



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 7, 2018 – 11:29 AM EDT

PDB ID : 6B7N
EMDB ID: : EMD-7063
Title : Cryo-electron microscopy structure of porcine delta coronavirus spike protein in the pre-fusion state
Authors : Shang, J.; Zheng, Y.; Yang, Y.; Liu, C.; Geng, Q.; Tai, W.; Du, L.; Zhou, Y.; Zhang, W.; Li, F.
Deposited on : 2017-10-04
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

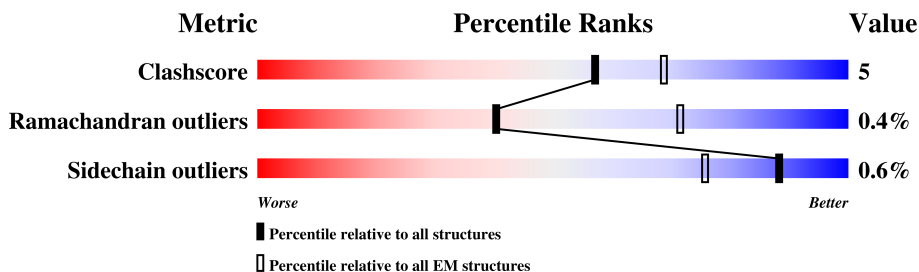
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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

Mol	Chain	Length	Quality of chain
1	A	1107	
1	B	1107	
1	C	1107	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22215 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	966	Total	C	N	O	S	0	0
			7139	4521	1184	1394	40		
1	B	966	Total	C	N	O	S	0	0
			7139	4521	1184	1394	40		
1	C	966	Total	C	N	O	S	0	0
			7139	4521	1184	1394	40		

There are 333 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ILE	VAL	conflict	UNP A0A075E3D7
A	553	ILE	THR	conflict	UNP A0A075E3D7
A	583	THR	ALA	conflict	UNP A0A075E3D7
A	642	LYS	GLN	conflict	UNP A0A075E3D7
A	1018	ASP	-	expression tag	UNP A0A075E3D7
A	1019	VAL	-	expression tag	UNP A0A075E3D7
A	1020	ASN	-	expression tag	UNP A0A075E3D7
A	1021	GLN	-	expression tag	UNP A0A075E3D7
A	1022	THR	-	expression tag	UNP A0A075E3D7
A	1023	VAL	-	expression tag	UNP A0A075E3D7
A	1024	SER	-	expression tag	UNP A0A075E3D7
A	1025	ASP	-	expression tag	UNP A0A075E3D7
A	1026	ILE	-	expression tag	UNP A0A075E3D7
A	1027	ILE	-	expression tag	UNP A0A075E3D7
A	1028	ASP	-	expression tag	UNP A0A075E3D7
A	1029	ASN	-	expression tag	UNP A0A075E3D7
A	1030	LEU	-	expression tag	UNP A0A075E3D7
A	1031	PRO	-	expression tag	UNP A0A075E3D7
A	1032	THR	-	expression tag	UNP A0A075E3D7
A	1033	ALA	-	expression tag	UNP A0A075E3D7
A	1034	THR	-	expression tag	UNP A0A075E3D7
A	1035	PRO	-	expression tag	UNP A0A075E3D7
A	1036	PRO	-	expression tag	UNP A0A075E3D7
A	1037	GLN	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1038	TRP	-	expression tag	UNP A0A075E3D7
A	1039	ASP	-	expression tag	UNP A0A075E3D7
A	1040	VAL	-	expression tag	UNP A0A075E3D7
A	1041	GLY	-	expression tag	UNP A0A075E3D7
A	1042	ILE	-	expression tag	UNP A0A075E3D7
A	1043	TYR	-	expression tag	UNP A0A075E3D7
A	1044	ASN	-	expression tag	UNP A0A075E3D7
A	1045	ASN	-	expression tag	UNP A0A075E3D7
A	1046	THR	-	expression tag	UNP A0A075E3D7
A	1047	ILE	-	expression tag	UNP A0A075E3D7
A	1048	LEU	-	expression tag	UNP A0A075E3D7
A	1049	ASN	-	expression tag	UNP A0A075E3D7
A	1050	LEU	-	expression tag	UNP A0A075E3D7
A	1051	THR	-	expression tag	UNP A0A075E3D7
A	1052	VAL	-	expression tag	UNP A0A075E3D7
A	1053	GLU	-	expression tag	UNP A0A075E3D7
A	1054	ILE	-	expression tag	UNP A0A075E3D7
A	1055	ASN	-	expression tag	UNP A0A075E3D7
A	1056	ASP	-	expression tag	UNP A0A075E3D7
A	1057	LEU	-	expression tag	UNP A0A075E3D7
A	1058	GLN	-	expression tag	UNP A0A075E3D7
A	1059	GLU	-	expression tag	UNP A0A075E3D7
A	1060	ARG	-	expression tag	UNP A0A075E3D7
A	1061	SER	-	expression tag	UNP A0A075E3D7
A	1062	LYS	-	expression tag	UNP A0A075E3D7
A	1063	ASN	-	expression tag	UNP A0A075E3D7
A	1064	LEU	-	expression tag	UNP A0A075E3D7
A	1065	SER	-	expression tag	UNP A0A075E3D7
A	1066	GLN	-	expression tag	UNP A0A075E3D7
A	1067	ILE	-	expression tag	UNP A0A075E3D7
A	1068	ALA	-	expression tag	UNP A0A075E3D7
A	1069	ASP	-	expression tag	UNP A0A075E3D7
A	1070	ARG	-	expression tag	UNP A0A075E3D7
A	1071	LEU	-	expression tag	UNP A0A075E3D7
A	1072	GLN	-	expression tag	UNP A0A075E3D7
A	1073	ASN	-	expression tag	UNP A0A075E3D7
A	1074	TYR	-	expression tag	UNP A0A075E3D7
A	1075	ILE	-	expression tag	UNP A0A075E3D7
A	1076	ASP	-	expression tag	UNP A0A075E3D7
A	1077	ASN	-	expression tag	UNP A0A075E3D7
A	1078	VAL	-	expression tag	UNP A0A075E3D7
A	1079	ASP	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1080	ILE	-	expression tag	UNP A0A075E3D7
A	1081	LYS	-	expression tag	UNP A0A075E3D7
A	1082	GLN	-	expression tag	UNP A0A075E3D7
A	1083	ILE	-	expression tag	UNP A0A075E3D7
A	1084	GLU	-	expression tag	UNP A0A075E3D7
A	1085	ASP	-	expression tag	UNP A0A075E3D7
A	1086	LYS	-	expression tag	UNP A0A075E3D7
A	1087	ILE	-	expression tag	UNP A0A075E3D7
A	1088	GLU	-	expression tag	UNP A0A075E3D7
A	1089	GLU	-	expression tag	UNP A0A075E3D7
A	1090	ILE	-	expression tag	UNP A0A075E3D7
A	1091	LEU	-	expression tag	UNP A0A075E3D7
A	1092	SER	-	expression tag	UNP A0A075E3D7
A	1093	LYS	-	expression tag	UNP A0A075E3D7
A	1094	ILE	-	expression tag	UNP A0A075E3D7
A	1095	TYR	-	expression tag	UNP A0A075E3D7
A	1096	HIS	-	expression tag	UNP A0A075E3D7
A	1097	ILE	-	expression tag	UNP A0A075E3D7
A	1098	GLU	-	expression tag	UNP A0A075E3D7
A	1099	ASN	-	expression tag	UNP A0A075E3D7
A	1100	GLU	-	expression tag	UNP A0A075E3D7
A	1101	ILE	-	expression tag	UNP A0A075E3D7
A	1102	ALA	-	expression tag	UNP A0A075E3D7
A	1103	ARG	-	expression tag	UNP A0A075E3D7
A	1104	ILE	-	expression tag	UNP A0A075E3D7
A	1105	LYS	-	expression tag	UNP A0A075E3D7
A	1106	LYS	-	expression tag	UNP A0A075E3D7
A	1107	LEU	-	expression tag	UNP A0A075E3D7
A	1108	ILE	-	expression tag	UNP A0A075E3D7
A	1109	GLY	-	expression tag	UNP A0A075E3D7
A	1110	GLU	-	expression tag	UNP A0A075E3D7
A	1111	ILE	-	expression tag	UNP A0A075E3D7
A	1112	GLY	-	expression tag	UNP A0A075E3D7
A	1113	GLY	-	expression tag	UNP A0A075E3D7
A	1114	GLY	-	expression tag	UNP A0A075E3D7
A	1115	GLY	-	expression tag	UNP A0A075E3D7
A	1116	SER	-	expression tag	UNP A0A075E3D7
A	1117	HIS	-	expression tag	UNP A0A075E3D7
A	1118	HIS	-	expression tag	UNP A0A075E3D7
A	1119	HIS	-	expression tag	UNP A0A075E3D7
A	1120	HIS	-	expression tag	UNP A0A075E3D7
A	1121	HIS	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1122	HIS	-	expression tag	UNP A0A075E3D7
A	1123	HIS	-	expression tag	UNP A0A075E3D7
A	1124	HIS	-	expression tag	UNP A0A075E3D7
B	111	ILE	VAL	conflict	UNP A0A075E3D7
B	553	ILE	THR	conflict	UNP A0A075E3D7
B	583	THR	ALA	conflict	UNP A0A075E3D7
B	642	LYS	GLN	conflict	UNP A0A075E3D7
B	1018	ASP	-	expression tag	UNP A0A075E3D7
B	1019	VAL	-	expression tag	UNP A0A075E3D7
B	1020	ASN	-	expression tag	UNP A0A075E3D7
B	1021	GLN	-	expression tag	UNP A0A075E3D7
B	1022	THR	-	expression tag	UNP A0A075E3D7
B	1023	VAL	-	expression tag	UNP A0A075E3D7
B	1024	SER	-	expression tag	UNP A0A075E3D7
B	1025	ASP	-	expression tag	UNP A0A075E3D7
B	1026	ILE	-	expression tag	UNP A0A075E3D7
B	1027	ILE	-	expression tag	UNP A0A075E3D7
B	1028	ASP	-	expression tag	UNP A0A075E3D7
B	1029	ASN	-	expression tag	UNP A0A075E3D7
B	1030	LEU	-	expression tag	UNP A0A075E3D7
B	1031	PRO	-	expression tag	UNP A0A075E3D7
B	1032	THR	-	expression tag	UNP A0A075E3D7
B	1033	ALA	-	expression tag	UNP A0A075E3D7
B	1034	THR	-	expression tag	UNP A0A075E3D7
B	1035	PRO	-	expression tag	UNP A0A075E3D7
B	1036	PRO	-	expression tag	UNP A0A075E3D7
B	1037	GLN	-	expression tag	UNP A0A075E3D7
B	1038	TRP	-	expression tag	UNP A0A075E3D7
B	1039	ASP	-	expression tag	UNP A0A075E3D7
B	1040	VAL	-	expression tag	UNP A0A075E3D7
B	1041	GLY	-	expression tag	UNP A0A075E3D7
B	1042	ILE	-	expression tag	UNP A0A075E3D7
B	1043	TYR	-	expression tag	UNP A0A075E3D7
B	1044	ASN	-	expression tag	UNP A0A075E3D7
B	1045	ASN	-	expression tag	UNP A0A075E3D7
B	1046	THR	-	expression tag	UNP A0A075E3D7
B	1047	ILE	-	expression tag	UNP A0A075E3D7
B	1048	LEU	-	expression tag	UNP A0A075E3D7
B	1049	ASN	-	expression tag	UNP A0A075E3D7
B	1050	LEU	-	expression tag	UNP A0A075E3D7
B	1051	THR	-	expression tag	UNP A0A075E3D7
B	1052	VAL	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1053	GLU	-	expression tag	UNP A0A075E3D7
B	1054	ILE	-	expression tag	UNP A0A075E3D7
B	1055	ASN	-	expression tag	UNP A0A075E3D7
B	1056	ASP	-	expression tag	UNP A0A075E3D7
B	1057	LEU	-	expression tag	UNP A0A075E3D7
B	1058	GLN	-	expression tag	UNP A0A075E3D7
B	1059	GLU	-	expression tag	UNP A0A075E3D7
B	1060	ARG	-	expression tag	UNP A0A075E3D7
B	1061	SER	-	expression tag	UNP A0A075E3D7
B	1062	LYS	-	expression tag	UNP A0A075E3D7
B	1063	ASN	-	expression tag	UNP A0A075E3D7
B	1064	LEU	-	expression tag	UNP A0A075E3D7
B	1065	SER	-	expression tag	UNP A0A075E3D7
B	1066	GLN	-	expression tag	UNP A0A075E3D7
B	1067	ILE	-	expression tag	UNP A0A075E3D7
B	1068	ALA	-	expression tag	UNP A0A075E3D7
B	1069	ASP	-	expression tag	UNP A0A075E3D7
B	1070	ARG	-	expression tag	UNP A0A075E3D7
B	1071	LEU	-	expression tag	UNP A0A075E3D7
B	1072	GLN	-	expression tag	UNP A0A075E3D7
B	1073	ASN	-	expression tag	UNP A0A075E3D7
B	1074	TYR	-	expression tag	UNP A0A075E3D7
B	1075	ILE	-	expression tag	UNP A0A075E3D7
B	1076	ASP	-	expression tag	UNP A0A075E3D7
B	1077	ASN	-	expression tag	UNP A0A075E3D7
B	1078	VAL	-	expression tag	UNP A0A075E3D7
B	1079	ASP	-	expression tag	UNP A0A075E3D7
B	1080	ILE	-	expression tag	UNP A0A075E3D7
B	1081	LYS	-	expression tag	UNP A0A075E3D7
B	1082	GLN	-	expression tag	UNP A0A075E3D7
B	1083	ILE	-	expression tag	UNP A0A075E3D7
B	1084	GLU	-	expression tag	UNP A0A075E3D7
B	1085	ASP	-	expression tag	UNP A0A075E3D7
B	1086	LYS	-	expression tag	UNP A0A075E3D7
B	1087	ILE	-	expression tag	UNP A0A075E3D7
B	1088	GLU	-	expression tag	UNP A0A075E3D7
B	1089	GLU	-	expression tag	UNP A0A075E3D7
B	1090	ILE	-	expression tag	UNP A0A075E3D7
B	1091	LEU	-	expression tag	UNP A0A075E3D7
B	1092	SER	-	expression tag	UNP A0A075E3D7
B	1093	LYS	-	expression tag	UNP A0A075E3D7
B	1094	ILE	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1095	TYR	-	expression tag	UNP A0A075E3D7
B	1096	HIS	-	expression tag	UNP A0A075E3D7
B	1097	ILE	-	expression tag	UNP A0A075E3D7
B	1098	GLU	-	expression tag	UNP A0A075E3D7
B	1099	ASN	-	expression tag	UNP A0A075E3D7
B	1100	GLU	-	expression tag	UNP A0A075E3D7
B	1101	ILE	-	expression tag	UNP A0A075E3D7
B	1102	ALA	-	expression tag	UNP A0A075E3D7
B	1103	ARG	-	expression tag	UNP A0A075E3D7
B	1104	ILE	-	expression tag	UNP A0A075E3D7
B	1105	LYS	-	expression tag	UNP A0A075E3D7
B	1106	LYS	-	expression tag	UNP A0A075E3D7
B	1107	LEU	-	expression tag	UNP A0A075E3D7
B	1108	ILE	-	expression tag	UNP A0A075E3D7
B	1109	GLY	-	expression tag	UNP A0A075E3D7
B	1110	GLU	-	expression tag	UNP A0A075E3D7
B	1111	ILE	-	expression tag	UNP A0A075E3D7
B	1112	GLY	-	expression tag	UNP A0A075E3D7
B	1113	GLY	-	expression tag	UNP A0A075E3D7
B	1114	GLY	-	expression tag	UNP A0A075E3D7
B	1115	GLY	-	expression tag	UNP A0A075E3D7
B	1116	SER	-	expression tag	UNP A0A075E3D7
B	1117	HIS	-	expression tag	UNP A0A075E3D7
B	1118	HIS	-	expression tag	UNP A0A075E3D7
B	1119	HIS	-	expression tag	UNP A0A075E3D7
B	1120	HIS	-	expression tag	UNP A0A075E3D7
B	1121	HIS	-	expression tag	UNP A0A075E3D7
B	1122	HIS	-	expression tag	UNP A0A075E3D7
B	1123	HIS	-	expression tag	UNP A0A075E3D7
B	1124	HIS	-	expression tag	UNP A0A075E3D7
C	111	ILE	VAL	conflict	UNP A0A075E3D7
C	553	ILE	THR	conflict	UNP A0A075E3D7
C	583	THR	ALA	conflict	UNP A0A075E3D7
C	642	LYS	GLN	conflict	UNP A0A075E3D7
C	1018	ASP	-	expression tag	UNP A0A075E3D7
C	1019	VAL	-	expression tag	UNP A0A075E3D7
C	1020	ASN	-	expression tag	UNP A0A075E3D7
C	1021	GLN	-	expression tag	UNP A0A075E3D7
C	1022	THR	-	expression tag	UNP A0A075E3D7
C	1023	VAL	-	expression tag	UNP A0A075E3D7
C	1024	SER	-	expression tag	UNP A0A075E3D7
C	1025	ASP	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1026	ILE	-	expression tag	UNP A0A075E3D7
C	1027	ILE	-	expression tag	UNP A0A075E3D7
C	1028	ASP	-	expression tag	UNP A0A075E3D7
C	1029	ASN	-	expression tag	UNP A0A075E3D7
C	1030	LEU	-	expression tag	UNP A0A075E3D7
C	1031	PRO	-	expression tag	UNP A0A075E3D7
C	1032	THR	-	expression tag	UNP A0A075E3D7
C	1033	ALA	-	expression tag	UNP A0A075E3D7
C	1034	THR	-	expression tag	UNP A0A075E3D7
C	1035	PRO	-	expression tag	UNP A0A075E3D7
C	1036	PRO	-	expression tag	UNP A0A075E3D7
C	1037	GLN	-	expression tag	UNP A0A075E3D7
C	1038	TRP	-	expression tag	UNP A0A075E3D7
C	1039	ASP	-	expression tag	UNP A0A075E3D7
C	1040	VAL	-	expression tag	UNP A0A075E3D7
C	1041	GLY	-	expression tag	UNP A0A075E3D7
C	1042	ILE	-	expression tag	UNP A0A075E3D7
C	1043	TYR	-	expression tag	UNP A0A075E3D7
C	1044	ASN	-	expression tag	UNP A0A075E3D7
C	1045	ASN	-	expression tag	UNP A0A075E3D7
C	1046	THR	-	expression tag	UNP A0A075E3D7
C	1047	ILE	-	expression tag	UNP A0A075E3D7
C	1048	LEU	-	expression tag	UNP A0A075E3D7
C	1049	ASN	-	expression tag	UNP A0A075E3D7
C	1050	LEU	-	expression tag	UNP A0A075E3D7
C	1051	THR	-	expression tag	UNP A0A075E3D7
C	1052	VAL	-	expression tag	UNP A0A075E3D7
C	1053	GLU	-	expression tag	UNP A0A075E3D7
C	1054	ILE	-	expression tag	UNP A0A075E3D7
C	1055	ASN	-	expression tag	UNP A0A075E3D7
C	1056	ASP	-	expression tag	UNP A0A075E3D7
C	1057	LEU	-	expression tag	UNP A0A075E3D7
C	1058	GLN	-	expression tag	UNP A0A075E3D7
C	1059	GLU	-	expression tag	UNP A0A075E3D7
C	1060	ARG	-	expression tag	UNP A0A075E3D7
C	1061	SER	-	expression tag	UNP A0A075E3D7
C	1062	LYS	-	expression tag	UNP A0A075E3D7
C	1063	ASN	-	expression tag	UNP A0A075E3D7
C	1064	LEU	-	expression tag	UNP A0A075E3D7
C	1065	SER	-	expression tag	UNP A0A075E3D7
C	1066	GLN	-	expression tag	UNP A0A075E3D7
C	1067	ILE	-	expression tag	UNP A0A075E3D7

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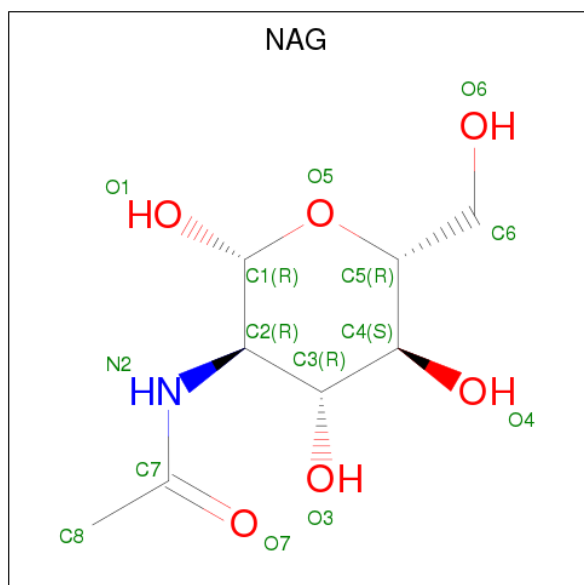
Chain	Residue	Modelled	Actual	Comment	Reference
C	1068	ALA	-	expression tag	UNP A0A075E3D7
C	1069	ASP	-	expression tag	UNP A0A075E3D7
C	1070	ARG	-	expression tag	UNP A0A075E3D7
C	1071	LEU	-	expression tag	UNP A0A075E3D7
C	1072	GLN	-	expression tag	UNP A0A075E3D7
C	1073	ASN	-	expression tag	UNP A0A075E3D7
C	1074	TYR	-	expression tag	UNP A0A075E3D7
C	1075	ILE	-	expression tag	UNP A0A075E3D7
C	1076	ASP	-	expression tag	UNP A0A075E3D7
C	1077	ASN	-	expression tag	UNP A0A075E3D7
C	1078	VAL	-	expression tag	UNP A0A075E3D7
C	1079	ASP	-	expression tag	UNP A0A075E3D7
C	1080	ILE	-	expression tag	UNP A0A075E3D7
C	1081	LYS	-	expression tag	UNP A0A075E3D7
C	1082	GLN	-	expression tag	UNP A0A075E3D7
C	1083	ILE	-	expression tag	UNP A0A075E3D7
C	1084	GLU	-	expression tag	UNP A0A075E3D7
C	1085	ASP	-	expression tag	UNP A0A075E3D7
C	1086	LYS	-	expression tag	UNP A0A075E3D7
C	1087	ILE	-	expression tag	UNP A0A075E3D7
C	1088	GLU	-	expression tag	UNP A0A075E3D7
C	1089	GLU	-	expression tag	UNP A0A075E3D7
C	1090	ILE	-	expression tag	UNP A0A075E3D7
C	1091	LEU	-	expression tag	UNP A0A075E3D7
C	1092	SER	-	expression tag	UNP A0A075E3D7
C	1093	LYS	-	expression tag	UNP A0A075E3D7
C	1094	ILE	-	expression tag	UNP A0A075E3D7
C	1095	TYR	-	expression tag	UNP A0A075E3D7
C	1096	HIS	-	expression tag	UNP A0A075E3D7
C	1097	ILE	-	expression tag	UNP A0A075E3D7
C	1098	GLU	-	expression tag	UNP A0A075E3D7
C	1099	ASN	-	expression tag	UNP A0A075E3D7
C	1100	GLU	-	expression tag	UNP A0A075E3D7
C	1101	ILE	-	expression tag	UNP A0A075E3D7
C	1102	ALA	-	expression tag	UNP A0A075E3D7
C	1103	ARG	-	expression tag	UNP A0A075E3D7
C	1104	ILE	-	expression tag	UNP A0A075E3D7
C	1105	LYS	-	expression tag	UNP A0A075E3D7
C	1106	LYS	-	expression tag	UNP A0A075E3D7
C	1107	LEU	-	expression tag	UNP A0A075E3D7
C	1108	ILE	-	expression tag	UNP A0A075E3D7
C	1109	GLY	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1110	GLU	-	expression tag	UNP A0A075E3D7
C	1111	ILE	-	expression tag	UNP A0A075E3D7
C	1112	GLY	-	expression tag	UNP A0A075E3D7
C	1113	GLY	-	expression tag	UNP A0A075E3D7
C	1114	GLY	-	expression tag	UNP A0A075E3D7
C	1115	GLY	-	expression tag	UNP A0A075E3D7
C	1116	SER	-	expression tag	UNP A0A075E3D7
C	1117	HIS	-	expression tag	UNP A0A075E3D7
C	1118	HIS	-	expression tag	UNP A0A075E3D7
C	1119	HIS	-	expression tag	UNP A0A075E3D7
C	1120	HIS	-	expression tag	UNP A0A075E3D7
C	1121	HIS	-	expression tag	UNP A0A075E3D7
C	1122	HIS	-	expression tag	UNP A0A075E3D7
C	1123	HIS	-	expression tag	UNP A0A075E3D7
C	1124	HIS	-	expression tag	UNP A0A075E3D7

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			266	152	19	95	
2	A	1	Total	C	N	O	0
			266	152	19	95	
2	A	1	Total	C	N	O	0
			266	152	19	95	
2	A	1	Total	C	N	O	0
			266	152	19	95	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	A	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0

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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	B	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0
2	C	1	Total 266	C 152	N 19	O 95	0

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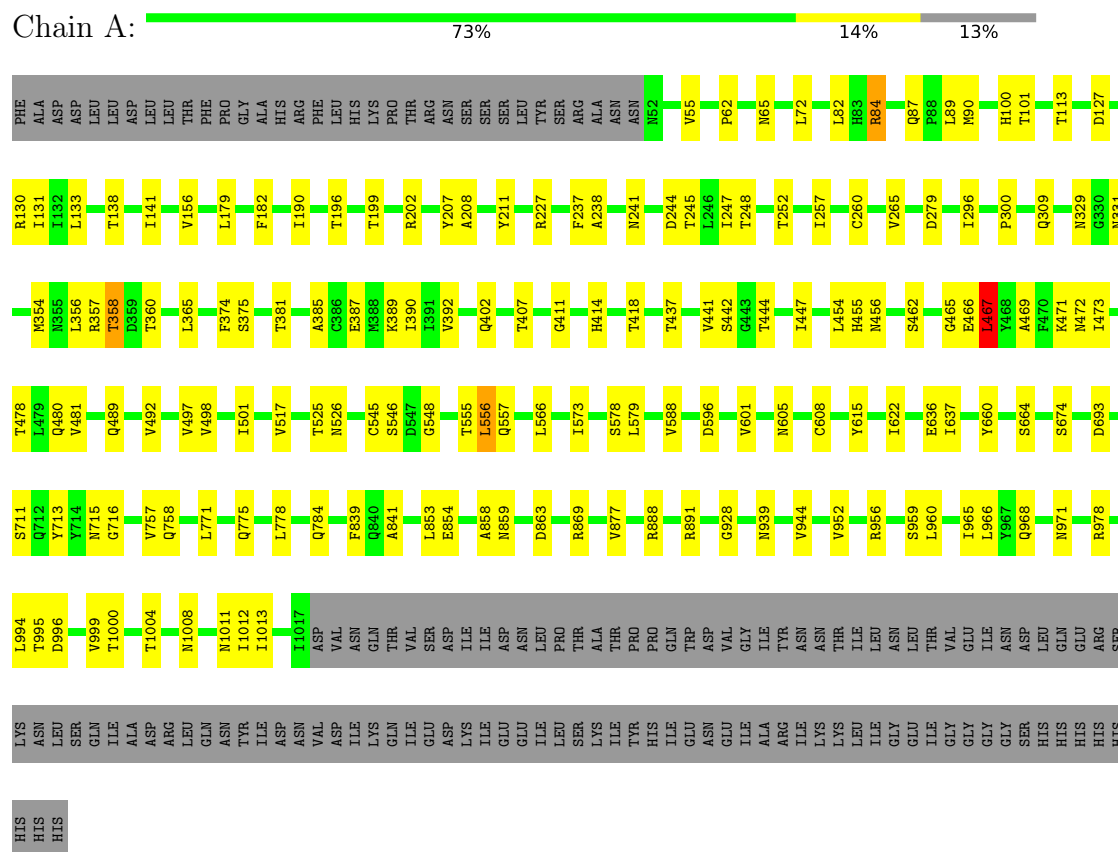
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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	
2	C	1	Total	C	N	O	0
			266	152	19	95	

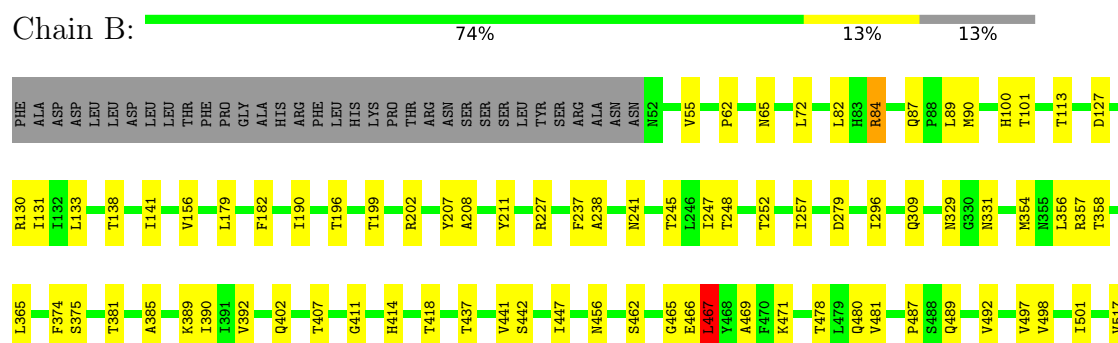
3 Residue-property plots

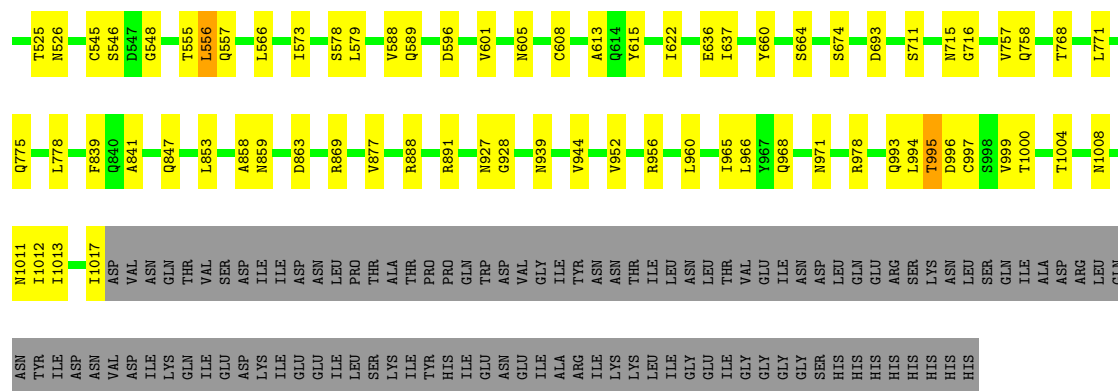
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: Spike protein

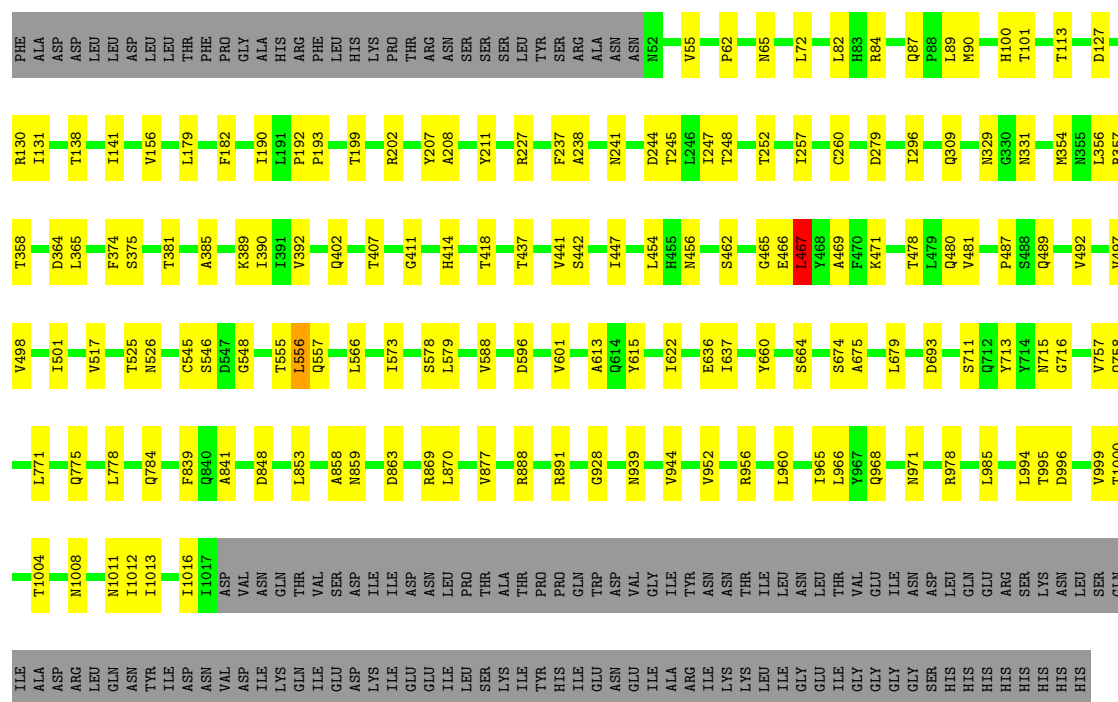


• Molecule 1: Spike protein





- Molecule 1: Spike protein



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	87002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.43	1/7270 (0.0%)	0.65	1/9959 (0.0%)
1	B	0.43	1/7270 (0.0%)	0.65	1/9959 (0.0%)
1	C	0.43	1/7270 (0.0%)	0.65	1/9959 (0.0%)
All	All	0.43	3/21810 (0.0%)	0.65	3/29877 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
All	All	0	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	517	VAL	C-N	-5.46	1.21	1.34
1	A	517	VAL	C-N	-5.44	1.21	1.34
1	B	517	VAL	C-N	-5.41	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	LEU	CA-CB-CG	9.88	138.02	115.30
1	A	467	LEU	CA-CB-CG	9.87	138.00	115.30
1	C	467	LEU	CA-CB-CG	9.86	137.98	115.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	THR	Peptide
1	A	358	THR	Peptide
1	A	418	THR	Peptide
1	A	466	GLU	Peptide
1	A	555	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7139	0	6840	86	0
1	B	7139	0	6840	83	0
1	C	7139	0	6840	83	0
2	A	266	0	241	3	0
2	B	266	0	241	1	0
2	C	266	0	241	2	0
All	All	22215	0	21243	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:ASN:O	1:A:863:ASP:HB2	1.87	0.74
1:B:859:ASN:O	1:B:863:ASP:HB2	1.87	0.74
1:C:859:ASN:O	1:C:863:ASP:HB2	1.87	0.74
1:B:456:ASN:ND2	1:C:252:THR:O	2.25	0.70
1:A:72:LEU:H	1:A:87:GLN:HE22	1.40	0.68

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	964/1107 (87%)	843 (87%)	117 (12%)	4 (0%)	36	69
1	B	964/1107 (87%)	844 (88%)	116 (12%)	4 (0%)	36	69
1	C	964/1107 (87%)	844 (88%)	116 (12%)	4 (0%)	36	69
All	All	2892/3321 (87%)	2531 (88%)	349 (12%)	12 (0%)	40	69

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	LEU
1	A	557	GLN
1	A	996	ASP
1	B	467	LEU
1	B	557	GLN

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	771/975 (79%)	766 (99%)	5 (1%)	87	92
1	B	771/975 (79%)	766 (99%)	5 (1%)	87	92
1	C	771/975 (79%)	766 (99%)	5 (1%)	87	92
All	All	2313/2925 (79%)	2298 (99%)	15 (1%)	88	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ARG
1	B	331	ASN
1	C	331	ASN
1	B	65	ASN
1	C	84	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	331	ASN
1	B	851	ASN
1	C	939	ASN
1	B	847	GLN
1	B	939	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](#)

57 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	1201	1,2	14,14,15	0.71	1 (7%)	17,19,21	2.60	4 (23%)
2	NAG	A	1202	2	14,14,15	0.28	0	17,19,21	0.68	1 (5%)
2	NAG	A	1203	1,2	14,14,15	0.27	0	17,19,21	0.58	0
2	NAG	A	1204	2	14,14,15	0.22	0	17,19,21	0.65	1 (5%)
2	NAG	A	1205	1	14,14,15	0.24	0	17,19,21	0.59	0
2	NAG	A	1206	1	14,14,15	0.58	0	17,19,21	0.69	0
2	NAG	A	1207	1	14,14,15	0.84	1 (7%)	17,19,21	2.18	3 (17%)
2	NAG	A	1208	1	14,14,15	0.21	0	17,19,21	0.53	0
2	NAG	A	1209	1	14,14,15	0.30	0	17,19,21	0.65	0
2	NAG	A	1210	1	14,14,15	0.41	0	17,19,21	0.44	0
2	NAG	A	1211	1	14,14,15	0.23	0	17,19,21	0.58	0
2	NAG	A	1212	1,2	14,14,15	0.33	0	17,19,21	0.72	0
2	NAG	A	1213	2	14,14,15	0.20	0	17,19,21	0.62	0
2	NAG	A	1214	1,2	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
2	NAG	A	1215	2	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	A	1216	2	14,14,15	0.45	0	17,19,21	0.70	1 (5%)
2	NAG	A	1217	1	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
2	NAG	A	1218	1,2	14,14,15	0.46	0	17,19,21	0.68	0
2	NAG	A	1219	2	14,14,15	0.22	0	17,19,21	0.54	0
2	NAG	B	1201	1,2	14,14,15	0.65	0	17,19,21	2.64	4 (23%)
2	NAG	B	1202	2	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
2	NAG	B	1203	1,2	14,14,15	0.28	0	17,19,21	0.56	0
2	NAG	B	1204	2	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	B	1205	1	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	B	1206	1	14,14,15	0.53	0	17,19,21	0.66	0
2	NAG	B	1207	1	14,14,15	0.81	1 (7%)	17,19,21	2.18	3 (17%)
2	NAG	B	1208	1	14,14,15	0.24	0	17,19,21	0.56	0
2	NAG	B	1209	1	14,14,15	0.25	0	17,19,21	0.63	0
2	NAG	B	1210	1	14,14,15	0.43	0	17,19,21	0.44	0
2	NAG	B	1211	1	14,14,15	0.27	0	17,19,21	0.58	0
2	NAG	B	1212	1,2	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
2	NAG	B	1213	2	14,14,15	0.18	0	17,19,21	0.61	0
2	NAG	B	1214	1,2	14,14,15	0.46	0	17,19,21	1.01	1 (5%)
2	NAG	B	1215	2	14,14,15	0.23	0	17,19,21	0.60	0
2	NAG	B	1216	2	14,14,15	0.45	0	17,19,21	0.67	0
2	NAG	B	1217	1	14,14,15	0.49	0	17,19,21	0.91	1 (5%)
2	NAG	B	1218	1,2	14,14,15	0.47	0	17,19,21	0.67	0
2	NAG	B	1219	2	14,14,15	0.20	0	17,19,21	0.57	0
2	NAG	C	1201	1,2	14,14,15	0.76	1 (7%)	17,19,21	2.61	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1202	2	14,14,15	0.28	0	17,19,21	0.65	1 (5%)
2	NAG	C	1203	1,2	14,14,15	0.32	0	17,19,21	0.57	0
2	NAG	C	1204	2	14,14,15	0.20	0	17,19,21	0.63	1 (5%)
2	NAG	C	1205	1	14,14,15	0.20	0	17,19,21	0.60	0
2	NAG	C	1206	1	14,14,15	0.49	0	17,19,21	0.71	1 (5%)
2	NAG	C	1207	1	14,14,15	0.81	1 (7%)	17,19,21	2.18	3 (17%)
2	NAG	C	1208	1	14,14,15	0.21	0	17,19,21	0.53	0
2	NAG	C	1209	1	14,14,15	0.37	0	17,19,21	0.62	0
2	NAG	C	1210	1	14,14,15	0.37	0	17,19,21	0.44	0
2	NAG	C	1211	1	14,14,15	0.27	0	17,19,21	0.58	0
2	NAG	C	1212	1,2	14,14,15	0.35	0	17,19,21	0.71	0
2	NAG	C	1213	2	14,14,15	0.20	0	17,19,21	0.62	0
2	NAG	C	1214	1,2	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
2	NAG	C	1215	2	14,14,15	0.22	0	17,19,21	0.60	0
2	NAG	C	1216	2	14,14,15	0.43	0	17,19,21	0.68	1 (5%)
2	NAG	C	1217	1	14,14,15	0.51	0	17,19,21	0.89	1 (5%)
2	NAG	C	1218	1,2	14,14,15	0.48	0	17,19,21	0.69	0
2	NAG	C	1219	2	14,14,15	0.22	0	17,19,21	0.54	0

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	1201	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1202	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1203	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1204	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1205	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1206	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1208	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1209	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1210	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1211	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1212	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1213	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1214	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1215	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1216	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1217	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1218	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1219	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1201	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1202	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1203	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1204	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1205	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1206	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1208	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1209	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1210	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1211	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1212	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1213	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1214	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1215	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1216	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1217	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1218	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1219	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1201	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1202	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1203	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1204	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1205	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1206	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1207	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1208	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1209	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1210	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1211	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1212	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1213	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1214	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1215	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1216	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1217	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1218	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1219	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	NAG	O5-C1	-2.37	1.39	1.43
2	A	1201	NAG	O5-C1	-2.20	1.40	1.43
2	B	1207	NAG	C1-C2	2.39	1.55	1.52
2	C	1207	NAG	C1-C2	2.45	1.55	1.52
2	A	1207	NAG	C1-C2	2.59	1.56	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	NAG	O4-C4-C5	-2.33	103.47	109.31
2	C	1201	NAG	O4-C4-C5	-2.33	103.47	109.31
2	B	1201	NAG	O4-C4-C5	-2.24	103.70	109.31
2	C	1216	NAG	C1-O5-C5	2.01	114.95	112.19
2	C	1204	NAG	C1-O5-C5	2.02	114.96	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1212	NAG	1	0
2	A	1214	NAG	1	0
2	A	1215	NAG	1	0
2	A	1217	NAG	1	0
2	B	1217	NAG	1	0
2	C	1212	NAG	1	0
2	C	1217	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.