



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 30, 2020 – 03:58 PM EST

PDB ID : 6V8Z
EMDB ID: : EMD-21112
Title : VRC03 and 10-1074 Bound BG505 F14 HIV-1 SOSIP Envelope Trimer Structure
Authors : Henderson, R.; Acharya, P.
Deposited on : 2019-12-12
Resolution : 2.90 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

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

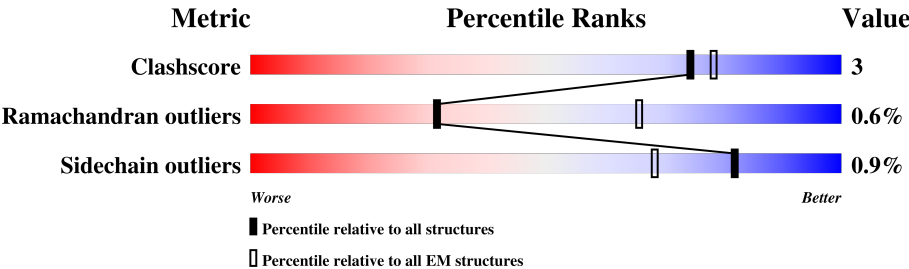
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 2.90 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	472	 86% 8% • 5%
1	G	472	 87% 7% • 5%
1	M	472	 87% 7% • 5%
2	B	147	 90% 9% •
2	H	147	 90% 9% ••
2	N	147	 90% 9% •
3	D	235	 88% 10% •
3	J	235	 87% 11% •
3	P	235	 88% 10% •

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Mol	Chain	Length	Quality of chain
4	E	211	 87% 13%
4	K	211	 87% 13%
4	Q	211	 87% 12%
5	C	231	 90% 8% .
5	I	231	 89% 9% .
5	O	231	 90% 8% .
6	F	208	 95% 5%
6	L	208	 95% 5%
6	R	208	 95% 5%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 35877 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3534	2227	618	659	30		
1	G	449	Total	C	N	O	S	0	0
			3534	2227	618	659	30		
1	M	449	Total	C	N	O	S	0	0
			3534	2227	618	659	30		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ILE	VAL	conflict	UNP Q2N0S6
A	142	ALA	ASN	conflict	UNP Q2N0S6
A	203	MET	GLN	conflict	UNP Q2N0S6
A	204	VAL	ALA	conflict	UNP Q2N0S6
A	208	LEU	VAL	conflict	UNP Q2N0S6
A	255	LEU	VAL	conflict	UNP Q2N0S6
A	300	LEU	ASN	conflict	UNP Q2N0S6
A	302	LEU	ASN	conflict	UNP Q2N0S6
A	320	MET	THR	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	422	MET	GLN	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
G	68	ILE	VAL	conflict	UNP Q2N0S6
G	142	ALA	ASN	conflict	UNP Q2N0S6
G	203	MET	GLN	conflict	UNP Q2N0S6
G	204	VAL	ALA	conflict	UNP Q2N0S6
G	208	LEU	VAL	conflict	UNP Q2N0S6
G	255	LEU	VAL	conflict	UNP Q2N0S6
G	300	LEU	ASN	conflict	UNP Q2N0S6
G	302	LEU	ASN	conflict	UNP Q2N0S6
G	320	MET	THR	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	422	MET	GLN	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	68	ILE	VAL	conflict	UNP Q2N0S6
M	142	ALA	ASN	conflict	UNP Q2N0S6
M	203	MET	GLN	conflict	UNP Q2N0S6
M	204	VAL	ALA	conflict	UNP Q2N0S6
M	208	LEU	VAL	conflict	UNP Q2N0S6
M	255	LEU	VAL	conflict	UNP Q2N0S6
M	300	LEU	ASN	conflict	UNP Q2N0S6
M	302	LEU	ASN	conflict	UNP Q2N0S6
M	320	MET	THR	conflict	UNP Q2N0S6
M	332	ASN	THR	conflict	UNP Q2N0S6
M	422	MET	GLN	conflict	UNP Q2N0S6
M	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	147	Total	C	N	O	S	0	0
			1171	740	205	220	6		
2	H	147	Total	C	N	O	S	0	0
			1171	740	205	220	6		
2	N	147	Total	C	N	O	S	0	0
			1171	740	205	220	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
H	559	PRO	ILE	conflict	UNP Q2N0S7
H	605	CYS	THR	conflict	UNP Q2N0S7
N	559	PRO	ILE	conflict	UNP Q2N0S7
N	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called 10-1074 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	230	Total	C	N	O	S	0	0
			1753	1108	293	345	7		
3	J	230	Total	C	N	O	S	0	0
			1753	1108	293	345	7		
3	P	230	Total	C	N	O	S	0	0
			1753	1108	293	345	7		

- Molecule 4 is a protein called 10-1074 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	211	Total	C	N	O	S	0	0
			1607	1006	281	314	6		
4	K	211	Total	C	N	O	S	0	0
			1607	1006	281	314	6		
4	Q	211	Total	C	N	O	S	0	0
			1607	1006	281	314	6		

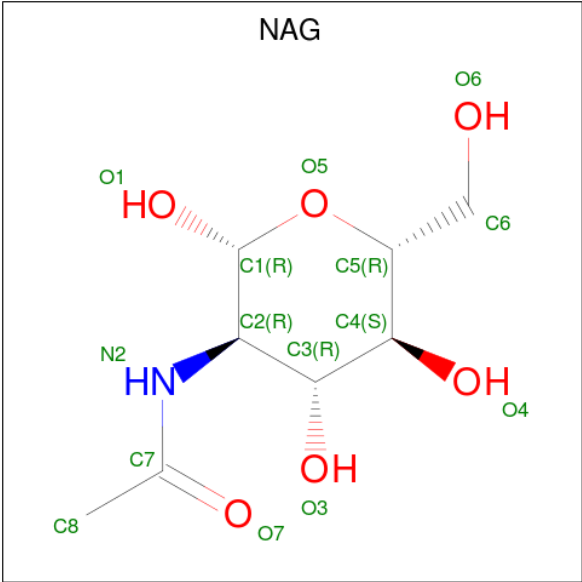
- Molecule 5 is a protein called VRC03 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	227	Total	C	N	O	S	0	0
			1739	1110	292	328	9		
5	I	227	Total	C	N	O	S	0	0
			1739	1110	292	328	9		
5	O	227	Total	C	N	O	S	0	0
			1739	1110	292	328	9		

- Molecule 6 is a protein called VRC03 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	208	Total	C	N	O	S	0	0
			1622	1020	276	321	5		
6	L	208	Total	C	N	O	S	0	0
			1622	1020	276	321	5		
6	R	208	Total	C	N	O	S	0	0
			1622	1020	276	321	5		

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



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	

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Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	A	1	Total	C	N	O	0
			392	224	28	140	
7	B	1	Total	C	N	O	0
			42	24	3	15	
7	B	1	Total	C	N	O	0
			42	24	3	15	
7	B	1	Total	C	N	O	0
			42	24	3	15	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	

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Mol	Chain	Residues	Atoms				AltConf
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	

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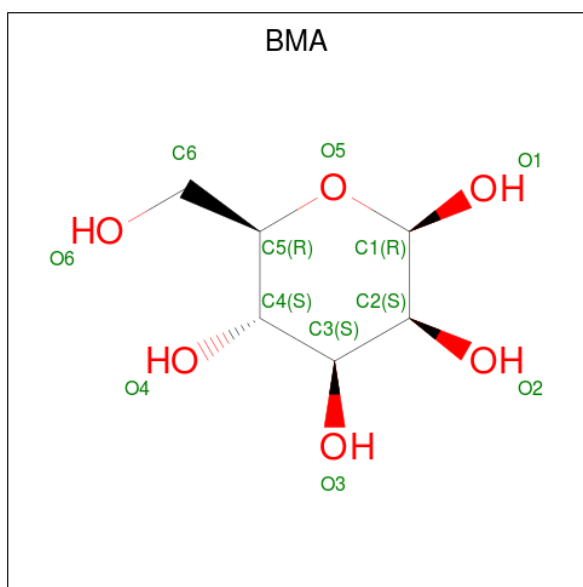
Mol	Chain	Residues	Atoms				AltConf
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	G	1	Total	C	N	O	0
			392	224	28	140	
7	H	1	Total	C	N	O	0
			42	24	3	15	
7	H	1	Total	C	N	O	0
			42	24	3	15	
7	H	1	Total	C	N	O	0
			42	24	3	15	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	

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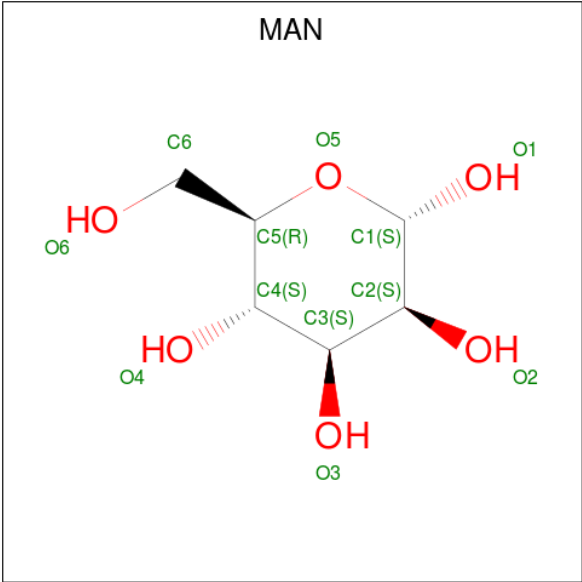
Mol	Chain	Residues	Atoms				AltConf
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	M	1	Total	C	N	O	0
			392	224	28	140	
7	N	1	Total	C	N	O	0
			42	24	3	15	
7	N	1	Total	C	N	O	0
			42	24	3	15	
7	N	1	Total	C	N	O	0
			42	24	3	15	

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			33	18	15	
8	A	1	Total	C	O	0
			33	18	15	
8	A	1	Total	C	O	0
			33	18	15	
8	G	1	Total	C	O	0
			33	18	15	
8	G	1	Total	C	O	0
			33	18	15	
8	G	1	Total	C	O	0
			33	18	15	
8	M	1	Total	C	O	0
			33	18	15	
8	M	1	Total	C	O	0
			33	18	15	
8	M	1	Total	C	O	0
			33	18	15	

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			66	36	30	
9	A	1	Total	C	O	0
			66	36	30	
9	A	1	Total	C	O	0
			66	36	30	
9	A	1	Total	C	O	0
			66	36	30	
9	A	1	Total	C	O	0
			66	36	30	
9	A	1	Total	C	O	0
			66	36	30	
9	G	1	Total	C	O	0
			66	36	30	
9	G	1	Total	C	O	0
			66	36	30	
9	G	1	Total	C	O	0
			66	36	30	
9	G	1	Total	C	O	0
			66	36	30	
9	G	1	Total	C	O	0
			66	36	30	
9	M	1	Total	C	O	0
			66	36	30	
9	M	1	Total	C	O	0
			66	36	30	

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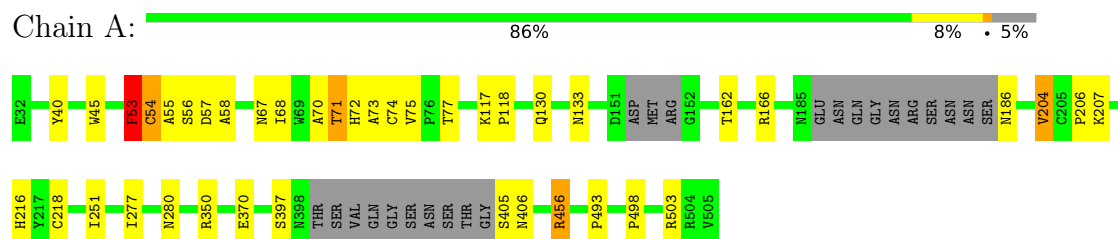
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Mol	Chain	Residues	Atoms			AltConf
9	M	1	Total	C	O	0
			66	36	30	
9	M	1	Total	C	O	0
			66	36	30	
9	M	1	Total	C	O	0
			66	36	30	
9	M	1	Total	C	O	0
			66	36	30	

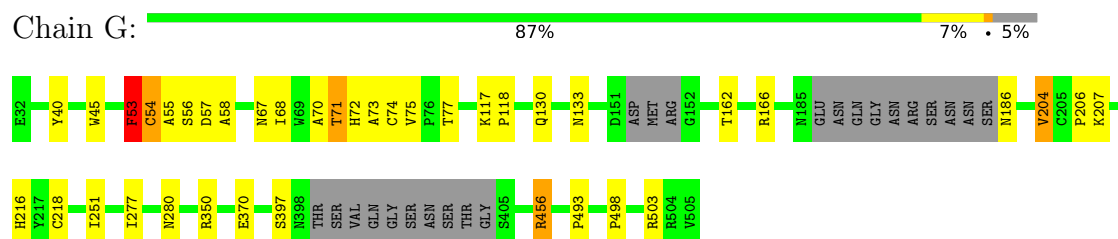
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

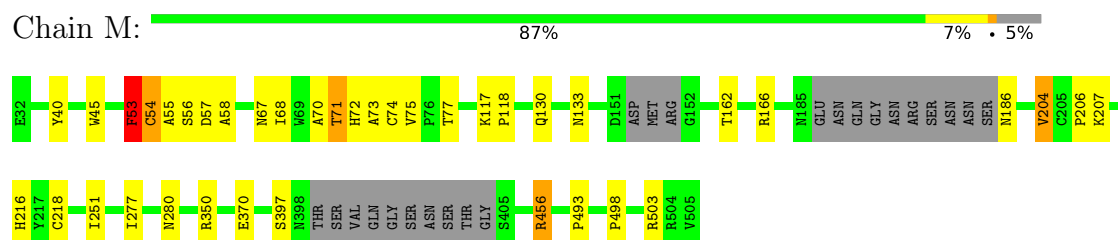
- Molecule 1: Envelope glycoprotein gp120



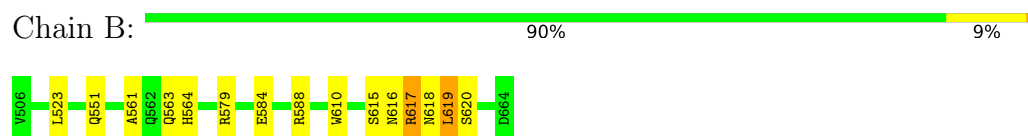
- Molecule 1: Envelope glycoprotein gp120



- Molecule 1: Envelope glycoprotein gp120



- Molecule 2: envelope glycoprotein gp41



- Molecule 2: envelope glycoprotein gp41





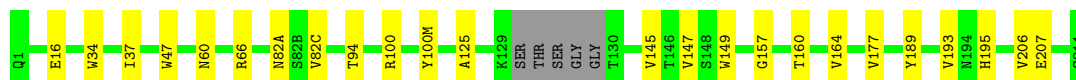
- Molecule 2: envelope glycoprotein gp41

Chain N: 90% 9% .



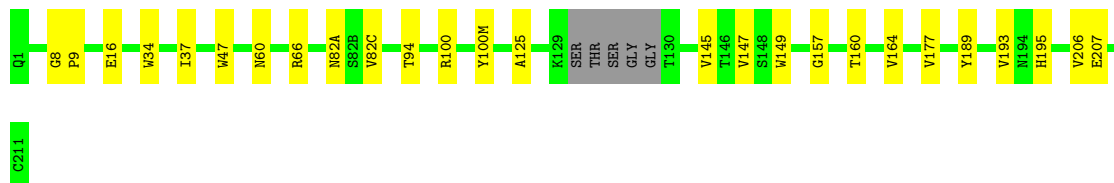
- Molecule 3: 10-1074 Fab Heavy Chain

Chain D: 88% 10% .



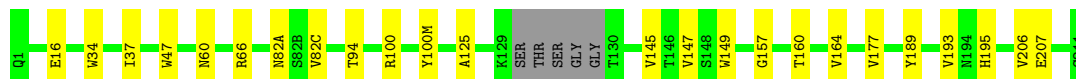
- Molecule 3: 10-1074 Fab Heavy Chain

Chain J: 87% 11% .



- Molecule 3: 10-1074 Fab Heavy Chain

Chain P: 88% 10% .



- Molecule 4: 10-1074 Fab Light Chain

Chain E: 87% 13% .




- Molecule 4: 10-1074 Fab Light Chain

Chain K: 87% 13% .



- Molecule 4: 10-1074 Fab Light Chain

Chain Q:  87% 12%




- Molecule 5: VRC03 Fab Heavy Chain

Chain C:  90% 8%



- Molecule 5: VRC03 Fab Heavy Chain

Chain I:  89% 9%



- Molecule 5: VRC03 Fab Heavy Chain

Chain O:  90% 8%



- Molecule 6: VRC03 Fab Light Chain

Chain F:  95% 5%



- Molecule 6: VRC03 Fab Light Chain

Chain L:  95% 5%



- Molecule 6: VRC03 Fab Light Chain

Chain R:  95% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	84378	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 ($e^-/\text{\AA}^2$)	54.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (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	0.50	0/3607	0.70	2/4894 (0.0%)
1	G	0.50	0/3607	0.70	2/4894 (0.0%)
1	M	0.50	0/3607	0.70	2/4894 (0.0%)
2	B	0.45	0/1192	0.69	2/1618 (0.1%)
2	H	0.45	0/1192	0.69	2/1618 (0.1%)
2	N	0.45	0/1192	0.69	2/1618 (0.1%)
3	D	0.39	0/1796	0.71	2/2450 (0.1%)
3	J	0.39	0/1796	0.71	2/2450 (0.1%)
3	P	0.39	0/1796	0.71	2/2450 (0.1%)
4	E	0.41	0/1649	0.68	0/2250
4	K	0.41	0/1649	0.68	0/2250
4	Q	0.41	0/1649	0.68	0/2250
5	C	0.47	0/1790	0.64	0/2444
5	I	0.47	0/1790	0.64	0/2444
5	O	0.47	0/1790	0.64	0/2444
6	F	0.42	0/1657	0.63	0/2244
6	L	0.42	0/1657	0.63	0/2244
6	R	0.42	0/1657	0.63	0/2244
All	All	0.45	0/35073	0.68	18/47700 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	H	0	2
2	N	0	2
4	E	0	1
4	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	Q	0	1
6	F	0	1
6	L	0	1
6	R	0	1
All	All	0	12

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	160	THR	C-N-CA	10.91	148.98	121.70
3	D	160	THR	C-N-CA	10.91	148.98	121.70
3	J	160	THR	C-N-CA	10.90	148.96	121.70
1	G	251	ILE	C-N-CA	8.21	142.23	121.70
1	A	251	ILE	C-N-CA	8.21	142.22	121.70
1	M	251	ILE	C-N-CA	8.21	142.21	121.70
1	M	53	PHE	CB-CA-C	-6.89	96.61	110.40
1	A	53	PHE	CB-CA-C	-6.89	96.63	110.40
1	G	53	PHE	CB-CA-C	-6.87	96.65	110.40
2	H	617	ARG	N-CA-CB	-6.58	98.76	110.60
2	B	617	ARG	N-CA-CB	-6.57	98.77	110.60
2	N	617	ARG	N-CA-CB	-6.56	98.79	110.60
2	H	619	LEU	CA-CB-CG	5.93	128.94	115.30
2	N	619	LEU	CA-CB-CG	5.92	128.91	115.30
2	B	619	LEU	CA-CB-CG	5.91	128.89	115.30
3	J	37	ILE	CG1-CB-CG2	-5.80	98.64	111.40
3	D	37	ILE	CG1-CB-CG2	-5.80	98.65	111.40
3	P	37	ILE	CG1-CB-CG2	-5.79	98.66	111.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	615	SER	Peptide
2	B	616	ASN	Peptide
4	E	140	PHE	Peptide
6	F	90	GLN	Peptide
2	H	615	SER	Peptide
2	H	616	ASN	Peptide
4	K	140	PHE	Peptide
6	L	90	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	N	615	SER	Peptide
2	N	616	ASN	Peptide
4	Q	140	PHE	Peptide
6	R	90	GLN	Peptide

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	3534	0	3488	28	0
1	G	3534	0	3488	27	0
1	M	3534	0	3488	27	0
2	B	1171	0	1158	10	0
2	H	1171	0	1158	11	0
2	N	1171	0	1158	10	0
3	D	1753	0	1720	16	0
3	J	1753	0	1720	17	0
3	P	1753	0	1720	16	0
4	E	1607	0	1552	19	0
4	K	1607	0	1552	19	0
4	Q	1607	0	1552	18	0
5	C	1739	0	1686	12	0
5	I	1739	0	1686	13	0
5	O	1739	0	1686	12	0
6	F	1622	0	1572	8	0
6	L	1622	0	1572	8	0
6	R	1622	0	1572	8	0
7	A	392	0	349	3	0
7	B	42	0	39	0	0
7	G	392	0	349	3	0
7	H	42	0	39	0	0
7	M	392	0	349	2	0
7	N	42	0	39	0	0
8	A	33	0	27	0	0
8	G	33	0	27	0	0
8	M	33	0	27	0	0
9	A	66	0	57	1	0
9	G	66	0	57	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	66	0	57	1	0
All	All	35877	0	34944	230	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (230) 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)
5:I:76(B):ASP:OD2	1:M:206:PRO:HG2	1.89	0.73
1:A:206:PRO:HG2	5:O:76(B):ASP:OD2	1.89	0.73
5:C:76(B):ASP:OD2	1:G:206:PRO:HG2	1.89	0.72
1:G:57:ASP:OD1	1:G:58:ALA:N	2.23	0.72
1:M:57:ASP:OD1	1:M:58:ALA:N	2.23	0.72
1:A:57:ASP:OD1	1:A:58:ALA:N	2.23	0.70
1:G:207:LYS:HZ1	2:H:563:GLN:HE21	1.41	0.69
1:A:207:LYS:NZ	2:B:563:GLN:HE21	1.91	0.68
1:G:207:LYS:NZ	2:H:563:GLN:HE21	1.91	0.68
1:M:207:LYS:NZ	2:N:563:GLN:HE21	1.91	0.67
1:M:207:LYS:HZ1	2:N:563:GLN:HE21	1.46	0.63
4:K:120:PRO:O	4:K:132:THR:OG1	2.19	0.61
1:A:117:LYS:HB2	1:A:118:PRO:HD3	1.83	0.60
4:Q:108:GLN:O	4:Q:141:TYR:CD2	2.55	0.60
1:M:117:LYS:HB2	1:M:118:PRO:HD3	1.83	0.60
1:G:117:LYS:HB2	1:G:118:PRO:HD3	1.83	0.59
4:K:108:GLN:O	4:K:141:TYR:CD2	2.55	0.59
4:E:108:GLN:O	4:E:141:TYR:CD2	2.55	0.59
6:F:186:TYR:O	6:F:192:TYR:OH	2.21	0.58
1:A:207:LYS:HZ1	2:B:563:GLN:HE21	1.51	0.58
6:L:186:TYR:O	6:L:192:TYR:OH	2.21	0.58
6:R:186:TYR:O	6:R:192:TYR:OH	2.21	0.57
6:R:108:ARG:NH1	6:R:170:ASP:O	2.37	0.57
2:B:584:GLU:OE2	2:H:579:ARG:NH2	2.38	0.57
6:L:108:ARG:NH1	6:L:170:ASP:O	2.37	0.57
2:H:584:GLU:OE2	2:N:579:ARG:NH2	2.38	0.56
2:B:579:ARG:NH2	2:N:584:GLU:OE2	2.38	0.56
6:F:108:ARG:NH1	6:F:170:ASP:O	2.37	0.56
4:Q:120:PRO:O	4:Q:132:THR:OG1	2.19	0.56
4:K:131:ALA:HB1	4:K:186:TRP:HE1	1.71	0.56
1:A:53:PHE:CZ	2:B:551:GLN:HG2	2.41	0.56
4:Q:131:ALA:HB1	4:Q:186:TRP:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:PHE:CZ	2:H:551:GLN:HG2	2.41	0.55
4:E:120:PRO:O	4:E:132:THR:OG1	2.18	0.55
4:E:131:ALA:HB1	4:E:186:TRP:HE1	1.71	0.55
1:A:56:SER:HB3	1:A:74:CYS:SG	2.47	0.54
1:G:56:SER:HB3	1:G:74:CYS:SG	2.48	0.54
4:Q:152:ASP:OD2	4:Q:190:ARG:HG2	2.08	0.54
4:K:152:ASP:OD2	4:K:190:ARG:HG2	2.08	0.54
1:M:53:PHE:CZ	2:N:551:GLN:HG2	2.41	0.54
4:E:152:ASP:OD2	4:E:190:ARG:HG2	2.08	0.54
1:M:55:ALA:HB3	1:M:216:HIS:O	2.08	0.53
1:G:55:ALA:HB3	1:G:216:HIS:O	2.08	0.53
1:A:55:ALA:HB3	1:A:216:HIS:O	2.08	0.53
1:G:498:PRO:HB3	2:H:610:TRP:CD2	2.44	0.53
2:N:618:ASN:O	2:N:620:SER:N	2.42	0.53
2:B:618:ASN:O	2:B:620:SER:N	2.42	0.53
1:M:56:SER:HB3	1:M:74:CYS:SG	2.47	0.53
1:M:130:GLN:OE1	1:M:186:ASN:N	2.42	0.52
3:D:100(M):TYR:OH	4:E:50:ASN:ND2	2.43	0.52
2:H:618:ASN:O	2:H:620:SER:N	2.42	0.52
3:P:100(M):TYR:OH	4:Q:50:ASN:ND2	2.43	0.52
1:A:498:PRO:HB3	2:B:610:TRP:CD2	2.44	0.52
1:M:498:PRO:HB3	2:N:610:TRP:CD2	2.44	0.52
1:A:130:GLN:OE1	1:A:186:ASN:N	2.42	0.52
3:D:66:ARG:NE	3:D:82(A):ASN:O	2.43	0.52
1:A:280:ASN:OD1	1:A:456:ARG:HD3	2.10	0.52
1:G:280:ASN:OD1	1:G:456:ARG:HD3	2.10	0.52
3:J:100(M):TYR:OH	4:K:50:ASN:ND2	2.43	0.52
1:G:130:GLN:OE1	1:G:186:ASN:N	2.42	0.51
7:G:603:NAG:O7	6:L:31:ASN:ND2	2.44	0.51
4:Q:89:HIS:CE1	4:Q:91:TRP:HE1	2.29	0.51
3:J:66:ARG:NE	3:J:82(A):ASN:O	2.43	0.51
5:C:134:LEU:HD22	5:C:190:TYR:CD2	2.46	0.51
7:M:603:NAG:O7	6:R:31:ASN:ND2	2.44	0.51
7:A:603:NAG:O7	6:F:31:ASN:ND2	2.44	0.50
5:O:134:LEU:HD22	5:O:190:TYR:CD2	2.46	0.50
6:L:181:LEU:HB2	6:L:186:TYR:CZ	2.47	0.50
1:M:280:ASN:OD1	1:M:456:ARG:HD3	2.10	0.50
5:O:35:HIS:CD2	5:O:100(F):TRP:HE1	2.29	0.50
5:C:35:HIS:CD2	5:C:100(F):TRP:HE1	2.29	0.50
5:I:134:LEU:HD22	5:I:190:TYR:CD2	2.46	0.50
3:P:145:VAL:HG13	3:P:195:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:181:LEU:HB2	6:F:186:TYR:CZ	2.47	0.50
3:D:145:VAL:HG13	3:D:195:HIS:CE1	2.47	0.50
1:G:54:CYS:O	1:G:216:HIS:O	2.30	0.49
4:K:89:HIS:CE1	4:K:91:TRP:HE1	2.29	0.49
1:M:54:CYS:O	1:M:216:HIS:O	2.30	0.49
3:P:66:ARG:NE	3:P:82(A):ASN:O	2.43	0.49
6:R:181:LEU:HB2	6:R:186:TYR:CZ	2.47	0.49
5:I:35:HIS:CD2	5:I:100(F):TRP:HE1	2.29	0.49
3:J:145:VAL:HG13	3:J:195:HIS:CE1	2.47	0.49
3:D:60:ASN:HA	4:E:96:TRP:CZ3	2.48	0.49
1:A:54:CYS:O	1:A:216:HIS:O	2.30	0.49
4:E:89:HIS:CE1	4:E:91:TRP:HE1	2.29	0.49
5:I:98:CYS:SG	6:L:49:TYR:OH	2.71	0.49
6:L:181:LEU:N	6:L:186:TYR:OH	2.43	0.49
3:P:47:TRP:HE3	4:Q:96:TRP:CD1	2.31	0.49
1:M:53:PHE:HB2	1:M:218:CYS:O	2.13	0.49
3:P:60:ASN:HA	4:Q:96:TRP:CZ3	2.48	0.49
1:A:53:PHE:HB2	1:A:218:CYS:O	2.13	0.48
5:O:98:CYS:SG	6:R:49:TYR:OH	2.71	0.48
3:D:47:TRP:HE3	4:E:96:TRP:CD1	2.31	0.48
3:J:60:ASN:HA	4:K:96:TRP:CZ3	2.48	0.48
1:G:53:PHE:HB2	1:G:218:CYS:O	2.13	0.48
9:M:625:MAN:O6	3:P:100:ARG:NH2	2.44	0.48
5:C:98:CYS:SG	6:F:49:TYR:OH	2.71	0.48
3:J:47:TRP:HE3	4:K:96:TRP:CD1	2.31	0.48
1:M:40:TYR:CE1	1:M:493:PRO:HB2	2.49	0.48
1:M:67:ASN:H	1:M:71:THR:HG21	1.79	0.47
6:R:181:LEU:N	6:R:186:TYR:OH	2.43	0.47
5:O:143:PRO:O	5:O:196:HIS:NE2	2.44	0.47
1:A:40:TYR:CE1	1:A:493:PRO:HB2	2.49	0.47
1:G:40:TYR:CE1	1:G:493:PRO:HB2	2.49	0.47
1:G:67:ASN:H	1:G:71:THR:HG21	1.79	0.47
4:K:131:ALA:CB	4:K:186:TRP:HE1	2.28	0.47
5:O:193:ASN:ND2	5:O:204:ASP:OD1	2.48	0.47
1:A:133:ASN:OD1	7:A:636:NAG:N2	2.49	0.46
4:E:131:ALA:CB	4:E:186:TRP:HE1	2.28	0.46
4:K:78:VAL:HG11	4:K:106:VAL:HG11	1.97	0.46
1:G:204:VAL:HG12	1:G:204:VAL:O	2.15	0.46
1:M:133:ASN:OD1	7:M:636:NAG:N2	2.49	0.46
3:J:47:TRP:CE3	4:K:96:TRP:CD1	3.04	0.46
3:D:149:TRP:CD1	3:D:177:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:204:VAL:HG12	1:M:204:VAL:O	2.15	0.46
3:P:47:TRP:CE3	4:Q:96:TRP:CD1	3.04	0.46
1:A:67:ASN:H	1:A:71:THR:HG21	1.79	0.46
9:G:625:MAN:O6	3:J:100:ARG:NH2	2.44	0.46
1:G:133:ASN:OD1	7:G:636:NAG:N2	2.49	0.46
3:J:149:TRP:CD1	3:J:177:VAL:HG21	2.51	0.46
4:Q:131:ALA:CB	4:Q:186:TRP:HE1	2.28	0.46
3:D:47:TRP:CE3	4:E:96:TRP:CD1	3.04	0.46
1:A:204:VAL:O	1:A:204:VAL:HG12	2.15	0.46
1:G:56:SER:CB	1:G:74:CYS:SG	3.04	0.46
5:I:193:ASN:ND2	5:I:204:ASP:OD1	2.48	0.45
3:P:149:TRP:CD1	3:P:177:VAL:HG21	2.51	0.45
1:A:162:THR:CG2	1:A:166:ARG:HA	2.47	0.45
1:A:56:SER:CB	1:A:74:CYS:SG	3.04	0.45
6:F:181:LEU:N	6:F:186:TYR:OH	2.43	0.45
4:Q:78:VAL:HG11	4:Q:106:VAL:HG11	1.97	0.45
9:A:625:MAN:O6	3:D:100:ARG:NH2	2.44	0.45
5:C:193:ASN:ND2	5:C:204:ASP:OD1	2.48	0.45
6:F:151:ASP:HB2	6:F:189:HIS:HB3	1.99	0.45
4:E:78:VAL:HG11	4:E:106:VAL:HG11	1.97	0.45
1:A:56:SER:HB3	1:A:74:CYS:CB	2.47	0.45
1:G:162:THR:CG2	1:G:166:ARG:HA	2.47	0.45
3:P:189:TYR:O	3:P:206:VAL:HG23	2.17	0.45
3:D:34:TRP:CD2	3:D:94:THR:HG22	2.52	0.45
6:L:151:ASP:HB2	6:L:189:HIS:HB3	1.99	0.45
1:M:56:SER:CB	1:M:74:CYS:SG	3.04	0.45
3:P:34:TRP:CD2	3:P:94:THR:HG22	2.52	0.45
6:R:151:ASP:HB2	6:R:189:HIS:HB3	1.99	0.45
1:M:162:THR:CG2	1:M:166:ARG:HA	2.47	0.44
4:E:20:ARG:NH1	4:E:74:THR:OG1	2.50	0.44
5:I:143:PRO:O	5:I:196:HIS:NE2	2.44	0.44
1:M:118:PRO:HB3	2:N:563:GLN:NE2	2.33	0.44
1:M:350:ARG:NH1	1:M:397:SER:OG	2.50	0.44
1:A:118:PRO:HB3	2:B:563:GLN:NE2	2.32	0.44
1:G:56:SER:HB3	1:G:74:CYS:CB	2.47	0.44
1:G:118:PRO:HB3	2:H:563:GLN:NE2	2.32	0.44
3:J:34:TRP:CD2	3:J:94:THR:HG22	2.52	0.44
4:Q:20:ARG:NH1	4:Q:74:THR:OG1	2.51	0.44
1:A:405:SER:OG	1:A:406:ASN:N	2.50	0.44
3:D:189:TYR:O	3:D:206:VAL:HG23	2.17	0.44
5:C:35:HIS:CE1	5:C:100(D):PHE:CE1	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:125:ALA:CB	3:J:207:GLU:O	2.66	0.44
3:J:189:TYR:O	3:J:206:VAL:HG23	2.17	0.44
4:K:152:ASP:OD1	4:K:191:SER:OG	2.35	0.44
5:O:119:PRO:HG3	5:O:196:HIS:HB2	2.00	0.44
3:P:164:VAL:HG21	4:Q:178:TYR:CB	2.48	0.44
5:O:35:HIS:CE1	5:O:100(D):PHE:CE1	3.06	0.44
5:I:119:PRO:HG3	5:I:196:HIS:HB2	2.00	0.43
4:K:20:ARG:NH1	4:K:74:THR:OG1	2.50	0.43
5:C:119:PRO:HG3	5:C:196:HIS:HB2	2.00	0.43
1:M:56:SER:HB3	1:M:74:CYS:CB	2.47	0.43
3:P:125:ALA:CB	3:P:207:GLU:O	2.66	0.43
5:C:143:PRO:O	5:C:196:HIS:NE2	2.44	0.43
5:C:162:PHE:CZ	6:F:176:SER:HB2	2.54	0.43
1:G:350:ARG:NH1	1:G:397:SER:OG	2.50	0.43
3:P:16:GLU:H	3:P:82(C):VAL:HG12	1.83	0.43
4:Q:140:PHE:HB2	4:Q:173:TYR:HB2	2.01	0.43
3:D:157:GLY:O	3:D:177:VAL:HA	2.19	0.43
5:I:35:HIS:CE1	5:I:100(D):PHE:CE1	3.06	0.43
3:D:125:ALA:CB	3:D:207:GLU:O	2.66	0.43
5:O:16:SER:OG	5:O:17:SER:N	2.52	0.43
4:E:140:PHE:HB2	4:E:173:TYR:HB2	2.01	0.43
4:E:83:GLU:OE1	4:E:167:LYS:NZ	2.47	0.43
3:J:34:TRP:CZ3	3:J:94:THR:HG23	2.54	0.43
1:A:350:ARG:NH1	1:A:397:SER:OG	2.50	0.43
4:E:119:PHE:CE2	4:E:136:LEU:HD12	2.54	0.43
3:J:147:VAL:HG22	3:J:193:VAL:HG22	2.01	0.43
1:M:117:LYS:CB	1:M:118:PRO:HD3	2.49	0.43
4:E:152:ASP:OD1	4:E:191:SER:OG	2.35	0.43
1:G:117:LYS:CB	1:G:118:PRO:HD3	2.49	0.42
5:C:20:ILE:CD1	5:C:90:TYR:HD2	2.32	0.42
3:J:164:VAL:HG21	4:K:178:TYR:CB	2.48	0.42
4:K:140:PHE:HB2	4:K:173:TYR:HB2	2.01	0.42
3:J:8:GLY:HA2	3:J:9:PRO:HD3	1.92	0.42
4:K:119:PHE:CE2	4:K:136:LEU:HD12	2.54	0.42
1:A:117:LYS:CB	1:A:118:PRO:HD3	2.49	0.42
3:P:147:VAL:HG22	3:P:193:VAL:HG22	2.01	0.42
4:Q:83:GLU:OE1	4:Q:167:LYS:NZ	2.47	0.42
3:J:16:GLU:H	3:J:82(C):VAL:HG12	1.83	0.42
3:D:164:VAL:HG21	4:E:178:TYR:CB	2.48	0.42
4:K:197:THR:HA	4:K:201:SER:O	2.20	0.42
4:Q:197:THR:HA	4:Q:201:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:20:ILE:CD1	5:O:90:TYR:HD2	2.32	0.42
5:O:162:PHE:CZ	6:R:176:SER:HB2	2.54	0.42
4:E:197:THR:HA	4:E:201:SER:O	2.20	0.42
5:I:162:PHE:CZ	6:L:176:SER:HB2	2.54	0.42
3:J:157:GLY:O	3:J:177:VAL:HA	2.19	0.42
3:P:157:GLY:O	3:P:177:VAL:HA	2.19	0.42
4:Q:119:PHE:CE2	4:Q:136:LEU:HD12	2.54	0.42
1:A:45:TRP:HE1	2:B:523:LEU:HD22	1.85	0.42
1:M:45:TRP:HE1	2:N:523:LEU:HD22	1.85	0.42
3:P:34:TRP:CZ3	3:P:94:THR:HG23	2.54	0.42
3:D:34:TRP:CZ3	3:D:94:THR:HG23	2.54	0.41
1:A:370:GLU:HG3	5:C:54:TRP:CZ3	2.56	0.41
5:C:16:SER:OG	5:C:17:SER:N	2.52	0.41
5:I:20:ILE:CD1	5:I:90:TYR:HD2	2.32	0.41
3:D:147:VAL:HG22	3:D:193:VAL:HG22	2.01	0.41
3:D:16:GLU:H	3:D:82(C):VAL:HG12	1.83	0.41
1:G:70:ALA:O	1:G:71:THR:O	2.39	0.41
1:M:70:ALA:O	1:M:71:THR:O	2.39	0.41
5:I:16:SER:OG	5:I:17:SER:N	2.52	0.41
7:A:632:NAG:H4	7:A:633:NAG:H2	1.92	0.41
1:A:70:ALA:O	1:A:71:THR:O	2.39	0.41
1:G:370:GLU:HG3	5:I:54:TRP:CZ3	2.56	0.41
1:G:45:TRP:HE1	2:H:523:LEU:HD22	1.85	0.41
5:I:7:SER:HA	5:I:8:GLY:HA2	1.88	0.41
1:M:45:TRP:HE1	2:N:523:LEU:CD2	2.34	0.41
1:G:45:TRP:HE1	2:H:523:LEU:CD2	2.34	0.41
4:E:108:GLN:HB3	4:E:141:TYR:CZ	2.56	0.41
4:K:108:GLN:HB3	4:K:141:TYR:CZ	2.56	0.40
7:G:632:NAG:H4	7:G:633:NAG:H2	1.92	0.40
4:K:83:GLU:OE1	4:K:167:LYS:NZ	2.47	0.40
1:A:45:TRP:HE1	2:B:523:LEU:CD2	2.34	0.40
2:H:617:ARG:HG3	2:H:618:ASN:H	1.86	0.40
4:Q:108:GLN:HB3	4:Q:141:TYR:CZ	2.56	0.40
1:M:370:GLU:HG3	5:O:54:TRP:CZ3	2.56	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	441/472 (93%)	399 (90%)	38 (9%)	4 (1%)	19	52
1	G	441/472 (93%)	399 (90%)	38 (9%)	4 (1%)	19	52
1	M	441/472 (93%)	399 (90%)	38 (9%)	4 (1%)	19	52
2	B	145/147 (99%)	131 (90%)	10 (7%)	4 (3%)	5	21
2	H	145/147 (99%)	131 (90%)	10 (7%)	4 (3%)	5	21
2	N	145/147 (99%)	131 (90%)	10 (7%)	4 (3%)	5	21
3	D	226/235 (96%)	213 (94%)	13 (6%)	0	100	100
3	J	226/235 (96%)	214 (95%)	12 (5%)	0	100	100
3	P	226/235 (96%)	213 (94%)	13 (6%)	0	100	100
4	E	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	31	65
4	K	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	31	65
4	Q	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	31	65
5	C	223/231 (96%)	208 (93%)	15 (7%)	0	100	100
5	I	223/231 (96%)	208 (93%)	15 (7%)	0	100	100
5	O	223/231 (96%)	208 (93%)	15 (7%)	0	100	100
6	F	206/208 (99%)	191 (93%)	15 (7%)	0	100	100
6	L	206/208 (99%)	191 (93%)	15 (7%)	0	100	100
6	R	206/208 (99%)	191 (93%)	15 (7%)	0	100	100
All	All	4350/4512 (96%)	3997 (92%)	326 (8%)	27 (1%)	31	61

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	503	ARG
2	B	617	ARG
1	G	71	THR

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Mol	Chain	Res	Type
1	G	503	ARG
2	H	617	ARG
1	M	71	THR
1	M	503	ARG
2	N	617	ARG
1	A	73	ALA
1	G	73	ALA
1	M	73	ALA
1	A	277	ILE
2	B	561	ALA
2	B	564	HIS
2	B	619	LEU
4	E	66(C)	ASN
1	G	277	ILE
2	H	561	ALA
2	H	564	HIS
2	H	619	LEU
4	K	66(C)	ASN
1	M	277	ILE
2	N	561	ALA
2	N	564	HIS
2	N	619	LEU
4	Q	66(C)	ASN

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	401/421 (95%)	393 (98%)	8 (2%)	58	85
1	G	401/421 (95%)	393 (98%)	8 (2%)	58	85
1	M	401/421 (95%)	393 (98%)	8 (2%)	58	85
2	B	127/127 (100%)	126 (99%)	1 (1%)	83	95
2	H	127/127 (100%)	126 (99%)	1 (1%)	83	95
2	N	127/127 (100%)	126 (99%)	1 (1%)	83	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	202/205 (98%)	202 (100%)	0	100	100
3	J	202/205 (98%)	202 (100%)	0	100	100
3	P	202/205 (98%)	202 (100%)	0	100	100
4	E	175/175 (100%)	174 (99%)	1 (1%)	87	96
4	K	175/175 (100%)	174 (99%)	1 (1%)	87	96
4	Q	175/175 (100%)	174 (99%)	1 (1%)	87	96
5	C	194/198 (98%)	193 (100%)	1 (0%)	90	97
5	I	194/198 (98%)	193 (100%)	1 (0%)	90	97
5	O	194/198 (98%)	193 (100%)	1 (0%)	90	97
6	F	181/181 (100%)	181 (100%)	0	100	100
6	L	181/181 (100%)	181 (100%)	0	100	100
6	R	181/181 (100%)	181 (100%)	0	100	100
All	All	3840/3921 (98%)	3807 (99%)	33 (1%)	82	94

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	54	CYS
1	A	68	ILE
1	A	72	HIS
1	A	75	VAL
1	A	77	THR
1	A	204	VAL
1	A	456	ARG
2	B	588	ARG
4	E	54	ARG
5	C	71	ARG
1	G	53	PHE
1	G	54	CYS
1	G	68	ILE
1	G	72	HIS
1	G	75	VAL
1	G	77	THR
1	G	204	VAL
1	G	456	ARG
2	H	588	ARG
4	K	54	ARG

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Mol	Chain	Res	Type
5	I	71	ARG
1	M	53	PHE
1	M	54	CYS
1	M	68	ILE
1	M	72	HIS
1	M	75	VAL
1	M	77	THR
1	M	204	VAL
1	M	456	ARG
2	N	588	ARG
4	Q	54	ARG
5	O	71	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
2	B	554	ASN
2	B	563	GLN
3	D	76	ASN
4	E	50	ASN
4	E	89	HIS
5	C	35	HIS
6	F	198	HIS
1	G	66	HIS
1	G	186	ASN
2	H	554	ASN
2	H	563	GLN
3	J	76	ASN
4	K	50	ASN
4	K	89	HIS
5	I	35	HIS
6	L	198	HIS
1	M	66	HIS
2	N	554	ASN
2	N	563	GLN
3	P	76	ASN
4	Q	50	ASN
4	Q	89	HIS
5	O	35	HIS
6	R	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

120 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	601	1,7	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
7	NAG	A	602	7	14,14,15	0.26	0	17,19,21	0.64	1 (5%)
7	NAG	A	603	1	14,14,15	0.41	0	17,19,21	0.53	0
7	NAG	A	604	1,7	14,14,15	0.21	0	17,19,21	0.47	0
7	NAG	A	605	8,7	14,14,15	0.33	0	17,19,21	0.50	0
8	BMA	A	606	7	11,11,12	0.84	0	15,15,17	0.76	0
7	NAG	A	607	1	14,14,15	0.33	0	17,19,21	0.45	0
7	NAG	A	608	1	14,14,15	0.46	0	17,19,21	0.96	1 (5%)
7	NAG	A	609	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
7	NAG	A	610	1,7	14,14,15	0.73	1 (7%)	17,19,21	1.16	1 (5%)
7	NAG	A	611	7	14,14,15	0.27	0	17,19,21	0.56	0
7	NAG	A	612	1,7	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
7	NAG	A	613	7	14,14,15	0.40	0	17,19,21	0.56	0
7	NAG	A	614	1,7	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
7	NAG	A	615	7	14,14,15	0.79	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	A	616	1,7	14,14,15	0.22	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	617	7	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	A	618	1,7	14,14,15	0.21	0	17,19,21	0.64	1 (5%)
7	NAG	A	619	7	14,14,15	0.25	0	17,19,21	0.42	0
7	NAG	A	620	1,7	14,14,15	0.58	0	17,19,21	0.55	0
7	NAG	A	621	8,7	14,14,15	0.24	0	17,19,21	0.66	0
8	BMA	A	622	9,7	11,11,12	0.97	0	15,15,17	1.92	4 (26%)
9	MAN	A	623	9,8	11,11,12	0.60	0	15,15,17	1.13	1 (6%)
9	MAN	A	624	9	11,11,12	0.72	0	15,15,17	1.24	2 (13%)
9	MAN	A	625	9,8	11,11,12	0.97	0	15,15,17	1.62	2 (13%)
9	MAN	A	626	9	11,11,12	0.63	0	15,15,17	1.05	1 (6%)
9	MAN	A	627	9	11,11,12	1.02	1 (9%)	15,15,17	1.57	2 (13%)
7	NAG	A	628	1,7	14,14,15	0.46	0	17,19,21	0.52	0
7	NAG	A	629	8,7	14,14,15	0.38	0	17,19,21	0.45	0
8	BMA	A	630	9,7	11,11,12	0.60	0	15,15,17	0.76	0
9	MAN	A	631	8	11,11,12	0.88	0	15,15,17	1.13	2 (13%)
7	NAG	A	632	1,7	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
7	NAG	A	633	7	14,14,15	0.59	0	17,19,21	0.80	1 (5%)
7	NAG	A	634	1,7	14,14,15	0.33	0	17,19,21	0.53	0
7	NAG	A	635	7	14,14,15	0.32	0	17,19,21	0.47	0
7	NAG	A	636	1,7	14,14,15	0.67	0	17,19,21	0.86	1 (5%)
7	NAG	A	637	7	14,14,15	0.52	0	17,19,21	0.94	1 (5%)
7	NAG	B	701	2	14,14,15	0.28	0	17,19,21	0.57	0
7	NAG	B	702	2	14,14,15	0.67	0	17,19,21	2.27	4 (23%)
7	NAG	B	703	2	14,14,15	0.70	0	17,19,21	2.21	3 (17%)
7	NAG	G	601	1,7	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
7	NAG	G	602	7	14,14,15	0.25	0	17,19,21	0.63	1 (5%)
7	NAG	G	603	1	14,14,15	0.40	0	17,19,21	0.53	0
7	NAG	G	604	1,7	14,14,15	0.21	0	17,19,21	0.47	0
7	NAG	G	605	8,7	14,14,15	0.33	0	17,19,21	0.50	0
8	BMA	G	606	7	11,11,12	0.84	0	15,15,17	0.75	0
7	NAG	G	607	1	14,14,15	0.32	0	17,19,21	0.45	0
7	NAG	G	608	1	14,14,15	0.47	0	17,19,21	0.96	1 (5%)
7	NAG	G	609	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
7	NAG	G	610	1,7	14,14,15	0.73	1 (7%)	17,19,21	1.16	1 (5%)
7	NAG	G	611	7	14,14,15	0.27	0	17,19,21	0.56	0
7	NAG	G	612	1,7	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
7	NAG	G	613	7	14,14,15	0.40	0	17,19,21	0.56	0
7	NAG	G	614	1,7	14,14,15	0.30	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	615	7	14,14,15	0.79	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	G	616	1,7	14,14,15	0.22	0	17,19,21	0.55	0
7	NAG	G	617	7	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	G	618	1,7	14,14,15	0.21	0	17,19,21	0.64	1 (5%)
7	NAG	G	619	7	14,14,15	0.25	0	17,19,21	0.43	0
7	NAG	G	620	1,7	14,14,15	0.57	0	17,19,21	0.55	0
7	NAG	G	621	8,7	14,14,15	0.25	0	17,19,21	0.66	0
8	BMA	G	622	9,7	11,11,12	0.98	0	15,15,17	1.92	4 (26%)
9	MAN	G	623	9,8	11,11,12	0.60	0	15,15,17	1.12	1 (6%)
9	MAN	G	624	9	11,11,12	0.73	0	15,15,17	1.23	2 (13%)
9	MAN	G	625	9,8	11,11,12	0.97	0	15,15,17	1.62	2 (13%)
9	MAN	G	626	9	11,11,12	0.64	0	15,15,17	1.06	1 (6%)
9	MAN	G	627	9	11,11,12	1.02	1 (9%)	15,15,17	1.57	2 (13%)
7	NAG	G	628	1,7	14,14,15	0.46	0	17,19,21	0.52	0
7	NAG	G	629	8,7	14,14,15	0.38	0	17,19,21	0.45	0
8	BMA	G	630	9,7	11,11,12	0.59	0	15,15,17	0.75	0
9	MAN	G	631	8	11,11,12	0.86	0	15,15,17	1.13	2 (13%)
7	NAG	G	632	1,7	14,14,15	0.38	0	17,19,21	0.74	1 (5%)
7	NAG	G	633	7	14,14,15	0.59	0	17,19,21	0.80	1 (5%)
7	NAG	G	634	1,7	14,14,15	0.33	0	17,19,21	0.54	0
7	NAG	G	635	7	14,14,15	0.32	0	17,19,21	0.46	0
7	NAG	G	636	1,7	14,14,15	0.66	0	17,19,21	0.86	1 (5%)
7	NAG	G	637	7	14,14,15	0.52	0	17,19,21	0.94	1 (5%)
7	NAG	H	701	2	14,14,15	0.28	0	17,19,21	0.57	0
7	NAG	H	702	2	14,14,15	0.66	0	17,19,21	2.26	4 (23%)
7	NAG	H	703	2	14,14,15	0.70	0	17,19,21	2.21	3 (17%)
7	NAG	M	601	1,7	14,14,15	0.50	0	17,19,21	0.99	0
7	NAG	M	602	7	14,14,15	0.25	0	17,19,21	0.64	1 (5%)
7	NAG	M	603	1	14,14,15	0.42	0	17,19,21	0.53	0
7	NAG	M	604	1,7	14,14,15	0.23	0	17,19,21	0.47	0
7	NAG	M	605	8,7	14,14,15	0.32	0	17,19,21	0.50	0
8	BMA	M	606	7	11,11,12	0.83	0	15,15,17	0.76	0
7	NAG	M	607	1	14,14,15	0.33	0	17,19,21	0.45	0
7	NAG	M	608	1	14,14,15	0.46	0	17,19,21	0.95	1 (5%)
7	NAG	M	609	1	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
7	NAG	M	610	1,7	14,14,15	0.74	1 (7%)	17,19,21	1.15	1 (5%)
7	NAG	M	611	7	14,14,15	0.28	0	17,19,21	0.56	0
7	NAG	M	612	1,7	14,14,15	0.29	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	M	613	7	14,14,15	0.40	0	17,19,21	0.56	0
7	NAG	M	614	1,7	14,14,15	0.29	0	17,19,21	0.96	1 (5%)
7	NAG	M	615	7	14,14,15	0.79	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	M	616	1,7	14,14,15	0.22	0	17,19,21	0.54	0
7	NAG	M	617	7	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	M	618	1,7	14,14,15	0.21	0	17,19,21	0.64	1 (5%)
7	NAG	M	619	7	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	M	620	1,7	14,14,15	0.58	0	17,19,21	0.55	0
7	NAG	M	621	8,7	14,14,15	0.25	0	17,19,21	0.66	0
8	BMA	M	622	9,7	11,11,12	0.96	0	15,15,17	1.92	4 (26%)
9	MAN	M	623	9,8	11,11,12	0.60	0	15,15,17	1.13	1 (6%)
9	MAN	M	624	9	11,11,12	0.73	0	15,15,17	1.24	2 (13%)
9	MAN	M	625	9,8	11,11,12	0.97	0	15,15,17	1.61	2 (13%)
9	MAN	M	626	9	11,11,12	0.62	0	15,15,17	1.05	1 (6%)
9	MAN	M	627	9	11,11,12	1.02	1 (9%)	15,15,17	1.56	2 (13%)
7	NAG	M	628	1,7	14,14,15	0.46	0	17,19,21	0.52	0
7	NAG	M	629	8,7	14,14,15	0.38	0	17,19,21	0.45	0
8	BMA	M	630	9,7	11,11,12	0.60	0	15,15,17	0.76	0
9	MAN	M	631	8	11,11,12	0.88	0	15,15,17	1.13	2 (13%)
7	NAG	M	632	1,7	14,14,15	0.38	0	17,19,21	0.75	1 (5%)
7	NAG	M	633	7	14,14,15	0.59	0	17,19,21	0.80	1 (5%)
7	NAG	M	634	1,7	14,14,15	0.34	0	17,19,21	0.53	0
7	NAG	M	635	7	14,14,15	0.33	0	17,19,21	0.46	0
7	NAG	M	636	1,7	14,14,15	0.68	0	17,19,21	0.86	1 (5%)
7	NAG	M	637	7	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
7	NAG	N	701	2	14,14,15	0.26	0	17,19,21	0.57	0
7	NAG	N	702	2	14,14,15	0.67	0	17,19,21	2.26	4 (23%)
7	NAG	N	703	2	14,14,15	0.70	0	17,19,21	2.21	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	601	1,7	-	3/6/23/26	0/1/1/1
7	NAG	A	602	7	-	2/6/23/26	0/1/1/1
7	NAG	A	603	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	604	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	605	8,7	-	1/6/23/26	0/1/1/1
8	BMA	A	606	7	-	0/2/19/22	0/1/1/1
7	NAG	A	607	1	-	2/6/23/26	0/1/1/1
7	NAG	A	608	1	-	1/6/23/26	0/1/1/1
7	NAG	A	609	1	-	0/6/23/26	0/1/1/1
7	NAG	A	610	1,7	-	3/6/23/26	0/1/1/1
7	NAG	A	611	7	-	2/6/23/26	0/1/1/1
7	NAG	A	612	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	613	7	-	2/6/23/26	0/1/1/1
7	NAG	A	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	615	7	-	3/6/23/26	0/1/1/1
7	NAG	A	616	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	617	7	-	0/6/23/26	0/1/1/1
7	NAG	A	618	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	619	7	-	0/6/23/26	0/1/1/1
7	NAG	A	620	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	621	8,7	-	0/6/23/26	0/1/1/1
8	BMA	A	622	9,7	-	2/2/19/22	0/1/1/1
9	MAN	A	623	9,8	-	1/2/19/22	0/1/1/1
9	MAN	A	624	9	-	2/2/19/22	0/1/1/1
9	MAN	A	625	9,8	-	2/2/19/22	0/1/1/1
9	MAN	A	626	9	-	1/2/19/22	0/1/1/1
9	MAN	A	627	9	-	2/2/19/22	0/1/1/1
7	NAG	A	628	1,7	-	1/6/23/26	0/1/1/1
7	NAG	A	629	8,7	-	2/6/23/26	0/1/1/1
8	BMA	A	630	9,7	-	1/2/19/22	0/1/1/1
9	MAN	A	631	8	-	2/2/19/22	1/1/1/1
7	NAG	A	632	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	633	7	-	2/6/23/26	0/1/1/1
7	NAG	A	634	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	635	7	-	2/6/23/26	0/1/1/1
7	NAG	A	636	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	637	7	-	3/6/23/26	0/1/1/1
7	NAG	B	701	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	5/6/23/26	0/1/1/1
7	NAG	B	703	2	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	601	1,7	-	3/6/23/26	0/1/1/1
7	NAG	G	602	7	-	2/6/23/26	0/1/1/1
7	NAG	G	603	1	-	1/6/23/26	0/1/1/1
7	NAG	G	604	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	605	8,7	-	1/6/23/26	0/1/1/1
8	BMA	G	606	7	-	0/2/19/22	0/1/1/1
7	NAG	G	607	1	-	2/6/23/26	0/1/1/1
7	NAG	G	608	1	-	1/6/23/26	0/1/1/1
7	NAG	G	609	1	-	0/6/23/26	0/1/1/1
7	NAG	G	610	1,7	-	3/6/23/26	0/1/1/1
7	NAG	G	611	7	-	2/6/23/26	0/1/1/1
7	NAG	G	612	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	613	7	-	2/6/23/26	0/1/1/1
7	NAG	G	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	615	7	-	3/6/23/26	0/1/1/1
7	NAG	G	616	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	617	7	-	0/6/23/26	0/1/1/1
7	NAG	G	618	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	619	7	-	0/6/23/26	0/1/1/1
7	NAG	G	620	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	621	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	622	9,7	-	2/2/19/22	0/1/1/1
9	MAN	G	623	9,8	-	1/2/19/22	0/1/1/1
9	MAN	G	624	9	-	2/2/19/22	0/1/1/1
9	MAN	G	625	9,8	-	2/2/19/22	0/1/1/1
9	MAN	G	626	9	-	1/2/19/22	0/1/1/1
9	MAN	G	627	9	-	2/2/19/22	0/1/1/1
7	NAG	G	628	1,7	-	1/6/23/26	0/1/1/1
7	NAG	G	629	8,7	-	2/6/23/26	0/1/1/1
8	BMA	G	630	9,7	-	1/2/19/22	0/1/1/1
9	MAN	G	631	8	-	2/2/19/22	1/1/1/1
7	NAG	G	632	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	633	7	-	2/6/23/26	0/1/1/1
7	NAG	G	634	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	635	7	-	2/6/23/26	0/1/1/1
7	NAG	G	636	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	637	7	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	H	701	2	-	0/6/23/26	0/1/1/1
7	NAG	H	702	2	-	5/6/23/26	0/1/1/1
7	NAG	H	703	2	-	5/6/23/26	0/1/1/1
7	NAG	M	601	1,7	-	3/6/23/26	0/1/1/1
7	NAG	M	602	7	-	2/6/23/26	0/1/1/1
7	NAG	M	603	1	-	1/6/23/26	0/1/1/1
7	NAG	M	604	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	605	8,7	-	1/6/23/26	0/1/1/1
8	BMA	M	606	7	-	0/2/19/22	0/1/1/1
7	NAG	M	607	1	-	2/6/23/26	0/1/1/1
7	NAG	M	608	1	-	1/6/23/26	0/1/1/1
7	NAG	M	609	1	-	0/6/23/26	0/1/1/1
7	NAG	M	610	1,7	-	3/6/23/26	0/1/1/1
7	NAG	M	611	7	-	2/6/23/26	0/1/1/1
7	NAG	M	612	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	613	7	-	2/6/23/26	0/1/1/1
7	NAG	M	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	M	615	7	-	3/6/23/26	0/1/1/1
7	NAG	M	616	1,7	-	0/6/23/26	0/1/1/1
7	NAG	M	617	7	-	0/6/23/26	0/1/1/1
7	NAG	M	618	1,7	-	0/6/23/26	0/1/1/1
7	NAG	M	619	7	-	0/6/23/26	0/1/1/1
7	NAG	M	620	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	621	8,7	-	0/6/23/26	0/1/1/1
8	BMA	M	622	9,7	-	2/2/19/22	0/1/1/1
9	MAN	M	623	9,8	-	1/2/19/22	0/1/1/1
9	MAN	M	624	9	-	2/2/19/22	0/1/1/1
9	MAN	M	625	9,8	-	2/2/19/22	0/1/1/1
9	MAN	M	626	9	-	2/2/19/22	0/1/1/1
9	MAN	M	627	9	-	2/2/19/22	0/1/1/1
7	NAG	M	628	1,7	-	1/6/23/26	0/1/1/1
7	NAG	M	629	8,7	-	2/6/23/26	0/1/1/1
8	BMA	M	630	9,7	-	1/2/19/22	0/1/1/1
9	MAN	M	631	8	-	2/2/19/22	1/1/1/1
7	NAG	M	632	1,7	-	0/6/23/26	0/1/1/1
7	NAG	M	633	7	-	2/6/23/26	0/1/1/1
7	NAG	M	634	1,7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	M	635	7	-	2/6/23/26	0/1/1/1
7	NAG	M	636	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	637	7	-	3/6/23/26	0/1/1/1
7	NAG	N	701	2	-	0/6/23/26	0/1/1/1
7	NAG	N	702	2	-	5/6/23/26	0/1/1/1
7	NAG	N	703	2	-	5/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	627	MAN	O5-C5	3.17	1.50	1.43
9	G	627	MAN	O5-C5	3.16	1.50	1.43
9	M	627	MAN	O5-C5	3.15	1.49	1.43
7	M	610	NAG	O5-C1	-2.59	1.39	1.43
7	G	610	NAG	O5-C1	-2.58	1.39	1.43
7	A	610	NAG	O5-C1	-2.56	1.39	1.43
7	G	615	NAG	C1-C2	2.37	1.55	1.52
7	M	615	NAG	C1-C2	2.35	1.55	1.52
7	A	615	NAG	C1-C2	2.35	1.55	1.52

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	702	NAG	C2-N2-C7	7.77	134.06	122.92
7	H	702	NAG	C2-N2-C7	7.76	134.03	122.92
7	N	702	NAG	C2-N2-C7	7.74	134.01	122.92
7	H	703	NAG	C2-N2-C7	7.64	133.87	122.92
7	B	703	NAG	C2-N2-C7	7.63	133.86	122.92
7	N	703	NAG	C2-N2-C7	7.63	133.85	122.92
9	G	625	MAN	C1-O5-C5	5.12	119.17	112.20
9	A	625	MAN	C1-O5-C5	5.12	119.16	112.20
9	M	625	MAN	C1-O5-C5	5.09	119.12	112.20
9	A	627	MAN	C1-O5-C5	4.85	118.79	112.20
9	G	627	MAN	C1-O5-C5	4.84	118.78	112.20
9	M	627	MAN	C1-O5-C5	4.82	118.75	112.20
8	M	622	BMA	C1-O5-C5	4.51	118.34	112.20
8	G	622	BMA	C1-O5-C5	4.51	118.33	112.20
8	A	622	BMA	C1-O5-C5	4.48	118.30	112.20
7	H	703	NAG	C1-C2-N2	3.83	117.03	110.49
7	B	703	NAG	C1-C2-N2	3.81	117.00	110.49
7	N	703	NAG	C1-C2-N2	3.81	116.99	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	624	MAN	C1-O5-C5	3.74	117.29	112.20
9	A	624	MAN	C1-O5-C5	3.74	117.29	112.20
9	G	624	MAN	C1-O5-C5	3.73	117.27	112.20
7	B	702	NAG	C1-C2-N2	3.45	116.39	110.49
7	N	702	NAG	C1-C2-N2	3.44	116.36	110.49
7	H	702	NAG	C1-C2-N2	3.43	116.34	110.49
7	G	610	NAG	C2-N2-C7	3.25	127.58	122.92
7	A	610	NAG	C2-N2-C7	3.25	127.57	122.92
7	M	610	NAG	C2-N2-C7	3.23	127.55	122.92
7	M	614	NAG	C1-O5-C5	3.18	116.52	112.20
7	A	614	NAG	C1-O5-C5	3.17	116.52	112.20
8	A	622	BMA	O5-C1-C2	3.17	115.67	110.79
8	M	622	BMA	O5-C1-C2	3.15	115.65	110.79
7	G	614	NAG	C1-O5-C5	3.15	116.48	112.20
8	G	622	BMA	O5-C1-C2	3.15	115.64	110.79
8	G	622	BMA	C1-C2-C3	3.03	113.38	109.66
8	A	622	BMA	C1-C2-C3	3.02	113.37	109.66
8	M	622	BMA	C1-C2-C3	3.02	113.37	109.66
7	M	615	NAG	C2-N2-C7	2.99	127.20	122.92
7	G	615	NAG	C2-N2-C7	2.97	127.18	122.92
7	A	615	NAG	C2-N2-C7	2.97	127.18	122.92
7	G	633	NAG	C1-O5-C5	2.97	116.24	112.20
7	M	633	NAG	C1-O5-C5	2.94	116.20	112.20
7	A	633	NAG	C1-O5-C5	2.94	116.20	112.20
7	G	637	NAG	C2-N2-C7	2.94	127.13	122.92
7	G	608	NAG	C2-N2-C7	2.93	127.13	122.92
7	M	637	NAG	C2-N2-C7	2.92	127.11	122.92
7	A	608	NAG	C2-N2-C7	2.92	127.10	122.92
7	A	637	NAG	C2-N2-C7	2.91	127.09	122.92
7	M	608	NAG	C2-N2-C7	2.91	127.09	122.92
9	M	631	MAN	C1-O5-C5	2.90	116.15	112.20
9	G	631	MAN	C1-O5-C5	2.90	116.14	112.20
9	A	631	MAN	C1-O5-C5	2.89	116.13	112.20
9	G	626	MAN	C1-O5-C5	2.87	116.10	112.20
9	A	626	MAN	C1-O5-C5	2.85	116.08	112.20
9	M	626	MAN	C1-O5-C5	2.83	116.05	112.20
7	M	612	NAG	C1-O5-C5	2.76	115.95	112.20
7	A	612	NAG	C1-O5-C5	2.75	115.94	112.20
7	G	612	NAG	C1-O5-C5	2.73	115.92	112.20
9	A	631	MAN	O2-C2-C3	-2.72	104.84	110.16
9	G	631	MAN	O2-C2-C3	-2.71	104.87	110.16
9	M	631	MAN	O2-C2-C3	-2.70	104.88	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	702	NAG	C1-O5-C5	2.63	115.77	112.20
7	B	702	NAG	C1-O5-C5	2.61	115.76	112.20
7	H	702	NAG	C1-O5-C5	2.59	115.73	112.20
9	G	627	MAN	C1-C2-C3	-2.38	106.73	109.66
9	A	624	MAN	O2-C2-C3	-2.36	105.55	110.16
9	M	624	MAN	O2-C2-C3	-2.36	105.55	110.16
9	G	624	MAN	O2-C2-C3	-2.36	105.56	110.16
9	A	627	MAN	C1-C2-C3	-2.35	106.77	109.66
9	A	623	MAN	O2-C2-C3	-2.35	105.58	110.16
9	M	627	MAN	C1-C2-C3	-2.34	106.78	109.66
9	G	623	MAN	O2-C2-C3	-2.34	105.59	110.16
9	M	623	MAN	O2-C2-C3	-2.34	105.59	110.16
7	H	703	NAG	C8-C7-N2	2.27	120.02	116.10
7	B	703	NAG	C8-C7-N2	2.26	120.00	116.10
7	M	602	NAG	C1-O5-C5	2.26	115.27	112.20
7	N	703	NAG	C8-C7-N2	2.26	119.99	116.10
7	A	602	NAG	C1-O5-C5	2.25	115.27	112.20
8	G	622	BMA	C3-C4-C5	-2.25	106.19	110.23
8	A	622	BMA	C3-C4-C5	-2.25	106.19	110.23
7	M	609	NAG	C1-O5-C5	2.24	115.25	112.20
7	A	609	NAG	C1-O5-C5	2.23	115.23	112.20
8	M	622	BMA	C3-C4-C5	-2.22	106.24	110.23
7	G	609	NAG	C1-O5-C5	2.22	115.22	112.20
7	G	602	NAG	C1-O5-C5	2.20	115.20	112.20
7	M	618	NAG	C1-O5-C5	2.18	115.17	112.20
9	G	625	MAN	O2-C2-C3	-2.18	105.91	110.16
9	M	625	MAN	O2-C2-C3	-2.18	105.91	110.16
7	G	618	NAG	C1-O5-C5	2.16	115.14	112.20
9	A	625	MAN	O2-C2-C3	-2.16	105.94	110.16
7	A	618	NAG	C1-O5-C5	2.16	115.13	112.20
7	M	636	NAG	O4-C4-C5	-2.14	103.94	109.29
7	A	636	NAG	O4-C4-C5	-2.13	103.97	109.29
7	G	636	NAG	O4-C4-C5	-2.12	103.98	109.29
7	N	702	NAG	C8-C7-N2	2.12	119.75	116.10
7	H	702	NAG	C8-C7-N2	2.11	119.75	116.10
7	B	702	NAG	C8-C7-N2	2.11	119.74	116.10
7	M	632	NAG	C1-O5-C5	2.04	114.97	112.20
7	A	632	NAG	C1-O5-C5	2.04	114.97	112.20
7	G	601	NAG	C1-O5-C5	2.03	114.96	112.20
7	G	632	NAG	C1-O5-C5	2.03	114.96	112.20
7	A	601	NAG	C1-O5-C5	2.01	114.94	112.20

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	624	MAN	O5-C5-C6-O6
9	G	624	MAN	O5-C5-C6-O6
9	A	624	MAN	O5-C5-C6-O6
7	M	613	NAG	C4-C5-C6-O6
7	A	613	NAG	C4-C5-C6-O6
7	G	613	NAG	C4-C5-C6-O6
7	B	703	NAG	O5-C5-C6-O6
7	H	703	NAG	O5-C5-C6-O6
7	N	703	NAG	O5-C5-C6-O6
7	M	620	NAG	O5-C5-C6-O6
7	M	613	NAG	O5-C5-C6-O6
7	A	613	NAG	O5-C5-C6-O6
7	G	613	NAG	O5-C5-C6-O6
7	G	620	NAG	O5-C5-C6-O6
7	A	620	NAG	O5-C5-C6-O6
7	G	637	NAG	C4-C5-C6-O6
7	M	637	NAG	C4-C5-C6-O6
7	A	637	NAG	C4-C5-C6-O6
7	N	702	NAG	O5-C5-C6-O6
7	B	702	NAG	O5-C5-C6-O6
7	H	702	NAG	O5-C5-C6-O6
7	A	607	NAG	O5-C5-C6-O6
7	G	607	NAG	O5-C5-C6-O6
7	M	607	NAG	O5-C5-C6-O6
7	A	610	NAG	O5-C5-C6-O6
7	G	615	NAG	O5-C5-C6-O6
7	M	615	NAG	O5-C5-C6-O6
7	G	610	NAG	O5-C5-C6-O6
7	M	610	NAG	O5-C5-C6-O6
7	A	615	NAG	O5-C5-C6-O6
7	A	604	NAG	O5-C5-C6-O6
7	G	604	NAG	O5-C5-C6-O6
7	M	604	NAG	O5-C5-C6-O6
9	M	624	MAN	C4-C5-C6-O6
9	G	624	MAN	C4-C5-C6-O6
9	A	624	MAN	C4-C5-C6-O6
9	G	631	MAN	O5-C5-C6-O6
7	G	635	NAG	O5-C5-C6-O6
9	M	631	MAN	O5-C5-C6-O6
9	A	631	MAN	O5-C5-C6-O6
7	M	635	NAG	O5-C5-C6-O6
7	A	635	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	G	637	NAG	O5-C5-C6-O6
7	M	637	NAG	O5-C5-C6-O6
7	A	637	NAG	O5-C5-C6-O6
7	B	703	NAG	C4-C5-C6-O6
7	H	703	NAG	C4-C5-C6-O6
7	N	703	NAG	C4-C5-C6-O6
7	M	601	NAG	C4-C5-C6-O6
7	A	601	NAG	C4-C5-C6-O6
7	G	601	NAG	C4-C5-C6-O6
7	G	615	NAG	C4-C5-C6-O6
7	M	615	NAG	C4-C5-C6-O6
7	A	615	NAG	C4-C5-C6-O6
7	A	607	NAG	C4-C5-C6-O6
7	G	607	NAG	C4-C5-C6-O6
7	M	607	NAG	C4-C5-C6-O6
7	A	604	NAG	C4-C5-C6-O6
7	G	604	NAG	C4-C5-C6-O6
7	M	604	NAG	C4-C5-C6-O6
7	M	634	NAG	O5-C5-C6-O6
7	G	634	NAG	O5-C5-C6-O6
7	A	634	NAG	O5-C5-C6-O6
8	M	622	BMA	C4-C5-C6-O6
7	G	635	NAG	C4-C5-C6-O6
7	N	702	NAG	C4-C5-C6-O6
7	B	702	NAG	C4-C5-C6-O6
7	H	702	NAG	C4-C5-C6-O6
9	M	627	MAN	C4-C5-C6-O6
8	G	622	BMA	C4-C5-C6-O6
9	G	627	MAN	C4-C5-C6-O6
7	M	635	NAG	C4-C5-C6-O6
8	A	622	BMA	C4-C5-C6-O6
7	A	635	NAG	C4-C5-C6-O6
9	A	627	MAN	C4-C5-C6-O6
7	B	703	NAG	C8-C7-N2-C2
7	B	703	NAG	O7-C7-N2-C2
7	N	702	NAG	C8-C7-N2-C2
7	N	702	NAG	O7-C7-N2-C2
7	B	702	NAG	C8-C7-N2-C2
7	B	702	NAG	O7-C7-N2-C2
7	H	702	NAG	C8-C7-N2-C2
7	H	702	NAG	O7-C7-N2-C2
7	H	703	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	H	703	NAG	O7-C7-N2-C2
7	N	703	NAG	C8-C7-N2-C2
7	N	703	NAG	O7-C7-N2-C2
7	M	601	NAG	O5-C5-C6-O6
7	A	601	NAG	O5-C5-C6-O6
7	G	601	NAG	O5-C5-C6-O6
7	M	620	NAG	C4-C5-C6-O6
7	G	620	NAG	C4-C5-C6-O6
7	A	620	NAG	C4-C5-C6-O6
7	A	610	NAG	C4-C5-C6-O6
7	G	610	NAG	C4-C5-C6-O6
7	M	610	NAG	C4-C5-C6-O6
7	M	629	NAG	O5-C5-C6-O6
7	A	629	NAG	O5-C5-C6-O6
7	G	629	NAG	O5-C5-C6-O6
9	G	631	MAN	C4-C5-C6-O6
9	M	631	MAN	C4-C5-C6-O6
7	G	634	NAG	C4-C5-C6-O6
9	A	631	MAN	C4-C5-C6-O6
7	G	633	NAG	O5-C5-C6-O6
7	M	633	NAG	O5-C5-C6-O6
7	A	633	NAG	O5-C5-C6-O6
7	M	634	NAG	C4-C5-C6-O6
7	A	634	NAG	C4-C5-C6-O6
7	A	602	NAG	O5-C5-C6-O6
7	G	602	NAG	O5-C5-C6-O6
7	M	602	NAG	O5-C5-C6-O6
7	G	633	NAG	C4-C5-C6-O6
7	M	633	NAG	C4-C5-C6-O6
7	A	633	NAG	C4-C5-C6-O6
9	M	627	MAN	O5-C5-C6-O6
9	G	627	MAN	O5-C5-C6-O6
9	A	627	MAN	O5-C5-C6-O6
7	A	602	NAG	C4-C5-C6-O6
7	G	602	NAG	C4-C5-C6-O6
7	M	602	NAG	C4-C5-C6-O6
9	M	625	MAN	O5-C5-C6-O6
8	G	630	BMA	O5-C5-C6-O6
8	M	630	BMA	O5-C5-C6-O6
8	A	630	BMA	O5-C5-C6-O6
9	A	625	MAN	O5-C5-C6-O6
9	G	625	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	M	625	MAN	C4-C5-C6-O6
9	G	625	MAN	C4-C5-C6-O6
9	A	625	MAN	C4-C5-C6-O6
7	M	611	NAG	C4-C5-C6-O6
7	G	611	NAG	C4-C5-C6-O6
7	A	611	NAG	C4-C5-C6-O6
9	M	623	MAN	O5-C5-C6-O6
9	A	623	MAN	O5-C5-C6-O6
9	G	623	MAN	O5-C5-C6-O6
7	G	612	NAG	O5-C5-C6-O6
7	A	612	NAG	O5-C5-C6-O6
7	M	612	NAG	O5-C5-C6-O6
8	M	622	BMA	O5-C5-C6-O6
7	G	603	NAG	O5-C5-C6-O6
8	G	622	BMA	O5-C5-C6-O6
8	A	622	BMA	O5-C5-C6-O6
7	M	603	NAG	O5-C5-C6-O6
7	A	603	NAG	O5-C5-C6-O6
7	G	605	NAG	O5-C5-C6-O6
7	M	605	NAG	O5-C5-C6-O6
7	A	605	NAG	O5-C5-C6-O6
7	M	611	NAG	O5-C5-C6-O6
7	G	611	NAG	O5-C5-C6-O6
7	A	611	NAG	O5-C5-C6-O6
9	M	626	MAN	C4-C5-C6-O6
9	G	626	MAN	C4-C5-C6-O6
9	A	626	MAN	C4-C5-C6-O6
7	M	629	NAG	C4-C5-C6-O6
7	A	629	NAG	C4-C5-C6-O6
7	G	629	NAG	C4-C5-C6-O6
7	G	628	NAG	C4-C5-C6-O6
7	A	628	NAG	C4-C5-C6-O6
7	A	610	NAG	C3-C2-N2-C7
7	N	702	NAG	C3-C2-N2-C7
7	B	702	NAG	C3-C2-N2-C7
7	H	702	NAG	C3-C2-N2-C7
7	G	615	NAG	C3-C2-N2-C7
7	A	608	NAG	C3-C2-N2-C7
7	M	615	NAG	C3-C2-N2-C7
7	G	608	NAG	C3-C2-N2-C7
7	G	610	NAG	C3-C2-N2-C7
7	M	610	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	A	615	NAG	C3-C2-N2-C7
7	M	608	NAG	C3-C2-N2-C7
7	M	628	NAG	C4-C5-C6-O6
7	A	636	NAG	C4-C5-C6-O6
7	G	636	NAG	C4-C5-C6-O6
7	M	636	NAG	C4-C5-C6-O6
7	M	601	NAG	C1-C2-N2-C7
7	A	601	NAG	C1-C2-N2-C7
7	G	601	NAG	C1-C2-N2-C7
7	A	612	NAG	C4-C5-C6-O6
7	G	612	NAG	C4-C5-C6-O6
7	M	612	NAG	C4-C5-C6-O6
7	A	636	NAG	O5-C5-C6-O6
7	M	636	NAG	O5-C5-C6-O6
7	G	636	NAG	O5-C5-C6-O6
7	G	637	NAG	C3-C2-N2-C7
7	B	703	NAG	C3-C2-N2-C7
7	H	703	NAG	C3-C2-N2-C7
7	M	637	NAG	C3-C2-N2-C7
7	A	637	NAG	C3-C2-N2-C7
7	N	703	NAG	C3-C2-N2-C7
9	M	626	MAN	O5-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	631	MAN	C1-C2-C3-C4-C5-O5
9	A	631	MAN	C1-C2-C3-C4-C5-O5
9	M	631	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	603	NAG	1	0
9	A	625	MAN	1	0
7	A	632	NAG	1	0
7	A	633	NAG	1	0
7	A	636	NAG	1	0
7	G	603	NAG	1	0
9	G	625	MAN	1	0
7	G	632	NAG	1	0
7	G	633	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	636	NAG	1	0
7	M	603	NAG	1	0
9	M	625	MAN	1	0
7	M	636	NAG	1	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.