



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

Feb 4, 2019 – 04:36 PM EST

PDB ID : 6E5P  
EMDB ID: : EMD-8981  
Title : Backbone model based on cryo-EM map at 8.5 Å of domain-swapped, glycan-reactive, neutralizing antibody 2G12 bound to HIV-1 Env BG505 DS-SOSIP, which was also bound to CD4-binding site antibody VRC03  
Authors : Acharya, P.; Kwong, P.D.  
Deposited on : 2018-07-21  
Resolution : 8.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

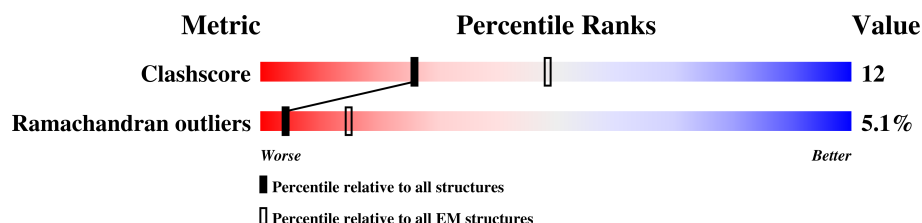
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.80 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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	212	88% 8% .
1	4	212	90% 8% .
1	K	212	86% 11% .
1	L	212	90% 8% .
1	Q	212	87% 10% .
1	T	212	91% 8% .
2	2	225	68% 26% 6%
2	3	225	74% 20% 5%
2	H	225	74% 20% 5%
2	M	225	68% 25% 7%
2	R	225	68% 25% 7%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	S	225	 74%20%5%
3	A	474	 94%••
3	C	474	 93%••
3	E	474	 94%••
4	B	170	 74%26%
4	D	170	 74%26%
4	F	170	 74%26%
5	I	227	 56%•44%
5	O	227	 56%•44%
5	V	227	 56%•44%
6	J	208	 49%51%
6	P	208	 49%51%
6	W	208	 49%51%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	2	301	-	-	X	-
7	MAN	2	303	-	-	X	-
7	MAN	2	304	X	-	-	-
7	MAN	3	704	-	-	X	-
7	MAN	3	708	-	-	X	-
7	MAN	3	709	X	-	-	-
7	MAN	3	713	-	-	X	-
7	MAN	3	714	-	-	X	-
7	MAN	3	715	-	-	X	-
7	MAN	A	608	-	-	X	-
7	MAN	A	609	-	-	X	-
7	MAN	A	610	-	-	X	-
7	MAN	C	608	-	-	X	-
7	MAN	C	610	-	-	X	-
7	MAN	H	704	-	-	X	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	H	708	-	-	X	-
7	MAN	H	709	X	-	-	-
7	MAN	M	301	-	-	X	-
7	MAN	M	303	-	-	X	-
7	MAN	M	304	X	-	-	-
7	MAN	R	301	-	-	X	-
7	MAN	R	303	-	-	X	-
7	MAN	R	304	X	-	-	-
7	MAN	S	704	-	-	X	-
7	MAN	S	708	-	-	X	-
7	MAN	S	709	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21252 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 2G12 Light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	212	Total	C	N	O	0	0
			848	424	212	212		
1	4	212	Total	C	N	O	0	0
			848	424	212	212		
1	K	212	Total	C	N	O	0	0
			848	424	212	212		
1	L	212	Total	C	N	O	0	0
			848	424	212	212		
1	Q	212	Total	C	N	O	0	0
			848	424	212	212		
1	T	212	Total	C	N	O	0	0
			848	424	212	212		

- Molecule 2 is a protein called 2G12 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	225	Total	C	N	O	0	0
			900	450	225	225		
2	3	225	Total	C	N	O	0	0
			900	450	225	225		
2	H	225	Total	C	N	O	0	0
			900	450	225	225		
2	M	225	Total	C	N	O	0	0
			900	450	225	225		
2	R	225	Total	C	N	O	0	0
			900	450	225	225		
2	S	225	Total	C	N	O	0	0
			900	450	225	225		

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	453	Total	C	N	O	0	0
			1812	906	453	453		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	453	Total	C	N	O	0	0
			1812	906	453	453		
3	E	453	Total	C	N	O	0	0
			1812	906	453	453		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	ILE	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	433	CYS	ALA	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	201	CYS	ILE	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	433	CYS	ALA	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
E	201	CYS	ILE	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	433	CYS	ALA	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	126	Total	C	N	O	0	0
			504	252	126	126		
4	D	126	Total	C	N	O	0	0
			504	252	126	126		
4	F	126	Total	C	N	O	0	0
			504	252	126	126		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S9
B	605	CYS	THR	conflict	UNP Q2N0S9
B	665	GLY	-	expression tag	UNP Q2N0S9
B	666	SER	-	expression tag	UNP Q2N0S9
B	667	ALA	-	expression tag	UNP Q2N0S9
B	668	PRO	-	expression tag	UNP Q2N0S9
B	669	THR	-	expression tag	UNP Q2N0S9
B	670	LYS	-	expression tag	UNP Q2N0S9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	671	ALA	-	expression tag	UNP Q2N0S9
B	672	LYS	-	expression tag	UNP Q2N0S9
B	673	ARG	-	expression tag	UNP Q2N0S9
B	674	ARG	-	expression tag	UNP Q2N0S9
B	675	VAL	-	expression tag	UNP Q2N0S9
B	676	VAL	-	expression tag	UNP Q2N0S9
B	677	GLN	-	expression tag	UNP Q2N0S9
B	678	ARG	-	expression tag	UNP Q2N0S9
B	679	GLU	-	expression tag	UNP Q2N0S9
B	680	LYS	-	expression tag	UNP Q2N0S9
B	681	ARG	-	expression tag	UNP Q2N0S9
D	559	PRO	ILE	conflict	UNP Q2N0S9
D	605	CYS	THR	conflict	UNP Q2N0S9
D	665	GLY	-	expression tag	UNP Q2N0S9
D	666	SER	-	expression tag	UNP Q2N0S9
D	667	ALA	-	expression tag	UNP Q2N0S9
D	668	PRO	-	expression tag	UNP Q2N0S9
D	669	THR	-	expression tag	UNP Q2N0S9
D	670	LYS	-	expression tag	UNP Q2N0S9
D	671	ALA	-	expression tag	UNP Q2N0S9
D	672	LYS	-	expression tag	UNP Q2N0S9
D	673	ARG	-	expression tag	UNP Q2N0S9
D	674	ARG	-	expression tag	UNP Q2N0S9
D	675	VAL	-	expression tag	UNP Q2N0S9
D	676	VAL	-	expression tag	UNP Q2N0S9
D	677	GLN	-	expression tag	UNP Q2N0S9
D	678	ARG	-	expression tag	UNP Q2N0S9
D	679	GLU	-	expression tag	UNP Q2N0S9
D	680	LYS	-	expression tag	UNP Q2N0S9
D	681	ARG	-	expression tag	UNP Q2N0S9
F	559	PRO	ILE	conflict	UNP Q2N0S9
F	605	CYS	THR	conflict	UNP Q2N0S9
F	665	GLY	-	expression tag	UNP Q2N0S9
F	666	SER	-	expression tag	UNP Q2N0S9
F	667	ALA	-	expression tag	UNP Q2N0S9
F	668	PRO	-	expression tag	UNP Q2N0S9
F	669	THR	-	expression tag	UNP Q2N0S9
F	670	LYS	-	expression tag	UNP Q2N0S9
F	671	ALA	-	expression tag	UNP Q2N0S9
F	672	LYS	-	expression tag	UNP Q2N0S9
F	673	ARG	-	expression tag	UNP Q2N0S9
F	674	ARG	-	expression tag	UNP Q2N0S9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	675	VAL	-	expression tag	UNP Q2N0S9
F	676	VAL	-	expression tag	UNP Q2N0S9
F	677	GLN	-	expression tag	UNP Q2N0S9
F	678	ARG	-	expression tag	UNP Q2N0S9
F	679	GLU	-	expression tag	UNP Q2N0S9
F	680	LYS	-	expression tag	UNP Q2N0S9
F	681	ARG	-	expression tag	UNP Q2N0S9

- Molecule 5 is a protein called VRC03 heavy chain.

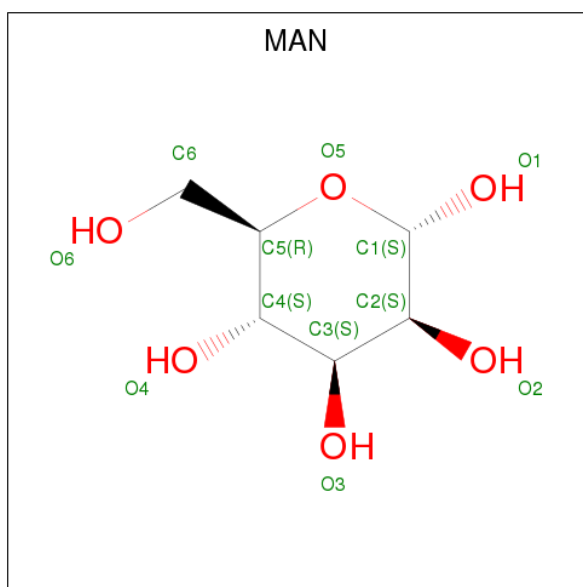
Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	128	Total	C	N	O	0	0
			512	256	128	128		
5	O	128	Total	C	N	O	0	0
			512	256	128	128		
5	V	128	Total	C	N	O	0	0
			512	256	128	128		

- Molecule 6 is a protein called VRC03 Light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	101	Total	C	N	O	0	0
			404	202	101	101		
6	P	101	Total	C	N	O	0	0
			404	202	101	101		
6	W	101	Total	C	N	O	0	0
			404	202	101	101		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			AltConf
7	2	1	Total	C	O	0
			77	42	35	
7	2	1	Total	C	O	0
			77	42	35	
7	2	1	Total	C	O	0
			77	42	35	
7	2	1	Total	C	O	0
			77	42	35	
7	2	1	Total	C	O	0
			77	42	35	
7	2	1	Total	C	O	0
			77	42	35	
7	3	1	Total	C	O	0
			110	60	50	
7	3	1	Total	C	O	0
			110	60	50	
7	3	1	Total	C	O	0
			110	60	50	
7	3	1	Total	C	O	0
			110	60	50	
7	3	1	Total	C	O	0
			110	60	50	
7	3	1	Total	C	O	0
			110	60	50	

*Continued on next page...*

*Continued from previous page...*

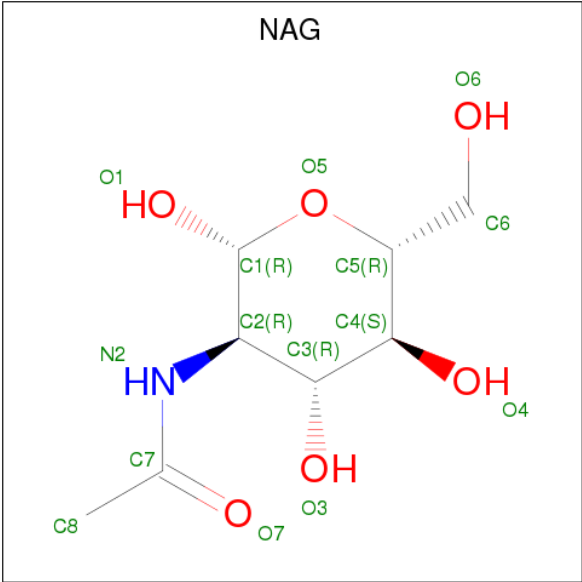
Mol	Chain	Residues	Atoms			AltConf
7	3	1	Total	C	O	0
			110	60	50	
7	3	1	Total	C	O	0
			110	60	50	
7	3	1	Total	C	O	0
			110	60	50	
7	A	1	Total	C	O	0
			55	30	25	
7	A	1	Total	C	O	0
			55	30	25	
7	A	1	Total	C	O	0
			55	30	25	
7	A	1	Total	C	O	0
			55	30	25	
7	A	1	Total	C	O	0
			55	30	25	
7	C	1	Total	C	O	0
			55	30	25	
7	C	1	Total	C	O	0
			55	30	25	
7	C	1	Total	C	O	0
			55	30	25	
7	C	1	Total	C	O	0
			55	30	25	
7	C	1	Total	C	O	0
			55	30	25	
7	E	1	Total	C	O	0
			11	6	5	
7	H	1	Total	C	O	0
			66	36	30	
7	H	1	Total	C	O	0
			66	36	30	
7	H	1	Total	C	O	0
			66	36	30	
7	H	1	Total	C	O	0
			66	36	30	
7	H	1	Total	C	O	0
			66	36	30	
7	H	1	Total	C	O	0
			66	36	30	
7	M	1	Total	C	O	0
			77	42	35	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
7	M	1	Total	C	O	0
			77	42	35	
7	M	1	Total	C	O	0
			77	42	35	
7	M	1	Total	C	O	0
			77	42	35	
7	M	1	Total	C	O	0
			77	42	35	
7	M	1	Total	C	O	0
			77	42	35	
7	R	1	Total	C	O	0
			77	42	35	
7	R	1	Total	C	O	0
			77	42	35	
7	R	1	Total	C	O	0
			77	42	35	
7	R	1	Total	C	O	0
			77	42	35	
7	R	1	Total	C	O	0
			77	42	35	
7	R	1	Total	C	O	0
			77	42	35	
7	R	1	Total	C	O	0
			77	42	35	
7	S	1	Total	C	O	0
			66	36	30	
7	S	1	Total	C	O	0
			66	36	30	
7	S	1	Total	C	O	0
			66	36	30	
7	S	1	Total	C	O	0
			66	36	30	
7	S	1	Total	C	O	0
			66	36	30	
7	S	1	Total	C	O	0
			66	36	30	

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



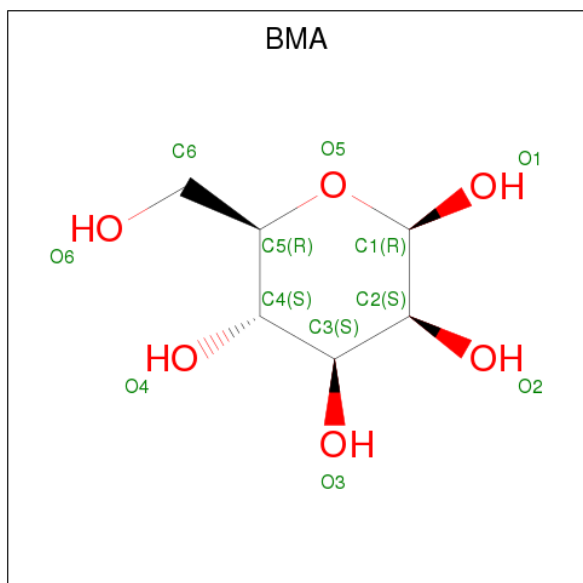
Mol	Chain	Residues	Atoms				AltConf
8	2	1	Total	C	N	O	0
			28	16	2	10	
8	2	1	Total	C	N	O	0
			28	16	2	10	
8	3	1	Total	C	N	O	0
			58	32	4	22	
8	3	1	Total	C	N	O	0
			58	32	4	22	
8	3	1	Total	C	N	O	0
			58	32	4	22	
8	3	1	Total	C	N	O	0
			58	32	4	22	
8	A	1	Total	C	N	O	0
			57	32	4	21	
8	A	1	Total	C	N	O	0
			57	32	4	21	
8	A	1	Total	C	N	O	0
			57	32	4	21	
8	A	1	Total	C	N	O	0
			57	32	4	21	
8	C	1	Total	C	N	O	0
			57	32	4	21	
8	C	1	Total	C	N	O	0
			57	32	4	21	
8	C	1	Total	C	N	O	0
			57	32	4	21	
8	C	1	Total	C	N	O	0
			57	32	4	21	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
8	E	1	Total	C	N	O	0
			28	16	2	10	
8	E	1	Total	C	N	O	0
			28	16	2	10	
8	H	1	Total	C	N	O	0
			29	16	2	11	
8	H	1	Total	C	N	O	0
			29	16	2	11	
8	M	1	Total	C	N	O	0
			28	16	2	10	
8	M	1	Total	C	N	O	0
			28	16	2	10	
8	R	1	Total	C	N	O	0
			28	16	2	10	
8	R	1	Total	C	N	O	0
			28	16	2	10	
8	S	1	Total	C	N	O	0
			29	16	2	11	
8	S	1	Total	C	N	O	0
			29	16	2	11	

- Molecule 9 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
9	2	1	Total	C	O	0
			11	6	5	

Continued on next page...

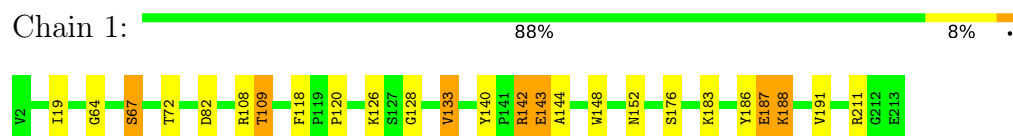
*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
9	3	1	Total	C	O	0
			22	12	10	
9	3	1	Total	C	O	0
			22	12	10	
9	A	1	Total	C	O	0
			22	12	10	
9	A	1	Total	C	O	0
			22	12	10	
9	C	1	Total	C	O	0
			22	12	10	
9	C	1	Total	C	O	0
			22	12	10	
9	E	1	Total	C	O	0
			11	6	5	
9	H	1	Total	C	O	0
			11	6	5	
9	M	1	Total	C	O	0
			11	6	5	
9	R	1	Total	C	O	0
			11	6	5	
9	S	1	Total	C	O	0
			11	6	5	

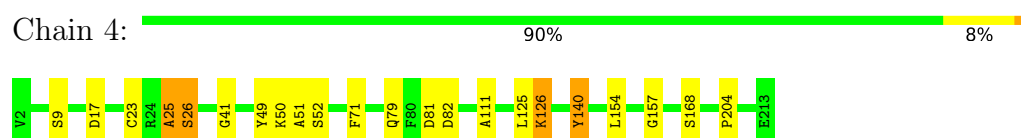
### 3 Residue-property plots

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.

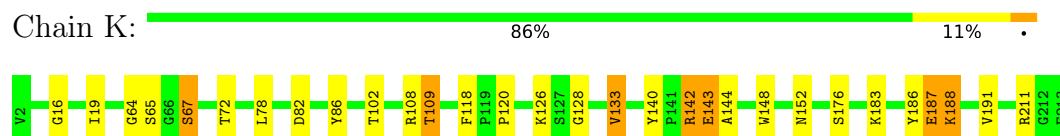
- Molecule 1: 2G12 Light chain



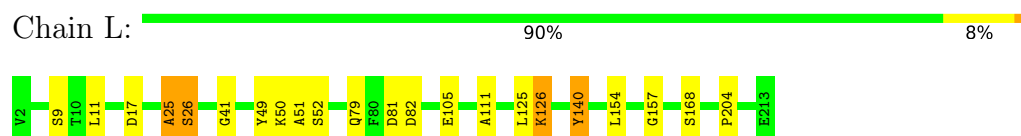
- Molecule 1: 2G12 Light chain



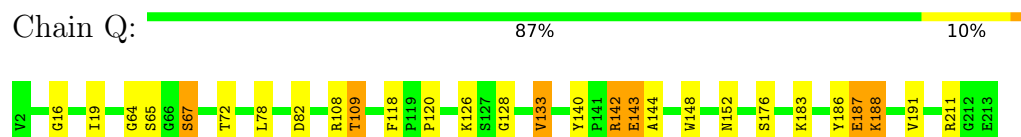
- Molecule 1: 2G12 Light chain



- Molecule 1: 2G12 Light chain



- Molecule 1: 2G12 Light chain

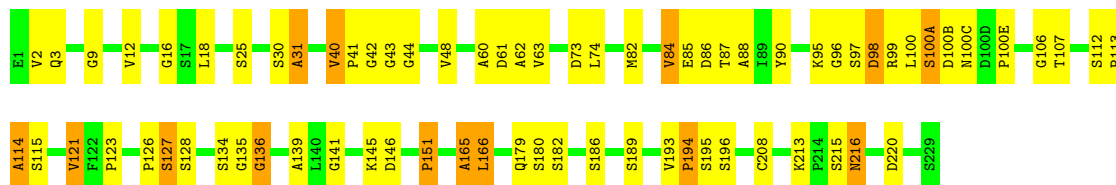


- Molecule 1: 2G12 Light chain

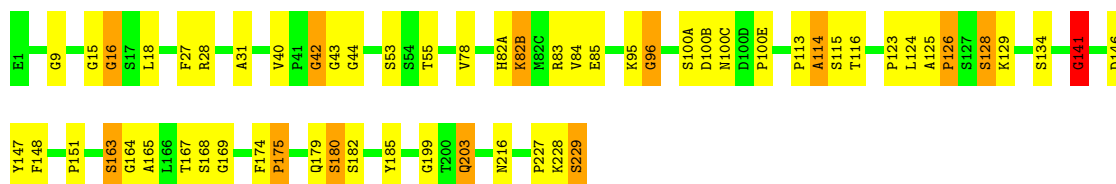




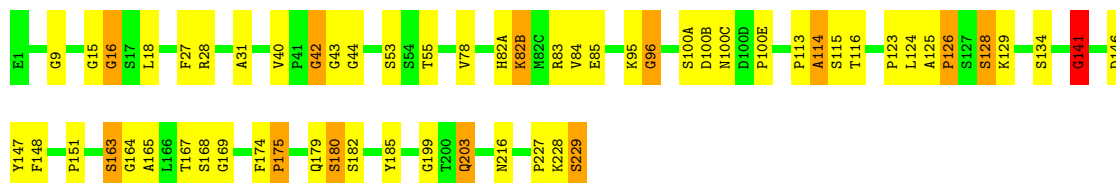
• Molecule 2: 2G12 heavy chain



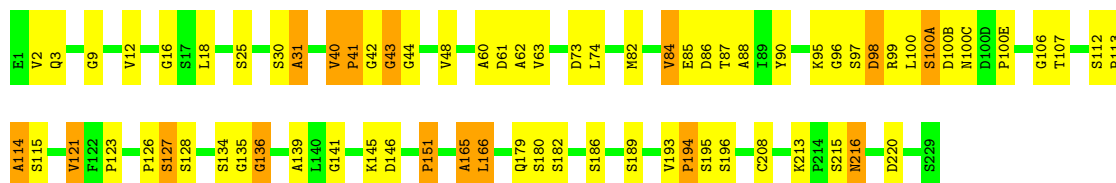
• Molecule 2: 2G12 heavy chain



• Molecule 2: 2G12 heavy chain



• Molecule 2: 2G12 heavy chain



• Molecule 2: 2G12 heavy chain

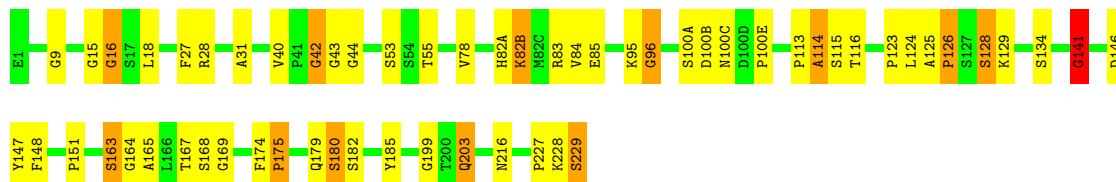






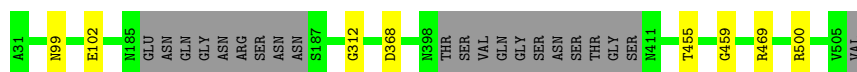
• Molecule 2: 2G12 heavy chain

Chain S: 74% 20% 5%



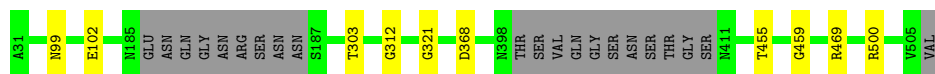
• Molecule 3: Envelope glycoprotein gp120

Chain A: 94% . .



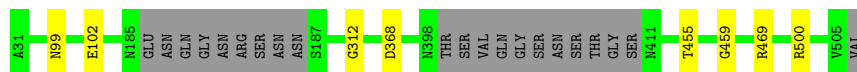
• Molecule 3: Envelope glycoprotein gp120

Chain C: 93% . .



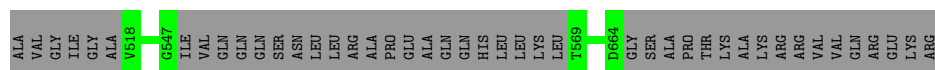
• Molecule 3: Envelope glycoprotein gp120

Chain E: 94% . .



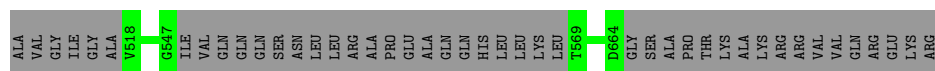
• Molecule 4: Envelope glycoprotein gp160

Chain B: 74% 26%



• Molecule 4: Envelope glycoprotein gp160

Chain D: 74% 26%

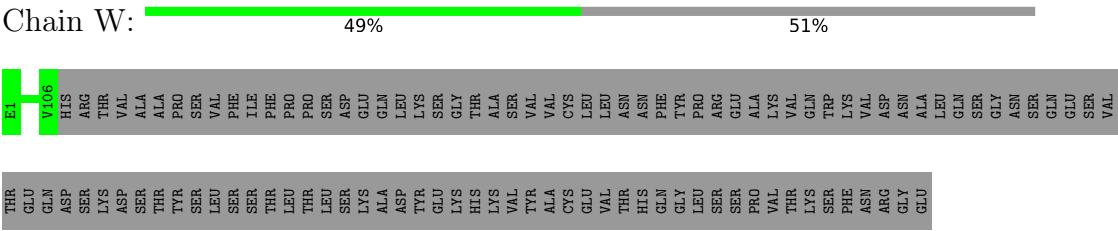


• Molecule 4: Envelope glycoprotein gp160

Chain F: 74% 26%



● Molecule 6: VRC03 Light chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	5245	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 ( $e^-/\text{\AA}^2$ )	63.84	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	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	1	1.16	1/847 (0.1%)	1.31	2/1057 (0.2%)
1	4	1.32	1/847 (0.1%)	1.35	2/1057 (0.2%)
1	K	1.16	1/847 (0.1%)	1.31	2/1057 (0.2%)
1	L	1.32	1/847 (0.1%)	1.35	2/1057 (0.2%)
1	Q	1.16	1/847 (0.1%)	1.31	2/1057 (0.2%)
1	T	1.32	1/847 (0.1%)	1.35	2/1057 (0.2%)
2	2	1.21	3/899 (0.3%)	1.45	4/1122 (0.4%)
2	3	1.35	3/899 (0.3%)	1.45	6/1122 (0.5%)
2	H	1.35	3/899 (0.3%)	1.44	6/1122 (0.5%)
2	M	1.21	3/899 (0.3%)	1.45	4/1122 (0.4%)
2	R	1.21	3/899 (0.3%)	1.45	4/1122 (0.4%)
2	S	1.35	3/899 (0.3%)	1.45	6/1122 (0.5%)
3	A	0.23	0/1809	0.48	0/2256
3	C	0.23	0/1809	0.48	0/2256
3	E	0.23	0/1809	0.48	0/2256
4	B	0.21	0/502	0.45	0/624
4	D	0.21	0/502	0.45	0/624
4	F	0.21	0/502	0.45	0/624
5	I	0.29	0/511	0.52	0/637
5	O	0.29	0/511	0.52	0/637
5	V	0.29	0/511	0.52	0/637
6	J	0.30	0/403	0.50	0/502
6	P	0.31	0/403	0.50	0/502
6	W	0.31	0/403	0.50	0/502
All	All	0.93	24/20151 (0.1%)	1.06	42/25131 (0.2%)

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
1	1	0	1
1	4	0	1
1	K	0	1
1	L	0	1
1	Q	0	1
1	T	0	1
2	2	0	9
2	3	0	4
2	H	0	4
2	M	0	9
2	R	0	9
2	S	0	4
All	All	0	45

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	123	PRO	C-O	9.53	1.42	1.23
2	H	123	PRO	C-O	9.52	1.42	1.23
2	3	123	PRO	C-O	9.49	1.42	1.23
2	2	44	GLY	N-CA	8.46	1.58	1.46
2	M	44	GLY	N-CA	8.42	1.58	1.46
2	R	44	GLY	N-CA	8.42	1.58	1.46
2	S	229	SER	C-O	7.76	1.38	1.23
2	H	229	SER	C-O	7.73	1.38	1.23
2	3	229	SER	C-O	7.71	1.38	1.23
2	M	43	GLY	N-CA	5.94	1.54	1.46
2	R	43	GLY	N-CA	5.92	1.54	1.46
2	2	43	GLY	N-CA	5.92	1.54	1.46
1	L	9	SER	C-O	5.59	1.33	1.23
1	T	9	SER	C-O	5.57	1.33	1.23
1	Q	67	SER	N-CA	5.56	1.57	1.46
1	4	9	SER	C-O	5.55	1.33	1.23
1	K	67	SER	N-CA	5.55	1.57	1.46
1	1	67	SER	N-CA	5.53	1.57	1.46
2	3	44	GLY	C-O	5.21	1.31	1.23
2	H	44	GLY	C-O	5.21	1.31	1.23
2	S	44	GLY	C-O	5.19	1.31	1.23
2	R	100(C)	ASN	C-N	5.14	1.45	1.34
2	2	100(C)	ASN	C-N	5.12	1.45	1.34
2	M	100(C)	ASN	C-N	5.12	1.45	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	96	GLY	N-CA-C	10.18	138.55	113.10
2	M	96	GLY	N-CA-C	10.18	138.54	113.10
2	R	96	GLY	N-CA-C	10.17	138.52	113.10
2	R	121	VAL	N-CA-C	6.86	129.53	111.00
2	M	121	VAL	N-CA-C	6.84	129.48	111.00
2	2	121	VAL	N-CA-C	6.84	129.47	111.00
2	3	95	LYS	C-N-CA	-6.50	108.66	122.30
2	H	95	LYS	C-N-CA	-6.48	108.68	122.30
2	S	95	LYS	C-N-CA	-6.47	108.70	122.30
1	1	148	TRP	N-CA-C	-6.47	93.53	111.00
1	K	148	TRP	N-CA-C	-6.45	93.59	111.00
1	Q	148	TRP	N-CA-C	-6.45	93.59	111.00
1	Q	133	VAL	N-CA-C	6.15	127.60	111.00
1	1	133	VAL	N-CA-C	6.14	127.58	111.00
1	K	133	VAL	N-CA-C	6.14	127.57	111.00
1	T	41	GLY	C-N-CA	-5.78	107.25	121.70
1	4	41	GLY	C-N-CA	-5.76	107.30	121.70
1	L	41	GLY	C-N-CA	-5.75	107.31	121.70
2	3	78	VAL	N-CA-C	-5.34	96.58	111.00
2	S	78	VAL	N-CA-C	-5.32	96.64	111.00
2	H	78	VAL	N-CA-C	-5.32	96.65	111.00
2	S	141	GLY	N-CA-C	5.20	126.10	113.10
2	H	141	GLY	N-CA-C	5.20	126.09	113.10
2	3	141	GLY	N-CA-C	5.19	126.08	113.10
2	R	95	LYS	N-CA-C	5.19	125.00	111.00
2	M	95	LYS	N-CA-C	5.18	124.99	111.00
2	2	95	LYS	N-CA-C	5.17	124.97	111.00
2	S	114	ALA	N-CA-C	-5.12	97.17	111.00
2	H	114	ALA	N-CA-C	-5.11	97.19	111.00
2	3	114	ALA	N-CA-C	-5.10	97.22	111.00
2	M	95	LYS	CA-C-N	5.10	126.39	116.20
2	2	95	LYS	CA-C-N	5.09	126.38	116.20
2	3	18	LEU	N-CA-C	-5.08	97.27	111.00
2	R	95	LYS	CA-C-N	5.08	126.36	116.20
2	H	18	LEU	N-CA-C	-5.07	97.33	111.00
2	S	18	LEU	N-CA-C	-5.06	97.34	111.00
2	H	96	GLY	N-CA-C	5.04	125.69	113.10
2	3	96	GLY	N-CA-C	5.03	125.68	113.10
2	S	96	GLY	N-CA-C	5.03	125.67	113.10
1	4	140	TYR	N-CA-C	-5.01	97.48	111.00
1	T	140	TYR	N-CA-C	-5.01	97.48	111.00
1	L	140	TYR	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	19	ILE	Peptide
2	2	100(A)	SER	Peptide
2	2	123	PRO	Peptide
2	2	145	LYS	Peptide
2	2	151	PRO	Peptide
2	2	215	SER	Peptide
2	2	40	VAL	Peptide
2	2	42	GLY	Peptide
2	2	88	ALA	Peptide
2	2	97	SER	Peptide
2	3	128	SER	Peptide
2	3	141	GLY	Peptide
2	3	42	GLY	Peptide
2	3	96	GLY	Peptide
1	4	25	ALA	Peptide
2	H	128	SER	Peptide
2	H	141	GLY	Peptide
2	H	42	GLY	Peptide
2	H	96	GLY	Peptide
1	K	19	ILE	Peptide
1	L	25	ALA	Peptide
2	M	100(A)	SER	Peptide
2	M	123	PRO	Peptide
2	M	145	LYS	Peptide
2	M	151	PRO	Peptide
2	M	215	SER	Peptide
2	M	40	VAL	Peptide
2	M	42	GLY	Peptide
2	M	88	ALA	Peptide
2	M	97	SER	Peptide
1	Q	19	ILE	Peptide
2	R	100(A)	SER	Peptide
2	R	123	PRO	Peptide
2	R	145	LYS	Peptide
2	R	151	PRO	Peptide
2	R	215	SER	Peptide
2	R	40	VAL	Peptide
2	R	42	GLY	Peptide
2	R	88	ALA	Peptide
2	R	97	SER	Peptide
2	S	128	SER	Peptide
2	S	141	GLY	Peptide

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	S	42	GLY	Peptide
2	S	96	GLY	Peptide
1	T	25	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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	1	848	0	230	8	0
1	4	848	0	230	7	0
1	K	848	0	230	11	0
1	L	848	0	230	7	0
1	Q	848	0	230	10	0
1	T	848	0	230	6	0
2	2	900	0	256	21	0
2	3	900	0	256	27	0
2	H	900	0	256	28	0
2	M	900	0	256	22	0
2	R	900	0	256	23	0
2	S	900	0	256	27	0
3	A	1812	0	482	12	0
3	C	1812	0	482	13	0
3	E	1812	0	482	11	0
4	B	504	0	143	0	0
4	D	504	0	143	0	0
4	F	504	0	143	0	0
5	I	512	0	147	9	0
5	O	512	0	147	10	0
5	V	512	0	147	10	0
6	J	404	0	121	0	0
6	P	404	0	121	0	0
6	W	404	0	121	0	0
7	2	77	0	64	16	0
7	3	110	0	93	33	0
7	A	55	0	48	24	0
7	C	55	0	48	22	0
7	E	11	0	10	4	0
7	H	66	0	55	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	77	0	64	17	0
7	R	77	0	64	16	0
7	S	66	0	55	15	0
8	2	28	0	24	0	0
8	3	58	0	52	0	0
8	A	57	0	50	0	0
8	C	57	0	50	0	0
8	E	28	0	24	0	0
8	H	29	0	26	0	0
8	M	28	0	24	0	0
8	R	28	0	24	0	0
8	S	29	0	26	0	0
9	2	11	0	9	0	0
9	3	22	0	16	9	0
9	A	22	0	17	5	0
9	C	22	0	17	4	0
9	E	11	0	9	0	0
9	H	11	0	8	3	0
9	M	11	0	9	0	0
9	R	11	0	9	0	0
9	S	11	0	8	4	0
All	All	21252	0	6498	339	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 12.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:459:GLY:CA	5:O:61:ARG:H	1.25	1.50
3:A:459:GLY:HA3	5:V:61:ARG:CA	1.44	1.47
3:C:459:GLY:HA3	5:O:61:ARG:CA	1.44	1.47
3:A:459:GLY:CA	5:V:61:ARG:H	1.25	1.46
3:E:459:GLY:CA	5:I:61:ARG:H	1.25	1.46
3:E:459:GLY:HA3	5:I:61:ARG:CA	1.44	1.45
3:E:459:GLY:CA	5:I:61:ARG:N	1.90	1.35
3:A:459:GLY:CA	5:V:61:ARG:N	1.89	1.32
3:C:459:GLY:CA	5:O:61:ARG:N	1.90	1.32
3:E:459:GLY:HA2	5:I:61:ARG:H	1.09	1.10
7:2:303:MAN:C1	7:3:713:MAN:O2	2.00	1.10
7:3:704:MAN:O2	7:3:708:MAN:C1	2.00	1.10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:608:MAN:O2	7:M:303:MAN:C1	2.00	1.10
7:S:704:MAN:O2	7:S:708:MAN:C1	2.00	1.10
7:H:704:MAN:O2	7:H:708:MAN:C1	2.00	1.09
3:C:459:GLY:HA2	5:O:61:ARG:H	1.09	1.08
7:C:608:MAN:O2	7:R:303:MAN:C1	2.00	1.08
3:A:459:GLY:HA2	5:V:61:ARG:N	1.66	1.06
3:A:459:GLY:HA2	5:V:61:ARG:H	1.09	1.04
3:E:459:GLY:CA	5:I:61:ARG:CA	2.32	1.03
3:A:459:GLY:CA	5:V:61:ARG:CA	2.32	1.01
9:H:703:BMA:H62	7:H:705:MAN:H3	1.43	1.00
3:E:459:GLY:HA2	5:I:61:ARG:N	1.66	1.00
9:S:703:BMA:H62	7:S:705:MAN:H3	1.43	1.00
9:3:712:BMA:H62	7:3:714:MAN:H3	1.43	1.00
3:C:459:GLY:HA3	5:O:61:ARG:N	1.60	0.99
9:3:703:BMA:H62	7:3:705:MAN:H3	1.43	0.99
3:C:459:GLY:HA2	5:O:61:ARG:N	1.66	0.98
9:C:607:BMA:H62	7:C:609:MAN:H3	1.43	0.98
3:A:459:GLY:HA3	5:V:61:ARG:N	1.60	0.97
3:C:459:GLY:CA	5:O:61:ARG:CA	2.32	0.97
9:A:607:BMA:H62	7:A:609:MAN:H3	1.43	0.97
7:A:608:MAN:HO2	7:M:303:MAN:C1	1.77	0.96
7:2:301:MAN:C1	7:E:604:MAN:O2	2.14	0.96
7:C:604:MAN:O2	7:R:301:MAN:C1	2.14	0.95
2:R:194:PRO:O	2:R:196:SER:N	1.99	0.95
7:C:608:MAN:HO2	7:R:303:MAN:C1	1.80	0.94
7:3:704:MAN:HO2	7:3:708:MAN:C1	1.78	0.94
2:M:194:PRO:O	2:M:196:SER:N	1.99	0.94
7:A:604:MAN:O2	7:M:301:MAN:C1	2.14	0.94
3:E:459:GLY:HA3	5:I:61:ARG:N	1.60	0.94
7:S:704:MAN:O2	7:S:708:MAN:C2	2.16	0.94
2:2:194:PRO:O	2:2:196:SER:N	1.99	0.94
7:A:608:MAN:O2	7:M:303:MAN:C2	2.16	0.94
7:C:608:MAN:O2	7:R:303:MAN:C2	2.16	0.93
7:2:303:MAN:C2	7:3:713:MAN:O2	2.16	0.93
7:H:704:MAN:O2	7:H:708:MAN:C2	2.16	0.93
7:3:704:MAN:O2	7:3:708:MAN:C2	2.16	0.92
3:A:459:GLY:N	5:V:61:ARG:H	1.68	0.90
2:H:100(A):SER:O	2:H:100(C):ASN:N	2.05	0.90
2:2:84:VAL:O	2:2:86:ASP:N	2.05	0.89
3:E:459:GLY:N	5:I:61:ARG:H	1.68	0.89
2:R:84:VAL:O	2:R:86:ASP:N	2.05	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:704:MAN:HO2	7:H:708:MAN:C1	1.83	0.89
2:S:100(A):SER:O	2:S:100(C):ASN:N	2.05	0.89
3:C:459:GLY:N	5:O:61:ARG:H	1.68	0.89
2:M:84:VAL:O	2:M:86:ASP:N	2.05	0.89
2:3:100(A):SER:O	2:3:100(C):ASN:N	2.05	0.89
2:M:90:TYR:N	2:M:107:THR:O	2.06	0.88
7:H:704:MAN:HO2	7:H:708:MAN:C2	1.87	0.88
2:R:90:TYR:N	2:R:107:THR:O	2.06	0.87
7:2:303:MAN:C1	7:3:713:MAN:HO2	1.86	0.87
7:S:704:MAN:HO2	7:S:708:MAN:C2	1.86	0.87
7:2:303:MAN:C2	7:3:713:MAN:HO2	1.86	0.86
2:2:90:TYR:N	2:2:107:THR:O	2.06	0.86
7:A:608:MAN:HO2	7:M:303:MAN:C2	1.89	0.86
7:3:704:MAN:HO2	7:3:708:MAN:C2	1.89	0.85
7:C:608:MAN:HO2	7:R:303:MAN:C2	1.88	0.85
7:S:704:MAN:HO2	7:S:708:MAN:C1	1.86	0.83
7:S:704:MAN:HO2	7:S:708:MAN:H2	1.44	0.83
7:2:303:MAN:H2	7:3:713:MAN:HO2	1.44	0.81
7:C:610:MAN:C6	2:S:28:ARG:H	1.94	0.81
9:3:703:BMA:C6	7:3:705:MAN:H3	2.12	0.80
7:H:704:MAN:HO2	7:H:708:MAN:H2	1.45	0.80
9:3:712:BMA:C6	7:3:714:MAN:H3	2.12	0.80
9:A:607:BMA:C6	7:A:609:MAN:H3	2.12	0.79
7:A:610:MAN:C6	2:H:28:ARG:H	1.94	0.79
9:S:703:BMA:C6	7:S:705:MAN:H3	2.12	0.79
2:3:28:ARG:H	7:3:715:MAN:C6	1.94	0.79
7:2:301:MAN:C2	7:E:604:MAN:O2	2.31	0.79
7:C:604:MAN:O2	7:R:301:MAN:C2	2.31	0.79
9:H:703:BMA:C6	7:H:705:MAN:H3	2.12	0.79
7:A:604:MAN:O2	7:M:301:MAN:C2	2.31	0.78
9:C:607:BMA:C6	7:C:609:MAN:H3	2.12	0.78
7:C:608:MAN:HO2	7:R:303:MAN:H2	1.48	0.76
2:M:31:ALA:O	7:M:301:MAN:O3	2.04	0.76
7:3:704:MAN:HO2	7:3:708:MAN:H2	1.49	0.76
2:2:31:ALA:O	7:2:301:MAN:O3	2.04	0.75
2:H:124:LEU:N	2:H:141:GLY:O	2.20	0.75
2:S:124:LEU:N	2:S:141:GLY:O	2.19	0.75
7:A:608:MAN:HO2	7:M:303:MAN:H2	1.50	0.75
2:R:31:ALA:O	7:R:301:MAN:O3	2.04	0.74
9:C:607:BMA:C6	7:C:609:MAN:C3	2.63	0.74
2:3:124:LEU:N	2:3:141:GLY:O	2.20	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:301:MAN:H2	7:E:604:MAN:O2	1.88	0.74
7:A:604:MAN:O2	7:M:301:MAN:H2	1.88	0.74
7:M:301:MAN:O3	7:M:302:MAN:C1	2.36	0.73
7:C:604:MAN:O2	7:R:301:MAN:H2	1.88	0.72
7:2:301:MAN:O3	7:2:302:MAN:C1	2.36	0.71
1:Q:186:TYR:O	1:Q:188:LYS:N	2.22	0.71
9:3:712:BMA:C6	7:3:714:MAN:C3	2.63	0.70
7:R:301:MAN:O3	7:R:302:MAN:C1	2.36	0.70
1:1:186:TYR:O	1:1:188:LYS:N	2.22	0.70
7:A:608:MAN:O2	7:M:303:MAN:C3	2.40	0.69
7:3:704:MAN:O2	7:3:708:MAN:C3	2.40	0.69
7:H:704:MAN:O2	7:H:708:MAN:C3	2.40	0.69
1:K:186:TYR:O	1:K:188:LYS:N	2.22	0.69
7:2:303:MAN:C3	7:3:713:MAN:O2	2.40	0.69
7:C:608:MAN:O2	7:R:303:MAN:C3	2.40	0.69
7:S:704:MAN:O2	7:S:708:MAN:C3	2.40	0.69
9:3:703:BMA:C6	7:3:705:MAN:C3	2.63	0.68
1:L:50:LYS:O	1:L:52:SER:N	2.29	0.66
1:T:50:LYS:O	1:T:52:SER:N	2.29	0.66
7:A:610:MAN:C1	7:A:611:MAN:O5	2.44	0.65
1:Q:142:ARG:O	1:Q:143:GLU:C	2.34	0.65
1:1:142:ARG:O	1:1:143:GLU:C	2.34	0.65
7:C:610:MAN:C1	7:C:611:MAN:O5	2.44	0.65
7:3:715:MAN:C1	7:3:716:MAN:O5	2.44	0.65
7:3:706:MAN:C1	7:3:707:MAN:O5	2.44	0.65
2:S:15:GLY:O	2:S:16:GLY:O	2.15	0.65
7:S:706:MAN:C1	7:S:707:MAN:O5	2.44	0.65
2:3:15:GLY:O	2:3:16:GLY:O	2.15	0.64
1:K:142:ARG:O	1:K:143:GLU:C	2.34	0.64
7:H:706:MAN:C1	7:H:707:MAN:O5	2.44	0.64
2:H:179:GLN:O	2:H:180:SER:C	2.36	0.64
2:H:15:GLY:O	2:H:16:GLY:O	2.15	0.64
2:3:179:GLN:O	2:3:180:SER:C	2.36	0.63
2:3:31:ALA:O	7:3:709:MAN:O2	2.09	0.63
2:S:179:GLN:O	2:S:180:SER:C	2.36	0.63
9:A:607:BMA:C6	7:A:609:MAN:C3	2.63	0.63
2:H:83:ARG:O	2:H:84:VAL:C	2.37	0.62
2:S:31:ALA:O	7:S:709:MAN:O2	2.09	0.61
1:4:50:LYS:O	1:4:52:SER:N	2.29	0.61
1:K:183:LYS:O	1:K:187:GLU:N	2.34	0.61
2:R:84:VAL:C	2:R:86:ASP:H	2.04	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:183:LYS:O	1:1:187:GLU:N	2.34	0.61
2:S:83:ARG:O	2:S:84:VAL:C	2.37	0.61
2:2:84:VAL:C	2:2:86:ASP:H	2.04	0.61
2:H:31:ALA:O	7:H:709:MAN:O2	2.09	0.60
2:R:126:PRO:O	2:R:127:SER:O	2.19	0.60
2:M:126:PRO:O	2:M:127:SER:O	2.20	0.60
2:M:84:VAL:C	2:M:86:ASP:H	2.04	0.60
7:A:608:MAN:O2	7:M:303:MAN:H3	2.02	0.60
1:L:79:GLN:O	1:L:82:ASP:N	2.31	0.60
7:H:704:MAN:O2	7:H:708:MAN:H3	2.02	0.59
7:2:303:MAN:H3	7:3:713:MAN:O2	2.02	0.59
2:2:126:PRO:O	2:2:127:SER:O	2.20	0.59
7:3:704:MAN:O2	7:3:708:MAN:H3	2.02	0.59
1:4:25:ALA:O	1:4:26:SER:C	2.41	0.59
7:C:608:MAN:O2	7:R:303:MAN:H3	2.02	0.59
2:3:83:ARG:O	2:3:84:VAL:C	2.37	0.59
1:4:79:GLN:O	1:4:82:ASP:N	2.31	0.59
2:M:165:ALA:O	2:M:166:LEU:C	2.42	0.59
1:1:118:PHE:N	1:1:133:VAL:O	2.36	0.58
2:2:165:ALA:O	2:2:166:LEU:C	2.42	0.58
2:M:141:GLY:HA3	2:M:189:SER:O	2.03	0.58
1:L:25:ALA:O	1:L:26:SER:C	2.41	0.58
7:S:704:MAN:O2	7:S:708:MAN:H3	2.02	0.58
1:T:79:GLN:O	1:T:82:ASP:N	2.31	0.58
2:3:113:PRO:O	2:3:114:ALA:C	2.41	0.58
1:Q:183:LYS:O	1:Q:187:GLU:N	2.34	0.58
2:R:141:GLY:HA3	2:R:189:SER:O	2.04	0.58
1:T:25:ALA:O	1:T:26:SER:C	2.41	0.58
1:Q:118:PHE:N	1:Q:133:VAL:O	2.36	0.57
2:R:165:ALA:O	2:R:166:LEU:C	2.42	0.57
2:2:141:GLY:HA3	2:2:189:SER:O	2.04	0.57
2:S:113:PRO:O	2:S:114:ALA:C	2.41	0.57
2:3:167:THR:O	2:3:168:SER:C	2.42	0.57
1:K:118:PHE:N	1:K:133:VAL:O	2.36	0.57
2:3:28:ARG:H	7:3:715:MAN:H61	1.68	0.57
7:C:610:MAN:H61	2:S:28:ARG:H	1.69	0.57
2:H:167:THR:O	2:H:168:SER:C	2.42	0.56
2:2:113:PRO:C	2:2:114:ALA:O	2.43	0.56
2:M:113:PRO:C	2:M:114:ALA:O	2.43	0.56
7:2:301:MAN:H2	7:E:604:MAN:HO2	1.70	0.55
2:R:113:PRO:C	2:R:114:ALA:O	2.43	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:610:MAN:H61	2:H:28:ARG:H	1.68	0.54
2:S:167:THR:O	2:S:168:SER:C	2.42	0.54
2:H:55:THR:O	7:M:309:MAN:H3	2.08	0.54
7:R:309:MAN:H3	2:S:55:THR:O	2.08	0.54
7:2:309:MAN:H3	2:3:55:THR:O	2.08	0.53
2:R:113:PRO:O	2:R:114:ALA:O	2.27	0.53
2:2:113:PRO:O	2:2:114:ALA:O	2.26	0.53
2:S:27:PHE:O	2:S:28:ARG:C	2.47	0.53
2:2:12:VAL:O	2:2:112:SER:N	2.39	0.53
2:R:134:SER:O	2:R:136:GLY:N	2.41	0.53
2:3:179:GLN:O	2:3:182:SER:N	2.42	0.53
2:2:134:SER:O	2:2:136:GLY:N	2.41	0.52
2:S:179:GLN:O	2:S:182:SER:N	2.42	0.52
2:H:113:PRO:O	2:H:114:ALA:C	2.48	0.52
2:M:113:PRO:O	2:M:114:ALA:O	2.27	0.52
2:H:179:GLN:O	2:H:182:SER:N	2.42	0.52
1:1:126:LYS:C	1:1:128:GLY:N	2.62	0.52
2:3:27:PHE:O	2:3:28:ARG:C	2.47	0.51
2:M:12:VAL:O	2:M:112:SER:N	2.39	0.51
2:R:60:ALA:O	2:R:63:VAL:N	2.40	0.51
2:2:60:ALA:O	2:2:63:VAL:N	2.40	0.51
2:H:27:PHE:O	2:H:28:ARG:C	2.47	0.51
2:M:134:SER:O	2:M:136:GLY:N	2.41	0.50
1:Q:126:LYS:C	1:Q:128:GLY:N	2.62	0.50
9:3:712:BMA:H62	7:3:714:MAN:C3	2.21	0.50
2:M:98:ASP:C	2:M:100:LEU:H	2.15	0.50
2:2:98:ASP:C	2:2:100:LEU:H	2.15	0.50
2:M:60:ALA:O	2:M:63:VAL:N	2.40	0.50
2:3:199:GLY:C	2:3:203:GLN:H	2.14	0.50
2:R:98:ASP:C	2:R:100:LEU:H	2.15	0.50
1:K:126:LYS:C	1:K:128:GLY:N	2.62	0.50
2:H:199:GLY:C	2:H:203:GLN:H	2.14	0.49
2:R:12:VAL:O	2:R:112:SER:N	2.40	0.49
2:S:199:GLY:C	2:S:203:GLN:H	2.14	0.49
2:M:213:LYS:O	2:M:216:ASN:N	2.38	0.49
2:H:163:SER:O	2:H:165:ALA:N	2.41	0.49
2:3:199:GLY:C	2:3:203:GLN:N	2.66	0.49
1:1:142:ARG:O	1:1:144:ALA:N	2.46	0.49
1:Q:142:ARG:O	1:Q:144:ALA:N	2.46	0.49
2:H:199:GLY:C	2:H:203:GLN:N	2.66	0.48
2:S:199:GLY:C	2:S:203:GLN:N	2.66	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:604:MAN:HO2	7:M:301:MAN:H2	1.75	0.48
2:2:213:LYS:O	2:2:216:ASN:N	2.38	0.48
7:C:604:MAN:HO2	7:R:301:MAN:H2	1.76	0.48
1:K:142:ARG:O	1:K:144:ALA:N	2.46	0.48
7:M:301:MAN:C2	7:M:302:MAN:C5	2.92	0.48
7:R:301:MAN:C2	7:R:302:MAN:C5	2.92	0.48
7:2:301:MAN:C2	7:2:302:MAN:C5	2.92	0.48
2:3:82(A):HIS:O	2:3:82(B):LYS:C	2.52	0.48
3:E:368:ASP:N	5:I:54:TRP:O	2.46	0.47
2:S:163:SER:O	2:S:165:ALA:N	2.41	0.47
2:R:208:CYS:O	2:R:220:ASP:CA	2.63	0.47
2:3:113:PRO:O	2:3:115:SER:N	2.48	0.47
2:H:174:PHE:O	2:H:175:PRO:C	2.53	0.47
2:M:208:CYS:O	2:M:220:ASP:CA	2.63	0.47
2:2:208:CYS:O	2:2:220:ASP:CA	2.63	0.47
2:3:163:SER:O	2:3:165:ALA:N	2.41	0.47
2:3:174:PHE:O	2:3:175:PRO:C	2.53	0.47
7:3:706:MAN:C1	7:3:707:MAN:C5	2.93	0.47
1:4:111:ALA:O	1:4:140:TYR:O	2.33	0.47
9:A:607:BMA:H61	7:A:609:MAN:H2	1.41	0.47
2:M:3:GLN:O	2:M:25:SER:N	2.47	0.47
7:A:610:MAN:C1	7:A:611:MAN:C5	2.93	0.46
7:3:715:MAN:C1	7:3:716:MAN:C5	2.93	0.46
3:A:455:THR:N	3:A:469:ARG:O	2.48	0.46
2:H:82(A):HIS:O	2:H:82(B):LYS:C	2.52	0.46
2:S:113:PRO:O	2:S:115:SER:N	2.48	0.46
7:S:706:MAN:C1	7:S:707:MAN:C5	2.93	0.46
2:3:125:ALA:O	2:3:126:PRO:C	2.54	0.46
2:H:125:ALA:O	2:H:126:PRO:C	2.54	0.46
2:R:213:LYS:O	2:R:216:ASN:N	2.38	0.46
2:R:3:GLN:O	2:R:25:SER:N	2.47	0.46
9:C:607:BMA:H61	7:C:609:MAN:H2	1.41	0.46
7:C:610:MAN:C1	7:C:611:MAN:C5	2.93	0.46
2:S:228:LYS:O	2:S:229:SER:O	2.34	0.46
2:H:228:LYS:O	2:H:229:SER:O	2.34	0.46
7:H:706:MAN:C1	7:H:707:MAN:C5	2.93	0.46
1:L:111:ALA:O	1:L:140:TYR:O	2.33	0.46
1:T:125:LEU:O	1:T:126:LYS:C	2.54	0.45
2:S:174:PHE:O	2:S:175:PRO:C	2.53	0.45
3:C:455:THR:N	3:C:469:ARG:O	2.48	0.45
3:C:368:ASP:N	5:O:54:TRP:O	2.46	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:125:ALA:O	2:S:126:PRO:C	2.54	0.45
1:T:111:ALA:O	1:T:140:TYR:O	2.33	0.45
1:4:125:LEU:O	1:4:126:LYS:C	2.54	0.45
1:L:125:LEU:O	1:L:126:LYS:C	2.54	0.45
1:Q:64:GLY:HA2	1:Q:72:THR:O	2.17	0.45
2:S:82(A):HIS:O	2:S:82(B):LYS:C	2.52	0.45
2:3:40:VAL:O	2:3:43:GLY:HA2	2.17	0.45
2:H:40:VAL:O	2:H:43:GLY:HA2	2.17	0.45
2:H:167:THR:O	2:H:169:GLY:N	2.51	0.44
1:K:108:ARG:O	1:K:109:THR:C	2.56	0.44
1:K:64:GLY:HA2	1:K:72:THR:O	2.17	0.44
1:1:64:GLY:HA2	1:1:72:THR:O	2.17	0.44
2:3:228:LYS:O	2:3:229:SER:O	2.34	0.44
9:3:712:BMA:H61	7:3:714:MAN:H2	1.41	0.44
9:H:703:BMA:H61	7:H:705:MAN:H2	1.41	0.44
1:Q:108:ARG:O	1:Q:109:THR:C	2.56	0.44
7:A:608:MAN:O2	7:M:303:MAN:H2	2.02	0.44
2:2:179:GLN:O	2:2:182:SER:N	2.51	0.44
2:2:3:GLN:O	2:2:25:SER:N	2.47	0.44
2:3:167:THR:O	2:3:169:GLY:N	2.51	0.44
2:R:179:GLN:O	2:R:182:SER:N	2.51	0.44
1:1:108:ARG:O	1:1:109:THR:C	2.56	0.44
3:E:455:THR:N	3:E:469:ARG:O	2.48	0.44
2:M:179:GLN:O	2:M:182:SER:N	2.51	0.44
7:M:301:MAN:C2	7:M:302:MAN:H5	2.48	0.44
2:2:98:ASP:C	2:2:100:LEU:N	2.71	0.44
1:L:49:TYR:O	1:L:50:LYS:C	2.56	0.43
2:R:98:ASP:C	2:R:100:LEU:N	2.71	0.43
2:M:98:ASP:C	2:M:100:LEU:N	2.71	0.43
2:S:40:VAL:O	2:S:43:GLY:HA2	2.17	0.43
2:S:147:TYR:O	2:S:185:TYR:N	2.51	0.43
9:S:703:BMA:C6	7:S:705:MAN:C3	2.63	0.43
3:A:368:ASP:N	5:V:54:TRP:O	2.46	0.43
7:2:301:MAN:C2	7:2:302:MAN:H5	2.48	0.43
1:4:49:TYR:O	1:4:50:LYS:C	2.56	0.43
2:H:147:TYR:O	2:H:185:TYR:N	2.51	0.43
1:4:23:CYS:O	1:4:71:PHE:N	2.49	0.43
2:R:18:LEU:N	2:R:82:MET:O	2.49	0.43
1:T:49:TYR:O	1:T:50:LYS:C	2.56	0.43
2:3:28:ARG:N	7:3:715:MAN:C6	2.74	0.43
2:3:147:TYR:O	2:3:185:TYR:N	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3:703:BMA:H61	7:3:705:MAN:H2	1.41	0.43
2:S:167:THR:O	2:S:169:GLY:N	2.51	0.43
9:S:703:BMA:H61	7:S:705:MAN:H2	1.41	0.43
7:R:301:MAN:C2	7:R:302:MAN:H5	2.48	0.43
2:3:28:ARG:N	7:3:715:MAN:O6	2.52	0.42
1:K:86:TYR:N	1:K:102:THR:O	2.39	0.42
2:R:41:PRO:C	2:R:43:GLY:N	2.72	0.42
2:2:18:LEU:N	2:2:82:MET:O	2.49	0.42
3:C:459:GLY:N	5:O:61:ARG:N	2.46	0.42
2:M:18:LEU:N	2:M:82:MET:O	2.49	0.42
3:A:99:ASN:O	3:A:102:GLU:N	2.53	0.42
3:C:99:ASN:O	3:C:102:GLU:N	2.53	0.42
3:A:459:GLY:N	5:V:61:ARG:N	2.46	0.42
2:H:113:PRO:O	2:H:115:SER:N	2.53	0.42
1:Q:16:GLY:N	1:Q:78:LEU:O	2.52	0.42
7:C:610:MAN:C6	2:S:28:ARG:N	2.74	0.41
7:A:610:MAN:O6	2:H:28:ARG:N	2.52	0.41
2:M:41:PRO:C	2:M:43:GLY:N	2.72	0.41
2:3:199:GLY:N	2:3:203:GLN:H	2.19	0.41
2:R:84:VAL:O	2:R:87:THR:N	2.53	0.41
2:H:163:SER:C	2:H:165:ALA:H	2.22	0.41
9:A:607:BMA:H62	7:A:609:MAN:C3	2.21	0.41
7:A:609:MAN:H61	7:A:610:MAN:C5	2.51	0.41
3:E:99:ASN:O	3:E:102:GLU:N	2.53	0.41
2:M:84:VAL:O	2:M:87:THR:N	2.53	0.41
2:2:84:VAL:O	2:2:87:THR:N	2.53	0.41
2:H:199:GLY:N	2:H:203:GLN:H	2.19	0.41
1:K:65:SER:N	1:K:72:THR:O	2.54	0.41
2:R:84:VAL:C	2:R:86:ASP:N	2.67	0.41
7:3:714:MAN:H61	7:3:715:MAN:C5	2.51	0.41
7:H:705:MAN:H61	7:H:706:MAN:C5	2.51	0.41
1:Q:65:SER:N	1:Q:72:THR:O	2.54	0.41
3:C:303:THR:O	3:C:321:GLY:N	2.49	0.41
1:K:16:GLY:N	1:K:78:LEU:O	2.52	0.41
1:L:11:LEU:O	1:L:105:GLU:N	2.39	0.41
7:S:705:MAN:H61	7:S:706:MAN:C5	2.51	0.41
2:S:199:GLY:N	2:S:203:GLN:H	2.19	0.40
7:C:609:MAN:H61	7:C:610:MAN:C5	2.51	0.40
7:A:610:MAN:C6	2:H:28:ARG:N	2.74	0.40
7:C:610:MAN:O6	2:S:28:ARG:N	2.52	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	1	210/212 (99%)	158 (75%)	39 (19%)	13 (6%)	1	21
1	4	210/212 (99%)	177 (84%)	24 (11%)	9 (4%)	3	28
1	K	210/212 (99%)	158 (75%)	39 (19%)	13 (6%)	1	21
1	L	210/212 (99%)	177 (84%)	24 (11%)	9 (4%)	3	28
1	Q	210/212 (99%)	158 (75%)	39 (19%)	13 (6%)	1	21
1	T	210/212 (99%)	177 (84%)	24 (11%)	9 (4%)	3	28
2	2	223/225 (99%)	157 (70%)	28 (13%)	38 (17%)	0	4
2	3	223/225 (99%)	160 (72%)	40 (18%)	23 (10%)	0	10
2	H	223/225 (99%)	159 (71%)	41 (18%)	23 (10%)	0	10
2	M	223/225 (99%)	157 (70%)	28 (13%)	38 (17%)	0	4
2	R	223/225 (99%)	157 (70%)	28 (13%)	38 (17%)	0	4
2	S	223/225 (99%)	159 (71%)	41 (18%)	23 (10%)	0	10
3	A	447/474 (94%)	406 (91%)	39 (9%)	2 (0%)	36	77
3	C	447/474 (94%)	406 (91%)	39 (9%)	2 (0%)	36	77
3	E	447/474 (94%)	406 (91%)	39 (9%)	2 (0%)	36	77
4	B	122/170 (72%)	109 (89%)	13 (11%)	0	100	100
4	D	122/170 (72%)	109 (89%)	13 (11%)	0	100	100
4	F	122/170 (72%)	109 (89%)	13 (11%)	0	100	100
5	I	126/227 (56%)	124 (98%)	2 (2%)	0	100	100
5	O	126/227 (56%)	125 (99%)	1 (1%)	0	100	100
5	V	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
6	J	99/208 (48%)	96 (97%)	3 (3%)	0	100	100
6	P	99/208 (48%)	96 (97%)	3 (3%)	0	100	100
6	W	99/208 (48%)	96 (97%)	3 (3%)	0	100	100
All	All	4980/5859 (85%)	4159 (84%)	566 (11%)	255 (5%)	4	25

All (255) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	152	ASN
1	1	176	SER
1	1	187	GLU
2	2	16	GLY
2	2	30	SER
2	2	48	VAL
2	2	74	LEU
2	2	85	GLU
2	2	98	ASP
2	2	100(A)	SER
2	2	114	ALA
2	2	115	SER
2	2	121	VAL
2	2	127	SER
2	2	139	ALA
2	2	146	ASP
2	2	165	ALA
2	2	166	LEU
2	2	180	SER
2	2	195	SER
2	3	16	GLY
2	3	53	SER
2	3	100(B)	ASP
2	3	129	LYS
2	3	180	SER
2	3	227	PRO
1	4	26	SER
1	4	51	ALA
1	4	168	SER
2	H	16	GLY
2	H	53	SER
2	H	100(B)	ASP
2	H	129	LYS
2	H	180	SER
2	H	227	PRO
1	K	152	ASN
1	K	176	SER
1	K	187	GLU
1	L	26	SER
1	L	51	ALA
1	L	168	SER
2	M	16	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	30	SER
2	M	48	VAL
2	M	74	LEU
2	M	85	GLU
2	M	98	ASP
2	M	100(A)	SER
2	M	114	ALA
2	M	115	SER
2	M	121	VAL
2	M	127	SER
2	M	139	ALA
2	M	146	ASP
2	M	165	ALA
2	M	166	LEU
2	M	180	SER
2	M	195	SER
1	Q	152	ASN
1	Q	176	SER
1	Q	187	GLU
2	R	16	GLY
2	R	30	SER
2	R	48	VAL
2	R	74	LEU
2	R	85	GLU
2	R	98	ASP
2	R	100(A)	SER
2	R	114	ALA
2	R	115	SER
2	R	121	VAL
2	R	127	SER
2	R	139	ALA
2	R	146	ASP
2	R	165	ALA
2	R	166	LEU
2	R	180	SER
2	R	195	SER
2	S	16	GLY
2	S	53	SER
2	S	100(B)	ASP
2	S	129	LYS
2	S	180	SER
2	S	227	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	T	26	SER
1	T	51	ALA
1	T	168	SER
1	1	82	ASP
1	1	109	THR
1	1	143	GLU
1	1	191	VAL
1	1	211	ARG
2	2	2	VAL
2	2	9	GLY
2	2	61	ASP
2	2	100(B)	ASP
2	2	106	GLY
2	2	135	GLY
2	2	136	GLY
2	2	186	SER
2	2	216	ASN
2	3	9	GLY
2	3	134	SER
2	3	163	SER
2	3	164	GLY
1	4	154	LEU
2	H	9	GLY
2	H	134	SER
2	H	163	SER
2	H	164	GLY
1	K	82	ASP
1	K	109	THR
1	K	143	GLU
1	K	188	LYS
1	K	191	VAL
1	K	211	ARG
1	L	154	LEU
2	M	2	VAL
2	M	9	GLY
2	M	61	ASP
2	M	100(B)	ASP
2	M	106	GLY
2	M	135	GLY
2	M	136	GLY
2	M	186	SER
2	M	216	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	82	ASP
1	Q	109	THR
1	Q	143	GLU
1	Q	188	LYS
1	Q	191	VAL
1	Q	211	ARG
2	R	2	VAL
2	R	9	GLY
2	R	61	ASP
2	R	100(B)	ASP
2	R	106	GLY
2	R	135	GLY
2	R	136	GLY
2	R	186	SER
2	R	216	ASN
2	S	9	GLY
2	S	134	SER
2	S	163	SER
2	S	164	GLY
1	T	154	LEU
1	1	67	SER
1	1	188	LYS
2	2	31	ALA
2	2	73	ASP
2	3	42	GLY
2	3	85	GLU
2	3	116	THR
1	4	126	LYS
2	H	42	GLY
2	H	85	GLU
2	H	116	THR
1	K	67	SER
1	L	126	LYS
2	M	31	ALA
2	M	73	ASP
1	Q	67	SER
2	R	31	ALA
2	R	73	ASP
2	S	42	GLY
2	S	85	GLU
2	S	116	THR
1	T	126	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	120	PRO
2	2	40	VAL
2	2	99	ARG
2	2	128	SER
2	2	151	PRO
2	2	193	VAL
2	3	146	ASP
2	3	175	PRO
1	4	17	ASP
1	4	157	GLY
3	A	500	ARG
3	C	500	ARG
3	E	500	ARG
2	H	146	ASP
2	H	175	PRO
1	K	120	PRO
1	L	17	ASP
1	L	157	GLY
2	M	40	VAL
2	M	99	ARG
2	M	128	SER
2	M	151	PRO
2	M	193	VAL
1	Q	120	PRO
1	Q	142	ARG
2	R	40	VAL
2	R	99	ARG
2	R	128	SER
2	R	151	PRO
2	R	193	VAL
2	S	146	ASP
2	S	175	PRO
1	T	17	ASP
1	T	157	GLY
1	1	142	ARG
2	2	62	ALA
2	3	82(B)	LYS
2	3	100(E)	PRO
2	3	128	SER
2	3	148	PHE
2	3	203	GLN
2	3	216	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	4	204	PRO
2	H	82(B)	LYS
2	H	100(E)	PRO
2	H	128	SER
2	H	148	PHE
2	H	203	GLN
2	H	216	ASN
1	K	142	ARG
1	L	204	PRO
2	M	62	ALA
2	R	62	ALA
2	S	82(B)	LYS
2	S	100(E)	PRO
2	S	128	SER
2	S	148	PHE
2	S	203	GLN
2	S	216	ASN
1	T	204	PRO
1	1	140	TYR
2	2	100(E)	PRO
1	4	81	ASP
1	K	140	TYR
1	L	81	ASP
2	M	100(E)	PRO
1	Q	140	TYR
2	R	100(E)	PRO
1	T	81	ASP
2	2	41	PRO
3	A	312	GLY
3	C	312	GLY
3	E	312	GLY
2	M	41	PRO
2	R	41	PRO
2	2	194	PRO
2	M	194	PRO
2	R	194	PRO
2	3	126	PRO
2	H	126	PRO
2	S	126	PRO
2	2	84	VAL
2	M	84	VAL
2	R	84	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	3	151	PRO
2	H	151	PRO
2	S	151	PRO

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

90 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	MAN	2	301	7	11,11,12	1.59	3 (27%)	15,15,17	3.43	9 (60%)
7	MAN	2	302	7	11,11,12	1.17	1 (9%)	15,15,17	3.54	8 (53%)
7	MAN	2	303	7	11,11,12	1.26	2 (18%)	15,15,17	4.20	10 (66%)
7	MAN	2	304	7	11,11,12	1.34	2 (18%)	15,15,17	3.32	7 (46%)
8	NAG	2	305	8	14,14,15	0.32	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	2	306	9,8	14,14,15	0.37	0	17,19,21	0.67	0
9	BMA	2	307	8,7	11,11,12	0.64	0	15,15,17	0.87	0
7	MAN	2	308	9,7	11,11,12	0.73	0	15,15,17	1.02	2 (13%)
7	MAN	2	309	7	11,11,12	0.77	1 (9%)	15,15,17	1.13	1 (6%)
7	MAN	2	310	7	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
8	NAG	3	701	8	15,15,15	1.20	1 (6%)	21,21,21	2.63	9 (42%)
8	NAG	3	702	9,8	14,14,15	0.89	0	17,19,21	2.19	5 (29%)
9	BMA	3	703	8,7	11,11,12	1.17	0	15,15,17	2.90	8 (53%)
7	MAN	3	704	9	11,11,12	1.46	2 (18%)	15,15,17	2.09	6 (40%)
7	MAN	3	705	9,7	11,11,12	0.92	0	15,15,17	2.40	5 (33%)
7	MAN	3	706	7	11,11,12	1.80	3 (27%)	15,15,17	3.68	10 (66%)
7	MAN	3	707	7	11,11,12	2.14	5 (45%)	15,15,17	2.69	4 (26%)
7	MAN	3	708	7	11,11,12	1.26	2 (18%)	15,15,17	4.19	10 (66%)
7	MAN	3	709	7	11,11,12	1.34	2 (18%)	15,15,17	3.33	7 (46%)
8	NAG	3	710	8	15,15,15	1.21	1 (6%)	21,21,21	2.64	9 (42%)
8	NAG	3	711	9,8	14,14,15	0.89	0	17,19,21	2.20	5 (29%)
9	BMA	3	712	8,7	11,11,12	1.18	0	15,15,17	2.90	8 (53%)
7	MAN	3	713	9	11,11,12	1.46	2 (18%)	15,15,17	2.07	6 (40%)
7	MAN	3	714	9,7	11,11,12	0.93	0	15,15,17	2.39	5 (33%)
7	MAN	3	715	7	11,11,12	1.81	3 (27%)	15,15,17	3.68	10 (66%)
7	MAN	3	716	7	11,11,12	2.14	5 (45%)	15,15,17	2.69	4 (26%)
8	NAG	A	601	8	14,14,15	1.60	4 (28%)	17,19,21	2.83	8 (47%)
8	NAG	A	602	9,8	14,14,15	0.98	1 (7%)	17,19,21	2.81	8 (47%)
9	BMA	A	603	8,7	11,11,12	1.33	2 (18%)	15,15,17	2.81	9 (60%)
7	MAN	A	604	9	11,11,12	1.09	1 (9%)	15,15,17	2.62	6 (40%)
8	NAG	A	605	8	15,15,15	1.21	1 (6%)	21,21,21	2.63	9 (42%)
8	NAG	A	606	9,8	14,14,15	0.89	0	17,19,21	2.20	5 (29%)
9	BMA	A	607	8,7	11,11,12	1.18	0	15,15,17	2.90	8 (53%)
7	MAN	A	608	9	11,11,12	1.46	2 (18%)	15,15,17	2.07	6 (40%)
7	MAN	A	609	9,7	11,11,12	0.93	0	15,15,17	2.39	5 (33%)
7	MAN	A	610	7	11,11,12	1.81	3 (27%)	15,15,17	3.68	10 (66%)
7	MAN	A	611	7	11,11,12	2.14	5 (45%)	15,15,17	2.69	4 (26%)
8	NAG	C	601	8	14,14,15	1.60	4 (28%)	17,19,21	2.83	8 (47%)
8	NAG	C	602	9,8	14,14,15	0.98	1 (7%)	17,19,21	2.81	8 (47%)
9	BMA	C	603	8,7	11,11,12	1.33	2 (18%)	15,15,17	2.80	9 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	C	604	9	11,11,12	1.09	1 (9%)	15,15,17	2.62	6 (40%)
8	NAG	C	605	8	15,15,15	1.21	1 (6%)	21,21,21	2.63	9 (42%)
8	NAG	C	606	9,8	14,14,15	0.89	0	17,19,21	2.20	5 (29%)
9	BMA	C	607	8,7	11,11,12	1.18	0	15,15,17	2.89	7 (46%)
7	MAN	C	608	9	11,11,12	1.46	2 (18%)	15,15,17	2.07	6 (40%)
7	MAN	C	609	9,7	11,11,12	0.93	0	15,15,17	2.39	5 (33%)
7	MAN	C	610	7	11,11,12	1.81	3 (27%)	15,15,17	3.68	10 (66%)
7	MAN	C	611	7	11,11,12	2.13	5 (45%)	15,15,17	2.69	4 (26%)
8	NAG	E	601	8	14,14,15	1.60	4 (28%)	17,19,21	2.83	8 (47%)
8	NAG	E	602	9,8	14,14,15	0.98	1 (7%)	17,19,21	2.82	8 (47%)
9	BMA	E	603	8,7	11,11,12	1.33	2 (18%)	15,15,17	2.81	9 (60%)
7	MAN	E	604	9	11,11,12	1.08	1 (9%)	15,15,17	2.62	6 (40%)
8	NAG	H	701	8	15,15,15	1.21	1 (6%)	21,21,21	2.63	9 (42%)
8	NAG	H	702	9,8	14,14,15	0.89	0	17,19,21	2.20	5 (29%)
9	BMA	H	703	8,7	11,11,12	1.17	0	15,15,17	2.90	8 (53%)
7	MAN	H	704	9	11,11,12	1.46	2 (18%)	15,15,17	2.08	6 (40%)
7	MAN	H	705	9,7	11,11,12	0.93	0	15,15,17	2.39	5 (33%)
7	MAN	H	706	7	11,11,12	1.80	3 (27%)	15,15,17	3.68	10 (66%)
7	MAN	H	707	7	11,11,12	2.14	5 (45%)	15,15,17	2.70	4 (26%)
7	MAN	H	708	7	11,11,12	1.26	2 (18%)	15,15,17	4.19	10 (66%)
7	MAN	H	709	7	11,11,12	1.34	2 (18%)	15,15,17	3.33	7 (46%)
7	MAN	M	301	7	11,11,12	1.59	3 (27%)	15,15,17	3.43	9 (60%)
7	MAN	M	302	7	11,11,12	1.18	1 (9%)	15,15,17	3.54	8 (53%)
7	MAN	M	303	7	11,11,12	1.27	2 (18%)	15,15,17	4.19	10 (66%)
7	MAN	M	304	7	11,11,12	1.34	2 (18%)	15,15,17	3.33	7 (46%)
8	NAG	M	305	8	14,14,15	0.31	0	17,19,21	0.49	0
8	NAG	M	306	9,8	14,14,15	0.38	0	17,19,21	0.66	0
9	BMA	M	307	8,7	11,11,12	0.64	0	15,15,17	0.88	0
7	MAN	M	308	9,7	11,11,12	0.72	0	15,15,17	1.01	2 (13%)
7	MAN	M	309	7	11,11,12	0.77	1 (9%)	15,15,17	1.12	1 (6%)
7	MAN	M	310	7	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
7	MAN	R	301	7	11,11,12	1.59	3 (27%)	15,15,17	3.43	9 (60%)
7	MAN	R	302	7	11,11,12	1.19	1 (9%)	15,15,17	3.54	8 (53%)
7	MAN	R	303	7	11,11,12	1.27	2 (18%)	15,15,17	4.19	10 (66%)
7	MAN	R	304	7	11,11,12	1.32	2 (18%)	15,15,17	3.33	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	R	305	8	14,14,15	0.32	0	17,19,21	0.49	0
8	NAG	R	306	9,8	14,14,15	0.39	0	17,19,21	0.66	0
9	BMA	R	307	8,7	11,11,12	0.64	0	15,15,17	0.88	0
7	MAN	R	308	9,7	11,11,12	0.73	0	15,15,17	1.02	2 (13%)
7	MAN	R	309	7	11,11,12	0.79	1 (9%)	15,15,17	1.13	1 (6%)
7	MAN	R	310	7	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
8	NAG	S	701	8	15,15,15	1.20	1 (6%)	21,21,21	2.63	9 (42%)
8	NAG	S	702	9,8	14,14,15	0.88	0	17,19,21	2.20	5 (29%)
9	BMA	S	703	8,7	11,11,12	1.18	0	15,15,17	2.90	7 (46%)
7	MAN	S	704	9	11,11,12	1.45	2 (18%)	15,15,17	2.08	6 (40%)
7	MAN	S	705	9,7	11,11,12	0.92	0	15,15,17	2.39	5 (33%)
7	MAN	S	706	7	11,11,12	1.79	3 (27%)	15,15,17	3.68	10 (66%)
7	MAN	S	707	7	11,11,12	2.15	5 (45%)	15,15,17	2.69	4 (26%)
7	MAN	S	708	7	11,11,12	1.26	2 (18%)	15,15,17	4.19	10 (66%)
7	MAN	S	709	7	11,11,12	1.34	2 (18%)	15,15,17	3.32	7 (46%)

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	MAN	2	301	7	-	0/2/19/22	0/1/1/1
7	MAN	2	302	7	-	0/2/19/22	0/1/1/1
7	MAN	2	303	7	-	0/2/19/22	0/1/1/1
7	MAN	2	304	7	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	2	305	8	-	0/6/23/26	0/1/1/1
8	NAG	2	306	9,8	-	0/6/23/26	0/1/1/1
9	BMA	2	307	8,7	-	0/2/19/22	0/1/1/1
7	MAN	2	308	9,7	-	0/2/19/22	0/1/1/1
7	MAN	2	309	7	-	0/2/19/22	0/1/1/1
7	MAN	2	310	7	-	0/2/19/22	0/1/1/1
8	NAG	3	701	8	-	0/6/26/26	0/1/1/1
8	NAG	3	702	9,8	-	0/6/23/26	0/1/1/1
9	BMA	3	703	8,7	-	0/2/19/22	0/1/1/1
7	MAN	3	704	9	-	0/2/19/22	0/1/1/1
7	MAN	3	705	9,7	-	0/2/19/22	0/1/1/1
7	MAN	3	706	7	-	0/2/19/22	0/1/1/1
7	MAN	3	707	7	-	0/2/19/22	0/1/1/1
7	MAN	3	708	7	-	0/2/19/22	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	3	709	7	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	3	710	8	-	0/6/26/26	0/1/1/1
8	NAG	3	711	9,8	-	0/6/23/26	0/1/1/1
9	BMA	3	712	8,7	-	0/2/19/22	0/1/1/1
7	MAN	3	713	9	-	0/2/19/22	0/1/1/1
7	MAN	3	714	9,7	-	0/2/19/22	0/1/1/1
7	MAN	3	715	7	-	0/2/19/22	0/1/1/1
7	MAN	3	716	7	-	0/2/19/22	0/1/1/1
8	NAG	A	601	8	-	0/6/23/26	0/1/1/1
8	NAG	A	602	9,8	-	0/6/23/26	0/1/1/1
9	BMA	A	603	8,7	-	0/2/19/22	0/1/1/1
7	MAN	A	604	9	-	0/2/19/22	0/1/1/1
8	NAG	A	605	8	-	0/6/26/26	0/1/1/1
8	NAG	A	606	9,8	-	0/6/23/26	0/1/1/1
9	BMA	A	607	8,7	-	0/2/19/22	0/1/1/1
7	MAN	A	608	9	-	0/2/19/22	0/1/1/1
7	MAN	A	609	9,7	-	0/2/19/22	0/1/1/1
7	MAN	A	610	7	-	0/2/19/22	0/1/1/1
7	MAN	A	611	7	-	0/2/19/22	0/1/1/1
8	NAG	C	601	8	-	0/6/23/26	0/1/1/1
8	NAG	C	602	9,8	-	0/6/23/26	0/1/1/1
9	BMA	C	603	8,7	-	0/2/19/22	0/1/1/1
7	MAN	C	604	9	-	0/2/19/22	0/1/1/1
8	NAG	C	605	8	-	0/6/26/26	0/1/1/1
8	NAG	C	606	9,8	-	0/6/23/26	0/1/1/1
9	BMA	C	607	8,7	-	0/2/19/22	0/1/1/1
7	MAN	C	608	9	-	0/2/19/22	0/1/1/1
7	MAN	C	609	9,7	-	0/2/19/22	0/1/1/1
7	MAN	C	610	7	-	0/2/19/22	0/1/1/1
7	MAN	C	611	7	-	0/2/19/22	0/1/1/1
8	NAG	E	601	8	-	0/6/23/26	0/1/1/1
8	NAG	E	602	9,8	-	0/6/23/26	0/1/1/1
9	BMA	E	603	8,7	-	0/2/19/22	0/1/1/1
7	MAN	E	604	9	-	0/2/19/22	0/1/1/1
8	NAG	H	701	8	-	0/6/26/26	0/1/1/1
8	NAG	H	702	9,8	-	0/6/23/26	0/1/1/1
9	BMA	H	703	8,7	-	0/2/19/22	0/1/1/1
7	MAN	H	704	9	-	0/2/19/22	0/1/1/1
7	MAN	H	705	9,7	-	0/2/19/22	0/1/1/1
7	MAN	H	706	7	-	0/2/19/22	0/1/1/1
7	MAN	H	707	7	-	0/2/19/22	0/1/1/1
7	MAN	H	708	7	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	H	709	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	M	301	7	-	0/2/19/22	0/1/1/1
7	MAN	M	302	7	-	0/2/19/22	0/1/1/1
7	MAN	M	303	7	-	0/2/19/22	0/1/1/1
7	MAN	M	304	7	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	M	305	8	-	0/6/23/26	0/1/1/1
8	NAG	M	306	9,8	-	0/6/23/26	0/1/1/1
9	BMA	M	307	8,7	-	0/2/19/22	0/1/1/1
7	MAN	M	308	9,7	-	0/2/19/22	0/1/1/1
7	MAN	M	309	7	-	0/2/19/22	0/1/1/1
7	MAN	M	310	7	-	0/2/19/22	0/1/1/1
7	MAN	R	301	7	-	0/2/19/22	0/1/1/1
7	MAN	R	302	7	-	0/2/19/22	0/1/1/1
7	MAN	R	303	7	-	0/2/19/22	0/1/1/1
7	MAN	R	304	7	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	R	305	8	-	0/6/23/26	0/1/1/1
8	NAG	R	306	9,8	-	0/6/23/26	0/1/1/1
9	BMA	R	307	8,7	-	0/2/19/22	0/1/1/1
7	MAN	R	308	9,7	-	0/2/19/22	0/1/1/1
7	MAN	R	309	7	-	0/2/19/22	0/1/1/1
7	MAN	R	310	7	-	0/2/19/22	0/1/1/1
8	NAG	S	701	8	-	0/6/26/26	0/1/1/1
8	NAG	S	702	9,8	-	0/6/23/26	0/1/1/1
9	BMA	S	703	8,7	-	0/2/19/22	0/1/1/1
7	MAN	S	704	9	-	0/2/19/22	0/1/1/1
7	MAN	S	705	9,7	-	0/2/19/22	0/1/1/1
7	MAN	S	706	7	-	0/2/19/22	0/1/1/1
7	MAN	S	707	7	-	0/2/19/22	0/1/1/1
7	MAN	S	708	7	-	0/2/19/22	0/1/1/1
7	MAN	S	709	7	1/1/4/5	0/2/19/22	0/1/1/1

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	301	MAN	O5-C1	-3.00	1.38	1.43
7	M	301	MAN	O5-C1	-2.98	1.38	1.43
7	2	301	MAN	O5-C1	-2.94	1.38	1.43
7	2	304	MAN	O4-C4	-2.91	1.35	1.43
7	S	709	MAN	O4-C4	-2.90	1.35	1.43
7	M	304	MAN	O4-C4	-2.88	1.35	1.43
7	H	709	MAN	O4-C4	-2.87	1.35	1.43
7	R	304	MAN	O4-C4	-2.87	1.35	1.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3	709	MAN	O4-C4	-2.86	1.35	1.43
7	2	301	MAN	C2-C3	-2.85	1.48	1.52
7	M	301	MAN	C2-C3	-2.84	1.48	1.52
7	R	301	MAN	C2-C3	-2.83	1.48	1.52
7	C	608	MAN	C4-C5	-2.81	1.47	1.53
7	A	608	MAN	C4-C5	-2.80	1.47	1.53
7	3	713	MAN	C4-C5	-2.80	1.47	1.53
7	H	704	MAN	C4-C5	-2.76	1.47	1.53
7	3	704	MAN	C4-C5	-2.75	1.47	1.53
7	S	704	MAN	C4-C5	-2.72	1.47	1.53
7	R	302	MAN	O5-C5	-2.65	1.37	1.43
7	M	302	MAN	O5-C5	-2.62	1.38	1.43
7	2	302	MAN	O5-C5	-2.60	1.38	1.43
9	A	603	BMA	C2-C3	-2.39	1.49	1.52
9	E	603	BMA	C2-C3	-2.38	1.49	1.52
9	C	603	BMA	C2-C3	-2.37	1.49	1.52
7	S	704	MAN	O5-C5	-2.35	1.38	1.43
9	C	603	BMA	O5-C5	-2.35	1.38	1.43
9	E	603	BMA	O5-C5	-2.35	1.38	1.43
7	A	608	MAN	O5-C5	-2.35	1.38	1.43
7	C	608	MAN	O5-C5	-2.34	1.38	1.43
7	3	713	MAN	O5-C5	-2.33	1.38	1.43
7	H	704	MAN	O5-C5	-2.33	1.38	1.43
9	A	603	BMA	O5-C5	-2.32	1.38	1.43
7	3	704	MAN	O5-C5	-2.31	1.38	1.43
7	H	708	MAN	O5-C5	-2.16	1.39	1.43
7	3	708	MAN	O5-C5	-2.15	1.39	1.43
7	S	708	MAN	O5-C5	-2.14	1.39	1.43
7	M	303	MAN	O5-C5	-2.13	1.39	1.43
7	2	303	MAN	O5-C5	-2.13	1.39	1.43
7	R	303	MAN	O5-C5	-2.12	1.39	1.43
7	R	301	MAN	O5-C5	-2.06	1.39	1.43
7	2	301	MAN	O5-C5	-2.05	1.39	1.43
7	M	301	MAN	O5-C5	-2.04	1.39	1.43
7	3	716	MAN	O5-C5	2.02	1.47	1.43
7	2	309	MAN	C1-C2	2.03	1.57	1.52
7	A	611	MAN	O5-C5	2.03	1.47	1.43
7	M	309	MAN	C1-C2	2.04	1.57	1.52
7	3	706	MAN	C2-C3	2.05	1.55	1.52
7	H	707	MAN	O5-C5	2.05	1.47	1.43
7	C	611	MAN	O5-C5	2.06	1.47	1.43
7	R	309	MAN	C1-C2	2.06	1.57	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	601	NAG	C4-C5	2.07	1.57	1.53
7	S	707	MAN	O5-C5	2.07	1.47	1.43
7	3	707	MAN	O5-C5	2.08	1.47	1.43
7	H	706	MAN	C2-C3	2.09	1.55	1.52
7	S	706	MAN	C2-C3	2.09	1.55	1.52
8	A	601	NAG	C4-C5	2.10	1.57	1.53
8	E	601	NAG	C4-C5	2.11	1.57	1.53
7	3	715	MAN	C2-C3	2.13	1.55	1.52
7	A	610	MAN	C2-C3	2.13	1.55	1.52
7	C	610	MAN	C2-C3	2.18	1.55	1.52
8	C	601	NAG	C3-C2	2.30	1.57	1.52
8	E	601	NAG	C3-C2	2.30	1.57	1.52
8	A	601	NAG	C3-C2	2.33	1.57	1.52
7	E	604	MAN	C1-C2	2.34	1.57	1.52
8	C	601	NAG	C2-N2	2.35	1.50	1.46
7	C	604	MAN	C1-C2	2.35	1.57	1.52
8	E	601	NAG	C2-N2	2.35	1.50	1.46
7	A	604	MAN	C1-C2	2.36	1.57	1.52
8	A	601	NAG	C2-N2	2.36	1.50	1.46
7	H	708	MAN	C1-C2	2.42	1.57	1.52
7	R	304	MAN	C2-C3	2.43	1.56	1.52
7	3	708	MAN	C1-C2	2.44	1.57	1.52
7	S	708	MAN	C1-C2	2.44	1.58	1.52
7	2	303	MAN	C1-C2	2.45	1.58	1.52
7	S	709	MAN	C2-C3	2.46	1.56	1.52
7	M	303	MAN	C1-C2	2.47	1.58	1.52
7	M	304	MAN	C2-C3	2.48	1.56	1.52
7	H	709	MAN	C2-C3	2.48	1.56	1.52
7	2	304	MAN	C2-C3	2.49	1.56	1.52
7	R	303	MAN	C1-C2	2.50	1.58	1.52
7	3	709	MAN	C2-C3	2.51	1.56	1.52
7	C	611	MAN	C2-C3	2.53	1.56	1.52
7	H	707	MAN	C2-C3	2.54	1.56	1.52
7	S	707	MAN	C2-C3	2.54	1.56	1.52
7	A	611	MAN	C2-C3	2.58	1.56	1.52
7	3	707	MAN	C2-C3	2.58	1.56	1.52
7	3	716	MAN	C2-C3	2.58	1.56	1.52
8	C	602	NAG	C1-C2	2.65	1.56	1.52
8	A	602	NAG	C1-C2	2.66	1.56	1.52
8	E	602	NAG	C1-C2	2.69	1.56	1.52
7	C	610	MAN	C1-C2	3.03	1.59	1.52
7	A	610	MAN	C1-C2	3.05	1.59	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3	715	MAN	C1-C2	3.06	1.59	1.52
7	H	706	MAN	C1-C2	3.07	1.59	1.52
7	S	706	MAN	C1-C2	3.08	1.59	1.52
7	3	706	MAN	C1-C2	3.10	1.59	1.52
7	A	611	MAN	C1-C2	3.15	1.59	1.52
7	C	611	MAN	C1-C2	3.15	1.59	1.52
7	3	716	MAN	C1-C2	3.16	1.59	1.52
7	3	707	MAN	C1-C2	3.17	1.59	1.52
7	S	707	MAN	C1-C2	3.18	1.59	1.52
7	H	707	MAN	C1-C2	3.18	1.59	1.52
8	3	710	NAG	C1-C2	3.21	1.56	1.52
8	S	701	NAG	C1-C2	3.23	1.56	1.52
8	3	701	NAG	C1-C2	3.24	1.56	1.52
8	C	605	NAG	C1-C2	3.24	1.56	1.52
8	H	701	NAG	C1-C2	3.25	1.56	1.52
8	A	605	NAG	C1-C2	3.28	1.56	1.52
7	3	716	MAN	O5-C1	3.37	1.49	1.43
7	A	611	MAN	O5-C1	3.39	1.49	1.43
7	C	611	MAN	O5-C1	3.39	1.49	1.43
7	3	707	MAN	O5-C1	3.40	1.49	1.43
7	H	707	MAN	O5-C1	3.43	1.49	1.43
7	S	707	MAN	O5-C1	3.46	1.49	1.43
7	3	707	MAN	C4-C5	3.55	1.60	1.53
7	C	611	MAN	C4-C5	3.56	1.60	1.53
7	S	707	MAN	C4-C5	3.57	1.60	1.53
7	H	707	MAN	C4-C5	3.58	1.60	1.53
7	A	611	MAN	C4-C5	3.58	1.60	1.53
7	3	716	MAN	C4-C5	3.60	1.60	1.53
7	S	706	MAN	C4-C5	3.61	1.60	1.53
7	3	715	MAN	C4-C5	3.63	1.60	1.53
7	C	610	MAN	C4-C5	3.64	1.60	1.53
7	A	610	MAN	C4-C5	3.64	1.60	1.53
7	3	706	MAN	C4-C5	3.65	1.60	1.53
7	H	706	MAN	C4-C5	3.65	1.60	1.53
8	A	601	NAG	C1-C2	3.84	1.57	1.52
8	E	601	NAG	C1-C2	3.85	1.57	1.52
8	C	601	NAG	C1-C2	3.88	1.57	1.52

All (541) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	3	709	MAN	C1-C2-C3	-8.83	98.49	109.66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	304	MAN	C1-C2-C3	-8.81	98.52	109.66
7	M	304	MAN	C1-C2-C3	-8.81	98.52	109.66
7	R	304	MAN	C1-C2-C3	-8.80	98.52	109.66
7	H	709	MAN	C1-C2-C3	-8.80	98.52	109.66
7	S	709	MAN	C1-C2-C3	-8.78	98.55	109.66
7	2	301	MAN	O2-C2-C3	-8.27	94.07	110.19
7	M	301	MAN	O2-C2-C3	-8.27	94.07	110.19
7	R	301	MAN	O2-C2-C3	-8.25	94.10	110.19
7	M	302	MAN	O5-C5-C6	-7.65	95.04	107.15
7	R	302	MAN	O5-C5-C6	-7.63	95.06	107.15
7	2	302	MAN	O5-C5-C6	-7.63	95.06	107.15
7	R	302	MAN	C1-C2-C3	-7.40	100.29	109.66
7	2	302	MAN	C1-C2-C3	-7.39	100.31	109.66
7	M	302	MAN	C1-C2-C3	-7.38	100.32	109.66
7	R	303	MAN	O3-C3-C4	-6.49	95.19	110.34
7	M	303	MAN	O3-C3-C4	-6.49	95.19	110.34
7	2	303	MAN	O3-C3-C4	-6.48	95.21	110.34
7	S	708	MAN	O3-C3-C4	-6.48	95.21	110.34
7	3	708	MAN	O3-C3-C4	-6.48	95.22	110.34
7	H	708	MAN	O3-C3-C4	-6.47	95.23	110.34
8	E	602	NAG	C1-O5-C5	-5.66	104.40	112.19
8	A	602	NAG	C1-O5-C5	-5.63	104.44	112.19
8	C	602	NAG	C1-O5-C5	-5.61	104.47	112.19
7	2	303	MAN	O4-C4-C3	-5.58	97.31	110.34
7	M	303	MAN	O4-C4-C3	-5.57	97.34	110.34
7	3	708	MAN	O4-C4-C3	-5.57	97.34	110.34
7	R	303	MAN	O4-C4-C3	-5.56	97.35	110.34
7	S	708	MAN	O4-C4-C3	-5.55	97.37	110.34
7	H	708	MAN	O4-C4-C3	-5.55	97.38	110.34
7	C	604	MAN	C1-O5-C5	-5.46	104.67	112.19
7	A	604	MAN	C1-O5-C5	-5.45	104.70	112.19
7	E	604	MAN	C1-O5-C5	-5.42	104.73	112.19
7	R	303	MAN	O5-C5-C6	-5.40	98.60	107.15
7	3	715	MAN	O5-C5-C6	-5.39	98.62	107.15
7	A	610	MAN	O5-C5-C6	-5.39	98.62	107.15
7	3	706	MAN	O5-C5-C6	-5.38	98.62	107.15
7	S	708	MAN	O5-C5-C6	-5.38	98.62	107.15
7	S	706	MAN	O5-C5-C6	-5.38	98.63	107.15
7	M	303	MAN	O5-C5-C6	-5.38	98.63	107.15
7	C	610	MAN	O5-C5-C6	-5.38	98.63	107.15
7	H	706	MAN	O5-C5-C6	-5.37	98.64	107.15
7	H	708	MAN	O5-C5-C6	-5.37	98.64	107.15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	303	MAN	O5-C5-C6	-5.37	98.64	107.15
7	3	708	MAN	O5-C5-C6	-5.35	98.67	107.15
7	M	301	MAN	C1-O5-C5	-5.30	104.90	112.19
7	2	301	MAN	C1-O5-C5	-5.30	104.90	112.19
7	R	301	MAN	C1-O5-C5	-5.29	104.91	112.19
7	A	609	MAN	C1-O5-C5	-5.24	104.98	112.19
7	3	714	MAN	C1-O5-C5	-5.23	104.99	112.19
7	C	609	MAN	C1-O5-C5	-5.23	105.00	112.19
8	3	711	NAG	C1-C2-N2	-5.21	101.58	110.49
7	3	705	MAN	C1-O5-C5	-5.21	105.02	112.19
8	A	606	NAG	C1-C2-N2	-5.21	101.58	110.49
8	C	606	NAG	C1-C2-N2	-5.21	101.59	110.49
8	H	702	NAG	C1-C2-N2	-5.20	101.61	110.49
8	3	702	NAG	C1-C2-N2	-5.20	101.61	110.49
8	S	702	NAG	C1-C2-N2	-5.19	101.61	110.49
7	H	705	MAN	C1-O5-C5	-5.19	105.05	112.19
7	S	705	MAN	C1-O5-C5	-5.16	105.08	112.19
9	E	603	BMA	C2-C3-C4	-5.06	102.08	110.87
9	C	603	BMA	C2-C3-C4	-5.05	102.10	110.87
9	A	603	BMA	C2-C3-C4	-5.04	102.10	110.87
9	A	603	BMA	O5-C5-C6	-4.85	99.46	107.15
8	S	701	NAG	C3-C2-N2	-4.85	101.27	110.58
9	E	603	BMA	O5-C5-C6	-4.85	99.47	107.15
7	S	706	MAN	O4-C4-C3	-4.84	99.04	110.34
7	C	610	MAN	O4-C4-C3	-4.84	99.04	110.34
8	3	701	NAG	C3-C2-N2	-4.84	101.29	110.58
8	H	701	NAG	C3-C2-N2	-4.84	101.29	110.58
8	3	710	NAG	C3-C2-N2	-4.83	101.30	110.58
7	3	715	MAN	O4-C4-C3	-4.83	99.05	110.34
7	A	610	MAN	O4-C4-C3	-4.83	99.06	110.34
8	C	605	NAG	C3-C2-N2	-4.83	101.31	110.58
9	C	603	BMA	O5-C5-C6	-4.83	99.51	107.15
7	H	706	MAN	O4-C4-C3	-4.81	99.11	110.34
8	A	605	NAG	C3-C2-N2	-4.81	101.35	110.58
7	3	706	MAN	O4-C4-C3	-4.80	99.13	110.34
9	E	603	BMA	O3-C3-C2	-4.64	101.40	110.04
9	C	603	BMA	O3-C3-C2	-4.64	101.40	110.04
9	A	603	BMA	O3-C3-C2	-4.63	101.42	110.04
8	E	602	NAG	C4-C3-C2	-4.56	104.34	111.02
8	A	602	NAG	C4-C3-C2	-4.53	104.38	111.02
9	C	607	BMA	C6-C5-C4	-4.51	102.33	112.99
9	A	607	BMA	C6-C5-C4	-4.50	102.36	112.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	703	BMA	C6-C5-C4	-4.50	102.37	112.99
8	C	602	NAG	C4-C3-C2	-4.50	104.43	111.02
9	H	703	BMA	C6-C5-C4	-4.49	102.37	112.99
9	3	712	BMA	C6-C5-C4	-4.49	102.38	112.99
9	3	703	BMA	C6-C5-C4	-4.49	102.38	112.99
7	R	301	MAN	O3-C3-C4	-4.46	99.94	110.34
7	M	301	MAN	O3-C3-C4	-4.45	99.96	110.34
7	2	301	MAN	O3-C3-C4	-4.44	99.98	110.34
7	R	303	MAN	C6-C5-C4	-4.06	103.41	112.99
7	S	708	MAN	C6-C5-C4	-4.05	103.42	112.99
7	2	303	MAN	C6-C5-C4	-4.05	103.42	112.99
7	H	708	MAN	C6-C5-C4	-4.05	103.43	112.99
7	3	708	MAN	C6-C5-C4	-4.04	103.44	112.99
7	M	303	MAN	C6-C5-C4	-4.04	103.44	112.99
9	3	712	BMA	O5-C5-C6	-3.99	100.84	107.15
9	A	607	BMA	O5-C5-C6	-3.97	100.86	107.15
9	C	607	BMA	O5-C5-C6	-3.95	100.89	107.15
9	H	703	BMA	O5-C5-C6	-3.94	100.90	107.15
9	S	703	BMA	O5-C5-C6	-3.94	100.91	107.15
9	3	703	BMA	O5-C5-C6	-3.93	100.92	107.15
8	C	602	NAG	O5-C1-C2	-3.89	106.15	111.52
8	E	602	NAG	O5-C1-C2	-3.88	106.16	111.52
8	A	602	NAG	O5-C1-C2	-3.88	106.17	111.52
7	R	301	MAN	O3-C3-C2	-3.79	102.98	110.04
7	2	301	MAN	O3-C3-C2	-3.78	103.01	110.04
7	M	301	MAN	O3-C3-C2	-3.78	103.01	110.04
7	2	303	MAN	C2-C3-C4	-3.74	104.38	110.87
7	M	303	MAN	C2-C3-C4	-3.72	104.40	110.87
7	H	708	MAN	C2-C3-C4	-3.72	104.40	110.87
7	3	708	MAN	C2-C3-C4	-3.72	104.40	110.87
7	R	303	MAN	C2-C3-C4	-3.71	104.42	110.87
7	S	708	MAN	C2-C3-C4	-3.71	104.42	110.87
7	3	709	MAN	O5-C5-C4	-3.55	102.19	110.83
7	H	709	MAN	O5-C5-C4	-3.54	102.21	110.83
7	R	304	MAN	O5-C5-C4	-3.53	102.23	110.83
7	S	709	MAN	O5-C5-C4	-3.53	102.23	110.83
7	M	304	MAN	O5-C5-C4	-3.53	102.24	110.83
7	2	304	MAN	O5-C5-C4	-3.52	102.27	110.83
7	3	708	MAN	O2-C2-C3	-3.51	103.35	110.19
7	H	708	MAN	O2-C2-C3	-3.50	103.37	110.19
7	M	303	MAN	O2-C2-C3	-3.50	103.37	110.19
7	2	303	MAN	O2-C2-C3	-3.49	103.38	110.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	708	MAN	O2-C2-C3	-3.49	103.38	110.19
7	R	303	MAN	O2-C2-C3	-3.49	103.39	110.19
7	A	604	MAN	O6-C6-C5	-3.38	99.48	111.29
7	E	604	MAN	O6-C6-C5	-3.38	99.50	111.29
7	C	604	MAN	O6-C6-C5	-3.36	99.55	111.29
9	E	603	BMA	O2-C2-C3	-3.36	103.64	110.19
9	A	603	BMA	O2-C2-C3	-3.35	103.65	110.19
9	C	603	BMA	O2-C2-C3	-3.35	103.66	110.19
7	2	302	MAN	O5-C5-C4	-3.32	102.76	110.83
7	M	302	MAN	O5-C5-C4	-3.30	102.80	110.83
7	R	302	MAN	O5-C5-C4	-3.29	102.82	110.83
9	C	607	BMA	O3-C3-C4	-3.14	103.00	110.34
9	A	607	BMA	O3-C3-C4	-3.13	103.02	110.34
9	H	703	BMA	O3-C3-C4	-3.13	103.03	110.34
9	S	703	BMA	O3-C3-C4	-3.13	103.04	110.34
9	3	712	BMA	O3-C3-C4	-3.13	103.04	110.34
9	3	703	BMA	O3-C3-C4	-3.13	103.04	110.34
7	3	704	MAN	O5-C5-C4	-2.96	103.62	110.83
7	S	704	MAN	O5-C5-C4	-2.96	103.63	110.83
7	H	704	MAN	O5-C5-C4	-2.96	103.64	110.83
7	C	608	MAN	O5-C5-C4	-2.95	103.66	110.83
7	3	713	MAN	O5-C5-C4	-2.94	103.67	110.83
7	A	608	MAN	O5-C5-C4	-2.94	103.69	110.83
7	3	714	MAN	O2-C2-C1	-2.89	103.34	109.17
7	H	705	MAN	O2-C2-C1	-2.88	103.37	109.17
7	S	705	MAN	O2-C2-C1	-2.87	103.38	109.17
7	3	705	MAN	O2-C2-C1	-2.87	103.38	109.17
7	C	609	MAN	O2-C2-C1	-2.86	103.40	109.17
7	A	609	MAN	O2-C2-C1	-2.86	103.41	109.17
7	S	704	MAN	O5-C1-C2	-2.85	106.33	110.78
7	R	301	MAN	C3-C4-C5	-2.85	105.14	110.24
7	C	608	MAN	O5-C1-C2	-2.85	106.33	110.78
7	3	713	MAN	O5-C1-C2	-2.85	106.33	110.78
7	H	704	MAN	O5-C1-C2	-2.84	106.35	110.78
8	C	601	NAG	C8-C7-N2	-2.84	111.12	116.10
7	3	704	MAN	O5-C1-C2	-2.84	106.35	110.78
7	M	301	MAN	C3-C4-C5	-2.83	105.18	110.24
7	A	608	MAN	O5-C1-C2	-2.82	106.38	110.78
7	2	301	MAN	C3-C4-C5	-2.82	105.20	110.24
8	A	601	NAG	C8-C7-N2	-2.81	111.17	116.10
9	C	603	BMA	O3-C3-C4	-2.80	103.80	110.34
9	A	603	BMA	O3-C3-C4	-2.80	103.80	110.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	601	NAG	C8-C7-N2	-2.79	111.22	116.10
9	E	603	BMA	O3-C3-C4	-2.79	103.83	110.34
8	E	601	NAG	O5-C5-C6	-2.77	102.76	107.15
8	A	601	NAG	O5-C5-C6	-2.75	102.79	107.15
8	C	601	NAG	O5-C5-C6	-2.75	102.79	107.15
7	R	301	MAN	O5-C5-C4	-2.74	104.15	110.83
7	2	301	MAN	O5-C5-C4	-2.74	104.16	110.83
7	M	301	MAN	O5-C5-C4	-2.74	104.16	110.83
9	C	603	BMA	C6-C5-C4	-2.72	106.57	112.99
9	E	603	BMA	C6-C5-C4	-2.71	106.58	112.99
7	3	704	MAN	O4-C4-C5	-2.71	102.52	109.31
8	S	702	NAG	O4-C4-C5	-2.71	102.52	109.31
8	3	702	NAG	O4-C4-C5	-2.71	102.53	109.31
9	A	603	BMA	C6-C5-C4	-2.70	106.60	112.99
9	3	703	BMA	O2-C2-C1	-2.70	103.73	109.17
8	H	702	NAG	O4-C4-C5	-2.70	102.54	109.31
7	H	704	MAN	O4-C4-C5	-2.69	102.56	109.31
9	A	607	BMA	O2-C2-C1	-2.69	103.75	109.17
9	3	712	BMA	O2-C2-C1	-2.69	103.75	109.17
7	C	608	MAN	O4-C4-C5	-2.69	102.57	109.31
7	3	713	MAN	O4-C4-C5	-2.69	102.57	109.31
7	S	704	MAN	O4-C4-C5	-2.69	102.58	109.31
8	3	711	NAG	O4-C4-C5	-2.69	102.58	109.31
8	A	606	NAG	O4-C4-C5	-2.68	102.58	109.31
9	H	703	BMA	O2-C2-C1	-2.68	103.76	109.17
9	S	703	BMA	O2-C2-C1	-2.68	103.78	109.17
8	C	606	NAG	O4-C4-C5	-2.67	102.61	109.31
7	A	608	MAN	O4-C4-C5	-2.67	102.61	109.31
9	C	607	BMA	O2-C2-C1	-2.66	103.81	109.17
7	H	704	MAN	C6-C5-C4	-2.58	106.89	112.99
7	S	704	MAN	C6-C5-C4	-2.58	106.89	112.99
8	C	602	NAG	C3-C4-C5	-2.57	105.64	110.24
7	3	704	MAN	C6-C5-C4	-2.57	106.92	112.99
8	E	602	NAG	C3-C4-C5	-2.56	105.67	110.24
9	E	603	BMA	O5-C1-C2	-2.55	106.80	110.78
8	A	602	NAG	C3-C4-C5	-2.55	105.68	110.24
7	A	608	MAN	C6-C5-C4	-2.55	106.97	112.99
9	A	603	BMA	O5-C1-C2	-2.55	106.81	110.78
9	C	603	BMA	O5-C1-C2	-2.54	106.81	110.78
7	3	713	MAN	C6-C5-C4	-2.54	107.00	112.99
7	C	608	MAN	C6-C5-C4	-2.53	107.02	112.99
7	R	302	MAN	O6-C6-C5	-2.41	102.88	111.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	302	MAN	O6-C6-C5	-2.41	102.89	111.29
7	2	302	MAN	O6-C6-C5	-2.41	102.90	111.29
7	A	604	MAN	O4-C4-C3	-2.40	104.73	110.34
7	E	604	MAN	O4-C4-C3	-2.40	104.74	110.34
7	C	604	MAN	O4-C4-C3	-2.39	104.75	110.34
7	M	310	MAN	O2-C2-C3	-2.39	105.53	110.19
7	R	310	MAN	O2-C2-C3	-2.38	105.55	110.19
7	2	310	MAN	O2-C2-C3	-2.37	105.56	110.19
7	2	308	MAN	O2-C2-C3	-2.37	105.57	110.19
7	R	303	MAN	O6-C6-C5	-2.36	103.07	111.29
7	M	308	MAN	O2-C2-C3	-2.35	105.60	110.19
7	2	303	MAN	O6-C6-C5	-2.35	103.08	111.29
7	M	303	MAN	O6-C6-C5	-2.35	103.08	111.29
7	S	708	MAN	O6-C6-C5	-2.35	103.09	111.29
7	H	708	MAN	O6-C6-C5	-2.35	103.10	111.29
7	3	708	MAN	O6-C6-C5	-2.34	103.11	111.29
7	R	308	MAN	O2-C2-C3	-2.34	105.63	110.19
9	E	603	BMA	O2-C2-C1	-2.21	104.72	109.17
9	A	603	BMA	O2-C2-C1	-2.21	104.72	109.17
9	C	603	BMA	O2-C2-C1	-2.19	104.75	109.17
7	2	309	MAN	O2-C2-C3	-2.14	106.01	110.19
7	M	309	MAN	O2-C2-C3	-2.14	106.01	110.19
7	R	309	MAN	O2-C2-C3	-2.14	106.02	110.19
7	C	609	MAN	O6-C6-C5	-2.07	104.06	111.29
7	H	705	MAN	O6-C6-C5	-2.07	104.06	111.29
7	A	609	MAN	O6-C6-C5	-2.07	104.07	111.29
7	3	705	MAN	O6-C6-C5	-2.07	104.08	111.29
7	3	714	MAN	O6-C6-C5	-2.06	104.10	111.29
7	S	705	MAN	O6-C6-C5	-2.06	104.10	111.29
9	E	603	BMA	O6-C6-C5	-2.04	104.18	111.29
9	A	603	BMA	O6-C6-C5	-2.03	104.21	111.29
9	C	603	BMA	O6-C6-C5	-2.03	104.21	111.29
9	H	703	BMA	C2-C3-C4	2.01	114.36	110.87
9	A	607	BMA	C2-C3-C4	2.02	114.38	110.87
7	M	302	MAN	O3-C3-C4	2.03	115.08	110.34
7	2	302	MAN	O3-C3-C4	2.03	115.08	110.34
9	3	712	BMA	C2-C3-C4	2.03	114.39	110.87
7	R	302	MAN	O3-C3-C4	2.03	115.09	110.34
9	3	703	BMA	C2-C3-C4	2.04	114.40	110.87
8	C	605	NAG	C1-O5-C5	2.05	117.64	113.69
8	3	710	NAG	C1-O5-C5	2.06	117.64	113.69
8	A	605	NAG	C1-O5-C5	2.06	117.65	113.69

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	701	NAG	C1-O5-C5	2.08	117.69	113.69
8	H	701	NAG	C1-O5-C5	2.09	117.71	113.69
8	S	701	NAG	C1-O5-C5	2.10	117.74	113.69
8	S	701	NAG	O3-C3-C4	2.21	115.50	110.34
8	3	701	NAG	O3-C3-C4	2.21	115.51	110.34
8	C	606	NAG	C1-O5-C5	2.22	115.24	112.19
8	H	701	NAG	O3-C3-C4	2.22	115.52	110.34
8	C	605	NAG	O3-C3-C4	2.22	115.53	110.34
8	A	606	NAG	C1-O5-C5	2.23	115.25	112.19
8	3	711	NAG	C1-O5-C5	2.25	115.28	112.19
8	A	605	NAG	O3-C3-C4	2.25	115.59	110.34
8	3	710	NAG	O3-C3-C4	2.25	115.59	110.34
8	S	702	NAG	C1-O5-C5	2.25	115.28	112.19
8	H	702	NAG	C1-O5-C5	2.25	115.28	112.19
8	3	702	NAG	C1-O5-C5	2.25	115.29	112.19
8	C	602	NAG	O3-C3-C4	2.27	115.64	110.34
8	A	602	NAG	O3-C3-C4	2.28	115.67	110.34
8	E	602	NAG	O3-C3-C4	2.28	115.67	110.34
7	2	310	MAN	C1-O5-C5	2.35	115.43	112.19
7	M	310	MAN	C1-O5-C5	2.40	115.49	112.19
7	R	310	MAN	C1-O5-C5	2.41	115.50	112.19
7	2	304	MAN	C3-C4-C5	2.42	114.58	110.24
7	R	302	MAN	O5-C1-C2	2.43	114.57	110.78
7	2	302	MAN	O5-C1-C2	2.44	114.58	110.78
7	M	304	MAN	C3-C4-C5	2.44	114.60	110.24
7	M	302	MAN	O5-C1-C2	2.45	114.60	110.78
7	R	304	MAN	C3-C4-C5	2.45	114.62	110.24
7	S	709	MAN	C3-C4-C5	2.45	114.63	110.24
7	H	709	MAN	C3-C4-C5	2.48	114.67	110.24
7	2	308	MAN	C1-O5-C5	2.49	115.61	112.19
7	M	308	MAN	C1-O5-C5	2.49	115.61	112.19
7	3	709	MAN	C3-C4-C5	2.49	114.70	110.24
7	R	308	MAN	C1-O5-C5	2.52	115.66	112.19
9	3	712	BMA	O2-C2-C3	2.62	115.29	110.19
9	S	703	BMA	O2-C2-C3	2.62	115.30	110.19
9	H	703	BMA	O2-C2-C3	2.62	115.30	110.19
7	3	715	MAN	C2-C3-C4	2.63	115.43	110.87
9	A	607	BMA	O2-C2-C3	2.63	115.32	110.19
7	C	610	MAN	C2-C3-C4	2.64	115.45	110.87
9	C	607	BMA	O2-C2-C3	2.64	115.34	110.19
9	3	703	BMA	O2-C2-C3	2.65	115.35	110.19
7	A	610	MAN	C2-C3-C4	2.65	115.46	110.87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	706	MAN	C2-C3-C4	2.66	115.48	110.87
8	3	701	NAG	C2-N2-C7	2.67	129.88	123.23
7	H	706	MAN	C2-C3-C4	2.68	115.51	110.87
8	C	605	NAG	C2-N2-C7	2.68	129.90	123.23
8	S	701	NAG	C2-N2-C7	2.68	129.90	123.23
8	A	605	NAG	C2-N2-C7	2.69	129.92	123.23
8	H	701	NAG	C2-N2-C7	2.69	129.92	123.23
8	3	710	NAG	C2-N2-C7	2.69	129.93	123.23
8	E	601	NAG	C1-C2-N2	2.70	115.10	110.49
7	3	706	MAN	C2-C3-C4	2.70	115.56	110.87
8	A	601	NAG	C1-C2-N2	2.71	115.12	110.49
7	R	304	MAN	O2-C2-C1	2.72	114.65	109.17
8	C	601	NAG	C1-C2-N2	2.72	115.13	110.49
7	M	304	MAN	O2-C2-C1	2.72	114.66	109.17
7	2	304	MAN	O2-C2-C1	2.74	114.70	109.17
7	H	709	MAN	O2-C2-C1	2.75	114.72	109.17
7	S	709	MAN	O2-C2-C1	2.76	114.74	109.17
7	3	709	MAN	O2-C2-C1	2.77	114.76	109.17
7	R	301	MAN	O5-C5-C6	2.84	111.65	107.15
7	M	301	MAN	O5-C5-C6	2.85	111.66	107.15
7	2	301	MAN	O5-C5-C6	2.86	111.68	107.15
7	R	301	MAN	C1-C2-C3	3.04	113.51	109.66
7	2	301	MAN	C1-C2-C3	3.06	113.54	109.66
7	M	301	MAN	C1-C2-C3	3.07	113.54	109.66
8	E	601	NAG	O7-C7-N2	3.10	127.80	121.94
8	C	601	NAG	O7-C7-N2	3.10	127.80	121.94
8	A	601	NAG	O7-C7-N2	3.11	127.81	121.94
7	R	301	MAN	O4-C4-C5	3.13	117.16	109.31
7	M	301	MAN	O4-C4-C5	3.13	117.16	109.31
8	S	702	NAG	O3-C3-C4	3.14	117.67	110.34
8	H	702	NAG	O3-C3-C4	3.14	117.68	110.34
7	2	301	MAN	O4-C4-C5	3.15	117.19	109.31
8	3	702	NAG	O3-C3-C4	3.15	117.69	110.34
8	C	606	NAG	O3-C3-C4	3.15	117.70	110.34
8	A	606	NAG	O3-C3-C4	3.17	117.74	110.34
8	C	602	NAG	O3-C3-C2	3.17	116.19	109.39
8	E	602	NAG	O3-C3-C2	3.18	116.21	109.39
8	A	602	NAG	O3-C3-C2	3.19	116.22	109.39
8	3	711	NAG	O3-C3-C4	3.19	117.80	110.34
7	3	706	MAN	C3-C4-C5	3.23	116.02	110.24
7	A	610	MAN	C3-C4-C5	3.24	116.04	110.24
7	H	706	MAN	C3-C4-C5	3.24	116.04	110.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	3	715	MAN	C3-C4-C5	3.25	116.05	110.24
7	S	706	MAN	C3-C4-C5	3.25	116.06	110.24
7	3	714	MAN	O5-C5-C6	3.25	112.30	107.15
7	C	610	MAN	C3-C4-C5	3.26	116.06	110.24
7	A	609	MAN	O5-C5-C6	3.26	112.31	107.15
7	3	705	MAN	O5-C5-C6	3.27	112.32	107.15
7	C	609	MAN	O5-C5-C6	3.27	112.33	107.15
7	H	705	MAN	O5-C5-C6	3.29	112.35	107.15
7	S	705	MAN	O5-C5-C6	3.29	112.35	107.15
7	C	608	MAN	C2-C3-C4	3.30	116.59	110.87
7	3	713	MAN	C2-C3-C4	3.32	116.63	110.87
7	A	608	MAN	C2-C3-C4	3.32	116.63	110.87
7	C	604	MAN	O5-C5-C6	3.32	112.40	107.15
7	S	704	MAN	C2-C3-C4	3.32	116.64	110.87
7	H	704	MAN	C2-C3-C4	3.33	116.64	110.87
7	3	704	MAN	C2-C3-C4	3.33	116.65	110.87
7	A	604	MAN	O5-C5-C6	3.35	112.44	107.15
7	E	604	MAN	O5-C5-C6	3.36	112.47	107.15
7	A	610	MAN	C1-O5-C5	3.40	116.86	112.19
7	H	706	MAN	C1-O5-C5	3.41	116.87	112.19
7	C	610	MAN	C1-O5-C5	3.41	116.87	112.19
7	S	706	MAN	C1-O5-C5	3.41	116.88	112.19
7	3	715	MAN	C1-O5-C5	3.42	116.89	112.19
8	S	701	NAG	O1-C1-C2	3.42	116.33	109.22
7	3	706	MAN	C1-O5-C5	3.42	116.90	112.19
8	A	605	NAG	O1-C1-C2	3.43	116.34	109.22
8	3	701	NAG	O1-C1-C2	3.43	116.35	109.22
8	C	605	NAG	O1-C1-C2	3.43	116.35	109.22
8	H	701	NAG	O1-C1-C2	3.44	116.36	109.22
9	C	607	BMA	C3-C4-C5	3.44	116.40	110.24
8	3	710	NAG	O1-C1-C2	3.45	116.38	109.22
9	A	607	BMA	C3-C4-C5	3.45	116.41	110.24
9	3	703	BMA	C3-C4-C5	3.45	116.42	110.24
9	3	712	BMA	C3-C4-C5	3.46	116.43	110.24
9	H	703	BMA	C3-C4-C5	3.47	116.45	110.24
7	3	706	MAN	O2-C2-C1	3.49	116.21	109.17
9	S	703	BMA	C3-C4-C5	3.49	116.49	110.24
7	3	715	MAN	O2-C2-C1	3.51	116.24	109.17
7	H	706	MAN	O2-C2-C1	3.52	116.27	109.17
7	S	706	MAN	O2-C2-C1	3.52	116.28	109.17
7	A	610	MAN	O2-C2-C1	3.52	116.28	109.17
7	C	610	MAN	O2-C2-C1	3.53	116.28	109.17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	601	NAG	O5-C1-C2	3.53	116.39	111.52
7	E	604	MAN	O5-C1-C2	3.53	116.29	110.78
7	A	604	MAN	O5-C1-C2	3.55	116.31	110.78
8	A	601	NAG	O5-C1-C2	3.55	116.42	111.52
8	C	601	NAG	O5-C1-C2	3.55	116.42	111.52
7	C	604	MAN	O5-C1-C2	3.57	116.35	110.78
7	S	709	MAN	O5-C1-C2	3.59	116.37	110.78
7	3	709	MAN	O5-C1-C2	3.60	116.39	110.78
7	H	709	MAN	O5-C1-C2	3.62	116.42	110.78
7	R	304	MAN	O5-C1-C2	3.62	116.42	110.78
7	S	708	MAN	C1-C2-C3	3.62	114.24	109.66
7	M	304	MAN	O5-C1-C2	3.62	116.43	110.78
7	2	304	MAN	O5-C1-C2	3.64	116.45	110.78
7	R	303	MAN	C1-C2-C3	3.65	114.28	109.66
7	3	708	MAN	C1-C2-C3	3.67	114.31	109.66
7	H	708	MAN	C1-C2-C3	3.67	114.31	109.66
7	M	303	MAN	C1-C2-C3	3.68	114.31	109.66
7	2	303	MAN	C1-C2-C3	3.69	114.33	109.66
7	3	714	MAN	C3-C4-C5	3.73	116.92	110.24
7	2	302	MAN	C2-C3-C4	3.73	117.35	110.87
7	M	302	MAN	C2-C3-C4	3.74	117.37	110.87
7	C	609	MAN	C3-C4-C5	3.75	116.96	110.24
7	H	705	MAN	C3-C4-C5	3.76	116.96	110.24
7	R	302	MAN	C2-C3-C4	3.76	117.39	110.87
7	A	609	MAN	C3-C4-C5	3.76	116.96	110.24
7	3	705	MAN	C3-C4-C5	3.76	116.97	110.24
7	S	705	MAN	C3-C4-C5	3.77	116.98	110.24
7	3	715	MAN	O5-C1-C2	3.80	116.71	110.78
7	S	706	MAN	O5-C1-C2	3.81	116.72	110.78
7	3	706	MAN	O5-C1-C2	3.82	116.73	110.78
7	A	610	MAN	O5-C1-C2	3.82	116.74	110.78
7	H	706	MAN	O5-C1-C2	3.82	116.74	110.78
7	C	610	MAN	O5-C1-C2	3.84	116.76	110.78
7	S	709	MAN	C1-O5-C5	3.86	117.50	112.19
7	C	608	MAN	C1-O5-C5	3.87	117.52	112.19
7	H	709	MAN	C1-O5-C5	3.88	117.52	112.19
7	A	608	MAN	C1-O5-C5	3.88	117.52	112.19
7	3	709	MAN	C1-O5-C5	3.88	117.53	112.19
7	2	304	MAN	C1-O5-C5	3.88	117.53	112.19
7	M	304	MAN	C1-O5-C5	3.89	117.53	112.19
7	3	713	MAN	C1-O5-C5	3.89	117.54	112.19
7	R	304	MAN	C1-O5-C5	3.91	117.56	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	704	MAN	C1-O5-C5	3.91	117.57	112.19
7	S	704	MAN	C1-O5-C5	3.93	117.59	112.19
8	3	710	NAG	C4-C3-C2	3.93	116.16	110.33
7	3	704	MAN	C1-O5-C5	3.94	117.61	112.19
8	C	605	NAG	C4-C3-C2	3.94	116.17	110.33
8	S	701	NAG	C4-C3-C2	3.95	116.18	110.33
8	H	701	NAG	C4-C3-C2	3.95	116.19	110.33
8	3	701	NAG	C4-C3-C2	3.95	116.19	110.33
8	A	605	NAG	C4-C3-C2	3.96	116.20	110.33
7	3	715	MAN	O4-C4-C5	3.99	119.31	109.31
7	3	706	MAN	O4-C4-C5	4.00	119.32	109.31
8	S	701	NAG	O5-C5-C4	4.00	117.04	109.69
7	H	706	MAN	O4-C4-C5	4.00	119.34	109.31
7	A	610	MAN	O4-C4-C5	4.01	119.36	109.31
7	S	706	MAN	O4-C4-C5	4.01	119.36	109.31
7	C	610	MAN	O4-C4-C5	4.02	119.38	109.31
8	3	701	NAG	O5-C5-C4	4.03	117.09	109.69
8	H	701	NAG	O5-C5-C4	4.03	117.10	109.69
8	A	605	NAG	O5-C5-C4	4.04	117.11	109.69
8	C	605	NAG	O5-C5-C4	4.05	117.13	109.69
8	3	710	NAG	O5-C5-C4	4.05	117.13	109.69
8	E	601	NAG	C4-C3-C2	4.06	116.97	111.02
8	A	601	NAG	C4-C3-C2	4.06	116.97	111.02
8	C	601	NAG	C4-C3-C2	4.07	116.98	111.02
7	S	707	MAN	O4-C4-C5	4.12	119.63	109.31
7	3	716	MAN	O4-C4-C5	4.12	119.63	109.31
7	A	611	MAN	C6-C5-C4	4.12	122.74	112.99
7	H	707	MAN	O4-C4-C5	4.12	119.64	109.31
7	C	611	MAN	C6-C5-C4	4.13	122.74	112.99
7	3	707	MAN	O4-C4-C5	4.13	119.64	109.31
7	A	611	MAN	O4-C4-C5	4.13	119.64	109.31
7	C	611	MAN	O4-C4-C5	4.13	119.66	109.31
7	3	716	MAN	C6-C5-C4	4.13	122.76	112.99
7	H	707	MAN	C6-C5-C4	4.15	122.79	112.99
7	3	707	MAN	C6-C5-C4	4.15	122.80	112.99
7	S	707	MAN	C6-C5-C4	4.16	122.82	112.99
8	E	602	NAG	O5-C5-C6	4.16	113.73	107.15
8	A	602	NAG	O5-C5-C6	4.17	113.75	107.15
8	C	602	NAG	O5-C5-C6	4.20	113.79	107.15
8	E	601	NAG	C1-O5-C5	4.20	117.97	112.19
8	A	601	NAG	C1-O5-C5	4.21	117.97	112.19
8	C	601	NAG	C1-O5-C5	4.22	117.99	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	710	NAG	C3-C4-C5	4.29	117.91	110.24
8	C	605	NAG	C3-C4-C5	4.29	117.92	110.24
8	A	605	NAG	C3-C4-C5	4.29	117.92	110.24
8	H	701	NAG	C3-C4-C5	4.29	117.92	110.24
8	3	701	NAG	C3-C4-C5	4.29	117.92	110.24
8	S	701	NAG	C3-C4-C5	4.30	117.94	110.24
8	C	602	NAG	C6-C5-C4	4.40	123.38	112.99
8	E	602	NAG	C6-C5-C4	4.40	123.38	112.99
8	A	602	NAG	C6-C5-C4	4.40	123.39	112.99
7	R	302	MAN	O2-C2-C1	4.84	118.93	109.17
7	2	302	MAN	O2-C2-C1	4.84	118.94	109.17
7	M	302	MAN	O2-C2-C1	4.84	118.94	109.17
7	2	304	MAN	O2-C2-C3	4.91	119.77	110.19
7	H	709	MAN	O2-C2-C3	4.94	119.82	110.19
7	3	709	MAN	O2-C2-C3	4.94	119.82	110.19
7	M	304	MAN	O2-C2-C3	4.94	119.83	110.19
7	S	709	MAN	O2-C2-C3	4.96	119.86	110.19
7	R	304	MAN	O2-C2-C3	4.96	119.87	110.19
8	3	702	NAG	O5-C1-C2	5.03	118.47	111.52
8	H	702	NAG	O5-C1-C2	5.05	118.50	111.52
8	3	711	NAG	O5-C1-C2	5.06	118.50	111.52
8	S	702	NAG	O5-C1-C2	5.06	118.51	111.52
8	A	606	NAG	O5-C1-C2	5.07	118.53	111.52
8	C	606	NAG	O5-C1-C2	5.08	118.54	111.52
7	3	716	MAN	C1-C2-C3	5.28	116.34	109.66
7	A	611	MAN	C1-C2-C3	5.30	116.37	109.66
7	C	611	MAN	C1-C2-C3	5.33	116.40	109.66
7	3	707	MAN	C1-C2-C3	5.34	116.41	109.66
7	H	707	MAN	C1-C2-C3	5.35	116.43	109.66
7	S	707	MAN	C1-C2-C3	5.35	116.43	109.66
7	C	604	MAN	O2-C2-C1	5.41	120.08	109.17
7	E	604	MAN	O2-C2-C1	5.41	120.08	109.17
7	A	604	MAN	O2-C2-C1	5.41	120.09	109.17
8	C	605	NAG	C1-C2-N2	5.62	117.24	110.73
8	H	701	NAG	C1-C2-N2	5.64	117.26	110.73
8	S	701	NAG	C1-C2-N2	5.64	117.26	110.73
8	A	605	NAG	C1-C2-N2	5.65	117.27	110.73
8	3	701	NAG	C1-C2-N2	5.65	117.28	110.73
8	3	710	NAG	C1-C2-N2	5.66	117.28	110.73
7	3	706	MAN	C1-C2-C3	5.90	117.13	109.66
7	H	706	MAN	C1-C2-C3	5.91	117.14	109.66
7	C	611	MAN	C1-O5-C5	5.92	120.33	112.19

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	707	MAN	C1-O5-C5	5.92	120.33	112.19
7	S	706	MAN	C1-C2-C3	5.92	117.15	109.66
7	C	610	MAN	C1-C2-C3	5.92	117.16	109.66
7	A	610	MAN	C1-C2-C3	5.93	117.16	109.66
7	A	611	MAN	C1-O5-C5	5.94	120.36	112.19
7	3	707	MAN	C1-O5-C5	5.94	120.36	112.19
7	H	707	MAN	C1-O5-C5	5.95	120.37	112.19
7	3	715	MAN	C1-C2-C3	5.95	117.19	109.66
7	3	716	MAN	C1-O5-C5	5.97	120.40	112.19
7	C	610	MAN	C6-C5-C4	6.29	127.87	112.99
7	A	610	MAN	C6-C5-C4	6.29	127.87	112.99
7	3	715	MAN	C6-C5-C4	6.31	127.90	112.99
7	H	706	MAN	C6-C5-C4	6.32	127.92	112.99
7	S	706	MAN	C6-C5-C4	6.32	127.92	112.99
7	3	706	MAN	C6-C5-C4	6.33	127.95	112.99
7	H	708	MAN	O5-C1-C2	6.56	121.01	110.78
7	R	303	MAN	O5-C1-C2	6.57	121.02	110.78
7	3	708	MAN	O5-C1-C2	6.57	121.02	110.78
7	M	303	MAN	O5-C1-C2	6.57	121.02	110.78
7	2	303	MAN	O5-C1-C2	6.58	121.03	110.78
7	S	708	MAN	O5-C1-C2	6.58	121.04	110.78
9	C	607	BMA	C1-O5-C5	6.63	121.31	112.19
9	A	607	BMA	C1-O5-C5	6.65	121.33	112.19
9	3	703	BMA	C1-O5-C5	6.65	121.34	112.19
9	3	712	BMA	C1-O5-C5	6.66	121.35	112.19
9	H	703	BMA	C1-O5-C5	6.66	121.36	112.19
9	S	703	BMA	C1-O5-C5	6.70	121.40	112.19
7	R	303	MAN	O4-C4-C5	6.90	126.60	109.31
8	C	601	NAG	C2-N2-C7	6.91	133.02	122.94
7	M	303	MAN	O4-C4-C5	6.92	126.63	109.31
7	2	303	MAN	O4-C4-C5	6.92	126.64	109.31
7	S	708	MAN	O4-C4-C5	6.93	126.65	109.31
7	H	708	MAN	O4-C4-C5	6.93	126.67	109.31
7	3	708	MAN	O4-C4-C5	6.94	126.69	109.31
8	A	601	NAG	C2-N2-C7	6.94	133.07	122.94
8	E	601	NAG	C2-N2-C7	6.96	133.10	122.94

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	3	709	MAN	C1
7	M	304	MAN	C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
7	H	709	MAN	C1
7	2	304	MAN	C1
7	S	709	MAN	C1
7	R	304	MAN	C1

There are no torsion outliers.

There are no ring outliers.

51 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	2	301	MAN	8	0
7	2	302	MAN	3	0
7	2	303	MAN	7	0
7	2	309	MAN	1	0
9	3	703	BMA	4	0
7	3	704	MAN	7	0
7	3	705	MAN	4	0
7	3	706	MAN	2	0
7	3	707	MAN	2	0
7	3	708	MAN	7	0
7	3	709	MAN	1	0
9	3	712	BMA	5	0
7	3	713	MAN	7	0
7	3	714	MAN	6	0
7	3	715	MAN	7	0
7	3	716	MAN	2	0
7	A	604	MAN	4	0
9	A	607	BMA	5	0
7	A	608	MAN	8	0
7	A	609	MAN	6	0
7	A	610	MAN	7	0
7	A	611	MAN	2	0
7	C	604	MAN	4	0
9	C	607	BMA	4	0
7	C	608	MAN	7	0
7	C	609	MAN	5	0
7	C	610	MAN	7	0
7	C	611	MAN	2	0
7	E	604	MAN	4	0
9	H	703	BMA	3	0
7	H	704	MAN	7	0
7	H	705	MAN	4	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	706	MAN	3	0
7	H	707	MAN	2	0
7	H	708	MAN	7	0
7	H	709	MAN	1	0
7	M	301	MAN	8	0
7	M	302	MAN	3	0
7	M	303	MAN	8	0
7	M	309	MAN	1	0
7	R	301	MAN	8	0
7	R	302	MAN	3	0
7	R	303	MAN	7	0
7	R	309	MAN	1	0
9	S	703	BMA	4	0
7	S	704	MAN	7	0
7	S	705	MAN	5	0
7	S	706	MAN	3	0
7	S	707	MAN	2	0
7	S	708	MAN	7	0
7	S	709	MAN	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.