



## wwPDB EM Validation Summary Report ⓘ

Mar 11, 2025 – 06:09 pm GMT

PDB ID : 9FR3  
EMDB ID : EMD-50707  
Title : Structure of the SARS-CoV-2 spike glycoprotein in complex with nanobody 7F  
Authors : Debski-Antoniak, O.; Hurdiss, D.L.  
Deposited on : 2024-06-18  
Resolution : 3.30 Å(reported)  
Based on initial model : 7R40

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

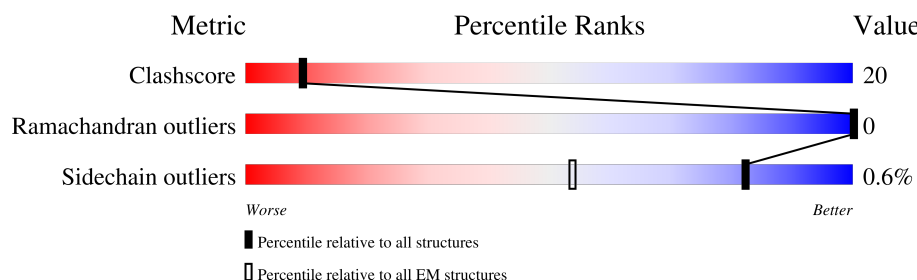
# 1 Overall quality at a glance

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	C	148	47% 34% 20%
1	E	148	47% 33% 20%
1	F	148	46% 34% 20%
1	I	148	47% 34% 20%
1	K	148	46% 34% 20%
1	L	148	47% 34% 20%
2	A	1275	57% 20% 23%
2	B	1275	57% 20% 23%
2	D	1275	56% 20% 23%

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Mol	Chain	Length	Quality of chain		
2	G	1275	<div><div></div></div>	57%	20% 23%
2	H	1275	<div><div></div></div>	56%	21% 23%
2	J	1275	<div><div></div></div>	57%	20% 23%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51750 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 Nanobody 7F.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	E	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	F	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	I	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	K	119	Total	C	N	O	S	0	0
			933	589	156	183	5		
1	L	119	Total	C	N	O	S	0	0
			933	589	156	183	5		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	B	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	D	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	G	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	H	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		
2	J	986	Total	C	N	O	S	0	0
			7594	4864	1261	1435	34		

There are 534 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	PHE	THR	conflict	UNP P0DTC2
A	607	GLU	GLN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	682	ALA	ARG	conflict	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	393	PHE	THR	conflict	UNP P0DTC2
B	607	GLU	GLN	conflict	UNP P0DTC2
B	682	ALA	ARG	conflict	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
D	393	PHE	THR	conflict	UNP P0DTC2
D	607	GLU	GLN	conflict	UNP P0DTC2
D	682	ALA	ARG	conflict	UNP P0DTC2
D	683	ALA	ARG	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	986	PRO	LYS	conflict	UNP P0DTC2
D	987	PRO	VAL	conflict	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLY	-	expression tag	UNP P0DTC2
D	1239	ARG	-	expression tag	UNP P0DTC2
D	1240	SER	-	expression tag	UNP P0DTC2
D	1241	LEU	-	expression tag	UNP P0DTC2
D	1242	GLU	-	expression tag	UNP P0DTC2
D	1243	VAL	-	expression tag	UNP P0DTC2
D	1244	LEU	-	expression tag	UNP P0DTC2
D	1245	PHE	-	expression tag	UNP P0DTC2
D	1246	GLN	-	expression tag	UNP P0DTC2
D	1247	GLY	-	expression tag	UNP P0DTC2
D	1248	PRO	-	expression tag	UNP P0DTC2
D	1249	GLY	-	expression tag	UNP P0DTC2
D	1250	HIS	-	expression tag	UNP P0DTC2
D	1251	HIS	-	expression tag	UNP P0DTC2
D	1252	HIS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	SER	-	expression tag	UNP P0DTC2
D	1259	ALA	-	expression tag	UNP P0DTC2
D	1260	TRP	-	expression tag	UNP P0DTC2
D	1261	SER	-	expression tag	UNP P0DTC2
D	1262	HIS	-	expression tag	UNP P0DTC2
D	1263	PRO	-	expression tag	UNP P0DTC2
D	1264	GLN	-	expression tag	UNP P0DTC2
D	1265	PHE	-	expression tag	UNP P0DTC2
D	1266	GLU	-	expression tag	UNP P0DTC2
D	1267	LYS	-	expression tag	UNP P0DTC2
D	1268	GLY	-	expression tag	UNP P0DTC2
D	1269	GLY	-	expression tag	UNP P0DTC2
D	1270	GLY	-	expression tag	UNP P0DTC2
D	1271	SER	-	expression tag	UNP P0DTC2
D	1272	GLY	-	expression tag	UNP P0DTC2
D	1273	GLY	-	expression tag	UNP P0DTC2
D	1274	GLY	-	expression tag	UNP P0DTC2
D	1275	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1276	SER	-	expression tag	UNP P0DTC2
D	1277	GLY	-	expression tag	UNP P0DTC2
D	1278	GLY	-	expression tag	UNP P0DTC2
D	1279	SER	-	expression tag	UNP P0DTC2
D	1280	ALA	-	expression tag	UNP P0DTC2
D	1281	TRP	-	expression tag	UNP P0DTC2
D	1282	SER	-	expression tag	UNP P0DTC2
D	1283	HIS	-	expression tag	UNP P0DTC2
D	1284	PRO	-	expression tag	UNP P0DTC2
D	1285	GLN	-	expression tag	UNP P0DTC2
D	1286	PHE	-	expression tag	UNP P0DTC2
D	1287	GLU	-	expression tag	UNP P0DTC2
D	1288	LYS	-	expression tag	UNP P0DTC2
G	393	PHE	THR	conflict	UNP P0DTC2
G	607	GLU	GLN	conflict	UNP P0DTC2
G	682	ALA	ARG	conflict	UNP P0DTC2
G	683	ALA	ARG	conflict	UNP P0DTC2
G	892	PRO	ALA	conflict	UNP P0DTC2
G	899	PRO	ALA	conflict	UNP P0DTC2
G	942	PRO	ALA	conflict	UNP P0DTC2
G	986	PRO	LYS	conflict	UNP P0DTC2
G	987	PRO	VAL	conflict	UNP P0DTC2
G	1209	GLY	-	expression tag	UNP P0DTC2
G	1210	SER	-	expression tag	UNP P0DTC2
G	1211	GLY	-	expression tag	UNP P0DTC2
G	1212	TYR	-	expression tag	UNP P0DTC2
G	1213	ILE	-	expression tag	UNP P0DTC2
G	1214	PRO	-	expression tag	UNP P0DTC2
G	1215	GLU	-	expression tag	UNP P0DTC2
G	1216	ALA	-	expression tag	UNP P0DTC2
G	1217	PRO	-	expression tag	UNP P0DTC2
G	1218	ARG	-	expression tag	UNP P0DTC2
G	1219	ASP	-	expression tag	UNP P0DTC2
G	1220	GLY	-	expression tag	UNP P0DTC2
G	1221	GLN	-	expression tag	UNP P0DTC2
G	1222	ALA	-	expression tag	UNP P0DTC2
G	1223	TYR	-	expression tag	UNP P0DTC2
G	1224	VAL	-	expression tag	UNP P0DTC2
G	1225	ARG	-	expression tag	UNP P0DTC2
G	1226	LYS	-	expression tag	UNP P0DTC2
G	1227	ASP	-	expression tag	UNP P0DTC2
G	1228	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1229	GLU	-	expression tag	UNP P0DTC2
G	1230	TRP	-	expression tag	UNP P0DTC2
G	1231	VAL	-	expression tag	UNP P0DTC2
G	1232	LEU	-	expression tag	UNP P0DTC2
G	1233	LEU	-	expression tag	UNP P0DTC2
G	1234	SER	-	expression tag	UNP P0DTC2
G	1235	THR	-	expression tag	UNP P0DTC2
G	1236	PHE	-	expression tag	UNP P0DTC2
G	1237	LEU	-	expression tag	UNP P0DTC2
G	1238	GLY	-	expression tag	UNP P0DTC2
G	1239	ARG	-	expression tag	UNP P0DTC2
G	1240	SER	-	expression tag	UNP P0DTC2
G	1241	LEU	-	expression tag	UNP P0DTC2
G	1242	GLU	-	expression tag	UNP P0DTC2
G	1243	VAL	-	expression tag	UNP P0DTC2
G	1244	LEU	-	expression tag	UNP P0DTC2
G	1245	PHE	-	expression tag	UNP P0DTC2
G	1246	GLN	-	expression tag	UNP P0DTC2
G	1247	GLY	-	expression tag	UNP P0DTC2
G	1248	PRO	-	expression tag	UNP P0DTC2
G	1249	GLY	-	expression tag	UNP P0DTC2
G	1250	HIS	-	expression tag	UNP P0DTC2
G	1251	HIS	-	expression tag	UNP P0DTC2
G	1252	HIS	-	expression tag	UNP P0DTC2
G	1253	HIS	-	expression tag	UNP P0DTC2
G	1254	HIS	-	expression tag	UNP P0DTC2
G	1255	HIS	-	expression tag	UNP P0DTC2
G	1256	HIS	-	expression tag	UNP P0DTC2
G	1257	HIS	-	expression tag	UNP P0DTC2
G	1258	SER	-	expression tag	UNP P0DTC2
G	1259	ALA	-	expression tag	UNP P0DTC2
G	1260	TRP	-	expression tag	UNP P0DTC2
G	1261	SER	-	expression tag	UNP P0DTC2
G	1262	HIS	-	expression tag	UNP P0DTC2
G	1263	PRO	-	expression tag	UNP P0DTC2
G	1264	GLN	-	expression tag	UNP P0DTC2
G	1265	PHE	-	expression tag	UNP P0DTC2
G	1266	GLU	-	expression tag	UNP P0DTC2
G	1267	LYS	-	expression tag	UNP P0DTC2
G	1268	GLY	-	expression tag	UNP P0DTC2
G	1269	GLY	-	expression tag	UNP P0DTC2
G	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1271	SER	-	expression tag	UNP P0DTC2
G	1272	GLY	-	expression tag	UNP P0DTC2
G	1273	GLY	-	expression tag	UNP P0DTC2
G	1274	GLY	-	expression tag	UNP P0DTC2
G	1275	GLY	-	expression tag	UNP P0DTC2
G	1276	SER	-	expression tag	UNP P0DTC2
G	1277	GLY	-	expression tag	UNP P0DTC2
G	1278	GLY	-	expression tag	UNP P0DTC2
G	1279	SER	-	expression tag	UNP P0DTC2
G	1280	ALA	-	expression tag	UNP P0DTC2
G	1281	TRP	-	expression tag	UNP P0DTC2
G	1282	SER	-	expression tag	UNP P0DTC2
G	1283	HIS	-	expression tag	UNP P0DTC2
G	1284	PRO	-	expression tag	UNP P0DTC2
G	1285	GLN	-	expression tag	UNP P0DTC2
G	1286	PHE	-	expression tag	UNP P0DTC2
G	1287	GLU	-	expression tag	UNP P0DTC2
G	1288	LYS	-	expression tag	UNP P0DTC2
H	393	PHE	THR	conflict	UNP P0DTC2
H	607	GLU	GLN	conflict	UNP P0DTC2
H	682	ALA	ARG	conflict	UNP P0DTC2
H	683	ALA	ARG	conflict	UNP P0DTC2
H	892	PRO	ALA	conflict	UNP P0DTC2
H	899	PRO	ALA	conflict	UNP P0DTC2
H	942	PRO	ALA	conflict	UNP P0DTC2
H	986	PRO	LYS	conflict	UNP P0DTC2
H	987	PRO	VAL	conflict	UNP P0DTC2
H	1209	GLY	-	expression tag	UNP P0DTC2
H	1210	SER	-	expression tag	UNP P0DTC2
H	1211	GLY	-	expression tag	UNP P0DTC2
H	1212	TYR	-	expression tag	UNP P0DTC2
H	1213	ILE	-	expression tag	UNP P0DTC2
H	1214	PRO	-	expression tag	UNP P0DTC2
H	1215	GLU	-	expression tag	UNP P0DTC2
H	1216	ALA	-	expression tag	UNP P0DTC2
H	1217	PRO	-	expression tag	UNP P0DTC2
H	1218	ARG	-	expression tag	UNP P0DTC2
H	1219	ASP	-	expression tag	UNP P0DTC2
H	1220	GLY	-	expression tag	UNP P0DTC2
H	1221	GLN	-	expression tag	UNP P0DTC2
H	1222	ALA	-	expression tag	UNP P0DTC2
H	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1224	VAL	-	expression tag	UNP P0DTC2
H	1225	ARG	-	expression tag	UNP P0DTC2
H	1226	LYS	-	expression tag	UNP P0DTC2
H	1227	ASP	-	expression tag	UNP P0DTC2
H	1228	GLY	-	expression tag	UNP P0DTC2
H	1229	GLU	-	expression tag	UNP P0DTC2
H	1230	TRP	-	expression tag	UNP P0DTC2
H	1231	VAL	-	expression tag	UNP P0DTC2
H	1232	LEU	-	expression tag	UNP P0DTC2
H	1233	LEU	-	expression tag	UNP P0DTC2
H	1234	SER	-	expression tag	UNP P0DTC2
H	1235	THR	-	expression tag	UNP P0DTC2
H	1236	PHE	-	expression tag	UNP P0DTC2
H	1237	LEU	-	expression tag	UNP P0DTC2
H	1238	GLY	-	expression tag	UNP P0DTC2
H	1239	ARG	-	expression tag	UNP P0DTC2
H	1240	SER	-	expression tag	UNP P0DTC2
H	1241	LEU	-	expression tag	UNP P0DTC2
H	1242	GLU	-	expression tag	UNP P0DTC2
H	1243	VAL	-	expression tag	UNP P0DTC2
H	1244	LEU	-	expression tag	UNP P0DTC2
H	1245	PHE	-	expression tag	UNP P0DTC2
H	1246	GLN	-	expression tag	UNP P0DTC2
H	1247	GLY	-	expression tag	UNP P0DTC2
H	1248	PRO	-	expression tag	UNP P0DTC2
H	1249	GLY	-	expression tag	UNP P0DTC2
H	1250	HIS	-	expression tag	UNP P0DTC2
H	1251	HIS	-	expression tag	UNP P0DTC2
H	1252	HIS	-	expression tag	UNP P0DTC2
H	1253	HIS	-	expression tag	UNP P0DTC2
H	1254	HIS	-	expression tag	UNP P0DTC2
H	1255	HIS	-	expression tag	UNP P0DTC2
H	1256	HIS	-	expression tag	UNP P0DTC2
H	1257	HIS	-	expression tag	UNP P0DTC2
H	1258	SER	-	expression tag	UNP P0DTC2
H	1259	ALA	-	expression tag	UNP P0DTC2
H	1260	TRP	-	expression tag	UNP P0DTC2
H	1261	SER	-	expression tag	UNP P0DTC2
H	1262	HIS	-	expression tag	UNP P0DTC2
H	1263	PRO	-	expression tag	UNP P0DTC2
H	1264	GLN	-	expression tag	UNP P0DTC2
H	1265	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1266	GLU	-	expression tag	UNP P0DTC2
H	1267	LYS	-	expression tag	UNP P0DTC2
H	1268	GLY	-	expression tag	UNP P0DTC2
H	1269	GLY	-	expression tag	UNP P0DTC2
H	1270	GLY	-	expression tag	UNP P0DTC2
H	1271	SER	-	expression tag	UNP P0DTC2
H	1272	GLY	-	expression tag	UNP P0DTC2
H	1273	GLY	-	expression tag	UNP P0DTC2
H	1274	GLY	-	expression tag	UNP P0DTC2
H	1275	GLY	-	expression tag	UNP P0DTC2
H	1276	SER	-	expression tag	UNP P0DTC2
H	1277	GLY	-	expression tag	UNP P0DTC2
H	1278	GLY	-	expression tag	UNP P0DTC2
H	1279	SER	-	expression tag	UNP P0DTC2
H	1280	ALA	-	expression tag	UNP P0DTC2
H	1281	TRP	-	expression tag	UNP P0DTC2
H	1282	SER	-	expression tag	UNP P0DTC2
H	1283	HIS	-	expression tag	UNP P0DTC2
H	1284	PRO	-	expression tag	UNP P0DTC2
H	1285	GLN	-	expression tag	UNP P0DTC2
H	1286	PHE	-	expression tag	UNP P0DTC2
H	1287	GLU	-	expression tag	UNP P0DTC2
H	1288	LYS	-	expression tag	UNP P0DTC2
J	393	PHE	THR	conflict	UNP P0DTC2
J	607	GLU	GLN	conflict	UNP P0DTC2
J	682	ALA	ARG	conflict	UNP P0DTC2
J	683	ALA	ARG	conflict	UNP P0DTC2
J	892	PRO	ALA	conflict	UNP P0DTC2
J	899	PRO	ALA	conflict	UNP P0DTC2
J	942	PRO	ALA	conflict	UNP P0DTC2
J	986	PRO	LYS	conflict	UNP P0DTC2
J	987	PRO	VAL	conflict	UNP P0DTC2
J	1209	GLY	-	expression tag	UNP P0DTC2
J	1210	SER	-	expression tag	UNP P0DTC2
J	1211	GLY	-	expression tag	UNP P0DTC2
J	1212	TYR	-	expression tag	UNP P0DTC2
J	1213	ILE	-	expression tag	UNP P0DTC2
J	1214	PRO	-	expression tag	UNP P0DTC2
J	1215	GLU	-	expression tag	UNP P0DTC2
J	1216	ALA	-	expression tag	UNP P0DTC2
J	1217	PRO	-	expression tag	UNP P0DTC2
J	1218	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1219	ASP	-	expression tag	UNP P0DTC2
J	1220	GLY	-	expression tag	UNP P0DTC2
J	1221	GLN	-	expression tag	UNP P0DTC2
J	1222	ALA	-	expression tag	UNP P0DTC2
J	1223	TYR	-	expression tag	UNP P0DTC2
J	1224	VAL	-	expression tag	UNP P0DTC2
J	1225	ARG	-	expression tag	UNP P0DTC2
J	1226	LYS	-	expression tag	UNP P0DTC2
J	1227	ASP	-	expression tag	UNP P0DTC2
J	1228	GLY	-	expression tag	UNP P0DTC2
J	1229	GLU	-	expression tag	UNP P0DTC2
J	1230	TRP	-	expression tag	UNP P0DTC2
J	1231	VAL	-	expression tag	UNP P0DTC2
J	1232	LEU	-	expression tag	UNP P0DTC2
J	1233	LEU	-	expression tag	UNP P0DTC2
J	1234	SER	-	expression tag	UNP P0DTC2
J	1235	THR	-	expression tag	UNP P0DTC2
J	1236	PHE	-	expression tag	UNP P0DTC2
J	1237	LEU	-	expression tag	UNP P0DTC2
J	1238	GLY	-	expression tag	UNP P0DTC2
J	1239	ARG	-	expression tag	UNP P0DTC2
J	1240	SER	-	expression tag	UNP P0DTC2
J	1241	LEU	-	expression tag	UNP P0DTC2
J	1242	GLU	-	expression tag	UNP P0DTC2
J	1243	VAL	-	expression tag	UNP P0DTC2
J	1244	LEU	-	expression tag	UNP P0DTC2
J	1245	PHE	-	expression tag	UNP P0DTC2
J	1246	GLN	-	expression tag	UNP P0DTC2
J	1247	GLY	-	expression tag	UNP P0DTC2
J	1248	PRO	-	expression tag	UNP P0DTC2
J	1249	GLY	-	expression tag	UNP P0DTC2
J	1250	HIS	-	expression tag	UNP P0DTC2
J	1251	HIS	-	expression tag	UNP P0DTC2
J	1252	HIS	-	expression tag	UNP P0DTC2
J	1253	HIS	-	expression tag	UNP P0DTC2
J	1254	HIS	-	expression tag	UNP P0DTC2
J	1255	HIS	-	expression tag	UNP P0DTC2
J	1256	HIS	-	expression tag	UNP P0DTC2
J	1257	HIS	-	expression tag	UNP P0DTC2
J	1258	SER	-	expression tag	UNP P0DTC2
J	1259	ALA	-	expression tag	UNP P0DTC2
J	1260	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1261	SER	-	expression tag	UNP P0DTC2
J	1262	HIS	-	expression tag	UNP P0DTC2
J	1263	PRO	-	expression tag	UNP P0DTC2
J	1264	GLN	-	expression tag	UNP P0DTC2
J	1265	PHE	-	expression tag	UNP P0DTC2
J	1266	GLU	-	expression tag	UNP P0DTC2
J	1267	LYS	-	expression tag	UNP P0DTC2
J	1268	GLY	-	expression tag	UNP P0DTC2
J	1269	GLY	-	expression tag	UNP P0DTC2
J	1270	GLY	-	expression tag	UNP P0DTC2
J	1271	SER	-	expression tag	UNP P0DTC2
J	1272	GLY	-	expression tag	UNP P0DTC2
J	1273	GLY	-	expression tag	UNP P0DTC2
J	1274	GLY	-	expression tag	UNP P0DTC2
J	1275	GLY	-	expression tag	UNP P0DTC2
J	1276	SER	-	expression tag	UNP P0DTC2
J	1277	GLY	-	expression tag	UNP P0DTC2
J	1278	GLY	-	expression tag	UNP P0DTC2
J	1279	SER	-	expression tag	UNP P0DTC2
J	1280	ALA	-	expression tag	UNP P0DTC2
J	1281	TRP	-	expression tag	UNP P0DTC2
J	1282	SER	-	expression tag	UNP P0DTC2
J	1283	HIS	-	expression tag	UNP P0DTC2
J	1284	PRO	-	expression tag	UNP P0DTC2
J	1285	GLN	-	expression tag	UNP P0DTC2
J	1286	PHE	-	expression tag	UNP P0DTC2
J	1287	GLU	-	expression tag	UNP P0DTC2
J	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	G	1	Total 14	C 8	N 1	O 5	0
3	H	1	Total 14	C 8	N 1	O 5	0
3	H	1	Total 14	C 8	N 1	O 5	0
3	H	1	Total 14	C 8	N 1	O 5	0
3	H	1	Total 14	C 8	N 1	O 5	0
3	H	1	Total 14	C 8	N 1	O 5	0
3	H	1	Total 14	C 8	N 1	O 5	0
3	H	1	Total 14	C 8	N 1	O 5	0

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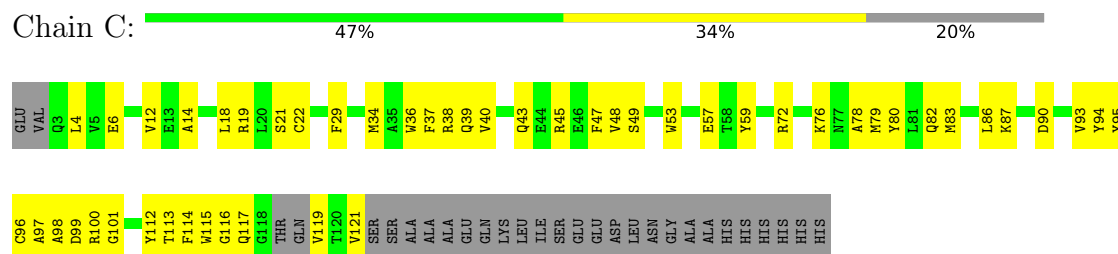
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Mol	Chain	Residues	Atoms				AltConf
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	
3	J	1	Total	C	N	O	0
			14	8	1	5	

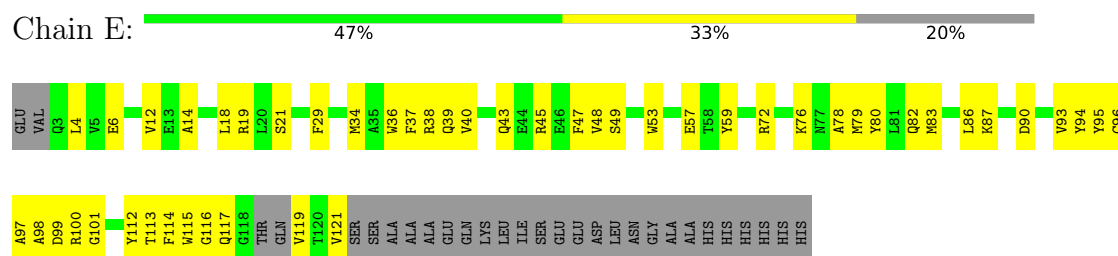
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

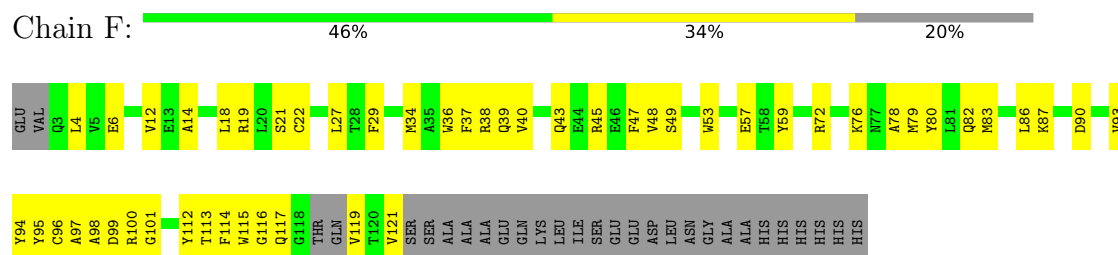
#### • Molecule 1: Nanobody 7F



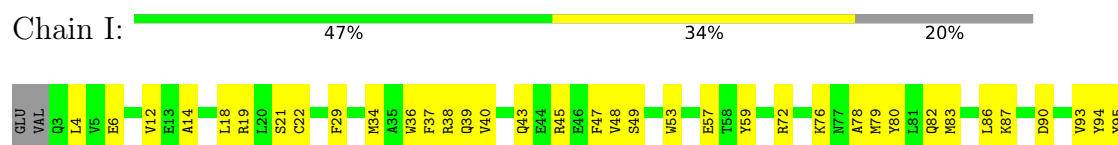
#### • Molecule 1: Nanobody 7F

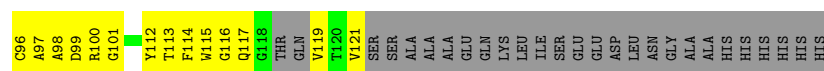


#### • Molecule 1: Nanobody 7F

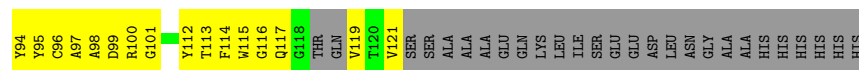
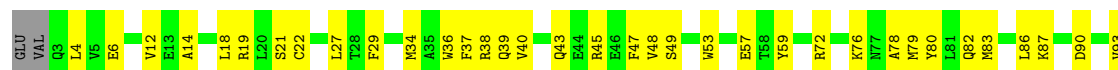


#### • Molecule 1: Nanobody 7F

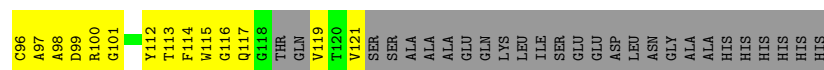




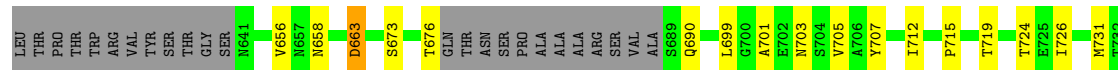
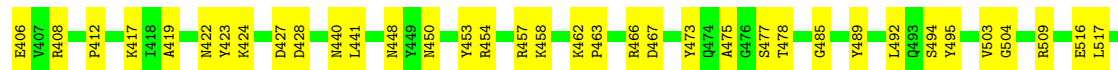
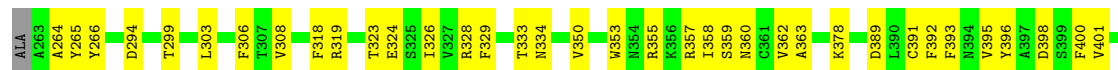
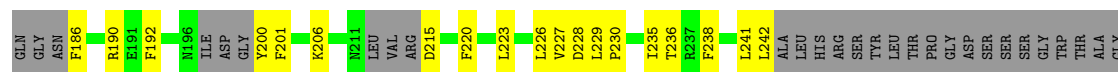
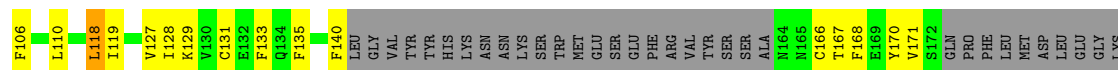
• Molecule 1: Nanobody 7F



• Molecule 1: Nanobody 7F



• Molecule 2: Spike glycoprotein

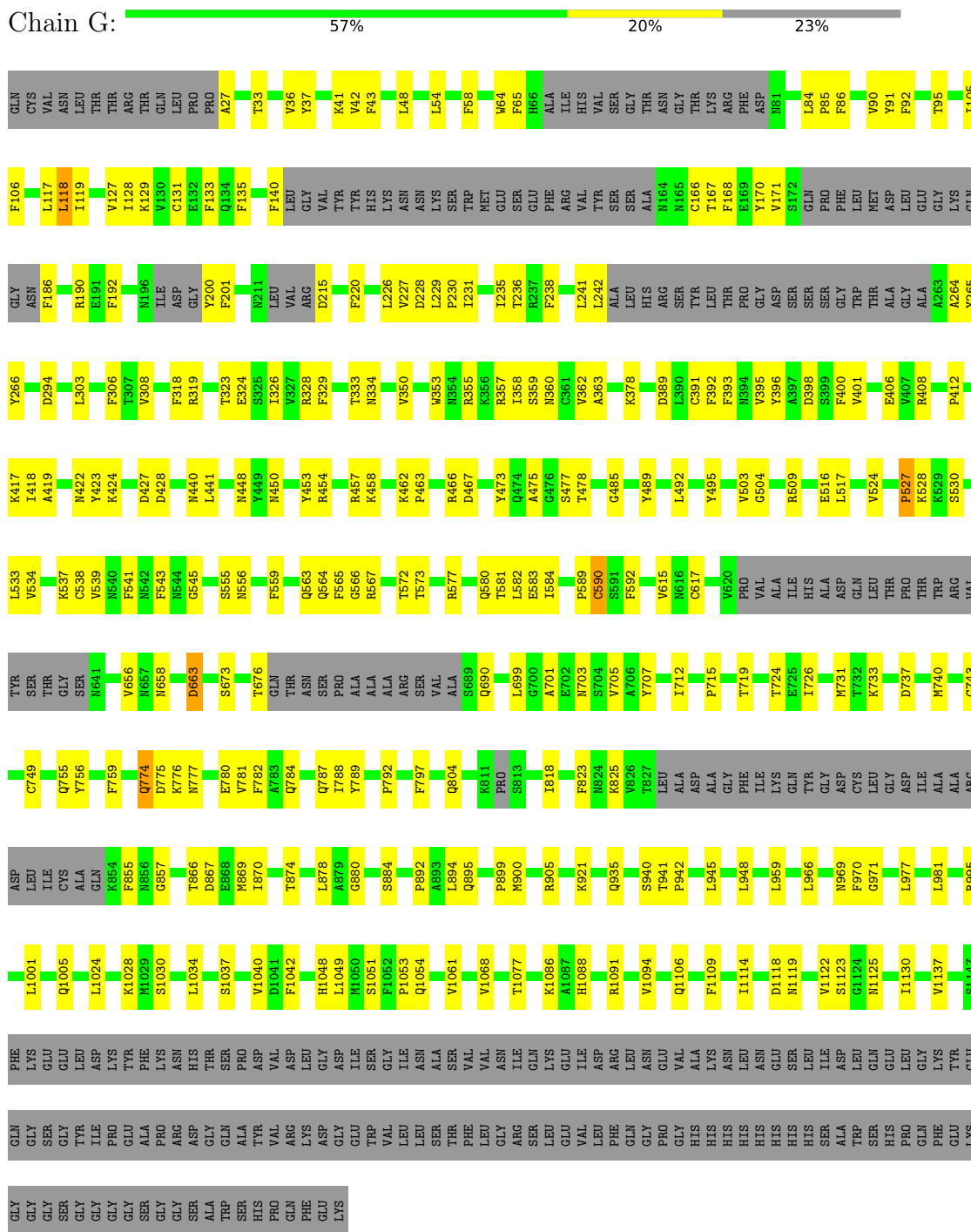








- Molecule 2: Spike glycoprotein



- Molecule 2: Spike glycoprotein

[illegible]

PRO	GLN	R995	ALA	M740	TRP	L533	K417	D294	ASN	F106
	GLY		ALA		ARG	V534	I418		F186	
	LYS	L1001	ARG	C743	VAL	K537	A419	T299		L118
	GLU	L1004	ASP		TYR	C538			R190	I119
	GLY	Q1005	ILE	C749	SER	V539	N422	L303	F192	
	GLY	L1024	CYS	Q755	THR	N540	Y423	F306		
	SER	GLY	ALA	Y756	GLY	F541	K424	T307	N196	
	GLY	LEU	GLN	F759	HE41	N542	D427	V308	ILE	V130
	GLY	K854				N544	D428		ASP	C131
	GLY	M1029	F855	F759	V656	N544		F318	GLY	F132
GLY	GLY	S1030	F855	Q774	N657	G545	N440	R319	Y200	F133
	LYS	L1034	G857	D775	N658	S555	L441		F201	F135
	LYS	L1037	K776	N777	D663	N556		T323		
	ASN	ASP		E780	S673	F559		S325	N211	F140
	GLY	V1040	D867	V781			N448	E324	VAL	LEU
	GLN	D1041	H869	F782	GLN	Q563	Y463	R328	ARG	GLY
	SER	F1042	H783	A783	THR	Q564	R454	F329	D215	VAL
	PRO	ALA		Q784	ASN	F565				TYR
	ASP	VAL	H784		SER	Q566	R457	T333	F220	HIS
	PRO	H1048	L878	Q787	PRO	R567	K458	N334	L226	LYS
GLN	GLN	L1049	L878	I788	ARG				V227	ASN
	LYS	M1050	K879	I788	THR	Q567			D228	ASN
	ASP	S1051	G880	Y789	ALA	T572	K462	V350	L229	LYS
	GLY	F1052	ASP	ALA	ALA	T573	P463		P230	SER
	ILE	Q1054	S884	P792	ALA	R577	R466	N353	TRP	SER
	SER	GLY		ARG	SER		D467	N354	GLY	MET
	GLY	VAL	P892	F797	GLN	Q580		R355	T235	GLU
	ILE	V1061	K893		VAL	T581	Y473	K356	T236	
	ASN	ALA	L894	Q804	ALA	L582	Q474	R357	R237	GLU
	SER	V1068	K895		S689	E583	A475	S359	F238	PHE
PHE	THR	SER		K811	Q690	I584				
	VAL	VAL	P899	PRO			G476	N360	L241	ARG
	LEU	N900	S813				S477	C361	L242	VAL
	GLY			L699		P589	T478	V362	ALA	TYR
	ASN	I1081		G780	THR	C590		A363	LEU	SER
	ILE	K1086	R905	A701	ARG	S591	G485		HIS	SER
	GLN	A1087	K921	E702	GLN	F592		K378	ALA	ALA
	LYS	H1088	Q924	S704	THR		Y469		ARG	ALA
	VAL	ILE	Q935	K825	V705	S605	D389	T391	TYR	N164
	ASP	R1091		V826	A786	N606	L492	L390	LEU	N165
PHE	LEU	ASP		T827	Y707			C391	THR	C166
	THR	GLN	S940	LEU		V615	Y495	F392	PRO	T167
	GLN	LEU	P942	ALA	I712	N616		F393	GLY	F168
	GLY	ASN		ASP	THR	C617	V503	N394	ASP	E169
	PRO	Q1106	ALA	ASP			G504	V395	GLY	Y170
	GLY	VAL	L945	ALA	F715			Y396	SER	V171
	ALA	F1109	GLY	GLY		V620		A397	SER	S172
	HIS	LYS	PHE	THR	T719	PRO	R509		SER	GLN
	HIS	I1114	ILE	GLY	VAL	VAL		D398	GLY	PRO
	ASN	I1115	LYS	LYS	T724	ALA	E516	S399	TRP	PHE
HIS	ASN		GLN	E725	ILE	L517		F400	THR	LEU
	GLY	D1118	N969	I726	HIS		V824	V401	ALA	MET
	SER	N1119	F970	GLY	ALA	ALA			GLY	ASP
	SER		ASP	THR	ASP	ASP		E406	ALA	LEU
	ILE	V1122	CYS	T732	GLN	GLN	P527	V407	A263	GLY
	ALA	S1123	LYS	K733	THR	LEU	K528	R408	A264	GLY
	THR	G1124	GLY	D737	THR	THR	K529		Y265	LYS
	SER	N1125	ASP	T15	PRO	PRO	S530	P412	Y266	GLN
	GLY									GLY

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43791	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C	0.27	0/956	0.51	0/1293
1	E	0.27	0/956	0.51	0/1293
1	F	0.26	0/956	0.51	0/1293
1	I	0.27	0/956	0.51	0/1293
1	K	0.27	0/956	0.51	0/1293
1	L	0.26	0/956	0.51	0/1293
2	A	0.38	0/7765	0.52	5/10575 (0.0%)
2	B	0.38	0/7765	0.52	5/10575 (0.0%)
2	D	0.38	0/7765	0.52	5/10575 (0.0%)
2	G	0.38	0/7765	0.52	5/10575 (0.0%)
2	H	0.38	0/7765	0.52	5/10575 (0.0%)
2	J	0.38	0/7765	0.52	5/10575 (0.0%)
All	All	0.37	0/52326	0.52	30/71208 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
2	B	0	1
2	D	0	1
2	G	0	1
2	H	0	1
2	J	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	527	PRO	O-C-N	-9.06	108.20	122.70
2	J	527	PRO	O-C-N	-9.06	108.20	122.70
2	G	527	PRO	O-C-N	-9.06	108.21	122.70
2	H	527	PRO	O-C-N	-9.06	108.21	122.70
2	A	527	PRO	O-C-N	-9.05	108.22	122.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	527	PRO	Mainchain
2	B	527	PRO	Mainchain
2	D	527	PRO	Mainchain
2	G	527	PRO	Mainchain
2	H	527	PRO	Mainchain

## 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	C	933	0	865	52	0
1	E	933	0	865	51	0
1	F	933	0	865	53	0
1	I	933	0	865	51	0
1	K	933	0	865	52	0
1	L	933	0	865	54	0
2	A	7594	0	7294	390	0
2	B	7594	0	7294	385	0
2	D	7594	0	7294	391	0
2	G	7594	0	7294	387	0
2	H	7594	0	7294	397	0
2	J	7594	0	7294	389	0
3	A	98	0	91	1	0
3	B	98	0	91	1	0
3	D	98	0	91	1	0
3	G	98	0	91	1	0
3	H	98	0	91	1	0
3	J	98	0	91	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	51750	0	49500	2000	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 20.

The worst 5 of 2000 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)
2:J:565:PHE:CE2	2:J:567:ARG:HG3	1.01	1.54
2:B:565:PHE:CE2	2:B:567:ARG:HG3	1.01	1.54
2:A:565:PHE:CE2	2:A:567:ARG:HG3	1.01	1.52
2:G:565:PHE:HE2	2:G:567:ARG:CG	1.22	1.52
2:G:565:PHE:CE2	2:G:567:ARG:HG3	1.01	1.51

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	C	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	E	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	F	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	I	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	K	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
1	L	117/148 (79%)	108 (92%)	9 (8%)	0	100	100
2	A	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	B	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	D	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	H	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
2	J	964/1275 (76%)	909 (94%)	55 (6%)	0	100	100
All	All	6486/8538 (76%)	6102 (94%)	384 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	C	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	E	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	F	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	I	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	K	96/119 (81%)	95 (99%)	1 (1%)	73	84
1	L	96/119 (81%)	95 (99%)	1 (1%)	73	84
2	A	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	B	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	D	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	G	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	H	831/1102 (75%)	826 (99%)	5 (1%)	84	90
2	J	831/1102 (75%)	826 (99%)	5 (1%)	84	90
All	All	5562/7326 (76%)	5526 (99%)	36 (1%)	82	90

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	774	GLN
2	J	1123	SER

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Mol	Chain	Res	Type
2	H	1123	SER
2	J	590	CYS
1	F	95	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	655	HIS
2	J	1048	HIS
2	D	360	ASN
2	B	1106	GLN
2	J	1071	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

42 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	$\# Z  > 2$
3	NAG	D	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	G	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	G	1303	2	14,14,15	0.75	0	17,19,21	0.83	0
3	NAG	J	1303	2	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	B	1305	2	14,14,15	0.70	0	17,19,21	1.24	2 (11%)
3	NAG	J	1302	2	14,14,15	0.68	0	17,19,21	1.01	1 (5%)
3	NAG	D	1303	2	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	B	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	J	1307	2	14,14,15	0.81	0	17,19,21	0.88	0
3	NAG	D	1307	2	14,14,15	0.81	0	17,19,21	0.88	0
3	NAG	H	1307	2	14,14,15	0.80	0	17,19,21	0.89	0
3	NAG	B	1304	2	14,14,15	0.71	0	17,19,21	0.91	0
3	NAG	A	1307	2	14,14,15	0.80	0	17,19,21	0.88	0
3	NAG	D	1304	2	14,14,15	0.71	0	17,19,21	0.91	0
3	NAG	A	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	A	1304	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	H	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	G	1304	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	D	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	J	1304	2	14,14,15	0.71	0	17,19,21	0.91	0
3	NAG	G	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	H	1305	2	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
3	NAG	H	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	J	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	B	1307	2	14,14,15	0.81	0	17,19,21	0.89	0
3	NAG	B	1302	2	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	NAG	A	1305	2	14,14,15	0.71	0	17,19,21	1.24	2 (11%)
3	NAG	A	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	G	1307	2	14,14,15	0.81	0	17,19,21	0.88	0
3	NAG	A	1301	2	14,14,15	0.69	0	17,19,21	1.13	1 (5%)
3	NAG	H	1304	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	D	1302	2	14,14,15	0.68	0	17,19,21	1.01	1 (5%)
3	NAG	A	1303	2	14,14,15	0.75	0	17,19,21	0.83	0
3	NAG	D	1305	2	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
3	NAG	H	1306	2	14,14,15	0.77	0	17,19,21	0.87	0
3	NAG	G	1305	2	14,14,15	0.70	0	17,19,21	1.24	2 (11%)
3	NAG	J	1305	2	14,14,15	0.70	0	17,19,21	1.25	2 (11%)
3	NAG	J	1306	2	14,14,15	0.76	0	17,19,21	0.87	0
3	NAG	B	1303	2	14,14,15	0.75	0	17,19,21	0.82	0
3	NAG	G	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1301	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
3	NAG	H	1303	2	14,14,15	0.74	0	17,19,21	0.82	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
3	NAG	D	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	G	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	J	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1307	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1304	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1302	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1305	2	-	1/6/23/26	0/1/1/1
3	NAG	J	1306	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	2	-	1/6/23/26	0/1/1/1
3	NAG	G	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	B	1301	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1303	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	NAG	C2-N2-C7	3.01	127.19	122.90
3	G	1301	NAG	C2-N2-C7	3.01	127.19	122.90
3	D	1301	NAG	C2-N2-C7	3.00	127.17	122.90
3	J	1301	NAG	C2-N2-C7	3.00	127.17	122.90
3	B	1301	NAG	C2-N2-C7	2.99	127.15	122.90

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	D	1306	NAG	O5-C5-C6-O6
3	G	1306	NAG	O5-C5-C6-O6
3	H	1306	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1302	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1302	NAG	1	0
3	A	1302	NAG	1	0
3	H	1302	NAG	1	0
3	B	1302	NAG	1	0
3	D	1302	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.