



wwPDB EM Map/Model Validation Report ⓘ

Oct 9, 2016 – 06:46 AM EDT

PDB ID : 5SZS
EMDB ID: : EMD-8331
Title : Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy
Authors : Walls, A.C.; Tortorici, M.A.; Frenz, B.; Snijder, J.; Li, W.; Rey, F.A.; DiMaio, F.; Bosch, B.J.; Veerler, D.
Deposited on : 2016-08-15
Resolution : 3.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

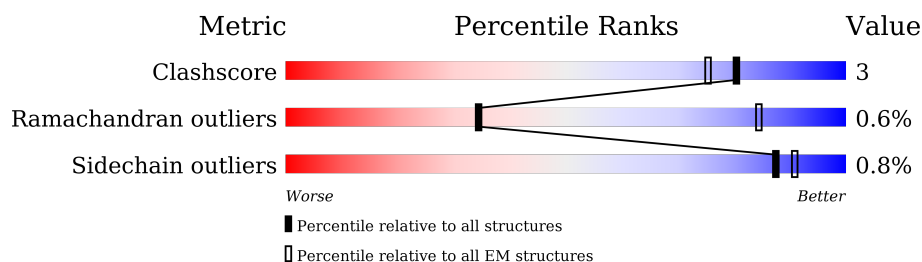
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	1325	
1	B	1325	
1	C	1325	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30306 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		
1	B	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		
1	C	1177	Total	C	N	O	S	0	0
			9141	5821	1532	1745	43		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1292	LEU	-	expression tag	UNP Q6Q1S2
A	1293	ILE	-	expression tag	UNP Q6Q1S2
A	1294	LYS	-	expression tag	UNP Q6Q1S2
A	1295	ARG	-	expression tag	UNP Q6Q1S2
A	1296	MET	-	expression tag	UNP Q6Q1S2
A	1297	LYS	-	expression tag	UNP Q6Q1S2
A	1298	GLN	-	expression tag	UNP Q6Q1S2
A	1299	ILE	-	expression tag	UNP Q6Q1S2
A	1300	GLU	-	expression tag	UNP Q6Q1S2
A	1301	ASP	-	expression tag	UNP Q6Q1S2
A	1302	LYS	-	expression tag	UNP Q6Q1S2
A	1303	ILE	-	expression tag	UNP Q6Q1S2
A	1304	GLU	-	expression tag	UNP Q6Q1S2
A	1305	GLU	-	expression tag	UNP Q6Q1S2
A	1306	ILE	-	expression tag	UNP Q6Q1S2
A	1307	GLU	-	expression tag	UNP Q6Q1S2
A	1308	SER	-	expression tag	UNP Q6Q1S2
A	1309	LYS	-	expression tag	UNP Q6Q1S2
A	1310	GLN	-	expression tag	UNP Q6Q1S2
A	1311	LYS	-	expression tag	UNP Q6Q1S2
A	1312	LYS	-	expression tag	UNP Q6Q1S2
A	1313	ILE	-	expression tag	UNP Q6Q1S2
A	1314	GLU	-	expression tag	UNP Q6Q1S2
A	1315	ASN	-	expression tag	UNP Q6Q1S2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1316	GLU	-	expression tag	UNP Q6Q1S2
A	1317	ILE	-	expression tag	UNP Q6Q1S2
A	1318	ALA	-	expression tag	UNP Q6Q1S2
A	1319	ARG	-	expression tag	UNP Q6Q1S2
A	1320	ILE	-	expression tag	UNP Q6Q1S2
A	1321	LYS	-	expression tag	UNP Q6Q1S2
A	1322	LYS	-	expression tag	UNP Q6Q1S2
A	1323	ILE	-	expression tag	UNP Q6Q1S2
A	1324	LYS	-	expression tag	UNP Q6Q1S2
A	1325	LEU	-	expression tag	UNP Q6Q1S2
A	1326	VAL	-	expression tag	UNP Q6Q1S2
A	1327	PRO	-	expression tag	UNP Q6Q1S2
A	1328	ARG	-	expression tag	UNP Q6Q1S2
A	1329	GLY	-	expression tag	UNP Q6Q1S2
A	1330	SER	-	expression tag	UNP Q6Q1S2
A	1331	LEU	-	expression tag	UNP Q6Q1S2
A	1332	GLU	-	expression tag	UNP Q6Q1S2
A	1333	TRP	-	expression tag	UNP Q6Q1S2
A	1334	SER	-	expression tag	UNP Q6Q1S2
A	1335	HIS	-	expression tag	UNP Q6Q1S2
A	1336	PRO	-	expression tag	UNP Q6Q1S2
A	1337	GLN	-	expression tag	UNP Q6Q1S2
A	1338	PHE	-	expression tag	UNP Q6Q1S2
A	1339	GLU	-	expression tag	UNP Q6Q1S2
A	1340	LYS	-	expression tag	UNP Q6Q1S2
B	1292	LEU	-	expression tag	UNP Q6Q1S2
B	1293	ILE	-	expression tag	UNP Q6Q1S2
B	1294	LYS	-	expression tag	UNP Q6Q1S2
B	1295	ARG	-	expression tag	UNP Q6Q1S2
B	1296	MET	-	expression tag	UNP Q6Q1S2
B	1297	LYS	-	expression tag	UNP Q6Q1S2
B	1298	GLN	-	expression tag	UNP Q6Q1S2
B	1299	ILE	-	expression tag	UNP Q6Q1S2
B	1300	GLU	-	expression tag	UNP Q6Q1S2
B	1301	ASP	-	expression tag	UNP Q6Q1S2
B	1302	LYS	-	expression tag	UNP Q6Q1S2
B	1303	ILE	-	expression tag	UNP Q6Q1S2
B	1304	GLU	-	expression tag	UNP Q6Q1S2
B	1305	GLU	-	expression tag	UNP Q6Q1S2
B	1306	ILE	-	expression tag	UNP Q6Q1S2
B	1307	GLU	-	expression tag	UNP Q6Q1S2
B	1308	SER	-	expression tag	UNP Q6Q1S2

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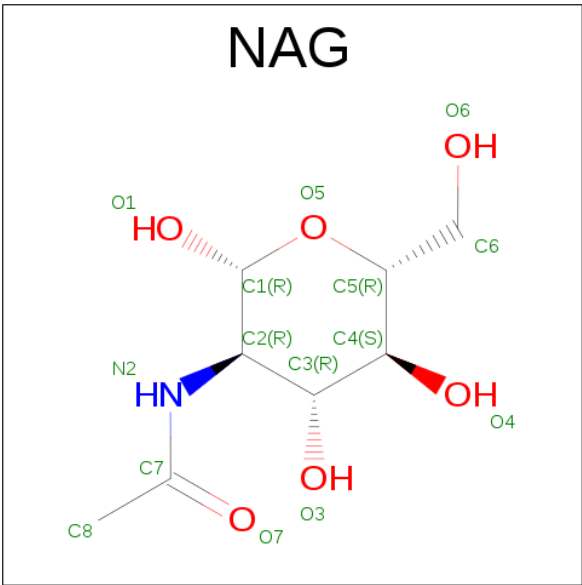
Chain	Residue	Modelled	Actual	Comment	Reference
B	1309	LYS	-	expression tag	UNP Q6Q1S2
B	1310	GLN	-	expression tag	UNP Q6Q1S2
B	1311	LYS	-	expression tag	UNP Q6Q1S2
B	1312	LYS	-	expression tag	UNP Q6Q1S2
B	1313	ILE	-	expression tag	UNP Q6Q1S2
B	1314	GLU	-	expression tag	UNP Q6Q1S2
B	1315	ASN	-	expression tag	UNP Q6Q1S2
B	1316	GLU	-	expression tag	UNP Q6Q1S2
B	1317	ILE	-	expression tag	UNP Q6Q1S2
B	1318	ALA	-	expression tag	UNP Q6Q1S2
B	1319	ARG	-	expression tag	UNP Q6Q1S2
B	1320	ILE	-	expression tag	UNP Q6Q1S2
B	1321	LYS	-	expression tag	UNP Q6Q1S2
B	1322	LYS	-	expression tag	UNP Q6Q1S2
B	1323	ILE	-	expression tag	UNP Q6Q1S2
B	1324	LYS	-	expression tag	UNP Q6Q1S2
B	1325	LEU	-	expression tag	UNP Q6Q1S2
B	1326	VAL	-	expression tag	UNP Q6Q1S2
B	1327	PRO	-	expression tag	UNP Q6Q1S2
B	1328	ARG	-	expression tag	UNP Q6Q1S2
B	1329	GLY	-	expression tag	UNP Q6Q1S2
B	1330	SER	-	expression tag	UNP Q6Q1S2
B	1331	LEU	-	expression tag	UNP Q6Q1S2
B	1332	GLU	-	expression tag	UNP Q6Q1S2
B	1333	TRP	-	expression tag	UNP Q6Q1S2
B	1334	SER	-	expression tag	UNP Q6Q1S2
B	1335	HIS	-	expression tag	UNP Q6Q1S2
B	1336	PRO	-	expression tag	UNP Q6Q1S2
B	1337	GLN	-	expression tag	UNP Q6Q1S2
B	1338	PHE	-	expression tag	UNP Q6Q1S2
B	1339	GLU	-	expression tag	UNP Q6Q1S2
B	1340	LYS	-	expression tag	UNP Q6Q1S2
C	1292	LEU	-	expression tag	UNP Q6Q1S2
C	1293	ILE	-	expression tag	UNP Q6Q1S2
C	1294	LYS	-	expression tag	UNP Q6Q1S2
C	1295	ARG	-	expression tag	UNP Q6Q1S2
C	1296	MET	-	expression tag	UNP Q6Q1S2
C	1297	LYS	-	expression tag	UNP Q6Q1S2
C	1298	GLN	-	expression tag	UNP Q6Q1S2
C	1299	ILE	-	expression tag	UNP Q6Q1S2
C	1300	GLU	-	expression tag	UNP Q6Q1S2
C	1301	ASP	-	expression tag	UNP Q6Q1S2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1302	LYS	-	expression tag	UNP Q6Q1S2
C	1303	ILE	-	expression tag	UNP Q6Q1S2
C	1304	GLU	-	expression tag	UNP Q6Q1S2
C	1305	GLU	-	expression tag	UNP Q6Q1S2
C	1306	ILE	-	expression tag	UNP Q6Q1S2
C	1307	GLU	-	expression tag	UNP Q6Q1S2
C	1308	SER	-	expression tag	UNP Q6Q1S2
C	1309	LYS	-	expression tag	UNP Q6Q1S2
C	1310	GLN	-	expression tag	UNP Q6Q1S2
C	1311	LYS	-	expression tag	UNP Q6Q1S2
C	1312	LYS	-	expression tag	UNP Q6Q1S2
C	1313	ILE	-	expression tag	UNP Q6Q1S2
C	1314	GLU	-	expression tag	UNP Q6Q1S2
C	1315	ASN	-	expression tag	UNP Q6Q1S2
C	1316	GLU	-	expression tag	UNP Q6Q1S2
C	1317	ILE	-	expression tag	UNP Q6Q1S2
C	1318	ALA	-	expression tag	UNP Q6Q1S2
C	1319	ARG	-	expression tag	UNP Q6Q1S2
C	1320	ILE	-	expression tag	UNP Q6Q1S2
C	1321	LYS	-	expression tag	UNP Q6Q1S2
C	1322	LYS	-	expression tag	UNP Q6Q1S2
C	1323	ILE	-	expression tag	UNP Q6Q1S2
C	1324	LYS	-	expression tag	UNP Q6Q1S2
C	1325	LEU	-	expression tag	UNP Q6Q1S2
C	1326	VAL	-	expression tag	UNP Q6Q1S2
C	1327	PRO	-	expression tag	UNP Q6Q1S2
C	1328	ARG	-	expression tag	UNP Q6Q1S2
C	1329	GLY	-	expression tag	UNP Q6Q1S2
C	1330	SER	-	expression tag	UNP Q6Q1S2
C	1331	LEU	-	expression tag	UNP Q6Q1S2
C	1332	GLU	-	expression tag	UNP Q6Q1S2
C	1333	TRP	-	expression tag	UNP Q6Q1S2
C	1334	SER	-	expression tag	UNP Q6Q1S2
C	1335	HIS	-	expression tag	UNP Q6Q1S2
C	1336	PRO	-	expression tag	UNP Q6Q1S2
C	1337	GLN	-	expression tag	UNP Q6Q1S2
C	1338	PHE	-	expression tag	UNP Q6Q1S2
C	1339	GLU	-	expression tag	UNP Q6Q1S2
C	1340	LYS	-	expression tag	UNP Q6Q1S2

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	
2	A	1	Total	C	N	O	0
			686	392	49	245	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	A	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0
2	B	1	Total 686	C 392	N 49	O 245	0

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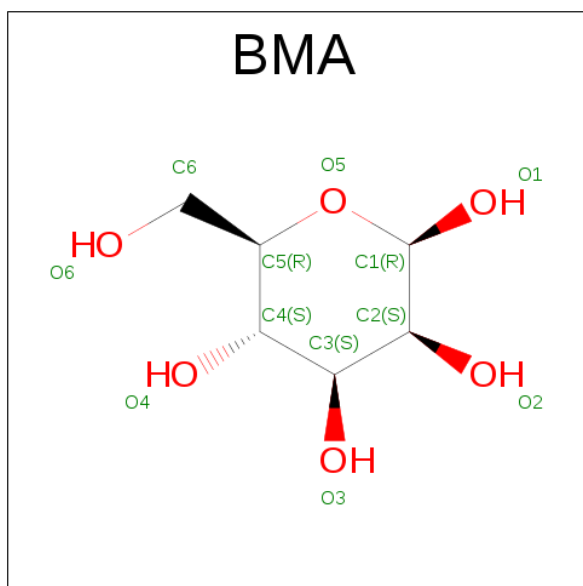
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			686	392	49	245	
2	C	1	Total	C	N	O	0
			686	392	49	245	
2	C	1	Total	C	N	O	0
			686	392	49	245	
2	C	1	Total	C	N	O	0
			686	392	49	245	
2	C	1	Total	C	N	O	0
			686	392	49	245	
2	C	1	Total	C	N	O	0
			686	392	49	245	

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	

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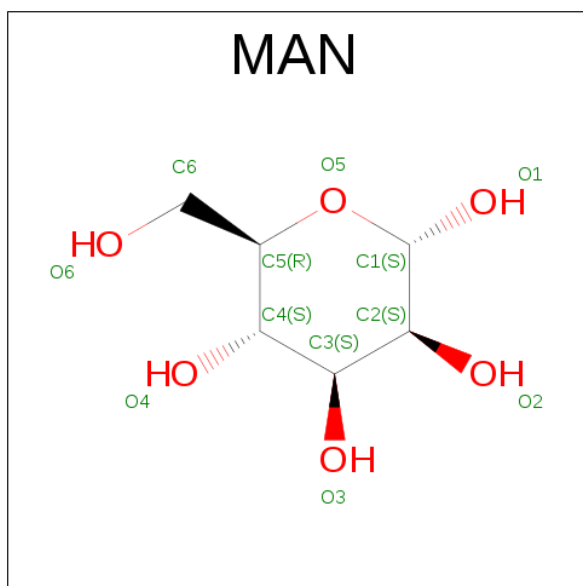
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	

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Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	
3	C	1	Total	C	O	0
			110	60	50	

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			165	90	75	
4	A	1	Total	C	O	0
			165	90	75	
4	A	1	Total	C	O	0
			165	90	75	
4	A	1	Total	C	O	0
			165	90	75	
4	A	1	Total	C	O	0
			165	90	75	
4	A	1	Total	C	O	0
			165	90	75	

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Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	A	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0

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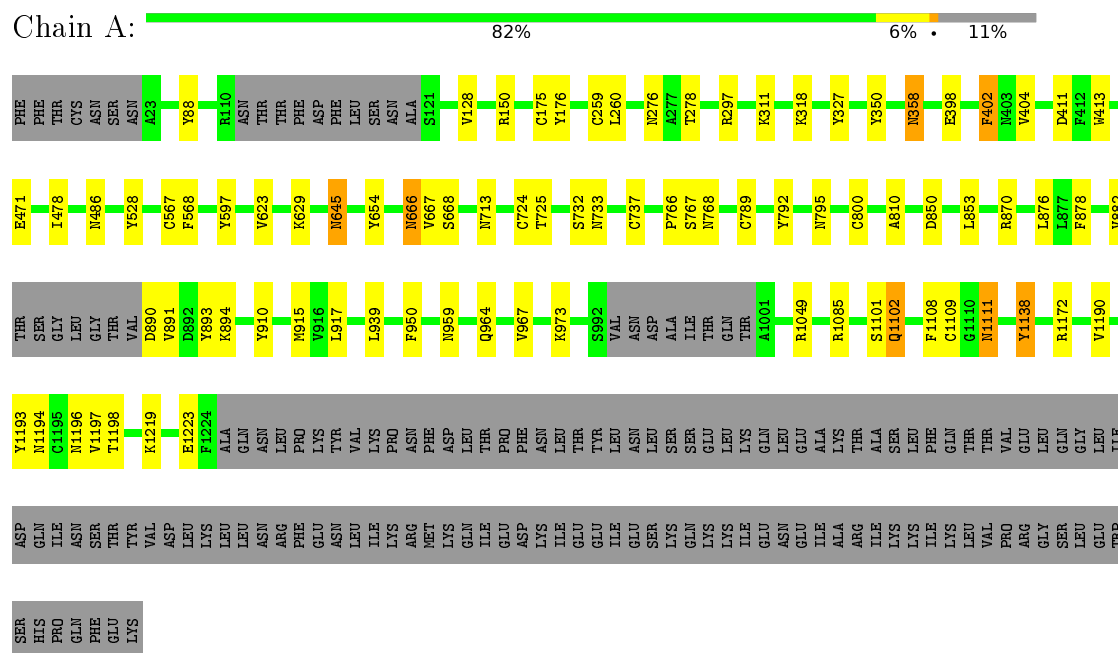
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Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0

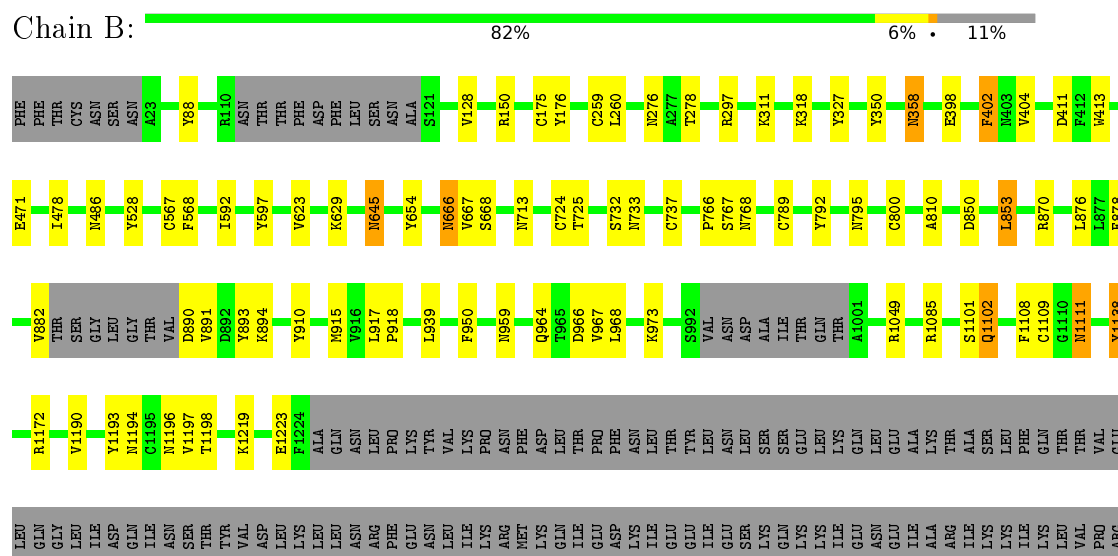
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Spike glycoprotein

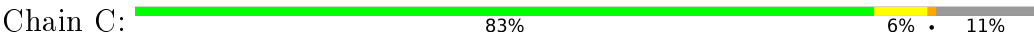


- Molecule 1: Spike glycoprotein



GLY
SER
LEU
GLU
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

- Molecule 1: Spike glycoprotein



PRO GLN PHE GLU LYS	ILE	ASN	SER	TYR	ASP	LEU	LYS	LEU	ASN	PHE	GLU	ASN	GLN	ILE	LYS	ARG	MET	LYS	GLN	ILE	GLU	ASP	LYS	ILE	GLU	GLU	ILE	GLU	ASN	GLU	SER	LYS	GLN	LYS	ILE	GLU	GLU	ASN	ILE	ALA	ARG	ILE	LYS	LYS	ILE	VAL	PRO	ARG	GLY	SER	LEU	GLU	TRP	SER	HIS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
	G1195	N1196	V1197	T1198	K1219	E1223	F1224	ALA	GLN	ASN	LEU	PRO	LYS	TYR	VAL	LYS	PRO	ASN	PHE	ASP	LEU	THR	PRO	LYS	ASN	LEU	TYR	ILE	LEU	ASN	LEU	SER	GLN	GLU	LYS	ILE	GLN	GLN	THR	VAL	GLU	GLU	ALA	LYS	THR	ALA	SER	LEU	PHE	GLN	LYS	LEU	VAL	PRO	ARG	GLY	SER	LEU	GLU	TRP	SER	HIS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	79667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
1	B	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
1	C	0.95	10/9345 (0.1%)	0.82	12/12747 (0.1%)
All	All	0.95	30/28035 (0.1%)	0.82	36/38241 (0.1%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	737	CYS	CB-SG	-8.38	1.68	1.82
1	C	737	CYS	CB-SG	-8.37	1.68	1.82
1	B	737	CYS	CB-SG	-8.34	1.68	1.82
1	C	800	CYS	CB-SG	-7.71	1.69	1.82
1	A	800	CYS	CB-SG	-7.70	1.69	1.82
1	B	800	CYS	CB-SG	-7.69	1.69	1.82
1	C	1193	TYR	CB-CG	-6.75	1.41	1.51
1	A	1193	TYR	CB-CG	-6.69	1.41	1.51
1	B	1193	TYR	CB-CG	-6.65	1.41	1.51
1	B	1190	VAL	C-N	5.62	1.47	1.34
1	B	666	ASN	CB-CG	5.61	1.64	1.51
1	C	666	ASN	CB-CG	5.61	1.64	1.51
1	A	666	ASN	CB-CG	5.61	1.64	1.51
1	A	1190	VAL	C-N	5.61	1.47	1.34
1	C	1190	VAL	C-N	5.61	1.47	1.34
1	C	128	VAL	CB-CG2	-5.58	1.41	1.52
1	A	128	VAL	CB-CG2	-5.58	1.41	1.52
1	B	128	VAL	CB-CG2	-5.56	1.41	1.52
1	A	950	PHE	CB-CG	-5.39	1.42	1.51
1	C	950	PHE	CB-CG	-5.38	1.42	1.51
1	B	950	PHE	CB-CG	-5.37	1.42	1.51
1	B	568	PHE	CB-CG	-5.33	1.42	1.51
1	C	568	PHE	CB-CG	-5.31	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	568	PHE	CB-CG	-5.31	1.42	1.51
1	C	413	TRP	CB-CG	-5.22	1.40	1.50
1	A	413	TRP	CB-CG	-5.21	1.40	1.50
1	C	597	TYR	CB-CG	-5.19	1.43	1.51
1	B	413	TRP	CB-CG	-5.18	1.41	1.50
1	B	597	TYR	CB-CG	-5.17	1.43	1.51
1	A	597	TYR	CB-CG	-5.16	1.44	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	C	297	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	297	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	C	1172	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	B	1172	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	B	810	ALA	CB-CA-C	8.49	122.84	110.10
1	A	1172	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	C	810	ALA	CB-CA-C	8.48	122.83	110.10
1	A	810	ALA	CB-CA-C	8.46	122.79	110.10
1	A	1193	TYR	CB-CG-CD2	-8.06	116.16	121.00
1	B	1193	TYR	CB-CG-CD2	-8.06	116.17	121.00
1	C	1193	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	B	1085	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	C	1085	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	1085	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	C	1198	THR	C-N-CA	7.10	139.45	121.70
1	A	1198	THR	C-N-CA	7.09	139.42	121.70
1	B	1198	THR	C-N-CA	7.08	139.40	121.70
1	B	297	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	297	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	297	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	1049	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	1049	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	1049	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	88	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	B	88	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	A	88	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	623	VAL	O-C-N	5.50	131.50	122.70
1	C	623	VAL	O-C-N	5.50	131.51	122.70
1	B	623	VAL	O-C-N	5.50	131.50	122.70
1	B	150	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	150	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	890	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	890	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	890	ASP	CB-CG-OD2	5.22	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

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	A	9141	0	8879	71	0
1	B	9141	0	8879	75	0
1	C	9141	0	8879	70	0
2	A	686	0	587	7	0
2	B	686	0	587	6	0
2	C	686	0	588	6	0
3	A	110	0	75	0	0
3	B	110	0	75	0	0
3	C	110	0	75	0	0
4	A	165	0	133	0	0
4	B	165	0	133	0	0
4	C	165	0	133	0	0
All	All	30306	0	29023	196	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 (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:TYR:O	1:B:792:TYR:CD2	2.00	1.15
1:C:792:TYR:CD2	1:C:792:TYR:O	2.00	1.15
1:A:792:TYR:CD2	1:A:792:TYR:O	2.00	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1111:ASN:OD1	1:B:1111:ASN:O	1.74	1.05
1:C:1111:ASN:O	1:C:1111:ASN:OD1	1.74	1.04
1:A:1111:ASN:OD1	1:A:1111:ASN:O	1.74	1.03
1:C:1197:VAL:HG22	2:C:1472:NAG:C7	1.99	0.92
1:A:276:ASN:O	1:A:276:ASN:OD1	1.88	0.92
1:B:1197:VAL:HG22	2:B:1472:NAG:C7	1.99	0.91
1:A:1197:VAL:HG22	2:A:1472:NAG:C7	1.99	0.90
1:C:276:ASN:OD1	1:C:276:ASN:O	1.88	0.90
1:B:276:ASN:OD1	1:B:276:ASN:O	1.88	0.90
1:B:891:VAL:HG11	1:B:893:TYR:CE2	2.07	0.90
1:A:891:VAL:HG11	1:A:893:TYR:CE2	2.07	0.89
1:C:891:VAL:HG11	1:C:893:TYR:CE2	2.07	0.87
1:C:1111:ASN:O	1:C:1111:ASN:CG	2.19	0.81
1:B:792:TYR:O	1:B:792:TYR:CG	2.35	0.80
1:B:1111:ASN:CG	1:B:1111:ASN:O	2.19	0.80
1:C:792:TYR:O	1:C:792:TYR:CG	2.35	0.79
1:A:1111:ASN:CG	1:A:1111:ASN:O	2.19	0.79
1:C:645:ASN:HD22	1:C:645:ASN:N	1.81	0.79
1:A:792:TYR:CG	1:A:792:TYR:O	2.35	0.79
1:A:645:ASN:N	1:A:645:ASN:HD22	1.81	0.78
1:B:645:ASN:HD22	1:B:645:ASN:N	1.81	0.77
1:B:878:PHE:O	1:B:882:VAL:HG23	1.87	0.75
1:C:878:PHE:O	1:C:882:VAL:HG23	1.87	0.75
1:A:878:PHE:O	1:A:882:VAL:HG23	1.87	0.74
1:A:967:VAL:HG11	1:B:1194:ASN:HB3	1.71	0.72
1:A:1194:ASN:HB3	1:C:967:VAL:HG11	1.71	0.72
1:C:1197:VAL:HG22	2:C:1472:NAG:O7	1.89	0.72
1:A:1197:VAL:HG22	2:A:1472:NAG:O7	1.89	0.72
1:B:967:VAL:HG11	1:C:1194:ASN:HB3	1.71	0.72
1:A:1197:VAL:HG22	2:A:1472:NAG:C8	2.20	0.71
1:C:1197:VAL:HG22	2:C:1472:NAG:C8	2.20	0.71
1:B:1197:VAL:HG22	2:B:1472:NAG:C8	2.20	0.71
1:B:1197:VAL:HG22	2:B:1472:NAG:O7	1.89	0.71
1:A:1196:ASN:HB2	1:C:967:VAL:HB	1.76	0.68
1:B:967:VAL:HB	1:C:1196:ASN:HB2	1.75	0.68
1:A:967:VAL:HB	1:B:1196:ASN:HB2	1.75	0.67
1:B:882:VAL:HG12	1:B:882:VAL:O	1.95	0.67
1:C:882:VAL:HG12	1:C:882:VAL:O	1.95	0.66
1:A:882:VAL:HG12	1:A:882:VAL:O	1.95	0.66
1:A:967:VAL:HG21	1:B:1194:ASN:HB3	1.78	0.66
1:B:967:VAL:HG21	1:C:1194:ASN:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1194:ASN:HB3	1:C:967:VAL:HG21	1.78	0.66
1:B:645:ASN:H	1:B:645:ASN:HD22	1.42	0.66
1:C:645:ASN:H	1:C:645:ASN:HD22	1.42	0.65
1:A:645:ASN:HD22	1:A:645:ASN:H	1.42	0.65
1:C:891:VAL:CG1	1:C:893:TYR:CE2	2.80	0.65
1:A:891:VAL:CG1	1:A:893:TYR:CE2	2.80	0.64
1:C:792:TYR:C	1:C:792:TYR:CD2	2.72	0.63
1:A:792:TYR:C	1:A:792:TYR:CD2	2.72	0.63
1:B:967:VAL:CG1	1:C:1194:ASN:HB3	2.29	0.62
1:B:891:VAL:CG1	1:B:893:TYR:CE2	2.80	0.62
1:A:967:VAL:CG1	1:B:1194:ASN:HB3	2.29	0.62
1:A:1194:ASN:HB3	1:C:967:VAL:CG1	2.29	0.62
1:A:471:GLU:OE2	1:A:629:LYS:HE3	2.00	0.62
1:C:471:GLU:OE2	1:C:629:LYS:HE3	2.00	0.62
1:B:471:GLU:OE2	1:B:629:LYS:HE3	2.00	0.61
2:A:1434:NAG:H5	2:A:1435:NAG:N2	2.15	0.61
2:C:1434:NAG:H5	2:C:1435:NAG:N2	2.15	0.61
1:B:792:TYR:CD2	1:B:792:TYR:C	2.72	0.60
2:B:1434:NAG:H5	2:B:1435:NAG:N2	2.15	0.60
1:A:311:LYS:NZ	1:A:411:ASP:OD1	2.37	0.58
1:B:967:VAL:CG2	1:C:1194:ASN:HB3	2.34	0.58
1:C:645:ASN:N	1:C:645:ASN:ND2	2.51	0.58
1:B:713:ASN:N	1:B:713:ASN:OD1	2.37	0.58
1:A:967:VAL:CG2	1:B:1194:ASN:HB3	2.33	0.58
1:C:311:LYS:NZ	1:C:411:ASP:OD1	2.37	0.58
1:B:311:LYS:NZ	1:B:411:ASP:OD1	2.36	0.57
1:A:713:ASN:N	1:A:713:ASN:OD1	2.37	0.57
1:C:1138:TYR:CD1	1:C:1138:TYR:N	2.73	0.57
1:A:1194:ASN:HB3	1:C:967:VAL:CG2	2.34	0.57
1:A:894:LYS:HB2	1:A:894:LYS:NZ	2.20	0.57
1:B:645:ASN:N	1:B:645:ASN:ND2	2.51	0.57
1:C:894:LYS:NZ	1:C:894:LYS:HB2	2.20	0.57
1:C:766:PRO:HA	1:C:1138:TYR:HB3	1.87	0.57
1:C:713:ASN:N	1:C:713:ASN:OD1	2.37	0.56
1:A:766:PRO:HA	1:A:1138:TYR:HB3	1.87	0.56
1:A:1138:TYR:N	1:A:1138:TYR:CD1	2.73	0.56
1:A:894:LYS:HZ2	1:A:894:LYS:HB2	1.70	0.56
1:B:1138:TYR:CD1	1:B:1138:TYR:N	2.73	0.56
1:B:766:PRO:HA	1:B:1138:TYR:HB3	1.87	0.56
1:A:870:ARG:NH1	1:A:878:PHE:CE1	2.74	0.56
1:B:894:LYS:HB2	1:B:894:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ASP:OD2	1:A:973:LYS:NZ	2.40	0.55
1:C:910:TYR:CE1	1:C:915:MET:HG2	2.42	0.55
1:B:870:ARG:NH1	1:B:878:PHE:CE1	2.74	0.55
1:B:894:LYS:HB2	1:B:894:LYS:HZ2	1.70	0.55
1:B:910:TYR:CE1	1:B:915:MET:HG2	2.42	0.55
1:A:1194:ASN:CB	1:C:967:VAL:HG11	2.37	0.55
1:C:870:ARG:NH1	1:C:878:PHE:CE1	2.74	0.55
1:A:910:TYR:CE1	1:A:915:MET:HG2	2.42	0.55
1:C:850:ASP:OD2	1:C:973:LYS:NZ	2.40	0.55
1:B:850:ASP:OD2	1:B:973:LYS:NZ	2.40	0.55
1:A:967:VAL:HG11	1:B:1194:ASN:CB	2.37	0.54
1:C:1197:VAL:CG2	2:C:1472:NAG:O7	2.56	0.54
1:B:1197:VAL:CG2	2:B:1472:NAG:O7	2.56	0.54
1:B:967:VAL:HG11	1:C:1194:ASN:CB	2.37	0.54
1:C:917:LEU:N	1:C:917:LEU:HD12	2.24	0.53
1:C:259:CYS:SG	1:C:260:LEU:N	2.82	0.53
1:A:259:CYS:SG	1:A:260:LEU:N	2.82	0.53
1:A:645:ASN:N	1:A:645:ASN:ND2	2.51	0.53
1:B:724:CYS:O	1:B:724:CYS:SG	2.67	0.52
1:C:724:CYS:O	1:C:724:CYS:SG	2.67	0.52
1:B:259:CYS:SG	1:B:260:LEU:N	2.82	0.52
1:B:917:LEU:N	1:B:917:LEU:HD12	2.24	0.52
1:B:318:LYS:HE2	1:B:398:GLU:OE1	2.10	0.52
1:A:917:LEU:HD12	1:A:917:LEU:N	2.24	0.52
1:C:318:LYS:HE2	1:C:398:GLU:OE1	2.10	0.52
1:A:666:ASN:O	1:A:668:SER:N	2.43	0.52
1:B:666:ASN:O	1:B:668:SER:N	2.43	0.52
1:C:666:ASN:O	1:C:668:SER:N	2.43	0.51
1:A:1197:VAL:CG2	2:A:1472:NAG:O7	2.56	0.51
1:A:724:CYS:SG	1:A:724:CYS:O	2.67	0.51
1:A:350:TYR:CD1	1:A:350:TYR:N	2.79	0.51
1:A:318:LYS:HE2	1:A:398:GLU:OE1	2.09	0.51
1:B:1196:ASN:ND2	1:B:1196:ASN:O	2.44	0.51
1:B:350:TYR:N	1:B:350:TYR:CD1	2.79	0.51
1:A:766:PRO:CA	1:A:1138:TYR:HB3	2.41	0.50
1:A:967:VAL:CG1	1:B:1194:ASN:CB	2.90	0.50
1:C:1196:ASN:ND2	1:C:1196:ASN:O	2.44	0.50
1:A:1194:ASN:CB	1:C:967:VAL:CG1	2.90	0.50
1:B:766:PRO:N	1:B:1138:TYR:HB3	2.27	0.50
1:B:766:PRO:CA	1:B:1138:TYR:HB3	2.41	0.50
1:C:766:PRO:CA	1:C:1138:TYR:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:ASN:O	1:A:1196:ASN:ND2	2.44	0.50
1:A:766:PRO:N	1:A:1138:TYR:HB3	2.27	0.49
1:A:1219:LYS:NZ	1:A:1223:GLU:OE2	2.44	0.49
1:B:967:VAL:CG1	1:C:1194:ASN:CB	2.90	0.49
1:A:358:ASN:OD1	1:A:358:ASN:N	2.45	0.49
1:C:766:PRO:N	1:C:1138:TYR:HB3	2.27	0.49
1:C:894:LYS:HB2	1:C:894:LYS:HZ2	1.75	0.49
1:C:276:ASN:OD1	1:C:276:ASN:C	2.51	0.49
1:C:882:VAL:O	1:C:882:VAL:CG1	2.60	0.49
1:A:882:VAL:CG1	1:A:882:VAL:O	2.60	0.49
1:C:350:TYR:N	1:C:350:TYR:CD1	2.79	0.49
1:C:654:TYR:CD1	1:C:654:TYR:N	2.81	0.48
1:B:1219:LYS:NZ	1:B:1223:GLU:OE2	2.44	0.48
1:B:358:ASN:OD1	1:B:358:ASN:N	2.46	0.48
1:C:939:LEU:O	1:C:939:LEU:HG	2.13	0.48
1:B:939:LEU:HG	1:B:939:LEU:O	2.13	0.48
1:C:358:ASN:OD1	1:C:358:ASN:N	2.45	0.48
1:A:654:TYR:N	1:A:654:TYR:CD1	2.81	0.48
1:B:882:VAL:O	1:B:882:VAL:CG1	2.60	0.48
1:A:176:TYR:N	1:A:176:TYR:CD1	2.82	0.48
1:A:767:SER:OG	1:A:768:ASN:N	2.46	0.48
1:C:1219:LYS:NZ	1:C:1223:GLU:OE2	2.44	0.48
1:C:767:SER:OG	1:C:768:ASN:N	2.46	0.47
1:A:1111:ASN:OD1	1:A:1111:ASN:C	2.49	0.47
1:A:939:LEU:O	1:A:939:LEU:HG	2.13	0.47
1:B:176:TYR:CD1	1:B:176:TYR:N	2.82	0.47
1:B:402:PHE:CD1	1:B:404:VAL:HG23	2.50	0.47
1:B:654:TYR:N	1:B:654:TYR:CD1	2.81	0.47
1:B:767:SER:OG	1:B:768:ASN:N	2.46	0.47
1:C:402:PHE:CD1	1:C:404:VAL:HG23	2.50	0.47
1:C:176:TYR:CD1	1:C:176:TYR:N	2.82	0.47
1:B:276:ASN:OD1	1:B:276:ASN:C	2.51	0.46
1:C:876:LEU:O	1:C:876:LEU:HD12	2.16	0.46
1:A:402:PHE:CD1	1:A:404:VAL:HG23	2.50	0.46
1:A:876:LEU:HD12	1:A:876:LEU:O	2.16	0.46
1:B:278:THR:HG21	2:B:1410:NAG:H82	1.99	0.45
1:B:876:LEU:HD12	1:B:876:LEU:O	2.16	0.45
1:A:278:THR:HG21	2:A:1410:NAG:H82	1.99	0.44
1:B:327:TYR:CD2	1:B:327:TYR:N	2.86	0.44
1:C:278:THR:HG21	2:C:1410:NAG:H82	1.99	0.44
1:C:795:ASN:N	1:C:795:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ILE:O	1:B:478:ILE:HG23	2.17	0.44
1:C:478:ILE:HG23	1:C:478:ILE:O	2.17	0.44
1:A:732:SER:OG	1:A:733:ASN:N	2.51	0.44
1:C:327:TYR:N	1:C:327:TYR:CD2	2.86	0.44
1:C:732:SER:OG	1:C:733:ASN:N	2.51	0.44
1:B:732:SER:OG	1:B:733:ASN:N	2.51	0.43
1:A:478:ILE:O	1:A:478:ILE:HG23	2.17	0.43
1:B:795:ASN:N	1:B:795:ASN:OD1	2.51	0.43
1:A:795:ASN:N	1:A:795:ASN:OD1	2.51	0.43
1:A:276:ASN:OD1	1:A:276:ASN:C	2.51	0.43
1:A:327:TYR:CD2	1:A:327:TYR:N	2.86	0.43
1:B:592:ILE:HA	1:B:592:ILE:HD13	1.84	0.43
1:B:910:TYR:HE1	1:B:915:MET:HG2	1.82	0.43
1:A:910:TYR:HE1	1:A:915:MET:HG2	1.82	0.41
1:B:1111:ASN:OD1	1:B:1111:ASN:C	2.49	0.41
1:A:959:ASN:OD1	1:A:964:GLN:HG2	2.20	0.41
1:C:910:TYR:HE1	1:C:915:MET:HG2	1.83	0.41
1:C:853:LEU:HA	1:C:853:LEU:HD12	1.90	0.41
1:A:1101:SER:O	1:A:1102:GLN:CB	2.68	0.41
1:A:528:TYR:CD1	1:A:528:TYR:C	2.93	0.41
1:B:1101:SER:O	1:B:1102:GLN:CB	2.69	0.41
1:B:528:TYR:C	1:B:528:TYR:CD1	2.93	0.41
1:B:918:PRO:O	1:C:731:TYR:OH	2.31	0.41
1:C:959:ASN:OD1	1:C:964:GLN:HG2	2.21	0.41
1:B:967:VAL:CB	1:C:1196:ASN:HB2	2.48	0.41
1:B:959:ASN:OD1	1:B:964:GLN:HG2	2.20	0.41
1:B:966:ASP:OD1	1:B:968:LEU:N	2.53	0.41
1:B:853:LEU:HD12	1:B:853:LEU:HA	1.90	0.40
1:A:1197:VAL:CG2	2:A:1472:NAG:C8	2.97	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	1169/1325 (88%)	1095 (94%)	67 (6%)	7 (1%)	30	72
1	B	1169/1325 (88%)	1096 (94%)	66 (6%)	7 (1%)	30	72
1	C	1169/1325 (88%)	1095 (94%)	67 (6%)	7 (1%)	30	72
All	All	3507/3975 (88%)	3286 (94%)	200 (6%)	21 (1%)	34	72

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	667	VAL
1	A	853	LEU
1	B	667	VAL
1	B	853	LEU
1	C	667	VAL
1	C	853	LEU
1	A	567	CYS
1	A	725	THR
1	A	1102	GLN
1	B	567	CYS
1	B	725	THR
1	B	1102	GLN
1	C	567	CYS
1	C	725	THR
1	C	1102	GLN
1	A	1109	CYS
1	B	1109	CYS
1	C	1109	CYS
1	A	1108	PHE
1	B	1108	PHE
1	C	1108	PHE

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	1031/1169 (88%)	1023 (99%)	8 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1031/1169 (88%)	1023 (99%)	8 (1%)	86	94
1	C	1031/1169 (88%)	1023 (99%)	8 (1%)	86	94
All	All	3093/3507 (88%)	3069 (99%)	24 (1%)	87	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	CYS
1	A	358	ASN
1	A	402	PHE
1	A	486	ASN
1	A	645	ASN
1	A	789	CYS
1	A	1111	ASN
1	A	1138	TYR
1	B	175	CYS
1	B	358	ASN
1	B	402	PHE
1	B	486	ASN
1	B	645	ASN
1	B	789	CYS
1	B	1111	ASN
1	B	1138	TYR
1	C	175	CYS
1	C	358	ASN
1	C	402	PHE
1	C	486	ASN
1	C	645	ASN
1	C	789	CYS
1	C	1111	ASN
1	C	1138	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	660	ASN
1	B	660	ASN
1	C	660	ASN

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 ⓘ

222 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$
2	NAG	A	1401	1	14,14,15	2.78	3 (21%)	15,19,21	1.83	2 (13%)
2	NAG	A	1402	1	14,14,15	2.66	4 (28%)	15,19,21	3.43	4 (26%)
2	NAG	A	1403	1	14,14,15	2.59	3 (21%)	15,19,21	3.85	5 (33%)
2	NAG	A	1404	1,2	14,14,15	2.61	3 (21%)	15,19,21	3.18	5 (33%)
2	NAG	A	1405	3,2	14,14,15	2.77	4 (28%)	15,19,21	4.89	6 (40%)
3	BMA	A	1406	2,4	11,11,12	1.92	3 (27%)	15,15,17	3.22	5 (33%)
4	MAN	A	1407	3,4	11,11,12	1.88	3 (27%)	15,15,17	4.11	5 (33%)
4	MAN	A	1408	4	11,11,12	2.57	6 (54%)	15,15,17	2.63	7 (46%)
4	MAN	A	1409	3	11,11,12	2.49	6 (54%)	15,15,17	3.23	6 (40%)
2	NAG	A	1410	1,2	14,14,15	2.81	3 (21%)	15,19,21	3.80	5 (33%)
2	NAG	A	1411	2	14,14,15	3.18	5 (35%)	15,19,21	3.06	4 (26%)
2	NAG	A	1412	1,2	14,14,15	2.67	3 (21%)	15,19,21	2.84	5 (33%)
2	NAG	A	1413	3,2	14,14,15	2.68	3 (21%)	15,19,21	6.76	5 (33%)
3	BMA	A	1414	2,4	11,11,12	1.80	2 (18%)	15,15,17	2.71	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	1415	3	11,11,12	1.96	3 (27%)	15,15,17	3.50	5 (33%)
2	NAG	A	1416	1,2	14,14,15	2.71	3 (21%)	15,19,21	2.45	4 (26%)
2	NAG	A	1417	2	14,14,15	2.77	3 (21%)	15,19,21	4.22	4 (26%)
2	NAG	A	1418	1,2	14,14,15	2.65	3 (21%)	15,19,21	2.94	5 (33%)
2	NAG	A	1419	3,2	14,14,15	2.88	3 (21%)	15,19,21	4.71	7 (46%)
3	BMA	A	1420	2,4	11,11,12	1.84	3 (27%)	15,15,17	3.65	4 (26%)
4	MAN	A	1421	3	11,11,12	1.87	3 (27%)	15,15,17	3.32	5 (33%)
2	NAG	A	1422	1,2	14,14,15	2.67	3 (21%)	15,19,21	4.17	5 (33%)
2	NAG	A	1423	2	14,14,15	2.88	3 (21%)	15,19,21	2.23	3 (20%)
2	NAG	A	1424	1,2	14,14,15	2.53	3 (21%)	15,19,21	4.89	7 (46%)
2	NAG	A	1425	2	14,14,15	2.65	3 (21%)	15,19,21	1.70	2 (13%)
2	NAG	A	1426	1,2	14,14,15	2.64	3 (21%)	15,19,21	3.77	5 (33%)
2	NAG	A	1427	3,2	14,14,15	2.77	4 (28%)	15,19,21	3.82	5 (33%)
3	BMA	A	1428	2,4	11,11,12	1.80	1 (9%)	15,15,17	5.66	6 (40%)
4	MAN	A	1429	3,4	11,11,12	1.67	2 (18%)	15,15,17	8.59	6 (40%)
4	MAN	A	1430	4	11,11,12	1.68	3 (27%)	15,15,17	4.08	5 (33%)
4	MAN	A	1431	4	11,11,12	1.91	3 (27%)	15,15,17	2.29	2 (13%)
4	MAN	A	1432	3,4	11,11,12	1.87	3 (27%)	15,15,17	5.14	7 (46%)
4	MAN	A	1433	4	11,11,12	2.49	6 (54%)	15,15,17	3.71	8 (53%)
2	NAG	A	1434	1,2	14,14,15	3.20	4 (28%)	15,19,21	5.77	5 (33%)
2	NAG	A	1435	3,2	14,14,15	2.95	4 (28%)	15,19,21	2.69	6 (40%)
3	BMA	A	1436	2	11,11,12	2.01	3 (27%)	15,15,17	3.88	5 (33%)
2	NAG	A	1437	1,2	14,14,15	2.74	3 (21%)	15,19,21	4.11	6 (40%)
2	NAG	A	1438	2	14,14,15	2.79	3 (21%)	15,19,21	2.03	3 (20%)
2	NAG	A	1439	1	14,14,15	2.43	3 (21%)	15,19,21	2.89	3 (20%)
2	NAG	A	1440	1	14,14,15	3.49	6 (42%)	15,19,21	3.03	7 (46%)
2	NAG	A	1441	1	14,14,15	2.95	4 (28%)	15,19,21	3.73	3 (20%)
2	NAG	A	1442	1,2	14,14,15	2.57	3 (21%)	15,19,21	3.22	5 (33%)
2	NAG	A	1443	3,2	14,14,15	2.73	3 (21%)	15,19,21	5.67	5 (33%)
3	BMA	A	1444	2,4	11,11,12	1.84	2 (18%)	15,15,17	2.85	5 (33%)
4	MAN	A	1445	3	11,11,12	2.02	3 (27%)	15,15,17	2.82	6 (40%)
4	MAN	A	1446	3	11,11,12	1.90	3 (27%)	15,15,17	3.00	4 (26%)
2	NAG	A	1447	1,2	14,14,15	2.79	3 (21%)	15,19,21	3.12	5 (33%)
2	NAG	A	1448	3,2	14,14,15	2.86	3 (21%)	15,19,21	3.81	6 (40%)
3	BMA	A	1449	2	11,11,12	1.90	2 (18%)	15,15,17	3.88	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1450	1,2	14,14,15	2.72	3 (21%)	15,19,21	3.62	5 (33%)
2	NAG	A	1451	2	14,14,15	2.75	3 (21%)	15,19,21	2.28	4 (26%)
2	NAG	A	1452	1,2	14,14,15	2.72	4 (28%)	15,19,21	4.80	6 (40%)
2	NAG	A	1453	2	14,14,15	2.77	2 (14%)	15,19,21	2.12	2 (13%)
2	NAG	A	1454	1,2	14,14,15	2.63	3 (21%)	15,19,21	3.66	6 (40%)
2	NAG	A	1455	2	14,14,15	2.89	3 (21%)	15,19,21	3.02	3 (20%)
2	NAG	A	1456	1,2	14,14,15	2.70	3 (21%)	15,19,21	4.10	5 (33%)
2	NAG	A	1457	2	14,14,15	2.64	4 (28%)	15,19,21	2.16	2 (13%)
2	NAG	A	1458	1,2	14,14,15	2.67	3 (21%)	15,19,21	4.07	4 (26%)
2	NAG	A	1459	2	14,14,15	2.85	3 (21%)	15,19,21	2.62	3 (20%)
2	NAG	A	1460	1,2	14,14,15	2.59	3 (21%)	15,19,21	5.15	4 (26%)
2	NAG	A	1461	3,2	14,14,15	2.80	3 (21%)	15,19,21	3.31	6 (40%)
3	BMA	A	1462	2,4	11,11,12	1.78	2 (18%)	15,15,17	4.45	5 (33%)
4	MAN	A	1463	3	11,11,12	1.95	3 (27%)	15,15,17	3.48	6 (40%)
2	NAG	A	1464	1,2	14,14,15	2.64	3 (21%)	15,19,21	4.34	5 (33%)
2	NAG	A	1465	3,2	14,14,15	2.70	3 (21%)	15,19,21	4.94	8 (53%)
3	BMA	A	1466	2,4	11,11,12	1.83	2 (18%)	15,15,17	4.56	6 (40%)
4	MAN	A	1467	3	11,11,12	2.00	4 (36%)	15,15,17	3.02	5 (33%)
4	MAN	A	1468	3	11,11,12	1.96	3 (27%)	15,15,17	3.58	4 (26%)
2	NAG	A	1469	1,2	14,14,15	2.79	3 (21%)	15,19,21	4.33	6 (40%)
2	NAG	A	1470	2	14,14,15	2.82	2 (14%)	15,19,21	1.53	2 (13%)
2	NAG	A	1471	1,2	14,14,15	2.68	3 (21%)	15,19,21	4.53	5 (33%)
2	NAG	A	1472	3,2	14,14,15	2.75	3 (21%)	15,19,21	5.19	8 (53%)
3	BMA	A	1473	2	11,11,12	1.99	3 (27%)	15,15,17	3.27	5 (33%)
2	NAG	A	1474	1	14,14,15	2.74	3 (21%)	15,19,21	2.96	4 (26%)
2	NAG	B	1401	1	14,14,15	2.77	3 (21%)	15,19,21	1.83	2 (13%)
2	NAG	B	1402	1	14,14,15	2.67	4 (28%)	15,19,21	3.43	4 (26%)
2	NAG	B	1403	1	14,14,15	2.59	3 (21%)	15,19,21	3.85	5 (33%)
2	NAG	B	1404	1,2	14,14,15	2.62	3 (21%)	15,19,21	3.18	5 (33%)
2	NAG	B	1405	3,2	14,14,15	2.77	4 (28%)	15,19,21	4.89	6 (40%)
3	BMA	B	1406	2,4	11,11,12	1.93	3 (27%)	15,15,17	3.22	5 (33%)
4	MAN	B	1407	3,4	11,11,12	1.88	3 (27%)	15,15,17	4.11	5 (33%)
4	MAN	B	1408	4	11,11,12	2.56	6 (54%)	15,15,17	2.64	7 (46%)
4	MAN	B	1409	3	11,11,12	2.49	6 (54%)	15,15,17	3.24	6 (40%)
2	NAG	B	1410	1,2	14,14,15	2.81	3 (21%)	15,19,21	3.81	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1411	2	14,14,15	3.18	5 (35%)	15,19,21	3.06	4 (26%)
2	NAG	B	1412	1,2	14,14,15	2.67	3 (21%)	15,19,21	2.84	5 (33%)
2	NAG	B	1413	3,2	14,14,15	2.67	3 (21%)	15,19,21	6.76	5 (33%)
3	BMA	B	1414	2,4	11,11,12	1.81	2 (18%)	15,15,17	2.72	4 (26%)
4	MAN	B	1415	3	11,11,12	1.95	3 (27%)	15,15,17	3.50	5 (33%)
2	NAG	B	1416	1,2	14,14,15	2.70	3 (21%)	15,19,21	2.45	4 (26%)
2	NAG	B	1417	2	14,14,15	2.77	3 (21%)	15,19,21	4.22	4 (26%)
2	NAG	B	1418	1,2	14,14,15	2.65	3 (21%)	15,19,21	2.94	5 (33%)
2	NAG	B	1419	3,2	14,14,15	2.88	3 (21%)	15,19,21	4.71	7 (46%)
3	BMA	B	1420	2,4	11,11,12	1.84	3 (27%)	15,15,17	3.65	4 (26%)
4	MAN	B	1421	3	11,11,12	1.87	3 (27%)	15,15,17	3.33	5 (33%)
2	NAG	B	1422	1,2	14,14,15	2.67	3 (21%)	15,19,21	4.17	5 (33%)
2	NAG	B	1423	2	14,14,15	2.87	3 (21%)	15,19,21	2.23	3 (20%)
2	NAG	B	1424	1,2	14,14,15	2.53	3 (21%)	15,19,21	4.90	7 (46%)
2	NAG	B	1425	2	14,14,15	2.65	3 (21%)	15,19,21	1.70	2 (13%)
2	NAG	B	1426	1,2	14,14,15	2.64	3 (21%)	15,19,21	3.77	5 (33%)
2	NAG	B	1427	3,2	14,14,15	2.77	4 (28%)	15,19,21	3.82	5 (33%)
3	BMA	B	1428	2,4	11,11,12	1.79	1 (9%)	15,15,17	5.66	6 (40%)
4	MAN	B	1429	3,4	11,11,12	1.67	2 (18%)	15,15,17	8.59	6 (40%)
4	MAN	B	1430	4	11,11,12	1.69	3 (27%)	15,15,17	4.08	5 (33%)
4	MAN	B	1431	4	11,11,12	1.91	3 (27%)	15,15,17	2.29	2 (13%)
4	MAN	B	1432	3,4	11,11,12	1.87	3 (27%)	15,15,17	5.14	7 (46%)
4	MAN	B	1433	4	11,11,12	2.49	6 (54%)	15,15,17	3.71	8 (53%)
2	NAG	B	1434	1,2	14,14,15	3.19	4 (28%)	15,19,21	5.76	5 (33%)
2	NAG	B	1435	3,2	14,14,15	2.96	4 (28%)	15,19,21	2.69	6 (40%)
3	BMA	B	1436	2	11,11,12	2.01	3 (27%)	15,15,17	3.88	5 (33%)
2	NAG	B	1437	1,2	14,14,15	2.73	3 (21%)	15,19,21	4.11	6 (40%)
2	NAG	B	1438	2	14,14,15	2.78	3 (21%)	15,19,21	2.03	3 (20%)
2	NAG	B	1439	1	14,14,15	2.42	3 (21%)	15,19,21	2.89	3 (20%)
2	NAG	B	1440	1	14,14,15	3.49	6 (42%)	15,19,21	3.03	7 (46%)
2	NAG	B	1441	1	14,14,15	2.95	4 (28%)	15,19,21	3.73	3 (20%)
2	NAG	B	1442	1,2	14,14,15	2.56	3 (21%)	15,19,21	3.22	5 (33%)
2	NAG	B	1443	3,2	14,14,15	2.73	3 (21%)	15,19,21	5.67	5 (33%)
3	BMA	B	1444	2,4	11,11,12	1.84	2 (18%)	15,15,17	2.85	5 (33%)
4	MAN	B	1445	3	11,11,12	2.02	3 (27%)	15,15,17	2.82	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	B	1446	3	11,11,12	1.90	3 (27%)	15,15,17	3.00	5 (33%)
2	NAG	B	1447	1,2	14,14,15	2.78	3 (21%)	15,19,21	3.12	5 (33%)
2	NAG	B	1448	3,2	14,14,15	2.86	3 (21%)	15,19,21	3.80	6 (40%)
3	BMA	B	1449	2	11,11,12	1.90	2 (18%)	15,15,17	3.88	5 (33%)
2	NAG	B	1450	1,2	14,14,15	2.72	3 (21%)	15,19,21	3.62	5 (33%)
2	NAG	B	1451	2	14,14,15	2.75	3 (21%)	15,19,21	2.28	4 (26%)
2	NAG	B	1452	1,2	14,14,15	2.72	3 (21%)	15,19,21	4.80	6 (40%)
2	NAG	B	1453	2	14,14,15	2.76	2 (14%)	15,19,21	2.12	2 (13%)
2	NAG	B	1454	1,2	14,14,15	2.63	3 (21%)	15,19,21	3.66	6 (40%)
2	NAG	B	1455	2	14,14,15	2.90	3 (21%)	15,19,21	3.02	3 (20%)
2	NAG	B	1456	1,2	14,14,15	2.70	3 (21%)	15,19,21	4.10	5 (33%)
2	NAG	B	1457	2	14,14,15	2.64	4 (28%)	15,19,21	2.17	2 (13%)
2	NAG	B	1458	1,2	14,14,15	2.68	3 (21%)	15,19,21	4.06	4 (26%)
2	NAG	B	1459	2	14,14,15	2.85	3 (21%)	15,19,21	2.62	3 (20%)
2	NAG	B	1460	1,2	14,14,15	2.59	3 (21%)	15,19,21	5.15	4 (26%)
2	NAG	B	1461	3,2	14,14,15	2.81	3 (21%)	15,19,21	3.31	6 (40%)
3	BMA	B	1462	2,4	11,11,12	1.79	2 (18%)	15,15,17	4.45	5 (33%)
4	MAN	B	1463	3	11,11,12	1.95	3 (27%)	15,15,17	3.48	6 (40%)
2	NAG	B	1464	1,2	14,14,15	2.64	3 (21%)	15,19,21	4.35	5 (33%)
2	NAG	B	1465	3,2	14,14,15	2.69	3 (21%)	15,19,21	4.95	8 (53%)
3	BMA	B	1466	2,4	11,11,12	1.82	2 (18%)	15,15,17	4.56	6 (40%)
4	MAN	B	1467	3	11,11,12	2.00	4 (36%)	15,15,17	3.02	5 (33%)
4	MAN	B	1468	3	11,11,12	1.97	3 (27%)	15,15,17	3.58	4 (26%)
2	NAG	B	1469	1,2	14,14,15	2.79	3 (21%)	15,19,21	4.33	6 (40%)
2	NAG	B	1470	2	14,14,15	2.82	2 (14%)	15,19,21	1.53	2 (13%)
2	NAG	B	1471	1,2	14,14,15	2.67	3 (21%)	15,19,21	4.53	5 (33%)
2	NAG	B	1472	3,2	14,14,15	2.76	3 (21%)	15,19,21	5.19	8 (53%)
3	BMA	B	1473	2	11,11,12	2.00	3 (27%)	15,15,17	3.27	5 (33%)
2	NAG	B	1474	1	14,14,15	2.73	3 (21%)	15,19,21	2.95	4 (26%)
2	NAG	C	1401	1	14,14,15	2.78	3 (21%)	15,19,21	1.82	2 (13%)
2	NAG	C	1402	1	14,14,15	2.66	4 (28%)	15,19,21	3.43	4 (26%)
2	NAG	C	1403	1	14,14,15	2.58	3 (21%)	15,19,21	3.85	5 (33%)
2	NAG	C	1404	1,2	14,14,15	2.61	3 (21%)	15,19,21	3.18	5 (33%)
2	NAG	C	1405	3,2	14,14,15	2.77	4 (28%)	15,19,21	4.89	6 (40%)
3	BMA	C	1406	2,4	11,11,12	1.93	3 (27%)	15,15,17	3.22	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	C	1407	3,4	11,11,12	1.88	3 (27%)	15,15,17	4.12	5 (33%)
4	MAN	C	1408	4	11,11,12	2.58	6 (54%)	15,15,17	2.63	7 (46%)
4	MAN	C	1409	3	11,11,12	2.48	6 (54%)	15,15,17	3.23	6 (40%)
2	NAG	C	1410	1,2	14,14,15	2.81	3 (21%)	15,19,21	3.81	5 (33%)
2	NAG	C	1411	2	14,14,15	3.17	5 (35%)	15,19,21	3.05	4 (26%)
2	NAG	C	1412	1,2	14,14,15	2.67	3 (21%)	15,19,21	2.83	5 (33%)
2	NAG	C	1413	3,2	14,14,15	2.68	3 (21%)	15,19,21	6.75	5 (33%)
3	BMA	C	1414	2,4	11,11,12	1.80	2 (18%)	15,15,17	2.71	4 (26%)
4	MAN	C	1415	3	11,11,12	1.96	3 (27%)	15,15,17	3.50	5 (33%)
2	NAG	C	1416	1,2	14,14,15	2.71	3 (21%)	15,19,21	2.45	4 (26%)
2	NAG	C	1417	2	14,14,15	2.78	3 (21%)	15,19,21	4.22	4 (26%)
2	NAG	C	1418	1,2	14,14,15	2.65	3 (21%)	15,19,21	2.94	5 (33%)
2	NAG	C	1419	3,2	14,14,15	2.88	3 (21%)	15,19,21	4.71	7 (46%)
3	BMA	C	1420	2,4	11,11,12	1.84	3 (27%)	15,15,17	3.65	4 (26%)
4	MAN	C	1421	3	11,11,12	1.86	3 (27%)	15,15,17	3.32	5 (33%)
2	NAG	C	1422	1,2	14,14,15	2.67	3 (21%)	15,19,21	4.17	5 (33%)
2	NAG	C	1423	2	14,14,15	2.87	3 (21%)	15,19,21	2.23	3 (20%)
2	NAG	C	1424	1,2	14,14,15	2.54	3 (21%)	15,19,21	4.90	7 (46%)
2	NAG	C	1425	2	14,14,15	2.66	3 (21%)	15,19,21	1.70	2 (13%)
2	NAG	C	1426	1,2	14,14,15	2.64	3 (21%)	15,19,21	3.77	5 (33%)
2	NAG	C	1427	3,2	14,14,15	2.76	4 (28%)	15,19,21	3.82	5 (33%)
3	BMA	C	1428	2,4	11,11,12	1.80	1 (9%)	15,15,17	5.66	6 (40%)
4	MAN	C	1429	3,4	11,11,12	1.66	2 (18%)	15,15,17	8.59	6 (40%)
4	MAN	C	1430	4	11,11,12	1.67	3 (27%)	15,15,17	4.08	5 (33%)
4	MAN	C	1431	4	11,11,12	1.92	3 (27%)	15,15,17	2.29	2 (13%)
4	MAN	C	1432	3,4	11,11,12	1.87	3 (27%)	15,15,17	5.14	7 (46%)
4	MAN	C	1433	4	11,11,12	2.49	6 (54%)	15,15,17	3.72	8 (53%)
2	NAG	C	1434	1,2	14,14,15	3.20	4 (28%)	15,19,21	5.77	5 (33%)
2	NAG	C	1435	3,2	14,14,15	2.95	4 (28%)	15,19,21	2.69	6 (40%)
3	BMA	C	1436	2	11,11,12	2.01	4 (36%)	15,15,17	3.89	5 (33%)
2	NAG	C	1437	1,2	14,14,15	2.74	3 (21%)	15,19,21	4.10	6 (40%)
2	NAG	C	1438	2	14,14,15	2.79	3 (21%)	15,19,21	2.04	3 (20%)
2	NAG	C	1439	1	14,14,15	2.43	3 (21%)	15,19,21	2.89	3 (20%)
2	NAG	C	1440	1	14,14,15	3.49	6 (42%)	15,19,21	3.03	7 (46%)
2	NAG	C	1441	1	14,14,15	2.94	4 (28%)	15,19,21	3.73	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1442	1,2	14,14,15	2.57	3 (21%)	15,19,21	3.22	5 (33%)
2	NAG	C	1443	3,2	14,14,15	2.73	3 (21%)	15,19,21	5.67	5 (33%)
3	BMA	C	1444	2,4	11,11,12	1.84	2 (18%)	15,15,17	2.85	5 (33%)
4	MAN	C	1445	3	11,11,12	2.02	3 (27%)	15,15,17	2.82	6 (40%)
4	MAN	C	1446	3	11,11,12	1.90	3 (27%)	15,15,17	3.00	4 (26%)
2	NAG	C	1447	1,2	14,14,15	2.79	3 (21%)	15,19,21	3.12	5 (33%)
2	NAG	C	1448	3,2	14,14,15	2.86	3 (21%)	15,19,21	3.81	6 (40%)
3	BMA	C	1449	2	11,11,12	1.90	2 (18%)	15,15,17	3.88	5 (33%)
2	NAG	C	1450	1,2	14,14,15	2.72	3 (21%)	15,19,21	3.62	5 (33%)
2	NAG	C	1451	2	14,14,15	2.74	3 (21%)	15,19,21	2.28	4 (26%)
2	NAG	C	1452	1,2	14,14,15	2.72	4 (28%)	15,19,21	4.80	6 (40%)
2	NAG	C	1453	2	14,14,15	2.77	2 (14%)	15,19,21	2.13	2 (13%)
2	NAG	C	1454	1,2	14,14,15	2.63	3 (21%)	15,19,21	3.66	6 (40%)
2	NAG	C	1455	2	14,14,15	2.89	3 (21%)	15,19,21	3.02	3 (20%)
2	NAG	C	1456	1,2	14,14,15	2.71	3 (21%)	15,19,21	4.11	5 (33%)
2	NAG	C	1457	2	14,14,15	2.63	4 (28%)	15,19,21	2.16	2 (13%)
2	NAG	C	1458	1,2	14,14,15	2.68	3 (21%)	15,19,21	4.07	4 (26%)
2	NAG	C	1459	2	14,14,15	2.85	3 (21%)	15,19,21	2.62	3 (20%)
2	NAG	C	1460	1,2	14,14,15	2.58	3 (21%)	15,19,21	5.15	4 (26%)
2	NAG	C	1461	3,2	14,14,15	2.80	3 (21%)	15,19,21	3.31	6 (40%)
3	BMA	C	1462	2,4	11,11,12	1.78	2 (18%)	15,15,17	4.45	5 (33%)
4	MAN	C	1463	3	11,11,12	1.94	3 (27%)	15,15,17	3.48	6 (40%)
2	NAG	C	1464	1,2	14,14,15	2.64	3 (21%)	15,19,21	4.35	5 (33%)
2	NAG	C	1465	3,2	14,14,15	2.70	4 (28%)	15,19,21	4.95	8 (53%)
3	BMA	C	1466	2,4	11,11,12	1.82	2 (18%)	15,15,17	4.56	6 (40%)
4	MAN	C	1467	3	11,11,12	2.00	4 (36%)	15,15,17	3.02	5 (33%)
4	MAN	C	1468	3	11,11,12	1.96	3 (27%)	15,15,17	3.59	4 (26%)
2	NAG	C	1469	1,2	14,14,15	2.78	3 (21%)	15,19,21	4.33	6 (40%)
2	NAG	C	1470	2	14,14,15	2.83	2 (14%)	15,19,21	1.53	2 (13%)
2	NAG	C	1471	1,2	14,14,15	2.68	3 (21%)	15,19,21	4.53	5 (33%)
2	NAG	C	1472	3,2	14,14,15	2.75	3 (21%)	15,19,21	5.20	8 (53%)
3	BMA	C	1473	2	11,11,12	1.99	3 (27%)	15,15,17	3.27	5 (33%)
2	NAG	C	1474	1	14,14,15	2.73	3 (21%)	15,19,21	2.96	4 (26%)

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
2	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1404	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1405	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1406	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1407	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1408	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1409	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1410	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1411	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1412	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1413	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1414	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1415	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1416	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1417	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1418	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1419	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1420	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1421	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1422	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1423	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1424	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1425	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1426	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1427	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1428	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1429	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1430	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1431	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1432	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1433	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1434	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1435	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1436	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1437	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1438	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1439	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1440	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1441	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1442	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1443	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1444	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1445	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1446	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1447	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1448	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1449	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1450	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1451	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1452	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1453	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1454	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1455	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1456	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1457	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1458	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1459	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1460	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1461	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1462	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1463	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1464	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1465	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1466	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1467	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1468	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1469	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1470	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1471	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1472	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1473	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1474	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1404	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1405	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1406	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1407	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1408	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	1409	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1410	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1411	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1412	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1413	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1414	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1415	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1416	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1417	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1418	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1419	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1420	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1421	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1422	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1423	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1424	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1425	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1426	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1427	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1428	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1429	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1430	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1431	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1432	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1433	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1434	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1435	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1436	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1437	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1438	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1439	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1440	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1441	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1442	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1443	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1444	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1445	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1446	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1447	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1448	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1449	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1450	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1451	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1452	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1453	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1454	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1455	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1456	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1457	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1458	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1459	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1460	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1461	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1462	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1463	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1464	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1465	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1466	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1467	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1468	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1469	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1470	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1471	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1472	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1473	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1474	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1404	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1405	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1406	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1407	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1408	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1409	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1410	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1411	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1412	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1413	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1414	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1415	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1416	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1417	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1418	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1419	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1420	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1421	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1422	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1423	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1424	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1425	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1426	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1427	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1428	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1429	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1430	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1431	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1432	3,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1433	4	-	0/2/19/22	0/1/1/1
2	NAG	C	1434	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1435	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1436	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1437	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1438	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1439	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1440	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1441	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1442	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1443	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1444	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1445	3	-	0/2/19/22	0/1/1/1
4	MAN	C	1446	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1447	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1448	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1449	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1450	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1451	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1452	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1453	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1454	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1455	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1456	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1457	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1458	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1459	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1460	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1461	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1462	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1463	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1464	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1465	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1466	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1467	3	-	0/2/19/22	0/1/1/1
4	MAN	C	1468	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1469	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1470	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1471	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1472	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1473	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1474	1	-	0/6/23/26	0/1/1/1

All (706) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1470	NAG	C2-N2	-7.10	1.33	1.46
2	A	1470	NAG	C2-N2	-7.08	1.33	1.46
2	B	1470	NAG	C2-N2	-7.06	1.33	1.46
2	B	1469	NAG	C2-N2	-7.04	1.33	1.46
2	A	1469	NAG	C2-N2	-7.02	1.33	1.46
2	C	1469	NAG	C2-N2	-6.99	1.33	1.46
2	A	1419	NAG	C2-N2	-6.71	1.34	1.46
2	B	1419	NAG	C2-N2	-6.70	1.34	1.46
2	B	1410	NAG	C2-N2	-6.70	1.34	1.46
2	A	1410	NAG	C2-N2	-6.69	1.34	1.46
2	C	1419	NAG	C2-N2	-6.69	1.34	1.46
2	C	1410	NAG	C2-N2	-6.68	1.34	1.46
2	A	1447	NAG	C2-N2	-6.66	1.34	1.46
2	C	1447	NAG	C2-N2	-6.65	1.34	1.46
2	B	1447	NAG	C2-N2	-6.64	1.34	1.46
2	B	1461	NAG	C2-N2	-6.41	1.34	1.46
2	C	1461	NAG	C2-N2	-6.39	1.34	1.46
2	A	1461	NAG	C2-N2	-6.38	1.34	1.46
2	B	1441	NAG	C2-N2	-6.34	1.35	1.46
2	A	1441	NAG	C2-N2	-6.34	1.35	1.46
2	A	1448	NAG	C2-N2	-6.33	1.35	1.46
2	C	1456	NAG	C2-N2	-6.33	1.35	1.46
2	B	1448	NAG	C2-N2	-6.33	1.35	1.46
2	C	1448	NAG	C2-N2	-6.33	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1456	NAG	C2-N2	-6.32	1.35	1.46
2	B	1456	NAG	C2-N2	-6.32	1.35	1.46
2	C	1437	NAG	C2-N2	-6.29	1.35	1.46
2	A	1437	NAG	C2-N2	-6.29	1.35	1.46
2	B	1437	NAG	C2-N2	-6.28	1.35	1.46
2	C	1441	NAG	C2-N2	-6.28	1.35	1.46
2	B	1472	NAG	C2-N2	-6.26	1.35	1.46
2	C	1443	NAG	C2-N2	-6.26	1.35	1.46
2	B	1443	NAG	C2-N2	-6.25	1.35	1.46
2	A	1472	NAG	C2-N2	-6.23	1.35	1.46
2	A	1412	NAG	C2-N2	-6.23	1.35	1.46
2	A	1443	NAG	C2-N2	-6.23	1.35	1.46
2	B	1412	NAG	C2-N2	-6.22	1.35	1.46
2	C	1472	NAG	C2-N2	-6.22	1.35	1.46
2	C	1412	NAG	C2-N2	-6.22	1.35	1.46
2	B	1413	NAG	C2-N2	-6.17	1.35	1.46
2	A	1413	NAG	C2-N2	-6.17	1.35	1.46
2	C	1413	NAG	C2-N2	-6.16	1.35	1.46
2	A	1455	NAG	C2-N2	-6.14	1.35	1.46
2	C	1459	NAG	C2-N2	-6.12	1.35	1.46
2	B	1455	NAG	C2-N2	-6.12	1.35	1.46
2	B	1422	NAG	C2-N2	-6.12	1.35	1.46
2	A	1450	NAG	C2-N2	-6.12	1.35	1.46
2	A	1459	NAG	C2-N2	-6.11	1.35	1.46
2	B	1459	NAG	C2-N2	-6.10	1.35	1.46
2	A	1422	NAG	C2-N2	-6.10	1.35	1.46
2	C	1455	NAG	C2-N2	-6.10	1.35	1.46
2	C	1422	NAG	C2-N2	-6.09	1.35	1.46
2	C	1450	NAG	C2-N2	-6.09	1.35	1.46
2	C	1416	NAG	C2-N2	-6.09	1.35	1.46
2	A	1434	NAG	C2-N2	-6.08	1.35	1.46
2	B	1450	NAG	C2-N2	-6.08	1.35	1.46
2	C	1434	NAG	C2-N2	-6.07	1.35	1.46
2	A	1416	NAG	C2-N2	-6.07	1.35	1.46
2	C	1452	NAG	C2-N2	-6.07	1.35	1.46
2	C	1471	NAG	C2-N2	-6.06	1.35	1.46
2	A	1471	NAG	C2-N2	-6.06	1.35	1.46
2	B	1434	NAG	C2-N2	-6.06	1.35	1.46
2	B	1452	NAG	C2-N2	-6.05	1.35	1.46
2	A	1452	NAG	C2-N2	-6.05	1.35	1.46
2	B	1416	NAG	C2-N2	-6.04	1.35	1.46
2	B	1427	NAG	C2-N2	-6.03	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1471	NAG	C2-N2	-6.03	1.35	1.46
2	A	1427	NAG	C2-N2	-6.03	1.35	1.46
2	B	1474	NAG	C2-N2	-6.02	1.35	1.46
2	A	1474	NAG	C2-N2	-6.02	1.35	1.46
2	C	1418	NAG	C2-N2	-6.01	1.35	1.46
2	A	1418	NAG	C2-N2	-6.01	1.35	1.46
2	C	1427	NAG	C2-N2	-6.00	1.35	1.46
2	C	1404	NAG	C2-N2	-6.00	1.35	1.46
2	B	1418	NAG	C2-N2	-5.98	1.35	1.46
2	C	1474	NAG	C2-N2	-5.98	1.35	1.46
2	A	1404	NAG	C2-N2	-5.98	1.35	1.46
2	C	1464	NAG	C2-N2	-5.95	1.35	1.46
2	B	1404	NAG	C2-N2	-5.95	1.35	1.46
2	A	1464	NAG	C2-N2	-5.93	1.35	1.46
2	B	1464	NAG	C2-N2	-5.93	1.35	1.46
2	B	1458	NAG	C2-N2	-5.92	1.35	1.46
2	A	1460	NAG	C2-N2	-5.90	1.35	1.46
2	C	1460	NAG	C2-N2	-5.90	1.35	1.46
2	A	1465	NAG	C2-N2	-5.89	1.35	1.46
2	B	1460	NAG	C2-N2	-5.89	1.35	1.46
2	C	1442	NAG	C2-N2	-5.88	1.35	1.46
2	A	1442	NAG	C2-N2	-5.87	1.35	1.46
2	C	1465	NAG	C2-N2	-5.87	1.35	1.46
2	B	1442	NAG	C2-N2	-5.87	1.35	1.46
2	C	1458	NAG	C2-N2	-5.87	1.35	1.46
2	A	1458	NAG	C2-N2	-5.87	1.35	1.46
2	B	1465	NAG	C2-N2	-5.86	1.35	1.46
2	A	1401	NAG	C2-N2	-5.86	1.35	1.46
2	C	1401	NAG	C2-N2	-5.86	1.35	1.46
2	B	1426	NAG	C2-N2	-5.86	1.35	1.46
2	A	1426	NAG	C2-N2	-5.85	1.35	1.46
2	B	1401	NAG	C2-N2	-5.84	1.35	1.46
2	C	1424	NAG	C2-N2	-5.83	1.35	1.46
2	C	1426	NAG	C2-N2	-5.83	1.35	1.46
2	B	1424	NAG	C2-N2	-5.81	1.35	1.46
2	A	1424	NAG	C2-N2	-5.80	1.35	1.46
2	A	1457	NAG	C2-N2	-5.78	1.36	1.46
2	C	1457	NAG	C2-N2	-5.78	1.36	1.46
2	B	1457	NAG	C2-N2	-5.77	1.36	1.46
2	C	1454	NAG	C2-N2	-5.77	1.36	1.46
2	A	1454	NAG	C2-N2	-5.77	1.36	1.46
2	B	1454	NAG	C2-N2	-5.75	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1417	NAG	C2-N2	-5.70	1.36	1.46
2	B	1417	NAG	C2-N2	-5.69	1.36	1.46
2	C	1417	NAG	C2-N2	-5.68	1.36	1.46
2	C	1451	NAG	C2-N2	-5.67	1.36	1.46
2	B	1451	NAG	C2-N2	-5.66	1.36	1.46
2	A	1451	NAG	C2-N2	-5.66	1.36	1.46
2	B	1438	NAG	C2-N2	-5.62	1.36	1.46
2	A	1438	NAG	C2-N2	-5.61	1.36	1.46
2	B	1440	NAG	C2-N2	-5.56	1.36	1.46
2	C	1438	NAG	C2-N2	-5.56	1.36	1.46
2	A	1440	NAG	C2-N2	-5.55	1.36	1.46
2	C	1440	NAG	C2-N2	-5.54	1.36	1.46
2	B	1423	NAG	C2-N2	-5.53	1.36	1.46
2	A	1423	NAG	C2-N2	-5.53	1.36	1.46
2	C	1423	NAG	C2-N2	-5.52	1.36	1.46
2	C	1453	NAG	C2-N2	-5.37	1.36	1.46
2	A	1453	NAG	C2-N2	-5.37	1.36	1.46
2	B	1453	NAG	C2-N2	-5.36	1.36	1.46
2	B	1405	NAG	C2-N2	-5.35	1.36	1.46
2	A	1405	NAG	C2-N2	-5.33	1.36	1.46
2	C	1405	NAG	C2-N2	-5.33	1.36	1.46
2	B	1402	NAG	C2-N2	-5.25	1.36	1.46
2	C	1425	NAG	C2-N2	-5.22	1.37	1.46
2	A	1402	NAG	C2-N2	-5.22	1.37	1.46
2	A	1425	NAG	C2-N2	-5.22	1.37	1.46
2	C	1402	NAG	C2-N2	-5.22	1.37	1.46
2	B	1425	NAG	C2-N2	-5.21	1.37	1.46
2	B	1435	NAG	C2-N2	-5.20	1.37	1.46
2	A	1435	NAG	C2-N2	-5.17	1.37	1.46
2	C	1435	NAG	C2-N2	-5.17	1.37	1.46
2	B	1403	NAG	C2-N2	-5.06	1.37	1.46
2	A	1403	NAG	C2-N2	-5.06	1.37	1.46
2	C	1403	NAG	C2-N2	-5.05	1.37	1.46
2	C	1439	NAG	C2-N2	-4.83	1.37	1.46
2	A	1439	NAG	C2-N2	-4.79	1.37	1.46
2	B	1439	NAG	C2-N2	-4.77	1.37	1.46
2	B	1411	NAG	C2-N2	-4.65	1.38	1.46
2	A	1411	NAG	C2-N2	-4.64	1.38	1.46
2	C	1411	NAG	C2-N2	-4.63	1.38	1.46
3	C	1428	BMA	O2-C2	-4.05	1.34	1.43
3	A	1428	BMA	O2-C2	-4.05	1.34	1.43
3	B	1428	BMA	O2-C2	-3.99	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1468	MAN	O2-C2	-3.99	1.34	1.43
4	A	1468	MAN	O2-C2	-3.99	1.34	1.43
3	B	1473	BMA	O2-C2	-3.97	1.34	1.43
3	A	1473	BMA	O2-C2	-3.97	1.34	1.43
4	C	1468	MAN	O2-C2	-3.96	1.34	1.43
3	C	1473	BMA	O2-C2	-3.94	1.34	1.43
4	C	1415	MAN	O2-C2	-3.94	1.34	1.43
4	A	1415	MAN	O2-C2	-3.94	1.34	1.43
4	B	1415	MAN	O2-C2	-3.91	1.34	1.43
4	C	1431	MAN	O2-C2	-3.89	1.34	1.43
4	B	1431	MAN	O2-C2	-3.88	1.34	1.43
4	A	1431	MAN	O2-C2	-3.88	1.34	1.43
3	C	1449	BMA	O2-C2	-3.88	1.34	1.43
3	A	1466	BMA	O2-C2	-3.86	1.34	1.43
3	B	1466	BMA	O2-C2	-3.86	1.34	1.43
3	A	1449	BMA	O2-C2	-3.85	1.34	1.43
3	C	1466	BMA	O2-C2	-3.85	1.34	1.43
3	B	1449	BMA	O2-C2	-3.85	1.34	1.43
4	B	1463	MAN	O2-C2	-3.84	1.34	1.43
4	A	1463	MAN	O2-C2	-3.84	1.34	1.43
3	B	1406	BMA	O2-C2	-3.83	1.34	1.43
4	C	1463	MAN	O2-C2	-3.83	1.34	1.43
3	C	1444	BMA	O2-C2	-3.81	1.34	1.43
3	A	1444	BMA	O2-C2	-3.80	1.34	1.43
3	B	1444	BMA	O2-C2	-3.80	1.34	1.43
3	C	1406	BMA	O2-C2	-3.79	1.34	1.43
3	A	1406	BMA	O2-C2	-3.79	1.34	1.43
3	C	1436	BMA	O2-C2	-3.77	1.35	1.43
3	A	1436	BMA	O2-C2	-3.77	1.35	1.43
4	A	1421	MAN	O2-C2	-3.77	1.35	1.43
4	B	1421	MAN	O2-C2	-3.77	1.35	1.43
3	B	1436	BMA	O2-C2	-3.76	1.35	1.43
3	A	1420	BMA	O2-C2	-3.76	1.35	1.43
3	B	1420	BMA	O2-C2	-3.76	1.35	1.43
4	C	1421	MAN	O2-C2	-3.75	1.35	1.43
3	C	1420	BMA	O2-C2	-3.75	1.35	1.43
4	C	1445	MAN	O2-C2	-3.74	1.35	1.43
4	A	1445	MAN	O2-C2	-3.74	1.35	1.43
4	B	1445	MAN	O2-C2	-3.73	1.35	1.43
4	C	1467	MAN	O2-C2	-3.73	1.35	1.43
3	B	1414	BMA	O2-C2	-3.73	1.35	1.43
4	B	1446	MAN	O2-C2	-3.72	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1462	BMA	O2-C2	-3.72	1.35	1.43
4	A	1446	MAN	O2-C2	-3.71	1.35	1.43
3	A	1414	BMA	O2-C2	-3.71	1.35	1.43
4	A	1467	MAN	O2-C2	-3.71	1.35	1.43
3	C	1414	BMA	O2-C2	-3.71	1.35	1.43
4	B	1433	MAN	O2-C2	-3.70	1.35	1.43
4	C	1446	MAN	O2-C2	-3.70	1.35	1.43
4	B	1467	MAN	O2-C2	-3.70	1.35	1.43
3	A	1462	BMA	O2-C2	-3.69	1.35	1.43
3	C	1462	BMA	O2-C2	-3.69	1.35	1.43
4	C	1433	MAN	O2-C2	-3.69	1.35	1.43
4	A	1433	MAN	O2-C2	-3.68	1.35	1.43
4	A	1409	MAN	O2-C2	-3.61	1.35	1.43
4	B	1409	MAN	O2-C2	-3.61	1.35	1.43
4	B	1408	MAN	O2-C2	-3.60	1.35	1.43
4	A	1408	MAN	O2-C2	-3.60	1.35	1.43
4	C	1408	MAN	O2-C2	-3.60	1.35	1.43
4	C	1409	MAN	O2-C2	-3.57	1.35	1.43
4	C	1432	MAN	O2-C2	-3.50	1.35	1.43
4	A	1432	MAN	O2-C2	-3.49	1.35	1.43
4	B	1432	MAN	O2-C2	-3.49	1.35	1.43
4	A	1429	MAN	O2-C2	-3.02	1.36	1.43
4	B	1429	MAN	O2-C2	-3.01	1.36	1.43
4	C	1429	MAN	O2-C2	-3.00	1.36	1.43
4	C	1407	MAN	O2-C2	-2.90	1.36	1.43
4	B	1407	MAN	O2-C2	-2.89	1.36	1.43
4	A	1407	MAN	O2-C2	-2.85	1.37	1.43
4	B	1430	MAN	O2-C2	-2.84	1.37	1.43
4	A	1430	MAN	O2-C2	-2.82	1.37	1.43
4	C	1430	MAN	O2-C2	-2.81	1.37	1.43
2	A	1469	NAG	C1-C2	-2.63	1.48	1.52
2	C	1469	NAG	C1-C2	-2.62	1.48	1.52
2	B	1469	NAG	C1-C2	-2.62	1.48	1.52
3	B	1444	BMA	C2-C3	-2.39	1.49	1.52
3	A	1444	BMA	C2-C3	-2.38	1.49	1.52
3	C	1444	BMA	C2-C3	-2.38	1.49	1.52
3	C	1466	BMA	C2-C3	-2.31	1.49	1.52
3	B	1466	BMA	C2-C3	-2.30	1.49	1.52
3	A	1466	BMA	C2-C3	-2.30	1.49	1.52
4	B	1430	MAN	C2-C3	-2.19	1.49	1.52
4	A	1430	MAN	C2-C3	-2.18	1.49	1.52
4	C	1430	MAN	C2-C3	-2.16	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1420	BMA	C2-C3	-2.05	1.49	1.52
3	B	1420	BMA	C2-C3	-2.05	1.49	1.52
3	A	1420	BMA	C2-C3	-2.03	1.49	1.52
3	C	1436	BMA	C6-C5	2.00	1.59	1.51
2	B	1442	NAG	C4-C3	2.00	1.57	1.52
2	A	1452	NAG	C4-C5	2.00	1.57	1.53
2	A	1442	NAG	C4-C3	2.01	1.57	1.52
2	C	1452	NAG	C4-C5	2.01	1.57	1.53
2	C	1465	NAG	C4-C5	2.02	1.57	1.53
4	C	1433	MAN	C1-C2	2.02	1.57	1.52
2	C	1442	NAG	C4-C3	2.03	1.57	1.52
4	B	1433	MAN	C1-C2	2.03	1.57	1.52
2	C	1427	NAG	C4-C5	2.03	1.57	1.53
4	A	1433	MAN	C1-C2	2.04	1.57	1.52
3	C	1462	BMA	O5-C1	2.04	1.47	1.43
3	B	1462	BMA	O5-C1	2.04	1.47	1.43
2	B	1416	NAG	C4-C3	2.05	1.57	1.52
2	B	1447	NAG	C4-C3	2.05	1.57	1.52
2	A	1427	NAG	C4-C5	2.05	1.57	1.53
2	C	1416	NAG	C4-C3	2.05	1.57	1.52
2	A	1447	NAG	C4-C3	2.05	1.57	1.52
2	C	1447	NAG	C4-C3	2.05	1.57	1.52
2	A	1416	NAG	C4-C3	2.05	1.57	1.52
3	A	1462	BMA	O5-C1	2.05	1.47	1.43
2	B	1427	NAG	C4-C5	2.06	1.57	1.53
2	A	1404	NAG	C4-C3	2.06	1.57	1.52
4	B	1431	MAN	C4-C5	2.06	1.57	1.53
4	C	1430	MAN	O5-C1	2.06	1.47	1.43
4	C	1409	MAN	C6-C5	2.07	1.59	1.51
2	B	1418	NAG	C4-C3	2.07	1.57	1.52
2	A	1418	NAG	C4-C3	2.08	1.57	1.52
2	C	1404	NAG	C4-C3	2.08	1.57	1.52
2	C	1418	NAG	C4-C3	2.08	1.57	1.52
2	B	1404	NAG	C4-C3	2.08	1.57	1.52
3	C	1436	BMA	C4-C5	2.08	1.57	1.53
4	A	1409	MAN	C6-C5	2.09	1.59	1.51
4	A	1467	MAN	C6-C5	2.09	1.59	1.51
2	C	1402	NAG	C4-C3	2.09	1.57	1.52
4	A	1431	MAN	C4-C5	2.09	1.57	1.53
4	B	1467	MAN	C6-C5	2.09	1.59	1.51
4	A	1430	MAN	O5-C1	2.09	1.47	1.43
4	B	1430	MAN	O5-C1	2.10	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1431	MAN	C4-C5	2.10	1.57	1.53
4	C	1467	MAN	C6-C5	2.10	1.59	1.51
4	B	1433	MAN	C6-C5	2.10	1.59	1.51
3	A	1436	BMA	C4-C5	2.10	1.57	1.53
4	B	1409	MAN	C6-C5	2.10	1.59	1.51
4	A	1433	MAN	C6-C5	2.10	1.59	1.51
2	A	1402	NAG	C4-C3	2.10	1.57	1.52
4	C	1433	MAN	C6-C5	2.10	1.59	1.51
2	C	1457	NAG	C4-C5	2.11	1.57	1.53
3	B	1436	BMA	C4-C5	2.11	1.57	1.53
2	B	1412	NAG	C4-C3	2.11	1.58	1.52
3	A	1473	BMA	C4-C5	2.11	1.57	1.53
2	C	1412	NAG	C4-C3	2.11	1.58	1.52
2	A	1457	NAG	C4-C5	2.12	1.57	1.53
2	B	1402	NAG	C4-C3	2.12	1.58	1.52
3	B	1473	BMA	C4-C5	2.12	1.57	1.53
3	C	1473	BMA	C4-C5	2.12	1.57	1.53
2	B	1457	NAG	C4-C5	2.12	1.57	1.53
2	A	1412	NAG	C4-C3	2.12	1.58	1.52
3	C	1420	BMA	O5-C1	2.13	1.47	1.43
2	A	1461	NAG	C4-C3	2.14	1.58	1.52
3	A	1420	BMA	O5-C1	2.14	1.47	1.43
3	B	1420	BMA	O5-C1	2.14	1.47	1.43
4	C	1415	MAN	C4-C5	2.15	1.57	1.53
2	B	1461	NAG	C4-C3	2.15	1.58	1.52
4	A	1415	MAN	C4-C5	2.15	1.57	1.53
4	C	1408	MAN	C6-C5	2.15	1.59	1.51
4	A	1408	MAN	C6-C5	2.15	1.59	1.51
2	C	1461	NAG	C4-C3	2.15	1.58	1.52
2	B	1474	NAG	C4-C3	2.15	1.58	1.52
4	B	1415	MAN	C4-C5	2.15	1.57	1.53
4	B	1408	MAN	C6-C5	2.16	1.59	1.51
4	A	1421	MAN	C4-C5	2.17	1.57	1.53
2	B	1438	NAG	C4-C3	2.17	1.58	1.52
4	B	1421	MAN	C4-C5	2.17	1.57	1.53
2	C	1438	NAG	C4-C3	2.17	1.58	1.52
4	C	1421	MAN	C4-C5	2.17	1.57	1.53
2	C	1474	NAG	C4-C3	2.18	1.58	1.52
2	C	1454	NAG	C4-C3	2.18	1.58	1.52
2	A	1474	NAG	C4-C3	2.18	1.58	1.52
2	A	1454	NAG	C4-C3	2.19	1.58	1.52
2	A	1438	NAG	C4-C3	2.20	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1454	NAG	C4-C3	2.21	1.58	1.52
2	C	1422	NAG	C4-C3	2.21	1.58	1.52
2	B	1403	NAG	C4-C3	2.22	1.58	1.52
2	B	1422	NAG	C4-C3	2.22	1.58	1.52
2	C	1471	NAG	C4-C3	2.22	1.58	1.52
2	B	1425	NAG	C4-C3	2.22	1.58	1.52
2	A	1458	NAG	C4-C3	2.22	1.58	1.52
2	B	1471	NAG	C4-C3	2.22	1.58	1.52
2	A	1425	NAG	C4-C3	2.22	1.58	1.52
2	A	1422	NAG	C4-C3	2.23	1.58	1.52
2	C	1425	NAG	C4-C3	2.23	1.58	1.52
2	B	1458	NAG	C4-C3	2.23	1.58	1.52
2	B	1437	NAG	C4-C3	2.23	1.58	1.52
4	C	1467	MAN	C4-C5	2.23	1.57	1.53
2	C	1458	NAG	C4-C3	2.23	1.58	1.52
2	A	1403	NAG	C4-C3	2.23	1.58	1.52
2	C	1437	NAG	C4-C3	2.23	1.58	1.52
2	B	1460	NAG	C4-C3	2.23	1.58	1.52
2	A	1437	NAG	C4-C3	2.23	1.58	1.52
4	A	1429	MAN	O5-C1	2.23	1.47	1.43
4	B	1429	MAN	O5-C1	2.23	1.47	1.43
2	C	1460	NAG	C4-C3	2.23	1.58	1.52
2	A	1451	NAG	C4-C3	2.24	1.58	1.52
2	A	1471	NAG	C4-C3	2.24	1.58	1.52
2	B	1451	NAG	C4-C3	2.24	1.58	1.52
2	A	1460	NAG	C4-C3	2.24	1.58	1.52
2	C	1410	NAG	C4-C3	2.25	1.58	1.52
2	C	1403	NAG	C4-C3	2.25	1.58	1.52
2	C	1441	NAG	C4-C5	2.25	1.58	1.53
3	B	1406	BMA	C4-C5	2.25	1.58	1.53
4	C	1429	MAN	O5-C1	2.25	1.47	1.43
2	C	1451	NAG	C4-C3	2.25	1.58	1.52
3	C	1414	BMA	O5-C1	2.25	1.47	1.43
2	B	1410	NAG	C4-C3	2.25	1.58	1.52
2	A	1441	NAG	C4-C5	2.26	1.58	1.53
2	B	1456	NAG	C4-C3	2.26	1.58	1.52
2	C	1401	NAG	C4-C3	2.26	1.58	1.52
2	A	1456	NAG	C4-C3	2.26	1.58	1.52
2	A	1410	NAG	C4-C3	2.26	1.58	1.52
4	B	1467	MAN	C4-C5	2.26	1.58	1.53
3	A	1406	BMA	C4-C5	2.26	1.58	1.53
4	A	1467	MAN	C4-C5	2.26	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1450	NAG	C4-C3	2.26	1.58	1.52
3	A	1414	BMA	O5-C1	2.27	1.47	1.43
2	C	1450	NAG	C4-C3	2.27	1.58	1.52
3	B	1414	BMA	O5-C1	2.27	1.47	1.43
3	C	1406	BMA	C4-C5	2.27	1.58	1.53
2	B	1450	NAG	C4-C3	2.28	1.58	1.52
2	C	1456	NAG	C4-C3	2.28	1.58	1.52
2	B	1401	NAG	C4-C3	2.28	1.58	1.52
2	A	1401	NAG	C4-C3	2.28	1.58	1.52
2	B	1464	NAG	C4-C3	2.28	1.58	1.52
2	C	1427	NAG	C4-C3	2.28	1.58	1.52
4	B	1432	MAN	C4-C5	2.28	1.58	1.53
2	B	1427	NAG	C4-C3	2.29	1.58	1.52
2	A	1464	NAG	C4-C3	2.29	1.58	1.52
2	A	1427	NAG	C4-C3	2.29	1.58	1.52
2	B	1441	NAG	C4-C5	2.30	1.58	1.53
2	C	1443	NAG	C4-C3	2.30	1.58	1.52
4	C	1432	MAN	C4-C5	2.30	1.58	1.53
2	C	1464	NAG	C4-C3	2.30	1.58	1.52
4	A	1432	MAN	C4-C5	2.31	1.58	1.53
4	A	1445	MAN	C4-C5	2.31	1.58	1.53
4	B	1463	MAN	C4-C5	2.32	1.58	1.53
4	C	1445	MAN	C4-C5	2.32	1.58	1.53
2	B	1423	NAG	C4-C3	2.32	1.58	1.52
2	C	1423	NAG	C4-C3	2.32	1.58	1.52
4	B	1445	MAN	C4-C5	2.32	1.58	1.53
2	A	1423	NAG	C4-C3	2.32	1.58	1.52
2	A	1443	NAG	C4-C3	2.33	1.58	1.52
4	A	1463	MAN	C4-C5	2.33	1.58	1.53
2	B	1402	NAG	C1-C2	2.33	1.55	1.52
2	C	1402	NAG	C1-C2	2.33	1.55	1.52
4	C	1463	MAN	C4-C5	2.34	1.58	1.53
2	B	1459	NAG	C4-C3	2.34	1.58	1.52
2	C	1459	NAG	C4-C3	2.34	1.58	1.52
2	C	1439	NAG	C4-C3	2.34	1.58	1.52
2	A	1402	NAG	C1-C2	2.34	1.55	1.52
2	A	1459	NAG	C4-C3	2.34	1.58	1.52
2	C	1426	NAG	C4-C3	2.34	1.58	1.52
2	B	1439	NAG	C4-C3	2.35	1.58	1.52
2	B	1426	NAG	C4-C3	2.35	1.58	1.52
2	A	1426	NAG	C4-C3	2.35	1.58	1.52
2	A	1439	NAG	C4-C3	2.35	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1448	NAG	C4-C3	2.36	1.58	1.52
2	B	1443	NAG	C4-C3	2.36	1.58	1.52
4	B	1446	MAN	C4-C5	2.37	1.58	1.53
2	A	1424	NAG	C4-C3	2.37	1.58	1.52
4	B	1468	MAN	C4-C5	2.37	1.58	1.53
4	A	1446	MAN	C4-C5	2.38	1.58	1.53
4	C	1468	MAN	C4-C5	2.38	1.58	1.53
2	C	1448	NAG	C4-C3	2.38	1.58	1.52
2	C	1424	NAG	C4-C3	2.38	1.58	1.52
2	B	1424	NAG	C4-C3	2.38	1.58	1.52
2	A	1448	NAG	C4-C3	2.39	1.58	1.52
2	B	1434	NAG	C4-C5	2.39	1.58	1.53
2	A	1455	NAG	C4-C3	2.39	1.58	1.52
2	B	1440	NAG	O5-C5	2.40	1.48	1.43
2	A	1440	NAG	O5-C5	2.40	1.48	1.43
2	C	1455	NAG	C4-C3	2.40	1.58	1.52
2	C	1440	NAG	O5-C5	2.40	1.48	1.43
4	C	1446	MAN	C4-C5	2.40	1.58	1.53
2	C	1434	NAG	C4-C5	2.41	1.58	1.53
2	B	1455	NAG	C4-C3	2.41	1.58	1.52
2	A	1434	NAG	C4-C5	2.41	1.58	1.53
4	A	1468	MAN	C4-C5	2.41	1.58	1.53
2	B	1413	NAG	C4-C3	2.42	1.58	1.52
2	B	1411	NAG	C1-C2	2.42	1.55	1.52
2	C	1411	NAG	C1-C2	2.42	1.55	1.52
2	A	1411	NAG	C1-C2	2.43	1.55	1.52
2	C	1413	NAG	C4-C3	2.43	1.58	1.52
2	A	1413	NAG	C4-C3	2.43	1.58	1.52
2	B	1457	NAG	C4-C3	2.48	1.58	1.52
2	C	1417	NAG	C4-C3	2.49	1.58	1.52
2	A	1417	NAG	C4-C3	2.49	1.59	1.52
4	A	1446	MAN	O5-C1	2.49	1.47	1.43
2	B	1417	NAG	C4-C3	2.49	1.59	1.52
2	A	1457	NAG	C4-C3	2.50	1.59	1.52
2	C	1457	NAG	C4-C3	2.52	1.59	1.52
4	B	1446	MAN	O5-C1	2.53	1.47	1.43
4	C	1446	MAN	O5-C1	2.53	1.47	1.43
3	B	1406	BMA	O5-C1	2.53	1.47	1.43
4	B	1408	MAN	C1-C2	2.53	1.58	1.52
4	A	1408	MAN	C1-C2	2.53	1.58	1.52
4	C	1408	MAN	C1-C2	2.54	1.58	1.52
4	C	1421	MAN	O5-C1	2.56	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1452	NAG	C4-C3	2.57	1.59	1.52
2	C	1452	NAG	C4-C3	2.57	1.59	1.52
2	B	1435	NAG	C4-C3	2.57	1.59	1.52
2	A	1435	NAG	C4-C3	2.57	1.59	1.52
2	C	1435	NAG	C4-C3	2.57	1.59	1.52
2	A	1452	NAG	C4-C3	2.57	1.59	1.52
3	C	1406	BMA	O5-C1	2.58	1.47	1.43
4	A	1421	MAN	O5-C1	2.58	1.47	1.43
3	A	1406	BMA	O5-C1	2.58	1.47	1.43
4	A	1468	MAN	O5-C1	2.58	1.47	1.43
4	B	1468	MAN	O5-C1	2.58	1.47	1.43
4	B	1421	MAN	O5-C1	2.59	1.47	1.43
4	A	1432	MAN	O5-C1	2.62	1.48	1.43
4	C	1432	MAN	O5-C1	2.62	1.48	1.43
4	C	1407	MAN	C4-C5	2.63	1.58	1.53
4	C	1468	MAN	O5-C1	2.63	1.48	1.43
4	B	1432	MAN	O5-C1	2.64	1.48	1.43
4	A	1407	MAN	C4-C5	2.65	1.58	1.53
2	B	1405	NAG	C4-C5	2.66	1.58	1.53
2	C	1405	NAG	C4-C5	2.66	1.58	1.53
4	B	1407	MAN	C4-C5	2.67	1.58	1.53
4	A	1409	MAN	C1-C2	2.68	1.58	1.52
4	C	1433	MAN	O5-C5	2.68	1.49	1.43
2	C	1419	NAG	C4-C3	2.68	1.59	1.52
2	A	1405	NAG	C4-C5	2.68	1.58	1.53
2	B	1419	NAG	C4-C3	2.68	1.59	1.52
2	A	1419	NAG	C4-C3	2.68	1.59	1.52
4	A	1433	MAN	O5-C5	2.68	1.49	1.43
4	B	1409	MAN	C1-C2	2.68	1.58	1.52
4	C	1409	MAN	O5-C5	2.69	1.49	1.43
2	C	1465	NAG	C4-C3	2.69	1.59	1.52
4	B	1433	MAN	O5-C5	2.69	1.49	1.43
4	C	1409	MAN	C1-C2	2.70	1.58	1.52
4	A	1409	MAN	O5-C5	2.71	1.49	1.43
4	B	1409	MAN	O5-C5	2.71	1.49	1.43
2	A	1465	NAG	C4-C3	2.72	1.59	1.52
2	B	1465	NAG	C4-C3	2.73	1.59	1.52
2	B	1435	NAG	C4-C5	2.75	1.59	1.53
4	B	1408	MAN	O5-C5	2.76	1.49	1.43
2	A	1435	NAG	C4-C5	2.76	1.59	1.53
4	A	1408	MAN	O5-C5	2.76	1.49	1.43
2	C	1435	NAG	C4-C5	2.76	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1408	MAN	O5-C5	2.80	1.49	1.43
2	C	1441	NAG	C4-C3	2.85	1.59	1.52
2	B	1441	NAG	C4-C3	2.86	1.59	1.52
2	A	1441	NAG	C4-C3	2.86	1.59	1.52
4	C	1463	MAN	O5-C1	2.87	1.48	1.43
4	A	1463	MAN	O5-C1	2.87	1.48	1.43
3	A	1473	BMA	O5-C1	2.88	1.48	1.43
4	B	1463	MAN	O5-C1	2.88	1.48	1.43
3	C	1473	BMA	O5-C1	2.90	1.48	1.43
3	B	1473	BMA	O5-C1	2.90	1.48	1.43
3	C	1449	BMA	O5-C1	2.92	1.48	1.43
2	A	1472	NAG	C4-C3	2.92	1.60	1.52
2	B	1472	NAG	C4-C3	2.93	1.60	1.52
2	C	1472	NAG	C4-C3	2.94	1.60	1.52
3	A	1449	BMA	O5-C1	2.96	1.48	1.43
3	B	1449	BMA	O5-C1	2.98	1.48	1.43
4	B	1431	MAN	O5-C1	3.04	1.48	1.43
4	A	1431	MAN	O5-C1	3.06	1.48	1.43
4	C	1431	MAN	O5-C1	3.08	1.48	1.43
4	B	1407	MAN	O5-C1	3.11	1.48	1.43
2	C	1405	NAG	C4-C3	3.11	1.60	1.52
4	B	1415	MAN	O5-C1	3.12	1.48	1.43
4	C	1415	MAN	O5-C1	3.12	1.48	1.43
2	B	1405	NAG	C4-C3	3.12	1.60	1.52
2	A	1405	NAG	C4-C3	3.13	1.60	1.52
2	A	1411	NAG	C4-C3	3.13	1.60	1.52
4	A	1415	MAN	O5-C1	3.13	1.48	1.43
2	B	1411	NAG	C4-C3	3.14	1.60	1.52
2	C	1411	NAG	C4-C3	3.15	1.60	1.52
4	A	1407	MAN	O5-C1	3.16	1.48	1.43
4	C	1407	MAN	O5-C1	3.17	1.48	1.43
4	B	1467	MAN	O5-C1	3.23	1.49	1.43
4	A	1467	MAN	O5-C1	3.24	1.49	1.43
4	C	1467	MAN	O5-C1	3.25	1.49	1.43
4	B	1445	MAN	O5-C1	3.28	1.49	1.43
4	A	1445	MAN	O5-C1	3.28	1.49	1.43
2	B	1411	NAG	C4-C5	3.29	1.60	1.53
2	C	1411	NAG	C4-C5	3.29	1.60	1.53
2	A	1411	NAG	C4-C5	3.29	1.60	1.53
4	C	1445	MAN	O5-C1	3.30	1.49	1.43
3	C	1436	BMA	O5-C1	3.40	1.49	1.43
3	A	1436	BMA	O5-C1	3.43	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1436	BMA	O5-C1	3.44	1.49	1.43
4	B	1409	MAN	O5-C1	3.44	1.49	1.43
4	C	1409	MAN	O5-C1	3.45	1.49	1.43
4	A	1409	MAN	O5-C1	3.49	1.49	1.43
2	C	1440	NAG	C1-C2	3.52	1.57	1.52
2	A	1440	NAG	C1-C2	3.53	1.57	1.52
2	B	1440	NAG	C1-C2	3.56	1.57	1.52
4	A	1433	MAN	C4-C5	3.57	1.60	1.53
4	B	1433	MAN	C4-C5	3.57	1.60	1.53
4	C	1433	MAN	C4-C5	3.58	1.60	1.53
2	B	1434	NAG	C4-C3	3.65	1.62	1.52
2	A	1434	NAG	C4-C3	3.66	1.62	1.52
2	C	1434	NAG	C4-C3	3.68	1.62	1.52
4	A	1408	MAN	C4-C5	3.88	1.61	1.53
4	A	1409	MAN	C4-C5	3.89	1.61	1.53
4	B	1409	MAN	C4-C5	3.90	1.61	1.53
4	C	1408	MAN	C4-C5	3.91	1.61	1.53
4	B	1408	MAN	C4-C5	3.91	1.61	1.53
4	C	1409	MAN	C4-C5	3.92	1.61	1.53
2	B	1440	NAG	C4-C5	4.03	1.61	1.53
4	B	1408	MAN	O5-C1	4.04	1.50	1.43
2	C	1440	NAG	C4-C5	4.04	1.61	1.53
2	A	1440	NAG	C4-C5	4.05	1.61	1.53
4	A	1408	MAN	O5-C1	4.10	1.50	1.43
4	C	1408	MAN	O5-C1	4.11	1.50	1.43
4	B	1433	MAN	O5-C1	4.14	1.50	1.43
4	A	1433	MAN	O5-C1	4.14	1.50	1.43
4	C	1433	MAN	O5-C1	4.15	1.50	1.43
2	C	1440	NAG	C4-C3	4.39	1.64	1.52
2	A	1440	NAG	C4-C3	4.39	1.64	1.52
2	B	1440	NAG	C4-C3	4.39	1.64	1.52
2	C	1469	NAG	O5-C1	6.34	1.54	1.43
2	A	1469	NAG	O5-C1	6.38	1.54	1.43
2	B	1469	NAG	O5-C1	6.39	1.54	1.43
2	B	1424	NAG	O5-C1	6.46	1.54	1.43
2	A	1424	NAG	O5-C1	6.49	1.54	1.43
2	C	1424	NAG	O5-C1	6.51	1.54	1.43
2	C	1460	NAG	O5-C1	6.56	1.54	1.43
2	A	1460	NAG	O5-C1	6.59	1.54	1.43
2	B	1460	NAG	O5-C1	6.60	1.54	1.43
2	C	1439	NAG	O5-C1	6.65	1.54	1.43
2	B	1439	NAG	O5-C1	6.65	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1439	NAG	O5-C1	6.66	1.54	1.43
2	B	1442	NAG	O5-C1	6.68	1.54	1.43
2	C	1442	NAG	O5-C1	6.72	1.54	1.43
2	A	1442	NAG	O5-C1	6.72	1.54	1.43
2	C	1404	NAG	O5-C1	6.78	1.54	1.43
2	B	1456	NAG	O5-C1	6.79	1.54	1.43
2	B	1413	NAG	O5-C1	6.81	1.54	1.43
2	B	1470	NAG	O5-C1	6.81	1.54	1.43
2	A	1456	NAG	O5-C1	6.81	1.54	1.43
2	A	1404	NAG	O5-C1	6.81	1.54	1.43
2	A	1413	NAG	O5-C1	6.81	1.54	1.43
2	A	1470	NAG	O5-C1	6.82	1.54	1.43
2	C	1412	NAG	O5-C1	6.83	1.54	1.43
2	B	1412	NAG	O5-C1	6.83	1.54	1.43
2	A	1412	NAG	O5-C1	6.83	1.54	1.43
2	A	1418	NAG	O5-C1	6.84	1.54	1.43
2	C	1413	NAG	O5-C1	6.84	1.54	1.43
2	C	1470	NAG	O5-C1	6.84	1.54	1.43
2	C	1456	NAG	O5-C1	6.85	1.54	1.43
2	B	1404	NAG	O5-C1	6.85	1.54	1.43
2	C	1418	NAG	O5-C1	6.86	1.54	1.43
2	B	1418	NAG	O5-C1	6.86	1.54	1.43
2	C	1464	NAG	O5-C1	6.88	1.54	1.43
2	B	1464	NAG	O5-C1	6.89	1.54	1.43
2	C	1457	NAG	O5-C1	6.90	1.55	1.43
2	A	1464	NAG	O5-C1	6.91	1.55	1.43
2	B	1422	NAG	O5-C1	6.92	1.55	1.43
2	C	1422	NAG	O5-C1	6.92	1.55	1.43
2	A	1422	NAG	O5-C1	6.93	1.55	1.43
2	A	1457	NAG	O5-C1	6.93	1.55	1.43
2	B	1457	NAG	O5-C1	6.94	1.55	1.43
2	B	1443	NAG	O5-C1	6.97	1.55	1.43
2	B	1426	NAG	O5-C1	6.97	1.55	1.43
2	B	1447	NAG	O5-C1	6.99	1.55	1.43
2	C	1443	NAG	O5-C1	6.99	1.55	1.43
2	C	1447	NAG	O5-C1	6.99	1.55	1.43
2	A	1443	NAG	O5-C1	6.99	1.55	1.43
2	C	1403	NAG	O5-C1	7.00	1.55	1.43
2	A	1454	NAG	O5-C1	7.00	1.55	1.43
2	A	1426	NAG	O5-C1	7.00	1.55	1.43
2	A	1447	NAG	O5-C1	7.00	1.55	1.43
2	C	1454	NAG	O5-C1	7.00	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1426	NAG	O5-C1	7.01	1.55	1.43
2	A	1403	NAG	O5-C1	7.02	1.55	1.43
2	B	1465	NAG	O5-C1	7.03	1.55	1.43
2	B	1454	NAG	O5-C1	7.03	1.55	1.43
2	A	1465	NAG	O5-C1	7.04	1.55	1.43
2	B	1403	NAG	O5-C1	7.05	1.55	1.43
2	B	1458	NAG	O5-C1	7.05	1.55	1.43
2	C	1465	NAG	O5-C1	7.06	1.55	1.43
2	A	1458	NAG	O5-C1	7.06	1.55	1.43
2	B	1471	NAG	O5-C1	7.08	1.55	1.43
2	C	1471	NAG	O5-C1	7.08	1.55	1.43
2	A	1472	NAG	O5-C1	7.08	1.55	1.43
2	B	1437	NAG	O5-C1	7.08	1.55	1.43
2	C	1472	NAG	O5-C1	7.08	1.55	1.43
2	A	1437	NAG	O5-C1	7.09	1.55	1.43
2	C	1458	NAG	O5-C1	7.10	1.55	1.43
2	A	1471	NAG	O5-C1	7.11	1.55	1.43
2	C	1437	NAG	O5-C1	7.11	1.55	1.43
2	B	1472	NAG	O5-C1	7.12	1.55	1.43
2	C	1450	NAG	O5-C1	7.12	1.55	1.43
2	B	1410	NAG	O5-C1	7.13	1.55	1.43
2	A	1410	NAG	O5-C1	7.13	1.55	1.43
2	A	1450	NAG	O5-C1	7.13	1.55	1.43
2	C	1410	NAG	O5-C1	7.14	1.55	1.43
2	B	1474	NAG	O5-C1	7.14	1.55	1.43
2	B	1450	NAG	O5-C1	7.14	1.55	1.43
2	A	1416	NAG	O5-C1	7.15	1.55	1.43
2	C	1416	NAG	O5-C1	7.16	1.55	1.43
2	B	1416	NAG	O5-C1	7.17	1.55	1.43
2	C	1452	NAG	O5-C1	7.18	1.55	1.43
2	A	1452	NAG	O5-C1	7.18	1.55	1.43
2	B	1452	NAG	O5-C1	7.18	1.55	1.43
2	C	1474	NAG	O5-C1	7.19	1.55	1.43
2	A	1474	NAG	O5-C1	7.20	1.55	1.43
2	C	1427	NAG	O5-C1	7.32	1.55	1.43
2	B	1427	NAG	O5-C1	7.32	1.55	1.43
2	B	1419	NAG	O5-C1	7.33	1.55	1.43
2	C	1419	NAG	O5-C1	7.33	1.55	1.43
2	C	1461	NAG	O5-C1	7.34	1.55	1.43
2	A	1419	NAG	O5-C1	7.34	1.55	1.43
2	A	1427	NAG	O5-C1	7.34	1.55	1.43
2	A	1461	NAG	O5-C1	7.37	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1402	NAG	O5-C1	7.37	1.55	1.43
2	B	1461	NAG	O5-C1	7.38	1.55	1.43
2	A	1402	NAG	O5-C1	7.38	1.55	1.43
2	C	1402	NAG	O5-C1	7.38	1.55	1.43
2	A	1405	NAG	O5-C1	7.48	1.55	1.43
2	C	1405	NAG	O5-C1	7.50	1.55	1.43
2	B	1405	NAG	O5-C1	7.50	1.55	1.43
2	A	1401	NAG	O5-C1	7.55	1.56	1.43
2	B	1401	NAG	O5-C1	7.55	1.56	1.43
2	C	1401	NAG	O5-C1	7.55	1.56	1.43
2	C	1448	NAG	O5-C1	7.59	1.56	1.43
2	B	1448	NAG	O5-C1	7.61	1.56	1.43
2	A	1448	NAG	O5-C1	7.61	1.56	1.43
2	B	1425	NAG	O5-C1	7.63	1.56	1.43
2	C	1451	NAG	O5-C1	7.63	1.56	1.43
2	A	1425	NAG	O5-C1	7.63	1.56	1.43
2	C	1425	NAG	O5-C1	7.64	1.56	1.43
2	B	1451	NAG	O5-C1	7.65	1.56	1.43
2	B	1417	NAG	O5-C1	7.67	1.56	1.43
2	A	1451	NAG	O5-C1	7.68	1.56	1.43
2	A	1417	NAG	O5-C1	7.68	1.56	1.43
2	C	1417	NAG	O5-C1	7.73	1.56	1.43
2	A	1459	NAG	O5-C1	7.79	1.56	1.43
2	C	1459	NAG	O5-C1	7.79	1.56	1.43
2	B	1459	NAG	O5-C1	7.79	1.56	1.43
2	B	1441	NAG	O5-C1	7.89	1.56	1.43
2	C	1441	NAG	O5-C1	7.89	1.56	1.43
2	A	1441	NAG	O5-C1	7.90	1.56	1.43
2	B	1438	NAG	O5-C1	7.94	1.56	1.43
2	A	1438	NAG	O5-C1	7.96	1.56	1.43
2	B	1453	NAG	O5-C1	7.98	1.56	1.43
2	A	1453	NAG	O5-C1	7.98	1.56	1.43
2	C	1438	NAG	O5-C1	7.99	1.56	1.43
2	C	1453	NAG	O5-C1	8.00	1.56	1.43
2	A	1455	NAG	O5-C1	8.01	1.56	1.43
2	C	1455	NAG	O5-C1	8.02	1.56	1.43
2	B	1455	NAG	O5-C1	8.05	1.56	1.43
2	B	1423	NAG	O5-C1	8.27	1.57	1.43
2	C	1423	NAG	O5-C1	8.28	1.57	1.43
2	A	1423	NAG	O5-C1	8.30	1.57	1.43
2	C	1435	NAG	O5-C1	8.55	1.57	1.43
2	A	1435	NAG	O5-C1	8.58	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1435	NAG	O5-C1	8.59	1.57	1.43
2	B	1434	NAG	O5-C1	8.74	1.58	1.43
2	A	1434	NAG	O5-C1	8.76	1.58	1.43
2	C	1434	NAG	O5-C1	8.78	1.58	1.43
2	B	1440	NAG	O5-C1	8.79	1.58	1.43
2	A	1440	NAG	O5-C1	8.79	1.58	1.43
2	C	1440	NAG	O5-C1	8.80	1.58	1.43
2	B	1411	NAG	O5-C1	9.04	1.58	1.43
2	C	1411	NAG	O5-C1	9.05	1.58	1.43
2	A	1411	NAG	O5-C1	9.06	1.58	1.43

All (1084) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1434	NAG	O4-C4-C3	-18.18	69.36	110.36
2	B	1434	NAG	O4-C4-C3	-18.18	69.37	110.36
2	C	1434	NAG	O4-C4-C3	-18.17	69.37	110.36
4	B	1429	MAN	O3-C3-C4	-17.67	70.52	110.36
4	C	1429	MAN	O3-C3-C4	-17.66	70.53	110.36
4	A	1429	MAN	O3-C3-C4	-17.66	70.54	110.36
2	B	1424	NAG	O5-C5-C6	-16.85	71.26	107.34
2	C	1424	NAG	O5-C5-C6	-16.85	71.27	107.34
2	A	1424	NAG	O5-C5-C6	-16.85	71.27	107.34
2	A	1413	NAG	O5-C5-C6	-15.14	74.93	107.34
2	B	1413	NAG	O5-C5-C6	-15.14	74.94	107.34
2	C	1413	NAG	O5-C5-C6	-15.12	74.97	107.34
2	B	1443	NAG	O5-C5-C6	-15.04	75.13	107.34
2	A	1443	NAG	O5-C5-C6	-15.04	75.14	107.34
2	C	1443	NAG	O5-C5-C6	-15.04	75.15	107.34
2	A	1469	NAG	O5-C5-C6	-14.59	76.11	107.34
2	B	1469	NAG	O5-C5-C6	-14.59	76.12	107.34
2	C	1469	NAG	O5-C5-C6	-14.58	76.12	107.34
2	B	1472	NAG	O5-C5-C6	-14.54	76.21	107.34
2	C	1472	NAG	O5-C5-C6	-14.54	76.21	107.34
2	A	1472	NAG	O5-C5-C6	-14.53	76.23	107.34
2	B	1460	NAG	O5-C5-C6	-14.26	76.82	107.34
2	A	1460	NAG	O5-C5-C6	-14.25	76.83	107.34
2	C	1460	NAG	O5-C5-C6	-14.24	76.86	107.34
4	B	1432	MAN	O3-C3-C2	-14.00	84.36	110.01
4	A	1432	MAN	O3-C3-C2	-13.99	84.37	110.01
4	C	1432	MAN	O3-C3-C2	-13.98	84.38	110.01
3	C	1462	BMA	O3-C3-C2	-13.98	84.39	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1462	BMA	O3-C3-C2	-13.97	84.40	110.01
3	B	1462	BMA	O3-C3-C2	-13.97	84.40	110.01
2	A	1422	NAG	O5-C5-C6	-13.48	78.48	107.34
2	B	1422	NAG	O5-C5-C6	-13.48	78.49	107.34
2	C	1422	NAG	O5-C5-C6	-13.46	78.52	107.34
2	C	1456	NAG	O4-C4-C3	-13.37	80.22	110.36
2	B	1456	NAG	O4-C4-C3	-13.37	80.22	110.36
2	A	1456	NAG	O4-C4-C3	-13.36	80.23	110.36
2	B	1405	NAG	O5-C5-C6	-13.35	78.77	107.34
2	A	1405	NAG	O5-C5-C6	-13.34	78.78	107.34
2	C	1405	NAG	O5-C5-C6	-13.34	78.79	107.34
2	B	1403	NAG	O5-C5-C6	-12.64	80.28	107.34
2	A	1403	NAG	O5-C5-C6	-12.63	80.29	107.34
2	C	1403	NAG	O5-C5-C6	-12.63	80.31	107.34
2	C	1417	NAG	O5-C5-C6	-11.90	81.87	107.34
2	A	1417	NAG	O5-C5-C6	-11.89	81.90	107.34
2	B	1417	NAG	O5-C5-C6	-11.88	81.91	107.34
2	B	1471	NAG	O4-C4-C3	-11.56	84.30	110.36
2	A	1471	NAG	O4-C4-C3	-11.55	84.31	110.36
2	C	1471	NAG	O4-C4-C3	-11.54	84.33	110.36
2	A	1437	NAG	O5-C5-C6	-11.53	82.66	107.34
2	C	1437	NAG	O5-C5-C6	-11.53	82.66	107.34
2	B	1437	NAG	O5-C5-C6	-11.52	82.67	107.34
4	A	1429	MAN	O5-C5-C6	-11.16	83.44	107.34
4	B	1429	MAN	O5-C5-C6	-11.16	83.44	107.34
4	C	1429	MAN	O5-C5-C6	-11.15	83.46	107.34
2	B	1413	NAG	O3-C3-C2	-10.91	86.02	109.37
2	A	1413	NAG	O3-C3-C2	-10.90	86.04	109.37
2	C	1413	NAG	O3-C3-C2	-10.90	86.05	109.37
4	B	1432	MAN	O5-C5-C6	-10.86	84.10	107.34
4	C	1432	MAN	O5-C5-C6	-10.85	84.12	107.34
4	A	1432	MAN	O5-C5-C6	-10.84	84.12	107.34
2	B	1452	NAG	O3-C3-C2	-10.75	86.37	109.37
2	C	1452	NAG	O3-C3-C2	-10.74	86.39	109.37
2	A	1452	NAG	O3-C3-C2	-10.73	86.41	109.37
2	A	1458	NAG	O5-C5-C6	-10.68	84.47	107.34
2	C	1458	NAG	O5-C5-C6	-10.68	84.47	107.34
2	B	1458	NAG	O5-C5-C6	-10.67	84.50	107.34
4	B	1430	MAN	O5-C5-C6	-10.66	84.51	107.34
4	A	1430	MAN	O5-C5-C6	-10.66	84.52	107.34
4	C	1430	MAN	O5-C5-C6	-10.66	84.53	107.34
2	B	1464	NAG	O4-C4-C3	-10.65	86.35	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1464	NAG	O4-C4-C3	-10.64	86.36	110.36
2	C	1464	NAG	O4-C4-C3	-10.63	86.38	110.36
2	B	1405	NAG	O4-C4-C3	-10.43	86.84	110.36
2	A	1460	NAG	O4-C4-C3	-10.43	86.85	110.36
2	A	1405	NAG	O4-C4-C3	-10.42	86.86	110.36
2	B	1460	NAG	O4-C4-C3	-10.42	86.86	110.36
2	C	1460	NAG	O4-C4-C3	-10.42	86.86	110.36
2	C	1405	NAG	O4-C4-C3	-10.41	86.88	110.36
2	B	1419	NAG	O5-C5-C6	-10.40	85.07	107.34
2	A	1419	NAG	O5-C5-C6	-10.40	85.08	107.34
2	C	1419	NAG	O5-C5-C6	-10.39	85.09	107.34
2	B	1465	NAG	O3-C3-C2	-10.27	87.40	109.37
2	C	1465	NAG	O3-C3-C2	-10.26	87.41	109.37
2	A	1465	NAG	O3-C3-C2	-10.26	87.42	109.37
3	B	1420	BMA	O3-C3-C4	-10.23	87.29	110.36
2	A	1402	NAG	O5-C5-C6	-10.23	85.44	107.34
2	C	1402	NAG	O5-C5-C6	-10.23	85.44	107.34
2	B	1402	NAG	O5-C5-C6	-10.22	85.45	107.34
3	C	1420	BMA	O3-C3-C4	-10.22	87.31	110.36
3	A	1420	BMA	O3-C3-C4	-10.22	87.31	110.36
2	A	1443	NAG	O4-C4-C3	-9.93	87.97	110.36
2	B	1443	NAG	O4-C4-C3	-9.93	87.97	110.36
2	C	1443	NAG	O4-C4-C3	-9.92	87.98	110.36
2	C	1450	NAG	O4-C4-C3	-9.92	88.00	110.36
2	B	1450	NAG	O4-C4-C3	-9.92	88.00	110.36
2	A	1450	NAG	O4-C4-C3	-9.91	88.00	110.36
3	C	1466	BMA	O2-C2-C1	-9.69	89.82	109.23
3	B	1466	BMA	O2-C2-C1	-9.69	89.83	109.23
3	A	1466	BMA	O2-C2-C1	-9.68	89.86	109.23
2	C	1471	NAG	O3-C3-C2	-9.66	88.70	109.37
2	B	1471	NAG	O3-C3-C2	-9.66	88.70	109.37
2	A	1471	NAG	O3-C3-C2	-9.65	88.71	109.37
4	C	1407	MAN	O5-C5-C6	-9.41	87.20	107.34
2	C	1441	NAG	O5-C5-C6	-9.41	87.20	107.34
2	B	1411	NAG	O5-C5-C6	-9.40	87.21	107.34
2	A	1441	NAG	O5-C5-C6	-9.40	87.22	107.34
2	A	1411	NAG	O5-C5-C6	-9.40	87.23	107.34
4	C	1468	MAN	O5-C5-C6	-9.39	87.23	107.34
4	A	1407	MAN	O5-C5-C6	-9.39	87.25	107.34
2	B	1441	NAG	O5-C5-C6	-9.38	87.26	107.34
2	C	1439	NAG	O5-C5-C6	-9.38	87.26	107.34
4	B	1407	MAN	O5-C5-C6	-9.38	87.26	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1468	MAN	O5-C5-C6	-9.38	87.26	107.34
2	B	1439	NAG	O5-C5-C6	-9.37	87.27	107.34
2	C	1411	NAG	O5-C5-C6	-9.37	87.27	107.34
2	A	1439	NAG	O5-C5-C6	-9.37	87.28	107.34
4	A	1468	MAN	O5-C5-C6	-9.37	87.28	107.34
4	B	1421	MAN	O5-C5-C6	-9.30	87.43	107.34
4	A	1421	MAN	O5-C5-C6	-9.30	87.43	107.34
4	C	1421	MAN	O5-C5-C6	-9.28	87.47	107.34
2	A	1474	NAG	O5-C5-C6	-9.28	87.47	107.34
2	C	1474	NAG	O5-C5-C6	-9.28	87.48	107.34
2	B	1474	NAG	O5-C5-C6	-9.28	87.48	107.34
2	A	1461	NAG	O5-C5-C6	-9.14	87.76	107.34
2	C	1461	NAG	O5-C5-C6	-9.14	87.77	107.34
2	B	1461	NAG	O5-C5-C6	-9.14	87.77	107.34
4	C	1415	MAN	O3-C3-C2	-9.01	93.49	110.01
4	B	1415	MAN	O3-C3-C2	-9.00	93.51	110.01
4	A	1415	MAN	O3-C3-C2	-9.00	93.52	110.01
2	A	1455	NAG	O5-C5-C6	-8.92	88.25	107.34
2	C	1455	NAG	O5-C5-C6	-8.91	88.26	107.34
2	B	1455	NAG	O5-C5-C6	-8.91	88.27	107.34
2	C	1434	NAG	O3-C3-C4	-8.89	90.31	110.36
2	B	1434	NAG	O3-C3-C4	-8.87	90.35	110.36
2	A	1434	NAG	O3-C3-C4	-8.87	90.36	110.36
2	B	1418	NAG	O3-C3-C2	-8.86	90.42	109.37
2	A	1418	NAG	O3-C3-C2	-8.86	90.42	109.37
2	C	1418	NAG	O3-C3-C2	-8.85	90.43	109.37
3	B	1428	BMA	O5-C5-C6	-8.84	88.40	107.34
3	A	1428	BMA	O5-C5-C6	-8.84	88.42	107.34
3	C	1428	BMA	O5-C5-C6	-8.83	88.43	107.34
2	B	1404	NAG	O5-C5-C6	-8.81	88.49	107.34
2	A	1404	NAG	O5-C5-C6	-8.80	88.49	107.34
2	C	1404	NAG	O5-C5-C6	-8.80	88.50	107.34
2	C	1410	NAG	O5-C5-C6	-8.59	88.95	107.34
2	B	1410	NAG	O5-C5-C6	-8.59	88.96	107.34
2	A	1410	NAG	O5-C5-C6	-8.58	88.97	107.34
4	A	1433	MAN	O5-C5-C6	-8.43	89.30	107.34
4	B	1433	MAN	O5-C5-C6	-8.43	89.30	107.34
4	C	1433	MAN	O5-C5-C6	-8.42	89.31	107.34
2	B	1465	NAG	O5-C5-C6	-8.40	89.36	107.34
2	A	1465	NAG	O5-C5-C6	-8.39	89.39	107.34
2	C	1465	NAG	O5-C5-C6	-8.38	89.39	107.34
2	C	1434	NAG	O5-C5-C6	-8.38	89.40	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1434	NAG	O5-C5-C6	-8.37	89.41	107.34
2	B	1434	NAG	O5-C5-C6	-8.37	89.42	107.34
4	A	1430	MAN	O3-C3-C4	-8.30	91.65	110.36
4	C	1430	MAN	O3-C3-C4	-8.29	91.66	110.36
4	B	1430	MAN	O3-C3-C4	-8.28	91.69	110.36
2	A	1440	NAG	O5-C5-C6	-8.27	89.63	107.34
2	B	1440	NAG	O5-C5-C6	-8.27	89.63	107.34
2	C	1440	NAG	O5-C5-C6	-8.27	89.63	107.34
2	B	1454	NAG	O5-C5-C6	-8.14	89.92	107.34
2	A	1454	NAG	O5-C5-C6	-8.13	89.93	107.34
2	C	1454	NAG	O5-C5-C6	-8.13	89.94	107.34
4	A	1467	MAN	O3-C3-C2	-7.93	95.48	110.01
4	B	1467	MAN	O3-C3-C2	-7.92	95.49	110.01
4	B	1431	MAN	O5-C5-C6	-7.91	90.40	107.34
4	C	1467	MAN	O3-C3-C2	-7.91	95.52	110.01
4	C	1431	MAN	O5-C5-C6	-7.90	90.42	107.34
4	A	1431	MAN	O5-C5-C6	-7.90	90.43	107.34
4	C	1433	MAN	O3-C3-C2	-7.87	95.59	110.01
4	A	1433	MAN	O3-C3-C2	-7.86	95.61	110.01
4	B	1433	MAN	O3-C3-C2	-7.84	95.65	110.01
4	A	1429	MAN	O4-C4-C5	-7.84	88.58	109.23
4	B	1429	MAN	O4-C4-C5	-7.83	88.59	109.23
4	C	1429	MAN	O4-C4-C5	-7.83	88.61	109.23
2	C	1442	NAG	O5-C5-C6	-7.82	90.60	107.34
2	A	1442	NAG	O5-C5-C6	-7.81	90.62	107.34
2	B	1442	NAG	O5-C5-C6	-7.80	90.64	107.34
3	C	1436	BMA	O3-C3-C2	-7.76	95.78	110.01
3	B	1436	BMA	O3-C3-C2	-7.76	95.79	110.01
3	A	1436	BMA	O3-C3-C2	-7.76	95.79	110.01
3	A	1449	BMA	O5-C5-C6	-7.70	90.86	107.34
3	B	1449	BMA	O5-C5-C6	-7.70	90.86	107.34
3	C	1449	BMA	O5-C5-C6	-7.69	90.88	107.34
2	A	1471	NAG	O3-C3-C4	-7.68	93.04	110.36
2	C	1471	NAG	O3-C3-C4	-7.67	93.06	110.36
2	B	1471	NAG	O3-C3-C4	-7.67	93.06	110.36
4	C	1407	MAN	O3-C3-C4	-7.64	93.12	110.36
4	B	1407	MAN	O3-C3-C4	-7.64	93.13	110.36
4	B	1409	MAN	O5-C5-C6	-7.64	90.99	107.34
2	B	1447	NAG	O4-C4-C3	-7.63	93.14	110.36
4	A	1409	MAN	O5-C5-C6	-7.63	91.00	107.34
4	A	1407	MAN	O3-C3-C4	-7.63	93.15	110.36
2	C	1447	NAG	O4-C4-C3	-7.63	93.15	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1447	NAG	O4-C4-C3	-7.63	93.15	110.36
4	C	1409	MAN	O5-C5-C6	-7.61	91.04	107.34
3	C	1462	BMA	O5-C5-C6	-7.61	91.05	107.34
3	B	1462	BMA	O5-C5-C6	-7.61	91.06	107.34
3	A	1462	BMA	O5-C5-C6	-7.60	91.06	107.34
2	C	1416	NAG	O3-C3-C2	-7.60	93.11	109.37
2	A	1416	NAG	O3-C3-C2	-7.59	93.14	109.37
2	B	1416	NAG	O3-C3-C2	-7.58	93.15	109.37
4	B	1445	MAN	O3-C3-C2	-7.49	96.29	110.01
4	C	1445	MAN	O3-C3-C2	-7.48	96.30	110.01
4	A	1445	MAN	O3-C3-C2	-7.47	96.31	110.01
3	B	1444	BMA	O5-C5-C6	-7.46	91.37	107.34
2	A	1412	NAG	O5-C5-C6	-7.46	91.37	107.34
2	B	1412	NAG	O5-C5-C6	-7.46	91.37	107.34
3	A	1444	BMA	O5-C5-C6	-7.46	91.37	107.34
3	C	1444	BMA	O5-C5-C6	-7.46	91.37	107.34
2	C	1412	NAG	O5-C5-C6	-7.45	91.39	107.34
3	C	1436	BMA	O2-C2-C1	-7.44	94.34	109.23
3	A	1436	BMA	O2-C2-C1	-7.43	94.37	109.23
3	B	1436	BMA	O2-C2-C1	-7.41	94.40	109.23
2	A	1447	NAG	O5-C5-C6	-7.37	91.56	107.34
2	C	1447	NAG	O5-C5-C6	-7.37	91.57	107.34
2	B	1447	NAG	O5-C5-C6	-7.36	91.57	107.34
2	B	1450	NAG	O5-C5-C6	-7.27	91.77	107.34
2	A	1450	NAG	O5-C5-C6	-7.27	91.77	107.34
2	C	1450	NAG	O5-C5-C6	-7.26	91.79	107.34
3	C	1436	BMA	O4-C4-C3	-7.16	94.22	110.36
3	A	1436	BMA	O4-C4-C3	-7.15	94.24	110.36
3	B	1436	BMA	O4-C4-C3	-7.14	94.26	110.36
3	A	1449	BMA	O2-C2-C1	-7.13	94.95	109.23
3	C	1449	BMA	O2-C2-C1	-7.13	94.96	109.23
3	B	1449	BMA	O2-C2-C1	-7.13	94.97	109.23
2	A	1426	NAG	O3-C3-C2	-7.11	94.16	109.37
2	B	1426	NAG	O3-C3-C2	-7.10	94.19	109.37
2	C	1426	NAG	O3-C3-C2	-7.10	94.19	109.37
2	B	1459	NAG	O5-C5-C6	-7.00	92.35	107.34
2	C	1459	NAG	O5-C5-C6	-7.00	92.35	107.34
2	A	1459	NAG	O5-C5-C6	-7.00	92.36	107.34
2	A	1451	NAG	O5-C5-C6	-6.95	92.46	107.34
2	B	1451	NAG	O5-C5-C6	-6.94	92.48	107.34
2	C	1451	NAG	O5-C5-C6	-6.92	92.53	107.34
4	A	1415	MAN	O5-C5-C6	-6.72	92.95	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1415	MAN	O5-C5-C6	-6.72	92.96	107.34
4	C	1415	MAN	O5-C5-C6	-6.71	92.97	107.34
2	C	1464	NAG	O5-C5-C6	-6.65	93.11	107.34
2	A	1464	NAG	O5-C5-C6	-6.64	93.12	107.34
2	B	1464	NAG	O5-C5-C6	-6.64	93.13	107.34
3	B	1414	BMA	O5-C5-C6	-6.55	93.31	107.34
3	A	1414	BMA	O5-C5-C6	-6.55	93.33	107.34
3	C	1414	BMA	O5-C5-C6	-6.54	93.34	107.34
4	C	1446	MAN	O5-C5-C6	-6.50	93.42	107.34
4	A	1446	MAN	O5-C5-C6	-6.50	93.42	107.34
4	B	1446	MAN	O5-C5-C6	-6.50	93.43	107.34
2	A	1442	NAG	O4-C4-C3	-6.43	95.86	110.36
2	B	1442	NAG	O4-C4-C3	-6.42	95.87	110.36
2	C	1442	NAG	O4-C4-C3	-6.42	95.88	110.36
4	B	1463	MAN	O5-C5-C6	-6.41	93.61	107.34
4	A	1463	MAN	O3-C3-C2	-6.41	98.26	110.01
4	C	1463	MAN	O3-C3-C2	-6.41	98.26	110.01
4	C	1463	MAN	O5-C5-C6	-6.40	93.63	107.34
4	A	1463	MAN	O5-C5-C6	-6.40	93.63	107.34
4	B	1463	MAN	O3-C3-C2	-6.40	98.28	110.01
2	B	1457	NAG	O5-C5-C6	-6.37	93.69	107.34
2	A	1448	NAG	O5-C5-C6	-6.36	93.71	107.34
2	A	1457	NAG	O5-C5-C6	-6.36	93.73	107.34
2	B	1448	NAG	O5-C5-C6	-6.35	93.74	107.34
2	C	1448	NAG	O5-C5-C6	-6.35	93.74	107.34
2	C	1457	NAG	O5-C5-C6	-6.33	93.78	107.34
4	A	1446	MAN	O3-C3-C2	-6.30	98.46	110.01
4	B	1446	MAN	O3-C3-C2	-6.30	98.46	110.01
4	C	1446	MAN	O3-C3-C2	-6.29	98.48	110.01
3	A	1449	BMA	O3-C3-C2	-6.25	98.55	110.01
3	B	1449	BMA	O3-C3-C2	-6.25	98.55	110.01
2	A	1423	NAG	O4-C4-C3	-6.24	96.29	110.36
2	B	1423	NAG	O4-C4-C3	-6.24	96.29	110.36
2	C	1423	NAG	O4-C4-C3	-6.24	96.29	110.36
3	C	1449	BMA	O3-C3-C2	-6.24	98.58	110.01
2	B	1403	NAG	O4-C4-C5	-6.18	92.94	109.23
2	A	1403	NAG	O4-C4-C5	-6.18	92.96	109.23
2	C	1403	NAG	O4-C4-C5	-6.17	92.96	109.23
4	B	1408	MAN	O3-C3-C2	-6.11	98.82	110.01
2	C	1456	NAG	O5-C5-C6	-6.10	94.28	107.34
4	A	1408	MAN	O3-C3-C2	-6.10	98.83	110.01
4	C	1408	MAN	O3-C3-C2	-6.10	98.84	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1456	NAG	O5-C5-C6	-6.09	94.29	107.34
2	B	1456	NAG	O5-C5-C6	-6.09	94.30	107.34
2	C	1452	NAG	O5-C5-C6	-6.00	94.50	107.34
2	A	1452	NAG	O5-C5-C6	-5.99	94.51	107.34
2	B	1452	NAG	O5-C5-C6	-5.99	94.52	107.34
3	B	1466	BMA	O4-C4-C5	-5.91	93.65	109.23
3	A	1466	BMA	O4-C4-C5	-5.91	93.66	109.23
3	C	1466	BMA	O4-C4-C5	-5.91	93.67	109.23
2	C	1438	NAG	O5-C5-C6	-5.83	94.87	107.34
2	A	1438	NAG	O5-C5-C6	-5.82	94.89	107.34
2	B	1438	NAG	O5-C5-C6	-5.80	94.91	107.34
2	A	1455	NAG	O4-C4-C5	-5.80	93.96	109.23
2	B	1455	NAG	O4-C4-C5	-5.79	93.96	109.23
2	C	1455	NAG	O4-C4-C5	-5.79	93.97	109.23
2	A	1435	NAG	O3-C3-C4	-5.75	97.40	110.36
2	B	1435	NAG	O3-C3-C4	-5.74	97.42	110.36
2	C	1435	NAG	O3-C3-C4	-5.74	97.42	110.36
2	C	1419	NAG	O3-C3-C2	-5.74	97.10	109.37
2	A	1419	NAG	O3-C3-C2	-5.73	97.10	109.37
2	B	1419	NAG	O3-C3-C2	-5.72	97.13	109.37
2	A	1401	NAG	O5-C5-C6	-5.69	95.17	107.34
2	B	1401	NAG	O5-C5-C6	-5.68	95.18	107.34
2	C	1401	NAG	O5-C5-C6	-5.67	95.19	107.34
2	C	1469	NAG	O4-C4-C3	-5.63	97.65	110.36
2	A	1469	NAG	O4-C4-C3	-5.63	97.67	110.36
2	B	1469	NAG	O4-C4-C3	-5.62	97.68	110.36
3	C	1406	BMA	O5-C5-C6	-5.54	95.49	107.34
3	A	1406	BMA	O5-C5-C6	-5.53	95.49	107.34
3	B	1406	BMA	O5-C5-C6	-5.53	95.49	107.34
2	B	1412	NAG	O4-C4-C3	-5.39	98.21	110.36
2	A	1412	NAG	O4-C4-C3	-5.38	98.22	110.36
2	C	1412	NAG	O4-C4-C3	-5.38	98.24	110.36
3	B	1428	BMA	O2-C2-C1	-5.33	98.56	109.23
3	A	1428	BMA	O2-C2-C1	-5.33	98.57	109.23
3	C	1428	BMA	O2-C2-C1	-5.31	98.60	109.23
2	B	1464	NAG	O3-C3-C2	-5.29	98.05	109.37
2	C	1464	NAG	O3-C3-C2	-5.28	98.07	109.37
2	A	1464	NAG	O3-C3-C2	-5.28	98.08	109.37
4	B	1445	MAN	O5-C5-C6	-5.15	96.31	107.34
4	C	1445	MAN	O5-C5-C6	-5.15	96.32	107.34
4	A	1445	MAN	O5-C5-C6	-5.14	96.33	107.34
3	B	1466	BMA	O5-C5-C6	-5.14	96.34	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1466	BMA	O5-C5-C6	-5.13	96.35	107.34
3	C	1466	BMA	O5-C5-C6	-5.13	96.36	107.34
4	C	1467	MAN	O5-C5-C6	-4.88	96.90	107.34
2	C	1440	NAG	O3-C3-C2	-4.87	98.95	109.37
4	B	1467	MAN	O5-C5-C6	-4.87	96.92	107.34
4	A	1467	MAN	O5-C5-C6	-4.86	96.93	107.34
2	A	1440	NAG	O3-C3-C2	-4.86	98.97	109.37
2	B	1440	NAG	O3-C3-C2	-4.85	98.99	109.37
2	C	1459	NAG	O4-C4-C3	-4.79	99.56	110.36
2	A	1459	NAG	O4-C4-C3	-4.79	99.57	110.36
2	B	1459	NAG	O4-C4-C3	-4.78	99.58	110.36
2	C	1411	NAG	O4-C4-C5	-4.77	96.65	109.23
2	A	1411	NAG	O4-C4-C5	-4.77	96.65	109.23
2	B	1411	NAG	O4-C4-C5	-4.76	96.67	109.23
2	A	1425	NAG	O5-C5-C6	-4.72	97.24	107.34
2	B	1425	NAG	O5-C5-C6	-4.71	97.25	107.34
2	C	1425	NAG	O5-C5-C6	-4.71	97.26	107.34
4	A	1463	MAN	O4-C4-C3	-4.67	99.84	110.36
4	C	1463	MAN	O4-C4-C3	-4.66	99.84	110.36
4	B	1463	MAN	O4-C4-C3	-4.65	99.88	110.36
2	A	1404	NAG	O3-C3-C2	-4.64	99.45	109.37
2	C	1404	NAG	O3-C3-C2	-4.63	99.45	109.37
2	B	1404	NAG	O3-C3-C2	-4.63	99.47	109.37
2	A	1453	NAG	O5-C5-C6	-4.59	97.52	107.34
2	C	1453	NAG	O5-C5-C6	-4.59	97.52	107.34
2	B	1453	NAG	O5-C5-C6	-4.58	97.53	107.34
3	B	1473	BMA	O3-C3-C2	-4.57	101.63	110.01
3	C	1473	BMA	O3-C3-C2	-4.57	101.64	110.01
3	A	1473	BMA	O3-C3-C2	-4.56	101.64	110.01
2	B	1435	NAG	O5-C5-C6	-4.56	97.59	107.34
2	C	1435	NAG	O5-C5-C6	-4.56	97.59	107.34
2	A	1435	NAG	O5-C5-C6	-4.55	97.60	107.34
2	C	1474	NAG	O4-C4-C3	-4.51	100.19	110.36
4	B	1468	MAN	O3-C3-C2	-4.50	101.77	110.01
2	A	1474	NAG	O4-C4-C3	-4.49	100.23	110.36
2	B	1474	NAG	O4-C4-C3	-4.49	100.24	110.36
3	B	1473	BMA	O5-C5-C6	-4.48	97.75	107.34
3	C	1473	BMA	O5-C5-C6	-4.47	97.77	107.34
3	A	1473	BMA	O5-C5-C6	-4.47	97.77	107.34
4	A	1468	MAN	O3-C3-C2	-4.46	101.83	110.01
4	C	1468	MAN	O3-C3-C2	-4.45	101.85	110.01
2	C	1404	NAG	O4-C4-C3	-4.29	100.68	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1404	NAG	O4-C4-C3	-4.29	100.68	110.36
2	B	1404	NAG	O4-C4-C3	-4.29	100.68	110.36
4	B	1421	MAN	O3-C3-C2	-4.29	102.14	110.01
4	A	1421	MAN	O3-C3-C2	-4.29	102.15	110.01
4	C	1421	MAN	O3-C3-C2	-4.29	102.15	110.01
4	C	1467	MAN	O4-C4-C3	-4.25	100.78	110.36
2	B	1426	NAG	O5-C5-C6	-4.24	98.25	107.34
4	B	1467	MAN	O4-C4-C3	-4.24	100.79	110.36
4	A	1467	MAN	O4-C4-C3	-4.24	100.79	110.36
2	A	1426	NAG	O5-C5-C6	-4.24	98.27	107.34
2	C	1426	NAG	O5-C5-C6	-4.23	98.29	107.34
2	B	1457	NAG	O4-C4-C5	-4.22	98.11	109.23
2	A	1457	NAG	O4-C4-C5	-4.20	98.17	109.23
2	C	1457	NAG	O4-C4-C5	-4.19	98.20	109.23
2	B	1410	NAG	O3-C3-C4	-4.13	101.05	110.36
2	C	1410	NAG	O3-C3-C4	-4.12	101.08	110.36
2	A	1410	NAG	O3-C3-C4	-4.11	101.08	110.36
3	B	1406	BMA	O3-C3-C2	-4.07	102.54	110.01
3	A	1406	BMA	O3-C3-C2	-4.07	102.55	110.01
3	C	1406	BMA	O3-C3-C2	-4.07	102.55	110.01
4	C	1430	MAN	O4-C4-C3	-3.93	101.50	110.36
4	A	1430	MAN	O4-C4-C3	-3.93	101.51	110.36
4	A	1432	MAN	O4-C4-C5	-3.92	98.91	109.23
4	C	1432	MAN	O4-C4-C5	-3.91	98.91	109.23
4	B	1432	MAN	O4-C4-C5	-3.91	98.92	109.23
4	B	1430	MAN	O4-C4-C3	-3.91	101.55	110.36
2	B	1437	NAG	O3-C3-C4	-3.79	101.80	110.36
2	C	1448	NAG	O3-C3-C2	-3.79	101.26	109.37
2	A	1437	NAG	O3-C3-C4	-3.79	101.81	110.36
2	C	1437	NAG	O3-C3-C4	-3.79	101.82	110.36
2	A	1448	NAG	O3-C3-C2	-3.79	101.27	109.37
2	B	1448	NAG	O3-C3-C2	-3.78	101.28	109.37
2	C	1470	NAG	O4-C4-C3	-3.78	101.85	110.36
2	A	1470	NAG	O4-C4-C3	-3.77	101.86	110.36
2	B	1470	NAG	O4-C4-C3	-3.76	101.87	110.36
2	C	1424	NAG	O4-C4-C3	-3.73	101.94	110.36
2	B	1424	NAG	O4-C4-C3	-3.73	101.95	110.36
2	A	1424	NAG	O4-C4-C3	-3.72	101.97	110.36
4	B	1409	MAN	O3-C3-C2	-3.69	103.25	110.01
4	C	1409	MAN	O3-C3-C2	-3.66	103.31	110.01
4	A	1409	MAN	O3-C3-C2	-3.64	103.34	110.01
2	A	1441	NAG	O3-C3-C2	-3.58	101.71	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1441	NAG	O3-C3-C2	-3.58	101.72	109.37
2	C	1441	NAG	O3-C3-C2	-3.57	101.74	109.37
2	A	1442	NAG	O3-C3-C4	-3.56	102.34	110.36
2	C	1442	NAG	O3-C3-C4	-3.56	102.34	110.36
2	B	1442	NAG	O3-C3-C4	-3.55	102.34	110.36
2	B	1440	NAG	O4-C4-C3	-3.55	102.36	110.36
2	A	1440	NAG	O4-C4-C3	-3.54	102.37	110.36
2	C	1440	NAG	O4-C4-C3	-3.54	102.37	110.36
2	A	1454	NAG	O4-C4-C3	-3.52	102.42	110.36
2	C	1454	NAG	O4-C4-C3	-3.52	102.42	110.36
2	B	1454	NAG	O4-C4-C3	-3.52	102.42	110.36
2	C	1448	NAG	O3-C3-C4	-3.52	102.43	110.36
2	B	1448	NAG	O3-C3-C4	-3.51	102.44	110.36
2	A	1448	NAG	O3-C3-C4	-3.51	102.44	110.36
2	C	1472	NAG	C2-N2-C7	-3.50	118.55	123.11
2	A	1472	NAG	C2-N2-C7	-3.50	118.56	123.11
2	B	1472	NAG	C2-N2-C7	-3.50	118.56	123.11
3	A	1473	BMA	O4-C4-C3	-3.44	102.60	110.36
3	C	1473	BMA	O4-C4-C3	-3.44	102.61	110.36
3	B	1473	BMA	O4-C4-C3	-3.43	102.62	110.36
2	C	1405	NAG	O3-C3-C2	-3.42	102.06	109.37
2	A	1405	NAG	O3-C3-C2	-3.42	102.06	109.37
2	B	1405	NAG	O3-C3-C2	-3.40	102.09	109.37
2	A	1426	NAG	O3-C3-C4	-3.34	102.83	110.36
2	C	1426	NAG	O3-C3-C4	-3.33	102.85	110.36
2	B	1426	NAG	O3-C3-C4	-3.32	102.87	110.36
2	B	1424	NAG	O3-C3-C2	-3.26	102.39	109.37
2	C	1424	NAG	O3-C3-C2	-3.26	102.40	109.37
2	A	1424	NAG	O3-C3-C2	-3.26	102.40	109.37
3	C	1466	BMA	O3-C3-C2	-3.25	104.06	110.01
2	C	1427	NAG	O5-C5-C6	-3.24	100.39	107.34
3	A	1466	BMA	O3-C3-C2	-3.24	104.06	110.01
3	B	1466	BMA	O3-C3-C2	-3.24	104.06	110.01
2	A	1427	NAG	O5-C5-C6	-3.23	100.42	107.34
2	B	1427	NAG	O5-C5-C6	-3.23	100.43	107.34
2	C	1419	NAG	C2-N2-C7	-3.21	118.93	123.11
2	A	1419	NAG	C2-N2-C7	-3.20	118.95	123.11
2	B	1419	NAG	C2-N2-C7	-3.19	118.96	123.11
2	A	1405	NAG	O3-C3-C4	-3.14	103.27	110.36
3	B	1462	BMA	O4-C4-C3	-3.14	103.28	110.36
2	C	1456	NAG	O3-C3-C4	-3.14	103.29	110.36
3	A	1462	BMA	O4-C4-C3	-3.14	103.29	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1462	BMA	O4-C4-C3	-3.14	103.29	110.36
2	C	1405	NAG	O3-C3-C4	-3.13	103.30	110.36
2	B	1405	NAG	O3-C3-C4	-3.13	103.30	110.36
2	A	1456	NAG	O3-C3-C4	-3.13	103.31	110.36
2	B	1456	NAG	O3-C3-C4	-3.12	103.33	110.36
2	C	1469	NAG	O3-C3-C4	-3.08	103.40	110.36
2	B	1469	NAG	O3-C3-C4	-3.08	103.41	110.36
2	B	1412	NAG	C2-N2-C7	-3.08	119.10	123.11
2	A	1412	NAG	C2-N2-C7	-3.08	119.10	123.11
2	A	1469	NAG	O3-C3-C4	-3.07	103.44	110.36
2	C	1412	NAG	C2-N2-C7	-3.07	119.11	123.11
2	B	1422	NAG	O7-C7-N2	-3.06	115.60	121.84
2	C	1422	NAG	O7-C7-N2	-3.06	115.60	121.84
2	A	1422	NAG	O7-C7-N2	-3.06	115.61	121.84
3	C	1428	BMA	C2-C3-C4	-2.97	105.86	111.05
2	B	1451	NAG	O4-C4-C5	-2.97	101.41	109.23
2	A	1451	NAG	O4-C4-C5	-2.96	101.42	109.23
2	C	1451	NAG	O4-C4-C5	-2.96	101.43	109.23
3	A	1428	BMA	C2-C3-C4	-2.95	105.91	111.05
3	B	1428	BMA	C2-C3-C4	-2.93	105.94	111.05
4	C	1408	MAN	O5-C5-C4	-2.90	105.33	110.13
2	C	1454	NAG	O3-C3-C2	-2.90	103.17	109.37
4	B	1408	MAN	O5-C5-C4	-2.89	105.35	110.13
2	A	1454	NAG	O3-C3-C2	-2.88	103.22	109.37
2	B	1454	NAG	O3-C3-C2	-2.87	103.22	109.37
4	A	1408	MAN	O5-C5-C4	-2.87	105.38	110.13
2	B	1469	NAG	C6-C5-C4	-2.86	105.81	112.99
2	C	1469	NAG	C6-C5-C4	-2.86	105.82	112.99
2	A	1469	NAG	C6-C5-C4	-2.85	105.84	112.99
4	B	1445	MAN	O4-C4-C3	-2.85	103.94	110.36
4	C	1445	MAN	O4-C4-C3	-2.84	103.94	110.36
4	A	1445	MAN	O4-C4-C3	-2.84	103.96	110.36
2	B	1472	NAG	O3-C3-C2	-2.81	103.36	109.37
2	A	1472	NAG	O3-C3-C2	-2.81	103.36	109.37
2	B	1410	NAG	C2-N2-C7	-2.81	119.45	123.11
2	C	1410	NAG	C2-N2-C7	-2.80	119.46	123.11
2	B	1418	NAG	O5-C5-C6	-2.80	101.34	107.34
2	C	1472	NAG	O3-C3-C2	-2.80	103.38	109.37
2	A	1418	NAG	O5-C5-C6	-2.79	101.36	107.34
2	C	1418	NAG	O5-C5-C6	-2.79	101.37	107.34
2	A	1410	NAG	C2-N2-C7	-2.78	119.48	123.11
2	C	1448	NAG	C2-N2-C7	-2.66	119.65	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1443	NAG	C2-N2-C7	-2.65	119.66	123.11
2	B	1443	NAG	C2-N2-C7	-2.65	119.66	123.11
2	C	1443	NAG	C2-N2-C7	-2.64	119.67	123.11
2	A	1448	NAG	C2-N2-C7	-2.63	119.68	123.11
2	B	1448	NAG	C2-N2-C7	-2.61	119.70	123.11
2	C	1469	NAG	C3-C4-C5	-2.60	105.59	110.23
2	B	1469	NAG	C3-C4-C5	-2.59	105.61	110.23
2	A	1469	NAG	C3-C4-C5	-2.57	105.64	110.23
2	B	1437	NAG	C2-N2-C7	-2.56	119.78	123.11
2	C	1437	NAG	C2-N2-C7	-2.52	119.82	123.11
2	A	1437	NAG	C2-N2-C7	-2.52	119.83	123.11
2	C	1438	NAG	O3-C3-C2	-2.51	104.01	109.37
4	B	1408	MAN	O5-C1-C2	-2.50	106.90	110.89
4	C	1408	MAN	O5-C1-C2	-2.50	106.90	110.89
4	A	1408	MAN	O5-C1-C2	-2.49	106.91	110.89
2	B	1438	NAG	O3-C3-C2	-2.49	104.04	109.37
2	C	1452	NAG	C3-C4-C5	-2.49	105.79	110.23
2	A	1438	NAG	O3-C3-C2	-2.49	104.05	109.37
2	A	1452	NAG	C3-C4-C5	-2.48	105.80	110.23
2	B	1452	NAG	C3-C4-C5	-2.48	105.81	110.23
2	C	1435	NAG	O5-C5-C4	-2.47	106.04	110.13
2	B	1435	NAG	O5-C5-C4	-2.46	106.06	110.13
2	A	1435	NAG	O5-C5-C4	-2.46	106.07	110.13
4	C	1421	MAN	O4-C4-C3	-2.42	104.91	110.36
4	B	1421	MAN	O4-C4-C3	-2.42	104.91	110.36
4	A	1421	MAN	O4-C4-C3	-2.41	104.92	110.36
3	C	1414	BMA	O2-C2-C1	-2.40	104.44	109.23
3	A	1414	BMA	O2-C2-C1	-2.39	104.44	109.23
3	B	1414	BMA	O2-C2-C1	-2.38	104.48	109.23
4	B	1415	MAN	O4-C4-C5	-2.37	102.98	109.23
4	C	1415	MAN	O4-C4-C5	-2.37	102.99	109.23
4	A	1415	MAN	O4-C4-C5	-2.37	102.99	109.23
4	A	1408	MAN	O5-C5-C6	-2.35	102.30	107.34
2	A	1403	NAG	O7-C7-C8	-2.35	117.75	122.07
4	C	1408	MAN	O5-C5-C6	-2.34	102.33	107.34
2	A	1469	NAG	C2-N2-C7	-2.34	120.07	123.11
2	B	1469	NAG	C2-N2-C7	-2.33	120.07	123.11
2	C	1461	NAG	C2-N2-C7	-2.33	120.07	123.11
2	C	1403	NAG	O7-C7-C8	-2.33	117.78	122.07
2	B	1403	NAG	O7-C7-C8	-2.33	117.78	122.07
2	A	1440	NAG	O4-C4-C5	-2.33	103.09	109.23
2	A	1427	NAG	C2-N2-C7	-2.33	120.07	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1440	NAG	O4-C4-C5	-2.33	103.10	109.23
2	C	1469	NAG	C2-N2-C7	-2.32	120.09	123.11
4	B	1408	MAN	O5-C5-C6	-2.32	102.38	107.34
2	B	1461	NAG	C2-N2-C7	-2.32	120.09	123.11
2	A	1461	NAG	C2-N2-C7	-2.32	120.09	123.11
2	B	1440	NAG	O4-C4-C5	-2.31	103.13	109.23
2	C	1427	NAG	C2-N2-C7	-2.30	120.11	123.11
2	C	1472	NAG	C3-C4-C5	-2.30	106.12	110.23
2	B	1427	NAG	C2-N2-C7	-2.29	120.12	123.11
2	C	1417	NAG	O4-C4-C5	-2.29	103.19	109.23
2	B	1472	NAG	C3-C4-C5	-2.29	106.14	110.23
2	A	1417	NAG	O4-C4-C5	-2.29	103.20	109.23
2	A	1472	NAG	C3-C4-C5	-2.29	106.15	110.23
2	B	1417	NAG	O4-C4-C5	-2.28	103.21	109.23
2	C	1425	NAG	O4-C4-C5	-2.28	103.22	109.23
2	B	1425	NAG	O4-C4-C5	-2.27	103.23	109.23
2	A	1425	NAG	O4-C4-C5	-2.27	103.25	109.23
4	C	1433	MAN	O5-C1-C2	-2.23	107.33	110.89
2	C	1402	NAG	C4-C3-C2	-2.22	107.89	111.34
4	B	1433	MAN	O5-C1-C2	-2.22	107.34	110.89
2	B	1413	NAG	C2-N2-C7	-2.22	120.22	123.11
4	A	1433	MAN	O5-C1-C2	-2.22	107.35	110.89
2	B	1443	NAG	O3-C3-C4	-2.21	105.37	110.36
2	A	1402	NAG	C4-C3-C2	-2.21	107.91	111.34
2	A	1413	NAG	C2-N2-C7	-2.21	120.23	123.11
2	A	1443	NAG	O3-C3-C4	-2.20	105.39	110.36
2	A	1465	NAG	C2-N2-C7	-2.20	120.24	123.11
2	C	1443	NAG	O3-C3-C4	-2.20	105.40	110.36
2	B	1465	NAG	C2-N2-C7	-2.20	120.24	123.11
4	C	1409	MAN	O5-C5-C4	-2.20	106.49	110.13
2	B	1402	NAG	C4-C3-C2	-2.20	107.93	111.34
2	C	1413	NAG	C2-N2-C7	-2.20	120.25	123.11
4	A	1409	MAN	O5-C5-C4	-2.20	106.50	110.13
2	C	1465	NAG	C2-N2-C7	-2.19	120.25	123.11
4	B	1409	MAN	O5-C5-C4	-2.19	106.51	110.13
2	A	1422	NAG	O7-C7-C8	-2.18	118.06	122.07
2	C	1422	NAG	O7-C7-C8	-2.18	118.07	122.07
2	B	1450	NAG	C2-N2-C7	-2.17	120.28	123.11
2	B	1424	NAG	C2-N2-C7	-2.17	120.28	123.11
2	A	1450	NAG	C2-N2-C7	-2.17	120.28	123.11
2	C	1434	NAG	O7-C7-C8	-2.17	118.08	122.07
2	A	1447	NAG	C2-N2-C7	-2.16	120.29	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1422	NAG	O7-C7-C8	-2.16	118.09	122.07
2	A	1434	NAG	O7-C7-C8	-2.16	118.09	122.07
2	C	1450	NAG	C2-N2-C7	-2.16	120.29	123.11
4	B	1433	MAN	O5-C5-C4	-2.16	106.56	110.13
4	C	1433	MAN	O5-C5-C4	-2.16	106.56	110.13
2	B	1447	NAG	C2-N2-C7	-2.15	120.30	123.11
2	C	1447	NAG	C2-N2-C7	-2.15	120.31	123.11
4	A	1433	MAN	O5-C5-C4	-2.15	106.57	110.13
2	C	1424	NAG	C2-N2-C7	-2.15	120.31	123.11
2	B	1434	NAG	O7-C7-C8	-2.15	118.11	122.07
2	A	1424	NAG	C2-N2-C7	-2.15	120.31	123.11
2	C	1465	NAG	C3-C4-C5	-2.12	106.45	110.23
2	B	1456	NAG	C2-N2-C7	-2.11	120.36	123.11
2	A	1465	NAG	C3-C4-C5	-2.11	106.47	110.23
2	A	1456	NAG	C2-N2-C7	-2.10	120.37	123.11
2	C	1458	NAG	C2-N2-C7	-2.10	120.37	123.11
2	C	1456	NAG	C2-N2-C7	-2.10	120.37	123.11
2	A	1419	NAG	C3-C4-C5	-2.10	106.48	110.23
2	C	1419	NAG	C3-C4-C5	-2.10	106.49	110.23
4	A	1431	MAN	O3-C3-C2	-2.10	106.17	110.01
2	B	1465	NAG	C3-C4-C5	-2.09	106.50	110.23
4	B	1431	MAN	O3-C3-C2	-2.09	106.18	110.01
2	B	1419	NAG	C3-C4-C5	-2.08	106.51	110.23
4	C	1431	MAN	O3-C3-C2	-2.08	106.20	110.01
2	A	1458	NAG	C2-N2-C7	-2.08	120.40	123.11
2	B	1458	NAG	C2-N2-C7	-2.07	120.41	123.11
4	B	1432	MAN	O5-C1-C2	-2.07	107.58	110.89
2	A	1454	NAG	C2-N2-C7	-2.07	120.41	123.11
2	B	1454	NAG	C2-N2-C7	-2.07	120.41	123.11
2	C	1454	NAG	C2-N2-C7	-2.06	120.42	123.11
4	A	1432	MAN	O5-C1-C2	-2.05	107.61	110.89
2	C	1461	NAG	O3-C3-C2	-2.05	104.98	109.37
2	A	1404	NAG	C2-N2-C7	-2.04	120.45	123.11
2	B	1418	NAG	O7-C7-C8	-2.04	118.31	122.07
4	C	1432	MAN	O5-C1-C2	-2.04	107.63	110.89
2	B	1404	NAG	C2-N2-C7	-2.04	120.45	123.11
2	C	1470	NAG	O5-C5-C6	-2.04	102.98	107.34
2	A	1461	NAG	O3-C3-C2	-2.04	105.02	109.37
2	A	1418	NAG	O7-C7-C8	-2.03	118.33	122.07
2	C	1404	NAG	C2-N2-C7	-2.03	120.46	123.11
2	A	1439	NAG	O4-C4-C3	-2.03	105.78	110.36
2	B	1417	NAG	C2-N2-C7	-2.03	120.47	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1461	NAG	O3-C3-C2	-2.03	105.03	109.37
2	C	1439	NAG	O4-C4-C3	-2.03	105.79	110.36
2	A	1470	NAG	O5-C5-C6	-2.03	103.00	107.34
2	C	1417	NAG	C2-N2-C7	-2.02	120.47	123.11
3	A	1462	BMA	O2-C2-C1	-2.02	105.18	109.23
2	B	1439	NAG	O4-C4-C3	-2.02	105.80	110.36
2	C	1418	NAG	O7-C7-C8	-2.02	118.35	122.07
3	B	1462	BMA	O2-C2-C1	-2.02	105.19	109.23
3	C	1462	BMA	O2-C2-C1	-2.01	105.20	109.23
2	A	1451	NAG	O7-C7-C8	-2.01	118.36	122.07
2	A	1417	NAG	C2-N2-C7	-2.01	120.49	123.11
2	B	1470	NAG	O5-C5-C6	-2.01	103.04	107.34
2	C	1451	NAG	O7-C7-C8	-2.01	118.38	122.07
2	B	1451	NAG	O7-C7-C8	-2.00	118.39	122.07
4	B	1446	MAN	O4-C4-C5	2.01	114.51	109.23
2	A	1416	NAG	C8-C7-N2	2.03	119.98	116.10
2	B	1416	NAG	C8-C7-N2	2.03	119.99	116.10
2	C	1416	NAG	C8-C7-N2	2.04	120.00	116.10
2	A	1419	NAG	C8-C7-N2	2.04	120.00	116.10
2	B	1419	NAG	C8-C7-N2	2.04	120.01	116.10
2	C	1419	NAG	C8-C7-N2	2.04	120.01	116.10
2	C	1461	NAG	O4-C4-C3	2.06	115.00	110.36
2	A	1461	NAG	O4-C4-C3	2.06	115.00	110.36
2	B	1461	NAG	O4-C4-C3	2.06	115.00	110.36
4	C	1445	MAN	O2-C2-C3	2.07	114.35	110.19
4	A	1445	MAN	O2-C2-C3	2.07	114.35	110.19
4	B	1445	MAN	O2-C2-C3	2.07	114.35	110.19
4	A	1407	MAN	C1-O5-C5	2.08	115.20	112.14
2	B	1460	NAG	C8-C7-N2	2.10	120.12	116.10
4	C	1407	MAN	C1-O5-C5	2.10	115.23	112.14
2	A	1460	NAG	C8-C7-N2	2.10	120.13	116.10
2	A	1452	NAG	C8-C7-N2	2.10	120.13	116.10
2	B	1426	NAG	C8-C7-N2	2.10	120.13	116.10
2	B	1452	NAG	C8-C7-N2	2.11	120.13	116.10
2	C	1460	NAG	C8-C7-N2	2.11	120.14	116.10
2	A	1426	NAG	C8-C7-N2	2.11	120.14	116.10
2	C	1426	NAG	C8-C7-N2	2.11	120.14	116.10
2	C	1452	NAG	C8-C7-N2	2.11	120.15	116.10
2	A	1411	NAG	C2-N2-C7	2.11	125.85	123.11
2	C	1440	NAG	C4-C3-C2	2.11	114.62	111.34
2	A	1440	NAG	C4-C3-C2	2.12	114.62	111.34
2	C	1411	NAG	C2-N2-C7	2.12	125.86	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1440	NAG	C4-C3-C2	2.12	114.62	111.34
4	B	1407	MAN	C1-O5-C5	2.13	115.27	112.14
2	C	1403	NAG	C8-C7-N2	2.13	120.19	116.10
2	B	1411	NAG	C2-N2-C7	2.14	125.88	123.11
2	B	1401	NAG	C6-C5-C4	2.14	118.34	112.99
2	A	1401	NAG	C6-C5-C4	2.14	118.36	112.99
2	C	1401	NAG	C6-C5-C4	2.15	118.37	112.99
2	A	1403	NAG	C8-C7-N2	2.15	120.22	116.10
2	B	1403	NAG	C8-C7-N2	2.16	120.24	116.10
3	B	1444	BMA	O4-C4-C5	2.23	115.10	109.23
3	A	1444	BMA	O4-C4-C5	2.25	115.15	109.23
2	C	1435	NAG	C1-O5-C5	2.25	115.45	112.14
2	A	1464	NAG	O3-C3-C4	2.25	115.44	110.36
2	C	1464	NAG	O3-C3-C4	2.25	115.44	110.36
2	B	1474	NAG	O3-C3-C2	2.25	114.20	109.37
2	C	1474	NAG	O3-C3-C2	2.26	114.20	109.37
2	B	1464	NAG	O3-C3-C4	2.26	115.45	110.36
3	C	1444	BMA	O4-C4-C5	2.26	115.18	109.23
2	A	1474	NAG	O3-C3-C2	2.26	114.22	109.37
2	A	1435	NAG	C1-O5-C5	2.27	115.47	112.14
2	B	1435	NAG	C1-O5-C5	2.27	115.47	112.14
2	B	1471	NAG	C8-C7-N2	2.28	120.46	116.10
2	A	1471	NAG	C8-C7-N2	2.29	120.48	116.10
2	A	1454	NAG	C8-C7-N2	2.29	120.49	116.10
2	C	1454	NAG	C8-C7-N2	2.29	120.49	116.10
2	B	1454	NAG	C8-C7-N2	2.30	120.50	116.10
2	C	1471	NAG	C8-C7-N2	2.31	120.53	116.10
2	B	1442	NAG	C8-C7-N2	2.32	120.54	116.10
2	A	1442	NAG	C8-C7-N2	2.33	120.55	116.10
2	C	1442	NAG	C8-C7-N2	2.34	120.58	116.10
2	C	1418	NAG	C8-C7-N2	2.34	120.59	116.10
2	C	1458	NAG	C8-C7-N2	2.36	120.61	116.10
2	A	1418	NAG	C8-C7-N2	2.36	120.62	116.10
2	B	1440	NAG	C6-C5-C4	2.36	118.91	112.99
2	B	1418	NAG	C8-C7-N2	2.37	120.63	116.10
2	B	1458	NAG	C8-C7-N2	2.37	120.64	116.10
2	C	1437	NAG	C8-C7-N2	2.37	120.64	116.10
2	A	1458	NAG	C8-C7-N2	2.37	120.64	116.10
2	B	1437	NAG	C8-C7-N2	2.37	120.64	116.10
2	A	1440	NAG	C6-C5-C4	2.38	118.94	112.99
2	B	1410	NAG	C8-C7-N2	2.38	120.65	116.10
2	A	1437	NAG	C8-C7-N2	2.38	120.67	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1440	NAG	C6-C5-C4	2.39	118.97	112.99
2	C	1410	NAG	C8-C7-N2	2.39	120.68	116.10
2	B	1424	NAG	C8-C7-N2	2.39	120.68	116.10
2	C	1424	NAG	C8-C7-N2	2.39	120.69	116.10
2	A	1410	NAG	C8-C7-N2	2.40	120.69	116.10
2	A	1424	NAG	C8-C7-N2	2.40	120.69	116.10
2	A	1465	NAG	C8-C7-N2	2.43	120.75	116.10
2	B	1465	NAG	C8-C7-N2	2.43	120.76	116.10
2	C	1465	NAG	C8-C7-N2	2.43	120.76	116.10
4	C	1432	MAN	C1-O5-C5	2.44	115.72	112.14
2	C	1472	NAG	C8-C7-N2	2.44	120.78	116.10
4	A	1432	MAN	C1-O5-C5	2.45	115.75	112.14
4	B	1432	MAN	C1-O5-C5	2.46	115.75	112.14
2	A	1472	NAG	C8-C7-N2	2.46	120.81	116.10
2	B	1472	NAG	C8-C7-N2	2.46	120.81	116.10
2	C	1447	NAG	C6-C5-C4	2.46	119.16	112.99
2	B	1447	NAG	C6-C5-C4	2.47	119.18	112.99
2	A	1447	NAG	C6-C5-C4	2.47	119.18	112.99
2	C	1423	NAG	O4-C4-C5	2.51	115.83	109.23
2	B	1423	NAG	O4-C4-C5	2.51	115.83	109.23
2	A	1423	NAG	O4-C4-C5	2.51	115.83	109.23
2	A	1412	NAG	C6-C5-C4	2.51	119.29	112.99
2	B	1412	NAG	C6-C5-C4	2.51	119.29	112.99
2	B	1434	NAG	C1-O5-C5	2.53	115.86	112.14
2	C	1412	NAG	C6-C5-C4	2.53	119.33	112.99
2	A	1434	NAG	C1-O5-C5	2.55	115.89	112.14
2	C	1472	NAG	O3-C3-C4	2.55	116.11	110.36
2	C	1434	NAG	C1-O5-C5	2.55	115.89	112.14
3	C	1449	BMA	C6-C5-C4	2.56	119.39	112.99
2	A	1472	NAG	O3-C3-C4	2.56	116.12	110.36
2	B	1472	NAG	O3-C3-C4	2.56	116.13	110.36
3	A	1449	BMA	C6-C5-C4	2.56	119.40	112.99
3	B	1449	BMA	C6-C5-C4	2.56	119.41	112.99
2	C	1424	NAG	C6-C5-C4	2.58	119.45	112.99
2	B	1424	NAG	C6-C5-C4	2.58	119.46	112.99
2	A	1424	NAG	C6-C5-C4	2.58	119.47	112.99
2	C	1471	NAG	C6-C5-C4	2.65	119.62	112.99
2	B	1471	NAG	C6-C5-C4	2.65	119.62	112.99
2	A	1471	NAG	C6-C5-C4	2.65	119.64	112.99
4	A	1433	MAN	O2-C2-C1	2.67	114.57	109.23
4	B	1433	MAN	O2-C2-C1	2.67	114.58	109.23
3	C	1414	BMA	O3-C3-C2	2.67	114.90	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1414	BMA	O3-C3-C2	2.67	114.91	110.01
3	B	1414	BMA	O3-C3-C2	2.68	114.92	110.01
4	C	1433	MAN	O2-C2-C1	2.69	114.61	109.23
4	C	1408	MAN	O2-C2-C3	2.81	115.85	110.19
4	A	1408	MAN	O2-C2-C3	2.82	115.86	110.19
2	A	1450	NAG	O3-C3-C4	2.82	116.72	110.36
4	B	1408	MAN	O2-C2-C3	2.82	115.87	110.19
2	B	1450	NAG	O3-C3-C4	2.83	116.73	110.36
2	C	1450	NAG	O3-C3-C4	2.84	116.76	110.36
2	B	1412	NAG	C8-C7-N2	2.85	121.55	116.10
2	C	1412	NAG	C8-C7-N2	2.85	121.56	116.10
4	C	1445	MAN	O2-C2-C1	2.85	114.94	109.23
4	A	1445	MAN	O2-C2-C1	2.85	114.94	109.23
2	A	1412	NAG	C8-C7-N2	2.85	121.56	116.10
4	B	1445	MAN	C6-C5-C4	2.86	120.15	112.99
4	B	1445	MAN	O2-C2-C1	2.86	114.96	109.23
4	C	1445	MAN	C6-C5-C4	2.86	120.16	112.99
4	A	1445	MAN	C6-C5-C4	2.86	120.17	112.99
3	C	1406	BMA	O2-C2-C3	2.87	115.96	110.19
3	A	1406	BMA	O2-C2-C3	2.87	115.97	110.19
4	B	1467	MAN	O2-C2-C1	2.87	114.99	109.23
3	B	1406	BMA	O2-C2-C3	2.88	116.00	110.19
2	C	1405	NAG	C1-O5-C5	2.90	116.40	112.14
2	A	1416	NAG	O5-C5-C6	2.90	113.55	107.34
2	C	1451	NAG	C6-C5-C4	2.90	120.25	112.99
2	B	1451	NAG	C6-C5-C4	2.90	120.25	112.99
2	C	1416	NAG	O5-C5-C6	2.90	113.55	107.34
4	A	1467	MAN	O2-C2-C1	2.90	115.04	109.23
2	A	1405	NAG	C1-O5-C5	2.90	116.41	112.14
2	A	1451	NAG	C6-C5-C4	2.90	120.26	112.99
2	B	1405	NAG	C1-O5-C5	2.91	116.42	112.14
2	B	1416	NAG	O5-C5-C6	2.91	113.56	107.34
4	C	1467	MAN	O2-C2-C1	2.91	115.07	109.23
4	B	1433	MAN	O2-C2-C3	2.94	116.10	110.19
4	A	1433	MAN	O2-C2-C3	2.95	116.13	110.19
4	C	1433	MAN	O2-C2-C3	2.96	116.14	110.19
2	C	1474	NAG	C6-C5-C4	2.99	120.47	112.99
2	B	1474	NAG	C6-C5-C4	2.99	120.48	112.99
2	A	1474	NAG	C6-C5-C4	2.99	120.48	112.99
2	A	1403	NAG	C6-C5-C4	2.99	120.49	112.99
2	C	1440	NAG	C2-N2-C7	3.00	127.00	123.11
2	C	1403	NAG	C6-C5-C4	3.00	120.50	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1440	NAG	C2-N2-C7	3.00	127.01	123.11
2	A	1416	NAG	C6-C5-C4	3.00	120.51	112.99
2	B	1403	NAG	C6-C5-C4	3.00	120.51	112.99
2	B	1440	NAG	C2-N2-C7	3.01	127.02	123.11
2	B	1416	NAG	C6-C5-C4	3.02	120.54	112.99
3	B	1428	BMA	O2-C2-C3	3.02	116.26	110.19
2	C	1416	NAG	C6-C5-C4	3.02	120.57	112.99
3	A	1428	BMA	O2-C2-C3	3.04	116.30	110.19
3	C	1428	BMA	O2-C2-C3	3.05	116.34	110.19
2	B	1455	NAG	O3-C3-C2	3.06	115.92	109.37
2	C	1455	NAG	O3-C3-C2	3.06	115.92	109.37
2	A	1455	NAG	O3-C3-C2	3.06	115.92	109.37
2	C	1465	NAG	O3-C3-C4	3.19	117.55	110.36
2	A	1465	NAG	O3-C3-C4	3.19	117.56	110.36
2	B	1465	NAG	O3-C3-C4	3.20	117.57	110.36
2	B	1472	NAG	C6-C5-C4	3.31	121.29	112.99
2	C	1472	NAG	C6-C5-C4	3.32	121.30	112.99
2	A	1472	NAG	C6-C5-C4	3.32	121.30	112.99
4	C	1467	MAN	C6-C5-C4	3.35	121.39	112.99
4	B	1467	MAN	C6-C5-C4	3.36	121.40	112.99
4	A	1467	MAN	C6-C5-C4	3.36	121.41	112.99
2	A	1438	NAG	C6-C5-C4	3.36	121.42	112.99
2	C	1438	NAG	C6-C5-C4	3.37	121.43	112.99
2	B	1438	NAG	C6-C5-C4	3.37	121.44	112.99
4	B	1446	MAN	O2-C2-C1	3.44	116.12	109.23
4	A	1446	MAN	O2-C2-C1	3.44	116.13	109.23
3	B	1473	BMA	O4-C4-C5	3.44	118.30	109.23
4	C	1446	MAN	O2-C2-C1	3.45	116.13	109.23
3	A	1473	BMA	O4-C4-C5	3.45	118.31	109.23
3	C	1473	BMA	O4-C4-C5	3.45	118.31	109.23
4	C	1408	MAN	C6-C5-C4	3.45	121.63	112.99
4	B	1408	MAN	C6-C5-C4	3.46	121.66	112.99
4	A	1408	MAN	C6-C5-C4	3.47	121.69	112.99
2	B	1456	NAG	C6-C5-C4	3.48	121.70	112.99
2	A	1456	NAG	C6-C5-C4	3.48	121.72	112.99
4	C	1421	MAN	C6-C5-C4	3.49	121.74	112.99
2	C	1456	NAG	C6-C5-C4	3.50	121.75	112.99
4	B	1421	MAN	C6-C5-C4	3.50	121.75	112.99
4	A	1421	MAN	C6-C5-C4	3.50	121.76	112.99
3	C	1444	BMA	O2-C2-C1	3.52	116.28	109.23
3	A	1444	BMA	O2-C2-C1	3.52	116.29	109.23
3	B	1444	BMA	O2-C2-C1	3.52	116.29	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1447	NAG	O3-C3-C4	3.60	118.47	110.36
2	A	1447	NAG	O3-C3-C4	3.60	118.47	110.36
2	C	1447	NAG	O3-C3-C4	3.60	118.49	110.36
4	C	1430	MAN	O3-C3-C2	3.64	116.67	110.01
4	A	1430	MAN	O3-C3-C2	3.64	116.67	110.01
4	B	1430	MAN	O3-C3-C2	3.66	116.71	110.01
3	C	1436	BMA	O4-C4-C5	3.70	118.97	109.23
3	A	1436	BMA	O4-C4-C5	3.70	118.98	109.23
3	B	1436	BMA	O4-C4-C5	3.71	119.00	109.23
2	C	1461	NAG	O3-C3-C4	3.71	118.73	110.36
2	B	1461	NAG	O3-C3-C4	3.72	118.75	110.36
2	A	1461	NAG	O3-C3-C4	3.73	118.76	110.36
2	B	1437	NAG	O3-C3-C2	3.73	117.36	109.37
2	C	1437	NAG	O3-C3-C2	3.74	117.37	109.37
2	A	1437	NAG	O3-C3-C2	3.75	117.39	109.37
4	B	1463	MAN	O4-C4-C5	3.76	119.13	109.23
2	B	1411	NAG	C1-O5-C5	3.76	117.67	112.14
4	A	1433	MAN	C1-O5-C5	3.76	117.67	112.14
4	B	1433	MAN	C1-O5-C5	3.76	117.67	112.14
2	A	1411	NAG	C1-O5-C5	3.77	117.68	112.14
4	C	1433	MAN	C1-O5-C5	3.77	117.68	112.14
4	C	1463	MAN	O4-C4-C5	3.77	119.16	109.23
4	A	1463	MAN	O4-C4-C5	3.78	119.19	109.23
2	C	1411	NAG	C1-O5-C5	3.78	117.70	112.14
4	A	1409	MAN	C1-O5-C5	3.79	117.71	112.14
4	B	1409	MAN	C1-O5-C5	3.80	117.72	112.14
2	C	1435	NAG	C6-C5-C4	3.81	122.54	112.99
2	B	1435	NAG	C6-C5-C4	3.81	122.54	112.99
4	C	1409	MAN	C1-O5-C5	3.83	117.78	112.14
2	A	1435	NAG	C6-C5-C4	3.84	122.60	112.99
2	B	1423	NAG	O3-C3-C2	4.10	118.16	109.37
2	A	1423	NAG	O3-C3-C2	4.11	118.16	109.37
2	C	1423	NAG	O3-C3-C2	4.11	118.17	109.37
2	A	1404	NAG	C6-C5-C4	4.19	123.50	112.99
2	C	1404	NAG	C6-C5-C4	4.19	123.50	112.99
2	B	1404	NAG	C6-C5-C4	4.20	123.50	112.99
3	B	1420	BMA	O4-C4-C3	4.20	119.83	110.36
3	C	1420	BMA	O4-C4-C3	4.20	119.83	110.36
2	C	1439	NAG	O3-C3-C2	4.21	118.37	109.37
3	A	1420	BMA	O4-C4-C3	4.21	119.84	110.36
2	A	1439	NAG	O3-C3-C2	4.22	118.40	109.37
2	B	1439	NAG	O3-C3-C2	4.23	118.42	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1409	MAN	C6-C5-C4	4.24	123.61	112.99
4	C	1409	MAN	C6-C5-C4	4.25	123.64	112.99
4	B	1409	MAN	C6-C5-C4	4.25	123.64	112.99
2	A	1402	NAG	C6-C5-C4	4.26	123.67	112.99
2	B	1402	NAG	C6-C5-C4	4.26	123.67	112.99
2	C	1402	NAG	C6-C5-C4	4.27	123.69	112.99
3	A	1444	BMA	O2-C2-C3	4.29	118.83	110.19
3	C	1444	BMA	O2-C2-C3	4.29	118.83	110.19
3	B	1444	BMA	O2-C2-C3	4.29	118.83	110.19
2	B	1435	NAG	O4-C4-C3	4.31	120.08	110.36
4	A	1468	MAN	O2-C2-C3	4.32	118.89	110.19
2	A	1435	NAG	O4-C4-C3	4.32	120.11	110.36
2	C	1435	NAG	O4-C4-C3	4.33	120.11	110.36
4	B	1468	MAN	O2-C2-C3	4.33	118.90	110.19
4	C	1468	MAN	O2-C2-C3	4.34	118.92	110.19
2	B	1450	NAG	C6-C5-C4	4.41	124.04	112.99
4	C	1415	MAN	O2-C2-C3	4.41	119.07	110.19
4	B	1415	MAN	O2-C2-C3	4.41	119.07	110.19
4	A	1415	MAN	O2-C2-C3	4.42	119.08	110.19
2	C	1450	NAG	C6-C5-C4	4.42	124.06	112.99
4	A	1432	MAN	C6-C5-C4	4.42	124.06	112.99
2	A	1450	NAG	C6-C5-C4	4.42	124.07	112.99
4	B	1432	MAN	C6-C5-C4	4.43	124.09	112.99
4	C	1432	MAN	C6-C5-C4	4.43	124.10	112.99
3	A	1462	BMA	O2-C2-C3	4.43	119.12	110.19
3	B	1462	BMA	O2-C2-C3	4.44	119.12	110.19
3	C	1462	BMA	O2-C2-C3	4.44	119.13	110.19
3	B	1420	BMA	O2-C2-C3	4.55	119.36	110.19
3	A	1420	BMA	O2-C2-C3	4.55	119.36	110.19
3	C	1420	BMA	O2-C2-C3	4.56	119.36	110.19
2	A	1459	NAG	C6-C5-C4	4.65	124.64	112.99
2	B	1459	NAG	C6-C5-C4	4.65	124.64	112.99
2	C	1459	NAG	C6-C5-C4	4.66	124.66	112.99
4	C	1463	MAN	C6-C5-C4	4.70	124.78	112.99
2	B	1427	NAG	C6-C5-C4	4.70	124.78	112.99
4	A	1463	MAN	C6-C5-C4	4.71	124.79	112.99
2	A	1427	NAG	C6-C5-C4	4.71	124.79	112.99
2	C	1427	NAG	C6-C5-C4	4.72	124.81	112.99
4	B	1463	MAN	C6-C5-C4	4.72	124.81	112.99
2	B	1418	NAG	C6-C5-C4	4.77	124.95	112.99
2	A	1418	NAG	C6-C5-C4	4.77	124.95	112.99
2	C	1418	NAG	C6-C5-C4	4.78	124.96	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1444	BMA	C6-C5-C4	4.79	125.00	112.99
3	C	1444	BMA	C6-C5-C4	4.80	125.01	112.99
3	B	1444	BMA	C6-C5-C4	4.81	125.04	112.99
4	C	1408	MAN	C1-O5-C5	4.85	119.28	112.14
4	A	1408	MAN	C1-O5-C5	4.86	119.28	112.14
4	B	1408	MAN	C1-O5-C5	4.89	119.32	112.14
4	C	1415	MAN	C6-C5-C4	4.91	125.29	112.99
4	B	1415	MAN	C6-C5-C4	4.92	125.31	112.99
4	A	1415	MAN	C6-C5-C4	4.92	125.32	112.99
2	B	1442	NAG	C6-C5-C4	4.96	125.42	112.99
2	A	1442	NAG	C6-C5-C4	4.96	125.42	112.99
2	C	1442	NAG	C6-C5-C4	4.96	125.43	112.99
2	A	1448	NAG	C6-C5-C4	4.97	125.45	112.99
2	C	1448	NAG	C6-C5-C4	4.98	125.47	112.99
2	B	1448	NAG	C6-C5-C4	4.98	125.47	112.99
4	A	1407	MAN	C6-C5-C4	5.00	125.51	112.99
4	C	1407	MAN	C6-C5-C4	5.01	125.55	112.99
4	B	1407	MAN	C6-C5-C4	5.02	125.57	112.99
2	A	1405	NAG	C6-C5-C4	5.04	125.63	112.99
2	B	1405	NAG	C6-C5-C4	5.05	125.64	112.99
2	C	1405	NAG	C6-C5-C4	5.06	125.66	112.99
4	C	1446	MAN	C6-C5-C4	5.07	125.70	112.99
4	A	1446	MAN	C6-C5-C4	5.08	125.71	112.99
4	B	1446	MAN	C6-C5-C4	5.08	125.71	112.99
2	A	1424	NAG	O3-C3-C4	5.09	121.83	110.36
2	C	1424	NAG	O3-C3-C4	5.09	121.84	110.36
2	B	1424	NAG	O3-C3-C4	5.09	121.84	110.36
4	A	1433	MAN	C6-C5-C4	5.19	126.00	112.99
4	C	1433	MAN	C6-C5-C4	5.19	126.00	112.99
4	B	1433	MAN	C6-C5-C4	5.19	126.01	112.99
3	C	1406	BMA	C6-C5-C4	5.23	126.11	112.99
3	B	1406	BMA	C6-C5-C4	5.24	126.13	112.99
3	A	1406	BMA	C6-C5-C4	5.25	126.15	112.99
2	B	1422	NAG	C8-C7-N2	5.33	126.31	116.10
2	A	1422	NAG	C8-C7-N2	5.34	126.33	116.10
2	C	1422	NAG	C8-C7-N2	5.34	126.33	116.10
4	A	1432	MAN	O2-C2-C3	5.40	121.06	110.19
4	B	1430	MAN	C6-C5-C4	5.40	126.51	112.99
4	C	1432	MAN	O2-C2-C3	5.40	121.06	110.19
4	C	1430	MAN	C6-C5-C4	5.41	126.54	112.99
4	A	1430	MAN	C6-C5-C4	5.41	126.55	112.99
4	B	1432	MAN	O2-C2-C3	5.42	121.09	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1453	NAG	C6-C5-C4	5.45	126.64	112.99
2	A	1453	NAG	C6-C5-C4	5.45	126.64	112.99
3	B	1466	BMA	O4-C4-C3	5.45	122.64	110.36
2	C	1453	NAG	C6-C5-C4	5.46	126.66	112.99
3	A	1466	BMA	O4-C4-C3	5.46	122.68	110.36
3	C	1466	BMA	O4-C4-C3	5.47	122.69	110.36
2	C	1422	NAG	C6-C5-C4	5.52	126.81	112.99
2	A	1422	NAG	C6-C5-C4	5.52	126.81	112.99
2	B	1422	NAG	C6-C5-C4	5.53	126.85	112.99
2	C	1465	NAG	C6-C5-C4	5.53	126.85	112.99
2	A	1465	NAG	C6-C5-C4	5.53	126.86	112.99
2	B	1465	NAG	C6-C5-C4	5.54	126.87	112.99
2	B	1452	NAG	C6-C5-C4	5.71	127.30	112.99
2	C	1452	NAG	C6-C5-C4	5.71	127.30	112.99
2	A	1452	NAG	C6-C5-C4	5.72	127.31	112.99
4	C	1429	MAN	O2-C2-C1	5.86	120.97	109.23
4	B	1429	MAN	O2-C2-C1	5.86	120.98	109.23
4	A	1429	MAN	O2-C2-C1	5.87	120.98	109.23
3	B	1436	BMA	O2-C2-C3	5.88	122.04	110.19
3	A	1436	BMA	O2-C2-C3	5.90	122.06	110.19
3	C	1436	BMA	O2-C2-C3	5.91	122.09	110.19
4	A	1463	MAN	O2-C2-C1	5.93	121.10	109.23
4	C	1463	MAN	O2-C2-C1	5.94	121.12	109.23
4	B	1463	MAN	O2-C2-C1	5.94	121.12	109.23
4	B	1421	MAN	O2-C2-C1	5.95	121.15	109.23
4	A	1421	MAN	O2-C2-C1	5.95	121.15	109.23
4	C	1421	MAN	O2-C2-C1	5.95	121.15	109.23
2	B	1402	NAG	O3-C3-C2	5.96	122.13	109.37
2	A	1402	NAG	O3-C3-C2	5.97	122.15	109.37
2	C	1402	NAG	O3-C3-C2	5.98	122.17	109.37
4	C	1409	MAN	O2-C2-C1	6.12	121.50	109.23
4	B	1409	MAN	O2-C2-C1	6.13	121.50	109.23
4	A	1409	MAN	O2-C2-C1	6.14	121.53	109.23
2	A	1461	NAG	C6-C5-C4	6.50	129.27	112.99
2	C	1461	NAG	C6-C5-C4	6.50	129.29	112.99
2	B	1461	NAG	C6-C5-C4	6.51	129.30	112.99
3	C	1420	BMA	O3-C3-C2	6.74	122.36	110.01
3	B	1420	BMA	O3-C3-C2	6.74	122.36	110.01
3	A	1420	BMA	O3-C3-C2	6.75	122.38	110.01
3	C	1414	BMA	O2-C2-C3	6.80	123.88	110.19
3	A	1414	BMA	O2-C2-C3	6.80	123.89	110.19
3	B	1414	BMA	O2-C2-C3	6.82	123.92	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1429	MAN	O4-C4-C3	6.91	125.93	110.36
4	C	1429	MAN	O4-C4-C3	6.91	125.94	110.36
4	B	1429	MAN	O4-C4-C3	6.91	125.95	110.36
2	B	1427	NAG	O3-C3-C4	7.26	126.73	110.36
2	A	1427	NAG	O3-C3-C4	7.27	126.75	110.36
2	C	1427	NAG	O3-C3-C4	7.28	126.77	110.36
4	B	1468	MAN	C6-C5-C4	7.29	131.25	112.99
4	A	1468	MAN	C6-C5-C4	7.30	131.28	112.99
4	C	1468	MAN	C6-C5-C4	7.32	131.33	112.99
3	A	1406	BMA	O2-C2-C1	7.69	124.64	109.23
3	B	1406	BMA	O2-C2-C1	7.70	124.65	109.23
3	C	1406	BMA	O2-C2-C1	7.70	124.66	109.23
3	B	1449	BMA	O2-C2-C3	7.72	125.74	110.19
3	A	1449	BMA	O2-C2-C3	7.73	125.76	110.19
3	C	1449	BMA	O2-C2-C3	7.76	125.82	110.19
4	B	1407	MAN	O2-C2-C1	8.22	125.70	109.23
4	A	1407	MAN	O2-C2-C1	8.22	125.70	109.23
4	C	1407	MAN	O2-C2-C1	8.27	125.80	109.23
2	B	1460	NAG	C6-C5-C4	8.28	133.73	112.99
2	C	1460	NAG	C6-C5-C4	8.28	133.73	112.99
2	A	1460	NAG	C6-C5-C4	8.28	133.73	112.99
2	C	1437	NAG	C6-C5-C4	8.30	133.79	112.99
2	B	1437	NAG	C6-C5-C4	8.31	133.81	112.99
2	A	1437	NAG	C6-C5-C4	8.31	133.81	112.99
2	A	1419	NAG	O4-C4-C3	8.45	129.42	110.36
2	C	1419	NAG	O4-C4-C3	8.45	129.43	110.36
2	B	1419	NAG	O4-C4-C3	8.46	129.43	110.36
2	C	1464	NAG	C6-C5-C4	8.92	135.36	112.99
2	A	1464	NAG	C6-C5-C4	8.92	135.36	112.99
2	B	1464	NAG	C6-C5-C4	8.93	135.36	112.99
3	C	1473	BMA	O2-C2-C3	9.26	128.84	110.19
3	A	1473	BMA	O2-C2-C3	9.27	128.86	110.19
3	B	1473	BMA	O2-C2-C3	9.28	128.89	110.19
2	B	1419	NAG	O3-C3-C4	9.68	132.19	110.36
2	C	1419	NAG	O3-C3-C4	9.69	132.21	110.36
2	A	1419	NAG	O3-C3-C4	9.70	132.22	110.36
2	C	1454	NAG	C6-C5-C4	9.80	137.55	112.99
2	B	1454	NAG	C6-C5-C4	9.81	137.57	112.99
2	A	1454	NAG	C6-C5-C4	9.82	137.60	112.99
2	B	1441	NAG	C6-C5-C4	9.87	137.72	112.99
2	A	1441	NAG	C6-C5-C4	9.87	137.73	112.99
2	C	1441	NAG	C6-C5-C4	9.88	137.76	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1410	NAG	O4-C4-C3	9.96	132.83	110.36
2	C	1410	NAG	O4-C4-C3	9.98	132.86	110.36
2	B	1410	NAG	O4-C4-C3	9.98	132.88	110.36
2	B	1417	NAG	C6-C5-C4	10.17	138.49	112.99
2	C	1417	NAG	C6-C5-C4	10.18	138.50	112.99
2	A	1417	NAG	C6-C5-C4	10.18	138.51	112.99
3	A	1466	BMA	O2-C2-C3	10.39	131.12	110.19
3	C	1466	BMA	O2-C2-C3	10.39	131.12	110.19
3	B	1466	BMA	O2-C2-C3	10.40	131.14	110.19
2	B	1448	NAG	O4-C4-C3	10.41	133.83	110.36
2	A	1448	NAG	O4-C4-C3	10.42	133.85	110.36
2	C	1448	NAG	O4-C4-C3	10.43	133.88	110.36
2	B	1458	NAG	C6-C5-C4	10.54	139.40	112.99
2	A	1458	NAG	C6-C5-C4	10.56	139.45	112.99
2	C	1458	NAG	C6-C5-C4	10.56	139.46	112.99
2	A	1413	NAG	O4-C4-C3	10.60	134.25	110.36
2	C	1413	NAG	O4-C4-C3	10.60	134.26	110.36
2	B	1413	NAG	O4-C4-C3	10.61	134.28	110.36
2	C	1426	NAG	C6-C5-C4	10.93	140.38	112.99
2	A	1426	NAG	C6-C5-C4	10.94	140.40	112.99
2	B	1426	NAG	C6-C5-C4	10.95	140.42	112.99
2	C	1427	NAG	O4-C4-C3	11.01	135.18	110.36
2	A	1427	NAG	O4-C4-C3	11.03	135.23	110.36
2	B	1427	NAG	O4-C4-C3	11.04	135.25	110.36
3	B	1428	BMA	C6-C5-C4	11.29	141.28	112.99
3	C	1428	BMA	C6-C5-C4	11.29	141.29	112.99
3	A	1428	BMA	C6-C5-C4	11.30	141.30	112.99
2	B	1465	NAG	O4-C4-C3	11.40	136.07	110.36
2	A	1465	NAG	O4-C4-C3	11.41	136.09	110.36
2	C	1465	NAG	O4-C4-C3	11.43	136.13	110.36
2	B	1443	NAG	C6-C5-C4	11.55	141.94	112.99
2	A	1443	NAG	C6-C5-C4	11.55	141.94	112.99
2	C	1443	NAG	C6-C5-C4	11.55	141.94	112.99
2	B	1472	NAG	O4-C4-C3	11.82	137.01	110.36
2	A	1472	NAG	O4-C4-C3	11.83	137.03	110.36
2	C	1472	NAG	O4-C4-C3	11.84	137.06	110.36
2	C	1452	NAG	O4-C4-C3	11.84	137.06	110.36
2	B	1452	NAG	O4-C4-C3	11.84	137.07	110.36
2	A	1452	NAG	O4-C4-C3	11.85	137.08	110.36
2	B	1413	NAG	C6-C5-C4	14.43	149.16	112.99
2	A	1413	NAG	C6-C5-C4	14.44	149.17	112.99
2	C	1413	NAG	C6-C5-C4	14.44	149.18	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1428	BMA	O3-C3-C2	14.65	136.85	110.01
3	A	1428	BMA	O3-C3-C2	14.66	136.87	110.01
3	C	1428	BMA	O3-C3-C2	14.69	136.92	110.01
4	A	1429	MAN	O3-C3-C2	22.75	151.70	110.01
4	B	1429	MAN	O3-C3-C2	22.77	151.73	110.01
4	C	1429	MAN	O3-C3-C2	22.77	151.74	110.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1410	NAG	1	0
2	A	1434	NAG	1	0
2	A	1435	NAG	1	0
2	A	1472	NAG	5	0
2	B	1410	NAG	1	0
2	B	1434	NAG	1	0
2	B	1435	NAG	1	0
2	B	1472	NAG	4	0
2	C	1410	NAG	1	0
2	C	1434	NAG	1	0
2	C	1435	NAG	1	0
2	C	1472	NAG	4	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.