1
5	NAG	A	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	606	5	-	0/6/23/26	0/1/1/1
5	NAG	A	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	608	5	-	0/6/23/26	0/1/1/1
5	NAG	A	609	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	610	5	-	0/6/23/26	0/1/1/1
5	NAG	A	611	1	-	0/6/23/26	0/1/1/1
5	NAG	A	612	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	613	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	614	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	615	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	616	7	-	0/2/19/22	0/1/1/1
7	MAN	A	617	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	618	7	-	0/2/19/22	0/1/1/1
5	NAG	A	619	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	620	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	621	5,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	622	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	623	7	-	0/2/19/22	0/1/1/1
7	MAN	A	624	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	625	7	-	0/2/19/22	0/1/1/1
7	MAN	A	626	7	-	0/2/19/22	0/1/1/1
5	NAG	A	627	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	628	5	-	0/6/23/26	0/1/1/1
5	NAG	A	629	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	630	5	-	0/6/23/26	0/1/1/1
5	NAG	A	631	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	632	5	-	0/6/23/26	0/1/1/1
5	NAG	A	633	1	-	0/6/23/26	0/1/1/1
5	NAG	A	634	1	-	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	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	637	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	638	6	-	0/2/19/22	0/1/1/1
7	MAN	A	639	7,6	-	0/2/19/22	0/1/1/1
7	MAN	A	640	7	-	0/2/19/22	0/1/1/1
5	NAG	A	641	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	642	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	643	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	644	6	-	0/2/19/22	0/1/1/1
5	NAG	A	645	1	-	0/6/23/26	0/1/1/1
5	NAG	A	646	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	647	5	-	0/6/23/26	0/1/1/1
5	NAG	B	701	2	-	0/6/23/26	0/1/1/1
5	NAG	B	702	2	-	0/6/23/26	0/1/1/1
5	NAG	F	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	602	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	603	5	-	0/2/19/22	0/1/1/1
5	NAG	F	604	1	-	0/6/23/26	0/1/1/1
5	NAG	F	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	606	5	-	0/6/23/26	0/1/1/1
5	NAG	F	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	608	5	-	0/6/23/26	0/1/1/1
5	NAG	F	609	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	610	5	-	0/6/23/26	0/1/1/1
5	NAG	F	611	1	-	0/6/23/26	0/1/1/1
5	NAG	F	612	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	613	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	614	5,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	F	615	7,6	-	0/2/19/22	0/1/1/1
7	MAN	F	616	7	-	0/2/19/22	0/1/1/1
7	MAN	F	617	7,6	-	0/2/19/22	0/1/1/1
7	MAN	F	618	7	-	0/2/19/22	0/1/1/1
5	NAG	F	619	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	620	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	621	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	622	7,6	-	0/2/19/22	0/1/1/1
7	MAN	F	623	7	-	0/2/19/22	0/1/1/1
7	MAN	F	624	7,6	-	0/2/19/22	0/1/1/1
7	MAN	F	625	7	-	0/2/19/22	0/1/1/1
7	MAN	F	626	7	-	0/2/19/22	0/1/1/1
5	NAG	F	627	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	628	5	-	0/6/23/26	0/1/1/1
5	NAG	F	629	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	630	5	-	0/6/23/26	0/1/1/1
5	NAG	F	631	1	-	0/6/23/26	0/1/1/1
5	NAG	F	632	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	633	5	-	0/6/23/26	0/1/1/1
5	NAG	F	634	1	-	0/6/23/26	0/1/1/1
5	NAG	F	635	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	636	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	637	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	638	6	-	0/2/19/22	0/1/1/1
7	MAN	F	639	7,6	-	0/2/19/22	0/1/1/1
7	MAN	F	640	7	-	0/2/19/22	0/1/1/1
5	NAG	F	641	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	642	5,6	-	0/6/23/26	0/1/1/1
6	BMA	F	643	5,7	-	0/2/19/22	0/1/1/1
7	MAN	F	644	6	-	0/2/19/22	0/1/1/1
5	NAG	F	645	1	-	0/6/23/26	0/1/1/1
5	NAG	F	646	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	647	5	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	602	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	603	5	-	0/2/19/22	0/1/1/1
5	NAG	G	604	1	-	0/6/23/26	0/1/1/1
5	NAG	G	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	606	5	-	0/6/23/26	0/1/1/1
5	NAG	G	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	608	5	-	0/6/23/26	0/1/1/1
5	NAG	G	609	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	610	5	-	0/6/23/26	0/1/1/1
5	NAG	G	611	1	-	0/6/23/26	0/1/1/1
5	NAG	G	612	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	613	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	614	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	615	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	616	7	-	0/2/19/22	0/1/1/1
7	MAN	G	617	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	618	7	-	0/2/19/22	0/1/1/1
5	NAG	G	619	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	620	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	621	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	622	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	623	7	-	0/2/19/22	0/1/1/1
7	MAN	G	624	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	625	7	-	0/2/19/22	0/1/1/1
7	MAN	G	626	7	-	0/2/19/22	0/1/1/1
5	NAG	G	627	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	628	5	-	0/6/23/26	0/1/1/1
5	NAG	G	629	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	630	5	-	0/6/23/26	0/1/1/1
5	NAG	G	631	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	632	5	-	0/6/23/26	0/1/1/1
5	NAG	G	633	1	-	0/6/23/26	0/1/1/1
5	NAG	G	634	1	-	0/6/23/26	0/1/1/1
5	NAG	G	635	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	636	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	637	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	638	6	-	0/2/19/22	0/1/1/1
7	MAN	G	639	7,6	-	0/2/19/22	0/1/1/1
7	MAN	G	640	7	-	0/2/19/22	0/1/1/1
5	NAG	G	641	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	642	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	643	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	644	6	-	0/2/19/22	0/1/1/1
5	NAG	G	645	1	-	0/6/23/26	0/1/1/1
5	NAG	G	646	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	647	5	-	0/6/23/26	0/1/1/1
5	NAG	I	701	2	-	0/6/23/26	0/1/1/1
5	NAG	I	702	2	-	0/6/23/26	0/1/1/1
5	NAG	J	701	2	-	0/6/23/26	0/1/1/1
5	NAG	J	702	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	L	301	5,4	-	0/6/23/26	0/1/1/1
5	NAG	L	302	5	-	0/6/23/26	0/1/1/1
5	NAG	T	301	5,4	-	0/6/23/26	0/1/1/1
5	NAG	T	302	5	-	0/6/23/26	0/1/1/1
5	NAG	U	301	5,4	-	0/6/23/26	0/1/1/1
5	NAG	U	302	5	-	0/6/23/26	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	619	NAG	O5-C1	-2.39	1.39	1.43
5	F	619	NAG	O5-C1	-2.38	1.39	1.43
5	A	619	NAG	O5-C1	-2.36	1.39	1.43
5	F	601	NAG	O5-C1	-2.31	1.39	1.43
5	A	601	NAG	O5-C1	-2.26	1.40	1.43
5	G	601	NAG	O5-C1	-2.26	1.40	1.43
6	A	603	BMA	C2-C3	2.06	1.55	1.52
6	F	603	BMA	C2-C3	2.07	1.55	1.52
6	G	603	BMA	C2-C3	2.07	1.55	1.52
7	F	623	MAN	O5-C5	2.09	1.47	1.43
7	A	623	MAN	O5-C5	2.13	1.47	1.43
7	G	623	MAN	O5-C5	2.14	1.48	1.43
6	G	621	BMA	C4-C5	2.19	1.57	1.53
6	F	621	BMA	C4-C5	2.20	1.57	1.53
6	A	621	BMA	C4-C5	2.20	1.57	1.53
6	F	621	BMA	O5-C5	2.23	1.48	1.43
6	G	621	BMA	O5-C5	2.24	1.48	1.43
6	A	621	BMA	O5-C5	2.24	1.48	1.43
6	F	603	BMA	C1-C2	2.35	1.57	1.52
6	A	603	BMA	C1-C2	2.36	1.57	1.52
6	G	603	BMA	C1-C2	2.36	1.57	1.52
7	G	622	MAN	C4-C5	2.45	1.58	1.53
7	F	622	MAN	C4-C5	2.45	1.58	1.53
7	A	622	MAN	C4-C5	2.45	1.58	1.53
7	G	622	MAN	C4-C3	2.47	1.58	1.52
7	A	622	MAN	C4-C3	2.48	1.58	1.52
7	F	622	MAN	C4-C3	2.50	1.58	1.52
6	G	621	BMA	C2-C3	2.67	1.56	1.52
6	A	621	BMA	C2-C3	2.69	1.56	1.52
6	F	621	BMA	C2-C3	2.70	1.56	1.52
7	F	622	MAN	O5-C5	2.90	1.49	1.43
7	G	622	MAN	O5-C5	2.93	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	622	MAN	O5-C5	2.94	1.49	1.43
7	F	623	MAN	C2-C3	3.21	1.56	1.52
7	A	623	MAN	C2-C3	3.24	1.56	1.52
7	G	623	MAN	C2-C3	3.25	1.56	1.52
5	G	641	NAG	O5-C1	3.46	1.49	1.43
5	A	641	NAG	O5-C1	3.49	1.49	1.43
5	F	641	NAG	O5-C1	3.50	1.49	1.43
7	G	623	MAN	C4-C3	3.72	1.61	1.52
7	A	623	MAN	C4-C3	3.75	1.61	1.52
7	F	623	MAN	C4-C3	3.75	1.61	1.52
7	F	623	MAN	C4-C5	4.33	1.62	1.53
7	G	623	MAN	C4-C5	4.34	1.62	1.53
7	A	623	MAN	C4-C5	4.35	1.62	1.53

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	612	NAG	O5-C1-C2	-8.50	99.65	111.47
5	U	301	NAG	O5-C1-C2	-8.50	99.65	111.47
5	A	612	NAG	O5-C1-C2	-8.48	99.68	111.47
5	F	612	NAG	O5-C1-C2	-8.47	99.68	111.47
5	F	609	NAG	O5-C1-C2	-8.47	99.68	111.47
5	L	301	NAG	O5-C1-C2	-8.47	99.69	111.47
5	T	301	NAG	O5-C1-C2	-8.47	99.69	111.47
5	A	609	NAG	O5-C1-C2	-8.46	99.70	111.47
5	G	609	NAG	O5-C1-C2	-8.44	99.72	111.47
7	F	626	MAN	C6-C5-C4	-5.05	101.17	113.00
7	A	626	MAN	C6-C5-C4	-5.05	101.18	113.00
7	G	626	MAN	C6-C5-C4	-5.05	101.19	113.00
7	F	640	MAN	O4-C4-C3	-4.25	101.11	110.36
7	A	640	MAN	O4-C4-C3	-4.24	101.13	110.36
7	G	640	MAN	O4-C4-C3	-4.23	101.15	110.36
7	G	616	MAN	O2-C2-C3	-4.19	101.94	110.17
7	A	618	MAN	O4-C4-C3	-4.19	101.24	110.36
7	F	618	MAN	O4-C4-C3	-4.18	101.26	110.36
7	A	616	MAN	O2-C2-C3	-4.18	101.97	110.17
7	G	618	MAN	O4-C4-C3	-4.18	101.27	110.36
7	F	625	MAN	O4-C4-C3	-4.17	101.29	110.36
7	F	616	MAN	O2-C2-C3	-4.16	102.00	110.17
7	G	625	MAN	O4-C4-C3	-4.16	101.30	110.36
7	A	625	MAN	O4-C4-C3	-4.16	101.31	110.36
7	A	617	MAN	C2-C3-C4	-4.10	103.72	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	617	MAN	C2-C3-C4	-4.10	103.72	110.88
7	G	617	MAN	C2-C3-C4	-4.09	103.74	110.88
7	G	644	MAN	C2-C3-C4	-4.07	103.77	110.88
7	F	624	MAN	C2-C3-C4	-4.07	103.77	110.88
7	A	624	MAN	C2-C3-C4	-4.07	103.78	110.88
7	A	644	MAN	C2-C3-C4	-4.07	103.78	110.88
7	G	624	MAN	C2-C3-C4	-4.06	103.80	110.88
7	F	644	MAN	C2-C3-C4	-4.04	103.84	110.88
7	F	639	MAN	C2-C3-C4	-4.03	103.85	110.88
7	G	639	MAN	C2-C3-C4	-4.02	103.86	110.88
7	A	639	MAN	C2-C3-C4	-4.00	103.90	110.88
7	G	626	MAN	O4-C4-C3	-3.82	102.04	110.36
7	A	626	MAN	O4-C4-C3	-3.81	102.07	110.36
7	F	626	MAN	O4-C4-C3	-3.80	102.09	110.36
7	F	617	MAN	O5-C1-C2	-3.43	105.41	110.79
7	G	617	MAN	O5-C1-C2	-3.41	105.45	110.79
7	A	617	MAN	O5-C1-C2	-3.41	105.45	110.79
7	G	624	MAN	O5-C1-C2	-3.40	105.47	110.79
7	F	624	MAN	O5-C1-C2	-3.38	105.49	110.79
7	A	644	MAN	O5-C1-C2	-3.38	105.50	110.79
7	A	624	MAN	O5-C1-C2	-3.37	105.51	110.79
7	G	644	MAN	O5-C1-C2	-3.37	105.51	110.79
7	F	644	MAN	O5-C1-C2	-3.35	105.55	110.79
7	G	639	MAN	O5-C1-C2	-3.34	105.56	110.79
7	A	639	MAN	O5-C1-C2	-3.34	105.56	110.79
7	F	639	MAN	O5-C1-C2	-3.32	105.58	110.79
7	F	623	MAN	C1-C2-C3	-3.19	105.60	109.65
7	F	626	MAN	C3-C4-C5	-3.19	104.60	110.22
7	A	623	MAN	C1-C2-C3	-3.18	105.61	109.65
7	G	623	MAN	C1-C2-C3	-3.18	105.62	109.65
7	A	626	MAN	C3-C4-C5	-3.18	104.62	110.22
7	G	626	MAN	C3-C4-C5	-3.15	104.66	110.22
7	F	626	MAN	O2-C2-C3	-3.03	104.23	110.17
7	A	626	MAN	O2-C2-C3	-3.02	104.24	110.17
7	G	626	MAN	O2-C2-C3	-3.02	104.25	110.17
7	A	616	MAN	O4-C4-C3	-2.89	104.06	110.36
7	F	616	MAN	O4-C4-C3	-2.89	104.07	110.36
7	G	616	MAN	O4-C4-C3	-2.88	104.09	110.36
5	L	301	NAG	O7-C7-C8	-2.86	116.85	122.06
5	U	301	NAG	O7-C7-C8	-2.86	116.85	122.06
5	T	301	NAG	O7-C7-C8	-2.84	116.89	122.06
5	A	612	NAG	O7-C7-C8	-2.80	116.95	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	612	NAG	O7-C7-C8	-2.80	116.97	122.06
5	G	612	NAG	O7-C7-C8	-2.80	116.97	122.06
5	A	609	NAG	O7-C7-C8	-2.78	117.01	122.06
5	G	609	NAG	O7-C7-C8	-2.76	117.03	122.06
5	F	610	NAG	O5-C1-C2	-2.76	107.63	111.47
5	F	609	NAG	O7-C7-C8	-2.76	117.03	122.06
5	U	301	NAG	C4-C3-C2	-2.76	106.98	111.02
5	G	610	NAG	O5-C1-C2	-2.74	107.67	111.47
5	A	610	NAG	O5-C1-C2	-2.73	107.67	111.47
5	T	301	NAG	C4-C3-C2	-2.72	107.04	111.02
5	L	301	NAG	C4-C3-C2	-2.71	107.04	111.02
5	G	613	NAG	O5-C1-C2	-2.71	107.70	111.47
5	A	613	NAG	O5-C1-C2	-2.71	107.70	111.47
5	A	609	NAG	C4-C3-C2	-2.70	107.06	111.02
5	G	609	NAG	C4-C3-C2	-2.69	107.08	111.02
5	F	613	NAG	O5-C1-C2	-2.68	107.74	111.47
5	F	609	NAG	C4-C3-C2	-2.68	107.09	111.02
5	U	302	NAG	O5-C1-C2	-2.68	107.75	111.47
5	L	302	NAG	O5-C1-C2	-2.67	107.75	111.47
5	F	612	NAG	C4-C3-C2	-2.65	107.14	111.02
5	A	612	NAG	C4-C3-C2	-2.65	107.14	111.02
5	T	302	NAG	O5-C1-C2	-2.64	107.79	111.47
5	G	612	NAG	C4-C3-C2	-2.62	107.17	111.02
6	G	637	BMA	O4-C4-C5	-2.60	102.72	109.28
6	F	637	BMA	O4-C4-C5	-2.60	102.73	109.28
6	A	637	BMA	O4-C4-C5	-2.59	102.77	109.28
6	F	643	BMA	O4-C4-C5	-2.57	102.81	109.28
6	A	643	BMA	O4-C4-C5	-2.57	102.82	109.28
6	F	614	BMA	O4-C4-C5	-2.56	102.84	109.28
6	G	643	BMA	O4-C4-C5	-2.56	102.84	109.28
6	A	614	BMA	O4-C4-C5	-2.55	102.86	109.28
6	G	614	BMA	O4-C4-C5	-2.55	102.87	109.28
6	F	614	BMA	C6-C5-C4	-2.47	107.23	113.00
6	A	614	BMA	C6-C5-C4	-2.46	107.25	113.00
6	G	614	BMA	C6-C5-C4	-2.45	107.27	113.00
6	G	643	BMA	C6-C5-C4	-2.44	107.30	113.00
6	F	643	BMA	C6-C5-C4	-2.43	107.31	113.00
6	A	643	BMA	C6-C5-C4	-2.42	107.34	113.00
7	G	618	MAN	O3-C3-C2	-2.42	105.63	110.02
6	F	637	BMA	C6-C5-C4	-2.41	107.36	113.00
7	F	618	MAN	O3-C3-C2	-2.41	105.64	110.02
6	A	637	BMA	C6-C5-C4	-2.40	107.39	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	640	MAN	O3-C3-C2	-2.40	105.67	110.02
7	A	618	MAN	O3-C3-C2	-2.39	105.67	110.02
6	G	637	BMA	C6-C5-C4	-2.39	107.40	113.00
7	A	640	MAN	O3-C3-C2	-2.38	105.69	110.02
7	A	625	MAN	O3-C3-C2	-2.37	105.70	110.02
7	G	640	MAN	O3-C3-C2	-2.37	105.72	110.02
7	G	625	MAN	O3-C3-C2	-2.37	105.72	110.02
7	F	625	MAN	O3-C3-C2	-2.37	105.72	110.02
7	F	622	MAN	O2-C2-C3	-2.31	105.64	110.17
7	G	622	MAN	O2-C2-C3	-2.31	105.64	110.17
7	A	622	MAN	O2-C2-C3	-2.30	105.65	110.17
5	L	302	NAG	C4-C3-C2	-2.21	107.78	111.02
5	A	613	NAG	C4-C3-C2	-2.20	107.80	111.02
5	F	610	NAG	C4-C3-C2	-2.20	107.80	111.02
5	A	610	NAG	C4-C3-C2	-2.20	107.80	111.02
5	U	302	NAG	C4-C3-C2	-2.19	107.81	111.02
5	F	613	NAG	C4-C3-C2	-2.19	107.81	111.02
5	G	613	NAG	C4-C3-C2	-2.18	107.82	111.02
5	T	302	NAG	C4-C3-C2	-2.18	107.83	111.02
5	G	610	NAG	C4-C3-C2	-2.17	107.84	111.02
7	F	615	MAN	O4-C4-C3	-2.14	105.70	110.36
7	G	615	MAN	O4-C4-C3	-2.14	105.70	110.36
5	F	602	NAG	O4-C4-C5	-2.13	103.91	109.28
7	A	615	MAN	O4-C4-C3	-2.13	105.72	110.36
5	A	602	NAG	O4-C4-C5	-2.13	103.91	109.28
7	F	638	MAN	O4-C4-C3	-2.13	105.73	110.36
7	A	638	MAN	O4-C4-C3	-2.12	105.74	110.36
5	G	602	NAG	O4-C4-C5	-2.12	103.94	109.28
5	A	631	NAG	O4-C4-C5	-2.10	103.98	109.28
7	G	638	MAN	O4-C4-C3	-2.10	105.78	110.36
5	G	631	NAG	O4-C4-C5	-2.10	104.00	109.28
5	F	632	NAG	O4-C4-C5	-2.09	104.01	109.28
7	G	626	MAN	C2-C3-C4	2.01	114.38	110.88
5	F	606	NAG	C1-O5-C5	2.01	114.94	112.17
5	A	606	NAG	C1-O5-C5	2.03	114.96	112.17
5	G	604	NAG	C1-O5-C5	2.03	114.96	112.17
5	F	604	NAG	C1-O5-C5	2.03	114.96	112.17
7	A	626	MAN	C2-C3-C4	2.03	114.41	110.88
5	A	604	NAG	C1-O5-C5	2.03	114.97	112.17
7	F	626	MAN	C2-C3-C4	2.04	114.43	110.88
7	F	618	MAN	O3-C3-C4	2.08	114.87	110.36
7	G	618	MAN	O3-C3-C4	2.08	114.88	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	618	MAN	O3-C3-C4	2.10	114.92	110.36
7	G	625	MAN	O3-C3-C4	2.11	114.94	110.36
7	A	625	MAN	O3-C3-C4	2.11	114.95	110.36
7	F	625	MAN	O3-C3-C4	2.12	114.97	110.36
7	G	618	MAN	C1-O5-C5	2.13	115.11	112.17
7	F	640	MAN	O3-C3-C4	2.15	115.04	110.36
7	A	640	MAN	O3-C3-C4	2.16	115.06	110.36
7	G	640	MAN	O3-C3-C4	2.16	115.06	110.36
5	F	636	NAG	C1-O5-C5	2.17	115.16	112.17
7	A	618	MAN	C1-O5-C5	2.17	115.16	112.17
7	F	618	MAN	C1-O5-C5	2.19	115.19	112.17
7	F	625	MAN	C1-O5-C5	2.20	115.20	112.17
7	A	625	MAN	C1-O5-C5	2.20	115.20	112.17
5	G	636	NAG	C1-O5-C5	2.22	115.22	112.17
7	F	623	MAN	O2-C2-C1	2.22	113.69	109.18
7	A	623	MAN	O2-C2-C1	2.22	113.70	109.18
7	G	625	MAN	C1-O5-C5	2.22	115.23	112.17
5	A	636	NAG	C1-O5-C5	2.23	115.23	112.17
7	F	640	MAN	C1-O5-C5	2.23	115.24	112.17
7	G	640	MAN	C1-O5-C5	2.24	115.25	112.17
7	G	623	MAN	O2-C2-C1	2.24	113.73	109.18
7	A	640	MAN	C1-O5-C5	2.24	115.26	112.17
7	G	638	MAN	O3-C3-C4	2.27	115.29	110.36
7	F	638	MAN	O3-C3-C4	2.27	115.30	110.36
7	A	638	MAN	O3-C3-C4	2.27	115.30	110.36
7	F	615	MAN	O3-C3-C4	2.29	115.34	110.36
7	F	616	MAN	O6-C6-C5	2.29	119.05	111.34
7	G	616	MAN	O6-C6-C5	2.29	119.06	111.34
7	A	615	MAN	O3-C3-C4	2.30	115.36	110.36
6	A	603	BMA	O5-C1-C2	2.30	114.39	110.79
7	A	616	MAN	O6-C6-C5	2.30	119.10	111.34
6	F	603	BMA	O5-C1-C2	2.31	114.40	110.79
6	G	603	BMA	O5-C1-C2	2.31	114.41	110.79
7	G	615	MAN	O3-C3-C4	2.31	115.38	110.36
5	F	601	NAG	C3-C4-C5	2.34	114.33	110.22
5	A	601	NAG	C3-C4-C5	2.35	114.35	110.22
5	F	602	NAG	C1-C2-N2	2.35	114.51	110.49
5	G	601	NAG	C3-C4-C5	2.36	114.37	110.22
5	A	602	NAG	C1-C2-N2	2.38	114.56	110.49
7	A	638	MAN	O5-C1-C2	2.40	114.55	110.79
7	G	638	MAN	O5-C1-C2	2.40	114.55	110.79
5	G	602	NAG	C1-C2-N2	2.41	114.60	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	638	MAN	O5-C1-C2	2.41	114.56	110.79
7	F	626	MAN	O2-C2-C1	2.43	114.13	109.18
7	F	615	MAN	O5-C1-C2	2.44	114.62	110.79
7	G	626	MAN	O2-C2-C1	2.45	114.15	109.18
7	A	626	MAN	O2-C2-C1	2.45	114.15	109.18
7	A	615	MAN	O5-C1-C2	2.46	114.64	110.79
7	G	615	MAN	O5-C1-C2	2.46	114.64	110.79
6	F	621	BMA	O2-C2-C1	2.50	114.27	109.18
6	G	621	BMA	O2-C2-C1	2.50	114.27	109.18
6	A	621	BMA	O2-C2-C1	2.50	114.27	109.18
7	A	623	MAN	O3-C3-C4	2.52	115.85	110.36
7	F	623	MAN	O3-C3-C4	2.53	115.85	110.36
7	G	623	MAN	O3-C3-C4	2.53	115.86	110.36
7	F	623	MAN	O5-C1-C2	2.56	114.81	110.79
7	G	623	MAN	O5-C1-C2	2.57	114.82	110.79
7	A	623	MAN	O5-C1-C2	2.58	114.83	110.79
6	G	643	BMA	O2-C2-C3	2.99	116.06	110.17
6	A	643	BMA	O2-C2-C3	3.00	116.06	110.17
6	F	643	BMA	O2-C2-C3	3.00	116.07	110.17
6	A	637	BMA	O2-C2-C3	3.08	116.22	110.17
6	A	614	BMA	O2-C2-C3	3.08	116.22	110.17
5	F	641	NAG	C1-O5-C5	3.08	116.41	112.17
6	F	614	BMA	O2-C2-C3	3.09	116.24	110.17
5	G	641	NAG	C1-O5-C5	3.09	116.43	112.17
6	F	637	BMA	O2-C2-C3	3.09	116.25	110.17
6	G	614	BMA	O2-C2-C3	3.09	116.25	110.17
5	A	641	NAG	C1-O5-C5	3.10	116.43	112.17
6	G	637	BMA	O2-C2-C3	3.11	116.28	110.17
7	F	625	MAN	O4-C4-C5	3.15	117.22	109.28
7	F	640	MAN	O4-C4-C5	3.16	117.25	109.28
7	A	625	MAN	O4-C4-C5	3.16	117.25	109.28
7	A	640	MAN	O4-C4-C5	3.16	117.25	109.28
7	G	640	MAN	O4-C4-C5	3.18	117.30	109.28
7	G	618	MAN	O4-C4-C5	3.18	117.31	109.28
7	A	618	MAN	O4-C4-C5	3.18	117.31	109.28
7	G	625	MAN	O4-C4-C5	3.18	117.31	109.28
7	F	618	MAN	O4-C4-C5	3.20	117.36	109.28
7	G	622	MAN	C1-O5-C5	3.68	117.23	112.17
7	A	622	MAN	C1-O5-C5	3.69	117.26	112.17
7	F	622	MAN	C1-O5-C5	3.72	117.29	112.17
7	A	623	MAN	C1-O5-C5	3.82	117.44	112.17
7	G	623	MAN	C1-O5-C5	3.84	117.46	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	623	MAN	C1-O5-C5	3.85	117.47	112.17
6	F	603	BMA	C1-O5-C5	3.93	117.58	112.17
6	G	603	BMA	C1-O5-C5	3.94	117.59	112.17
6	A	603	BMA	C1-O5-C5	3.94	117.60	112.17
5	G	602	NAG	C2-N2-C7	4.32	129.24	122.94
5	A	602	NAG	C2-N2-C7	4.35	129.29	122.94
5	F	602	NAG	C2-N2-C7	4.37	129.31	122.94
7	G	616	MAN	C1-O5-C5	4.68	118.61	112.17
7	A	616	MAN	C1-O5-C5	4.70	118.65	112.17
7	F	616	MAN	C1-O5-C5	4.73	118.69	112.17
7	F	616	MAN	O2-C2-C1	5.03	119.40	109.18
7	A	616	MAN	O2-C2-C1	5.03	119.41	109.18
7	G	616	MAN	O2-C2-C1	5.04	119.43	109.18
6	G	621	BMA	C1-O5-C5	5.55	119.81	112.17
6	F	621	BMA	C1-O5-C5	5.58	119.86	112.17
6	A	621	BMA	C1-O5-C5	5.60	119.88	112.17
7	F	639	MAN	C1-C2-C3	6.71	118.15	109.65
7	G	639	MAN	C1-C2-C3	6.72	118.17	109.65
7	A	639	MAN	C1-C2-C3	6.72	118.17	109.65
7	G	617	MAN	C1-C2-C3	6.74	118.19	109.65
7	F	624	MAN	C1-C2-C3	6.76	118.22	109.65
7	G	644	MAN	C1-C2-C3	6.76	118.22	109.65
7	A	617	MAN	C1-C2-C3	6.77	118.23	109.65
7	F	617	MAN	C1-C2-C3	6.77	118.23	109.65
7	F	644	MAN	C1-C2-C3	6.77	118.23	109.65
7	A	624	MAN	C1-C2-C3	6.77	118.23	109.65
7	G	624	MAN	C1-C2-C3	6.78	118.25	109.65
7	A	644	MAN	C1-C2-C3	6.78	118.25	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

48 monomers are involved in 140 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	NAG	2	0
5	A	602	NAG	1	0
5	A	605	NAG	6	0
5	A	607	NAG	6	0
5	A	619	NAG	2	0
5	A	620	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	627	NAG	13	0
5	A	629	NAG	1	0
5	A	630	NAG	1	0
5	A	631	NAG	5	0
5	A	635	NAG	1	0
5	A	641	NAG	1	0
5	A	646	NAG	2	0
5	A	647	NAG	2	0
5	B	701	NAG	1	0
5	B	702	NAG	5	0
5	F	601	NAG	2	0
5	F	602	NAG	1	0
5	F	605	NAG	6	0
5	F	607	NAG	6	0
5	F	619	NAG	2	0
5	F	620	NAG	2	0
5	F	627	NAG	13	0
5	F	629	NAG	1	0
5	F	630	NAG	1	0
5	F	632	NAG	5	0
5	F	635	NAG	1	0
5	F	641	NAG	1	0
5	F	646	NAG	2	0
5	F	647	NAG	2	0
5	G	601	NAG	2	0
5	G	602	NAG	1	0
5	G	605	NAG	6	0
5	G	607	NAG	6	0
5	G	619	NAG	2	0
5	G	620	NAG	2	0
5	G	627	NAG	12	0
5	G	629	NAG	1	0
5	G	630	NAG	1	0
5	G	631	NAG	5	0
5	G	635	NAG	1	0
5	G	641	NAG	1	0
5	G	646	NAG	2	0
5	G	647	NAG	2	0
5	I	701	NAG	1	0
5	I	702	NAG	5	0
5	J	701	NAG	1	0
5	J	702	NAG	5	0

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.