



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.; Veerle, 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

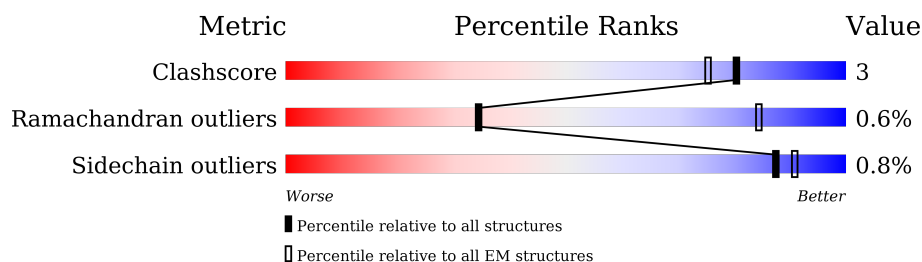
1 Overall quality at a glance

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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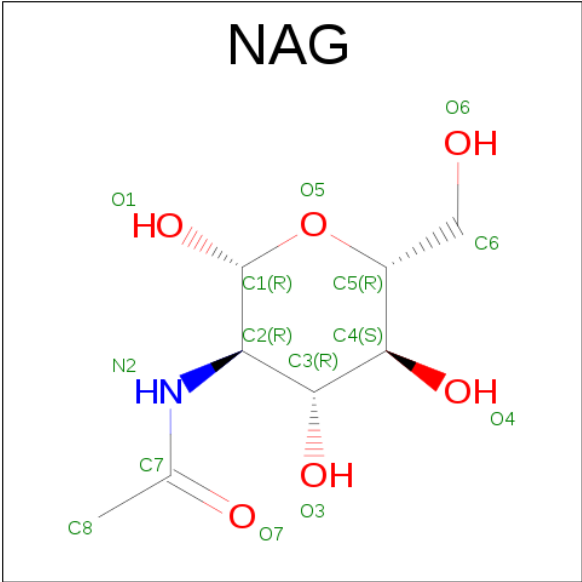
Chain	Residue	Modelled	Actual	Comment	Reference
B	1309	LYS	-	expression tag	UNP Q6Q1S2
B	1310	GLN	-	expression tag	UNP Q6Q1S2
B	1311	LYS	-	expression tag	UNP Q6Q1S2
B	1312	LYS	-	expression tag	UNP Q6Q1S2
B	1313	ILE	-	expression tag	UNP Q6Q1S2
B	1314	GLU	-	expression tag	UNP Q6Q1S2
B	1315	ASN	-	expression 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	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	
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
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
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	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	
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	
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	

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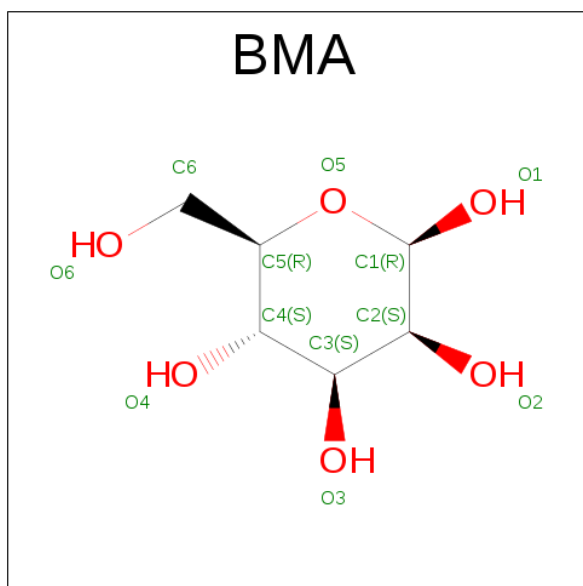
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	N 49	O 245	0
2	C	1	Total 686	C 392	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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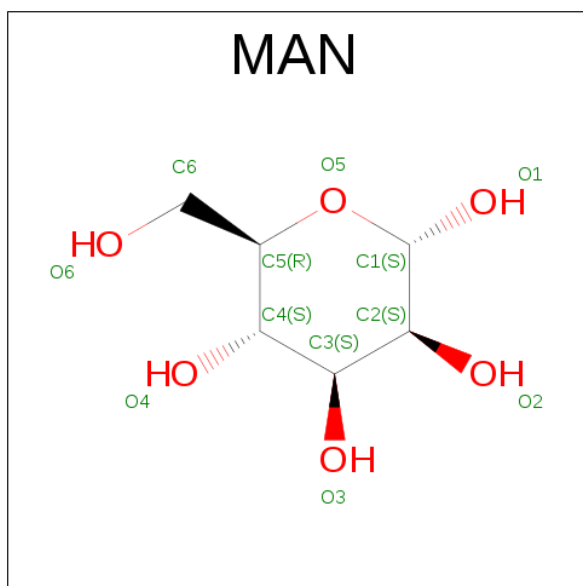
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	A	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	C	O	0
			110	60	50	
3	B	1	Total	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: $C_6H_{12}O_6$).



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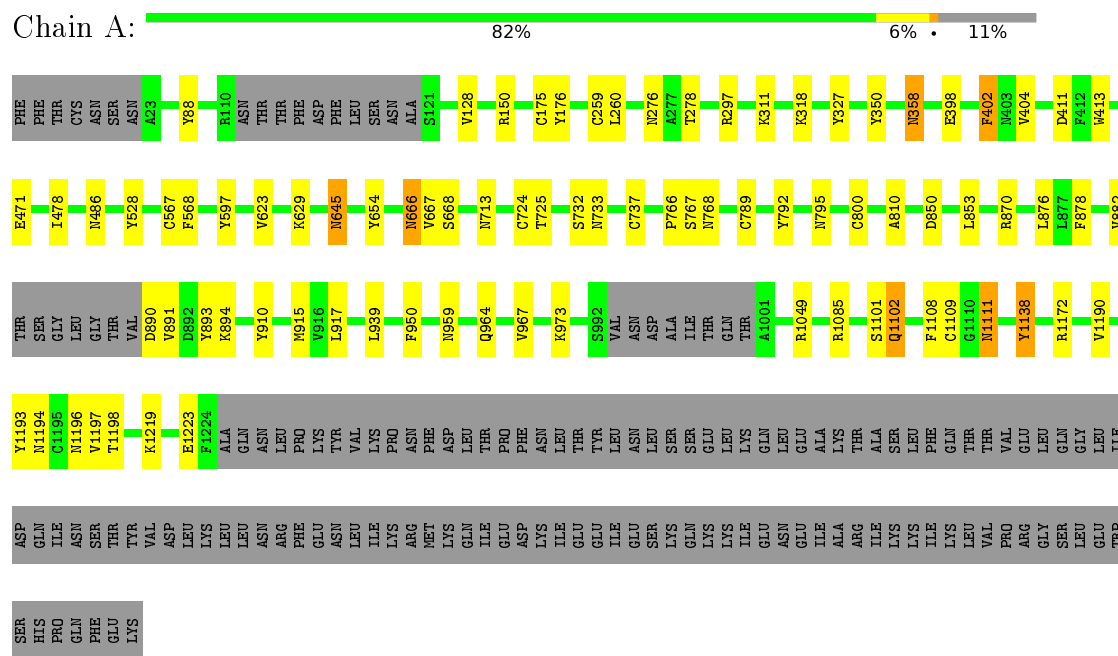
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Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	B	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C 90	O 75	0
4	C	1	Total 165	C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

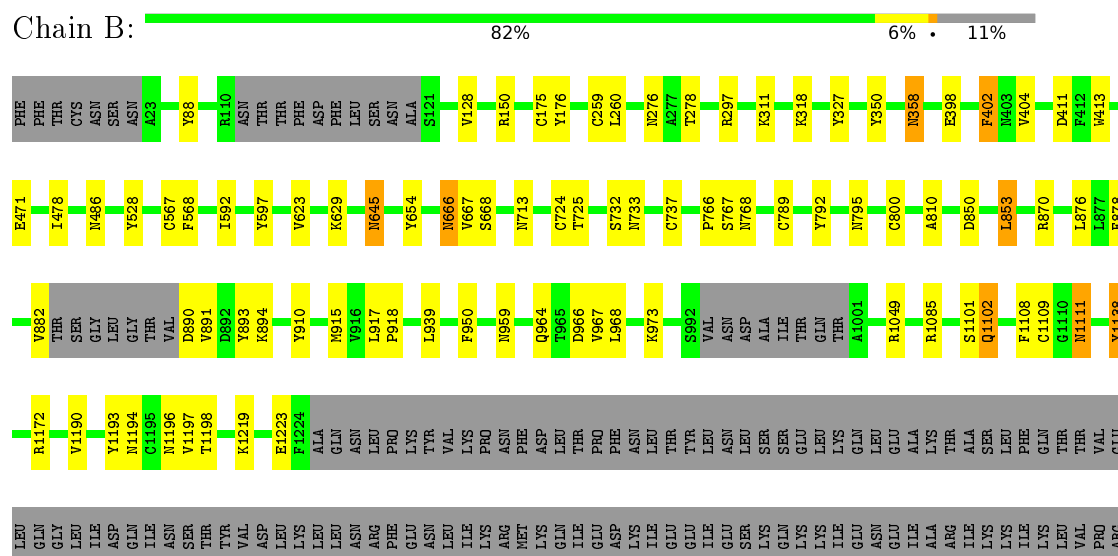
3 Residue-property plots

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

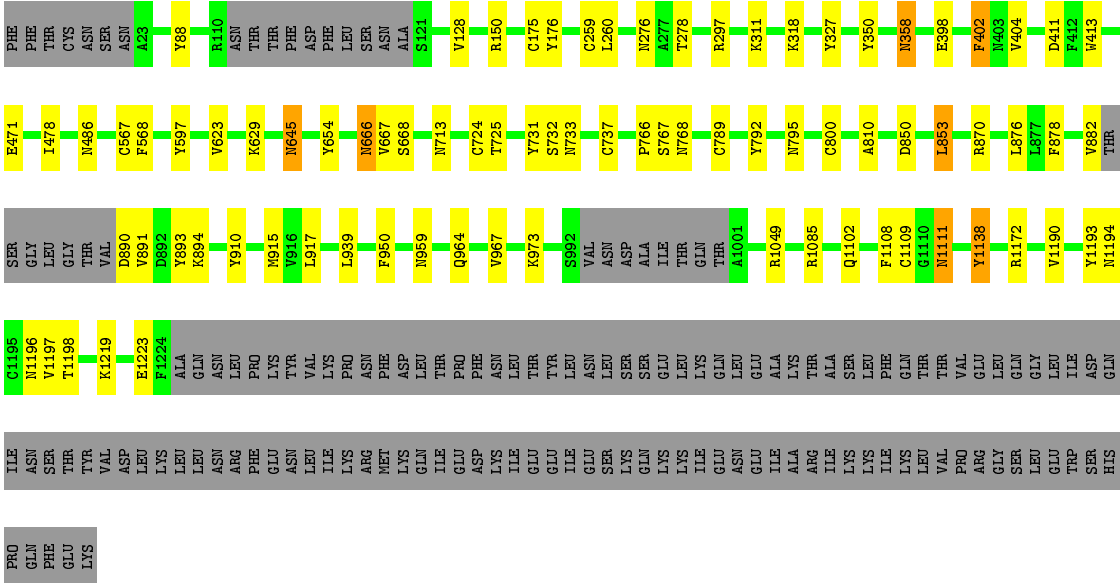
Chain C:

83%

6%

•

11%



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 [i](#)

5.1 Standard geometry [i](#)

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%)

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

The worst 5 of 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
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

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

5 of 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

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
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

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	402	PHE
1	B	789	CYS
1	C	1111	ASN
1	B	486	ASN
1	B	645	ASN

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1429	MAN	O3-C3-C4	-17.66	70.53	110.36

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.