



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Nov 2, 2017 – 06:40 AM EDT

PDB ID : 5W9K
EMDB ID: : EMD-8786
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : unknown
Resolution : 4.60 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

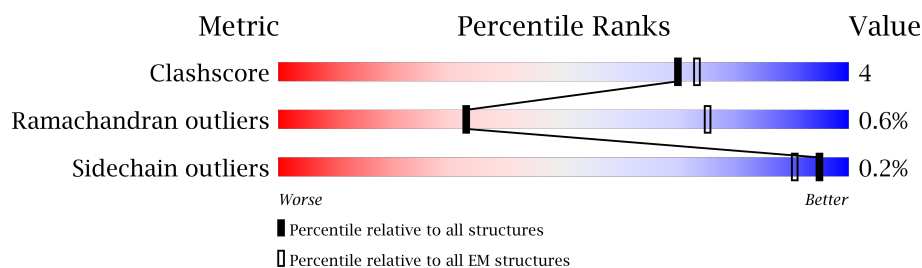
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1329	33% 65%
1	D	1329	33% 65%
1	G	1329	33% 65%
1	J	1329	51% 46%
1	K	1329	51% 46%
1	L	1329	50% 46%
2	B	233	51% 49%
2	E	233	51% 49%
2	H	233	51% 49%

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Mol	Chain	Length	Quality of chain
3	C	218	<div><div></div><div>49%</div><div></div><div></div><div>49%</div></div>
3	F	218	<div><div></div><div>50%</div><div></div><div></div><div>49%</div></div>
3	I	218	<div><div></div><div>50%</div><div></div><div></div><div>49%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32873 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	461	Total	C	N	O	S	0	0
			3531	2233	598	683	17		
1	D	462	Total	C	N	O	S	0	0
			3538	2238	599	684	17		
1	G	460	Total	C	N	O	S	0	0
			3527	2231	597	682	17		
1	J	724	Total	C	N	O	S	0	0
			5645	3593	924	1094	34		
1	K	724	Total	C	N	O	S	0	0
			5645	3593	924	1094	34		
1	L	723	Total	C	N	O	S	0	0
			5638	3589	923	1092	34		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	conflict	UNP W5ZZF5
A	1061	PRO	LEU	conflict	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
D	506	PHE	LEU	conflict	UNP W5ZZF5
D	748	ALA	ARG	conflict	UNP W5ZZF5
D	751	GLY	ARG	conflict	UNP W5ZZF5
D	1060	PRO	VAL	conflict	UNP W5ZZF5
D	1061	PRO	LEU	conflict	UNP W5ZZF5
D	1292	GLY	-	expression tag	UNP W5ZZF5
D	1293	SER	-	expression tag	UNP W5ZZF5
D	1294	GLY	-	expression tag	UNP W5ZZF5
D	1295	TYR	-	expression tag	UNP W5ZZF5
D	1296	ILE	-	expression tag	UNP W5ZZF5
D	1297	PRO	-	expression tag	UNP W5ZZF5
D	1298	GLU	-	expression tag	UNP W5ZZF5
D	1299	ALA	-	expression tag	UNP W5ZZF5
D	1300	PRO	-	expression tag	UNP W5ZZF5
D	1301	ARG	-	expression tag	UNP W5ZZF5
D	1302	ASP	-	expression tag	UNP W5ZZF5
D	1303	GLY	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1304	GLN	-	expression tag	UNP W5ZZF5
D	1305	ALA	-	expression tag	UNP W5ZZF5
D	1306	TYR	-	expression tag	UNP W5ZZF5
D	1307	VAL	-	expression tag	UNP W5ZZF5
D	1308	ARG	-	expression tag	UNP W5ZZF5
D	1309	LYS	-	expression tag	UNP W5ZZF5
D	1310	ASP	-	expression tag	UNP W5ZZF5
D	1311	GLY	-	expression tag	UNP W5ZZF5
D	1312	GLU	-	expression tag	UNP W5ZZF5
D	1313	TRP	-	expression tag	UNP W5ZZF5
D	1314	VAL	-	expression tag	UNP W5ZZF5
D	1315	LEU	-	expression tag	UNP W5ZZF5
D	1316	LEU	-	expression tag	UNP W5ZZF5
D	1317	SER	-	expression tag	UNP W5ZZF5
D	1318	THR	-	expression tag	UNP W5ZZF5
D	1319	PHE	-	expression tag	UNP W5ZZF5
D	1320	LEU	-	expression tag	UNP W5ZZF5
D	1321	GLY	-	expression tag	UNP W5ZZF5
D	1322	ARG	-	expression tag	UNP W5ZZF5
D	1323	SER	-	expression tag	UNP W5ZZF5
D	1324	LEU	-	expression tag	UNP W5ZZF5
D	1325	GLU	-	expression tag	UNP W5ZZF5
D	1326	VAL	-	expression tag	UNP W5ZZF5
D	1327	LEU	-	expression tag	UNP W5ZZF5
D	1328	PHE	-	expression tag	UNP W5ZZF5
D	1329	GLN	-	expression tag	UNP W5ZZF5
G	506	PHE	LEU	conflict	UNP W5ZZF5
G	748	ALA	ARG	conflict	UNP W5ZZF5
G	751	GLY	ARG	conflict	UNP W5ZZF5
G	1060	PRO	VAL	conflict	UNP W5ZZF5
G	1061	PRO	LEU	conflict	UNP W5ZZF5
G	1292	GLY	-	expression tag	UNP W5ZZF5
G	1293	SER	-	expression tag	UNP W5ZZF5
G	1294	GLY	-	expression tag	UNP W5ZZF5
G	1295	TYR	-	expression tag	UNP W5ZZF5
G	1296	ILE	-	expression tag	UNP W5ZZF5
G	1297	PRO	-	expression tag	UNP W5ZZF5
G	1298	GLU	-	expression tag	UNP W5ZZF5
G	1299	ALA	-	expression tag	UNP W5ZZF5
G	1300	PRO	-	expression tag	UNP W5ZZF5
G	1301	ARG	-	expression tag	UNP W5ZZF5
G	1302	ASP	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1303	GLY	-	expression tag	UNP W5ZZF5
G	1304	GLN	-	expression tag	UNP W5ZZF5
G	1305	ALA	-	expression tag	UNP W5ZZF5
G	1306	TYR	-	expression tag	UNP W5ZZF5
G	1307	VAL	-	expression tag	UNP W5ZZF5
G	1308	ARG	-	expression tag	UNP W5ZZF5
G	1309	LYS	-	expression tag	UNP W5ZZF5
G	1310	ASP	-	expression tag	UNP W5ZZF5
G	1311	GLY	-	expression tag	UNP W5ZZF5
G	1312	GLU	-	expression tag	UNP W5ZZF5
G	1313	TRP	-	expression tag	UNP W5ZZF5
G	1314	VAL	-	expression tag	UNP W5ZZF5
G	1315	LEU	-	expression tag	UNP W5ZZF5
G	1316	LEU	-	expression tag	UNP W5ZZF5
G	1317	SER	-	expression tag	UNP W5ZZF5
G	1318	THR	-	expression tag	UNP W5ZZF5
G	1319	PHE	-	expression tag	UNP W5ZZF5
G	1320	LEU	-	expression tag	UNP W5ZZF5
G	1321	GLY	-	expression tag	UNP W5ZZF5
G	1322	ARG	-	expression tag	UNP W5ZZF5
G	1323	SER	-	expression tag	UNP W5ZZF5
G	1324	LEU	-	expression tag	UNP W5ZZF5
G	1325	GLU	-	expression tag	UNP W5ZZF5
G	1326	VAL	-	expression tag	UNP W5ZZF5
G	1327	LEU	-	expression tag	UNP W5ZZF5
G	1328	PHE	-	expression tag	UNP W5ZZF5
G	1329	GLN	-	expression tag	UNP W5ZZF5
J	506	PHE	LEU	conflict	UNP W5ZZF5
J	748	ALA	ARG	conflict	UNP W5ZZF5
J	751	GLY	ARG	conflict	UNP W5ZZF5
J	1060	PRO	VAL	conflict	UNP W5ZZF5
J	1061	PRO	LEU	conflict	UNP W5ZZF5
J	1292	GLY	-	expression tag	UNP W5ZZF5
J	1293	SER	-	expression tag	UNP W5ZZF5
J	1294	GLY	-	expression tag	UNP W5ZZF5
J	1295	TYR	-	expression tag	UNP W5ZZF5
J	1296	ILE	-	expression tag	UNP W5ZZF5
J	1297	PRO	-	expression tag	UNP W5ZZF5
J	1298	GLU	-	expression tag	UNP W5ZZF5
J	1299	ALA	-	expression tag	UNP W5ZZF5
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1302	ASP	-	expression tag	UNP W5ZZF5
J	1303	GLY	-	expression tag	UNP W5ZZF5
J	1304	GLN	-	expression tag	UNP W5ZZF5
J	1305	ALA	-	expression tag	UNP W5ZZF5
J	1306	TYR	-	expression tag	UNP W5ZZF5
J	1307	VAL	-	expression tag	UNP W5ZZF5
J	1308	ARG	-	expression tag	UNP W5ZZF5
J	1309	LYS	-	expression tag	UNP W5ZZF5
J	1310	ASP	-	expression tag	UNP W5ZZF5
J	1311	GLY	-	expression tag	UNP W5ZZF5
J	1312	GLU	-	expression tag	UNP W5ZZF5
J	1313	TRP	-	expression tag	UNP W5ZZF5
J	1314	VAL	-	expression tag	UNP W5ZZF5
J	1315	LEU	-	expression tag	UNP W5ZZF5
J	1316	LEU	-	expression tag	UNP W5ZZF5
J	1317	SER	-	expression tag	UNP W5ZZF5
J	1318	THR	-	expression tag	UNP W5ZZF5
J	1319	PHE	-	expression tag	UNP W5ZZF5
J	1320	LEU	-	expression tag	UNP W5ZZF5
J	1321	GLY	-	expression tag	UNP W5ZZF5
J	1322	ARG	-	expression tag	UNP W5ZZF5
J	1323	SER	-	expression tag	UNP W5ZZF5
J	1324	LEU	-	expression tag	UNP W5ZZF5
J	1325	GLU	-	expression tag	UNP W5ZZF5
J	1326	VAL	-	expression tag	UNP W5ZZF5
J	1327	LEU	-	expression tag	UNP W5ZZF5
J	1328	PHE	-	expression tag	UNP W5ZZF5
J	1329	GLN	-	expression tag	UNP W5ZZF5
K	506	PHE	LEU	conflict	UNP W5ZZF5
K	748	ALA	ARG	conflict	UNP W5ZZF5
K	751	GLY	ARG	conflict	UNP W5ZZF5
K	1060	PRO	VAL	conflict	UNP W5ZZF5
K	1061	PRO	LEU	conflict	UNP W5ZZF5
K	1292	GLY	-	expression tag	UNP W5ZZF5
K	1293	SER	-	expression tag	UNP W5ZZF5
K	1294	GLY	-	expression tag	UNP W5ZZF5
K	1295	TYR	-	expression tag	UNP W5ZZF5
K	1296	ILE	-	expression tag	UNP W5ZZF5
K	1297	PRO	-	expression tag	UNP W5ZZF5
K	1298	GLU	-	expression tag	UNP W5ZZF5
K	1299	ALA	-	expression tag	UNP W5ZZF5
K	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1301	ARG	-	expression tag	UNP W5ZZF5
K	1302	ASP	-	expression tag	UNP W5ZZF5
K	1303	GLY	-	expression tag	UNP W5ZZF5
K	1304	GLN	-	expression tag	UNP W5ZZF5
K	1305	ALA	-	expression tag	UNP W5ZZF5
K	1306	TYR	-	expression tag	UNP W5ZZF5
K	1307	VAL	-	expression tag	UNP W5ZZF5
K	1308	ARG	-	expression tag	UNP W5ZZF5
K	1309	LYS	-	expression tag	UNP W5ZZF5
K	1310	ASP	-	expression tag	UNP W5ZZF5
K	1311	GLY	-	expression tag	UNP W5ZZF5
K	1312	GLU	-	expression tag	UNP W5ZZF5
K	1313	TRP	-	expression tag	UNP W5ZZF5
K	1314	VAL	-	expression tag	UNP W5ZZF5
K	1315	LEU	-	expression tag	UNP W5ZZF5
K	1316	LEU	-	expression tag	UNP W5ZZF5
K	1317	SER	-	expression tag	UNP W5ZZF5
K	1318	THR	-	expression tag	UNP W5ZZF5
K	1319	PHE	-	expression tag	UNP W5ZZF5
K	1320	LEU	-	expression tag	UNP W5ZZF5
K	1321	GLY	-	expression tag	UNP W5ZZF5
K	1322	ARG	-	expression tag	UNP W5ZZF5
K	1323	SER	-	expression tag	UNP W5ZZF5
K	1324	LEU	-	expression tag	UNP W5ZZF5
K	1325	GLU	-	expression tag	UNP W5ZZF5
K	1326	VAL	-	expression tag	UNP W5ZZF5
K	1327	LEU	-	expression tag	UNP W5ZZF5
K	1328	PHE	-	expression tag	UNP W5ZZF5
K	1329	GLN	-	expression tag	UNP W5ZZF5
L	506	PHE	LEU	conflict	UNP W5ZZF5
L	748	ALA	ARG	conflict	UNP W5ZZF5
L	751	GLY	ARG	conflict	UNP W5ZZF5
L	1060	PRO	VAL	conflict	UNP W5ZZF5
L	1061	PRO	LEU	conflict	UNP W5ZZF5
L	1292	GLY	-	expression tag	UNP W5ZZF5
L	1293	SER	-	expression tag	UNP W5ZZF5
L	1294	GLY	-	expression tag	UNP W5ZZF5
L	1295	TYR	-	expression tag	UNP W5ZZF5
L	1296	ILE	-	expression tag	UNP W5ZZF5
L	1297	PRO	-	expression tag	UNP W5ZZF5
L	1298	GLU	-	expression tag	UNP W5ZZF5
L	1299	ALA	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1300	PRO	-	expression tag	UNP W5ZZF5
L	1301	ARG	-	expression tag	UNP W5ZZF5
L	1302	ASP	-	expression tag	UNP W5ZZF5
L	1303	GLY	-	expression tag	UNP W5ZZF5
L	1304	GLN	-	expression tag	UNP W5ZZF5
L	1305	ALA	-	expression tag	UNP W5ZZF5
L	1306	TYR	-	expression tag	UNP W5ZZF5
L	1307	VAL	-	expression tag	UNP W5ZZF5
L	1308	ARG	-	expression tag	UNP W5ZZF5
L	1309	LYS	-	expression tag	UNP W5ZZF5
L	1310	ASP	-	expression tag	UNP W5ZZF5
L	1311	GLY	-	expression tag	UNP W5ZZF5
L	1312	GLU	-	expression tag	UNP W5ZZF5
L	1313	TRP	-	expression tag	UNP W5ZZF5
L	1314	VAL	-	expression tag	UNP W5ZZF5
L	1315	LEU	-	expression tag	UNP W5ZZF5
L	1316	LEU	-	expression tag	UNP W5ZZF5
L	1317	SER	-	expression tag	UNP W5ZZF5
L	1318	THR	-	expression tag	UNP W5ZZF5
L	1319	PHE	-	expression tag	UNP W5ZZF5
L	1320	LEU	-	expression tag	UNP W5ZZF5
L	1321	GLY	-	expression tag	UNP W5ZZF5
L	1322	ARG	-	expression tag	UNP W5ZZF5
L	1323	SER	-	expression tag	UNP W5ZZF5
L	1324	LEU	-	expression tag	UNP W5ZZF5
L	1325	GLU	-	expression tag	UNP W5ZZF5
L	1326	VAL	-	expression tag	UNP W5ZZF5
L	1327	LEU	-	expression tag	UNP W5ZZF5
L	1328	PHE	-	expression tag	UNP W5ZZF5
L	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	H	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

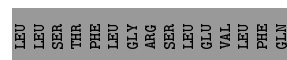
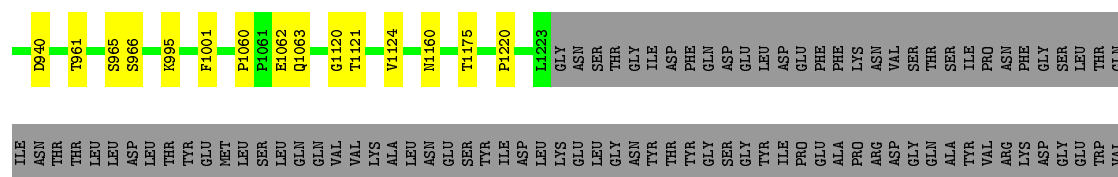
- Molecule 3 is a protein called G4 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	F	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	I	111	Total 835	C 522	N 143	O 166	S 4	0	0

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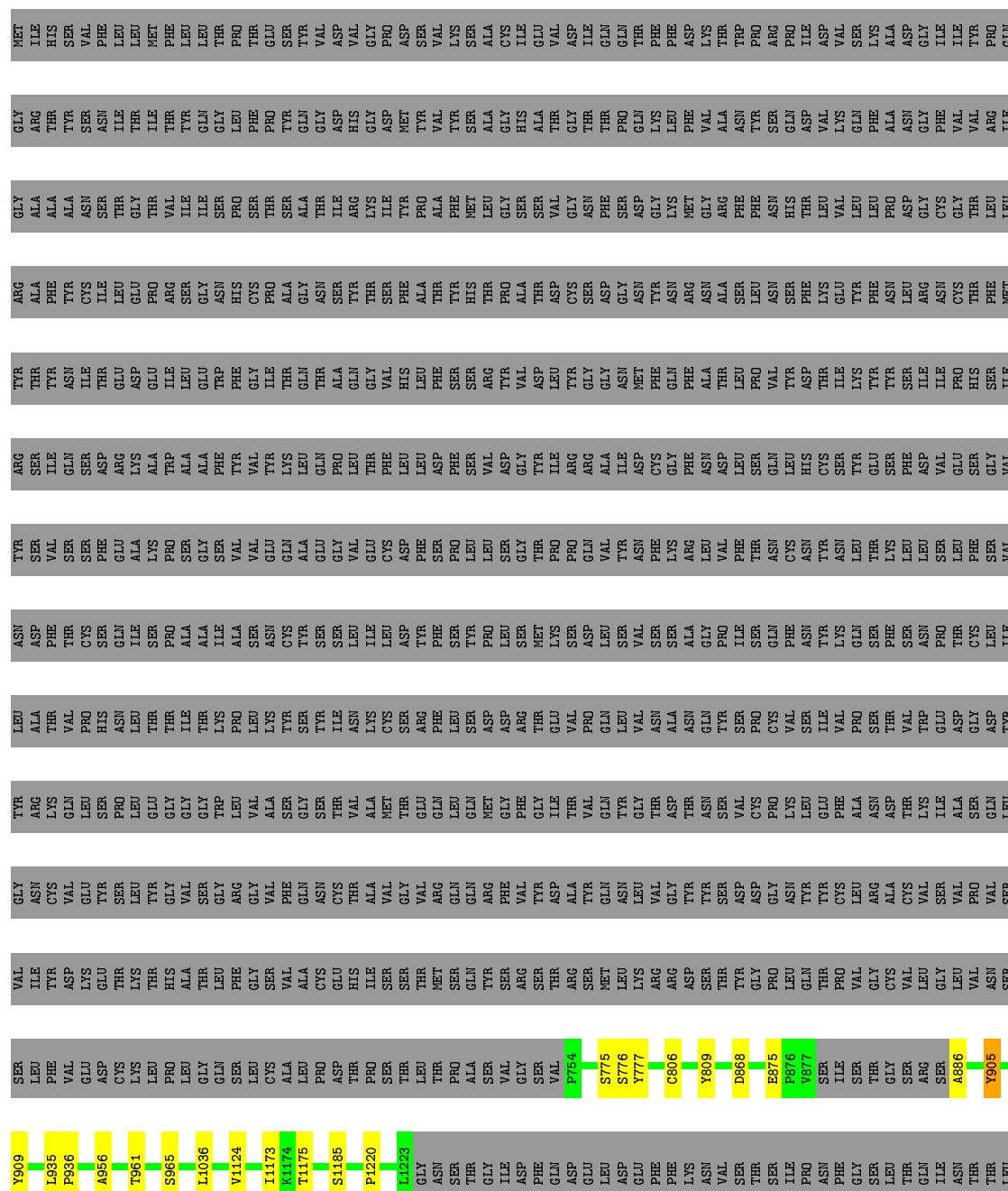
- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein

Chain D:  33% 65%



[illegible]

- Molecule 1: Spike glycoprotein

Chain G: 33% 65%

C912	THR	LEU	ASN	VAL	GLY	TYR	LEU	ASN	THR	LEU	ASN	THR	ARG	THR	ARG	THR	GLY	MET
C925	LEU	LEU	THR	ILE	ASN	ARG	ALA	ASP	SER	ALA	ASP	SER	SER	THR	ALA	ARG	ILE	THR
Y932	ASP	ASP	VAL	ASP	VAL	GLN	VAL	GLU	THR	PRO	THR	GLN	GLN	THR	TYR	THR	ASN	VAL
D940	THR	THR	GLU	THR	TYR	SER	ASN	SER	PRO	ASN	GLN	GLN	ARG	GLU	GLY	THR	ILE	LEU
T961	MET	THR	THR	HIS	GLY	GLY	ILE	THR	PRO	THR	ILE	ALA	TRP	ILE	ARG	THR	ILE	THR
S965	SER	LEU	ALA	THR	VAL	GLY	THR	THR	ILE	ALA	ALA	SER	SER	ALA	SER	ILE	TYR	LEU
S966	LEU	LEU	GLY	GLN	GLY	TRP	THR	THR	LYS	THR	ILE	GLY	PHE	GLY	GLY	GLY	GLN	LEU
F1001	GLN	GLN	ARG	PHE	GLY	LEU	PRO	ALA	SER	ALA	ILE	VAL	TYR	THR	THR	SER	THR	THR
P1060	VAL	VAL	GLY	THR	GLY	VAL	LEU	ALA	SER	LEU	VAL	VAL	VAL	GLY	VAL	PHE	PHE	PRO
Q1063	LYS	ALA	PHE	VAL	PHE	SER	TYR	CYS	TYR	TYR	CYS	GLN	LYS	THR	ALA	SER	TYR	TYR
V1124	ASN	LEU	ASN	CYS	ASN	THR	TYR	SER	SER	SER	SER	GLY	GLN	THR	GLY	ASN	GLN	VAL
T1175	SER	GLU	THR	HIS	THR	VAL	ASN	ILE	ILE	ILE	ILE	VAL	THR	GLY	THR	ARG	HIS	VAL
P1220	TYR	TYR	SER	SER	VAL	MET	CYS	SER	ASP	ASP	ASP	CYS	ASP	VAL	PHE	THR	ILE	PRO
L1423	ASP	ASP	LEU	THR	VAL	GLU	ARG	THR	THR	ARG	TYR	PHE	PHE	LEU	LEU	ALA	THR	SER
GLY	LEU	THR	THR	MET	ARG	GLN	PHE	PHE	PHE	ASN	ASN	SER	SER	THR	THR	ALA	TYR	VAL
ASN	GLU	GLU	ALA	SER	GLN	LEU	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	SER
SER	LEU	LEU	THR	TYR	ARG	MET	ASP	GLY	GLY	ASP	LEU	LEU	VAL	ARG	THR	ALA	ALA	ALA
THR	GLY	GLY	ASN	SER	PHE	GLY	THR	PHE	THR	THR	THR	THR	GLY	GLY	THR	GLY	GLY	GLY
ASN	ILE	TYR	SER	SER	TYR	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	THR	PHE	VAL	THR	ALA	ILE	THR	ASP	ILE	VAL	VAL	GLY	CYS	GLY	GLY	VAL	VAL	VAL
GLN	SER	GLY	GLY	THR	THR	VAL	PRO	SER	ARG	PRO	GLN	GLN	ARG	GLY	GLY	ASN	ASN	ASN
ASP	THR	ASP	PHE	ARG	TYR	THR	ASN	ASP	THR	LEU	LEU	VAL	ALA	PHE	THR	THR	THR	THR
PHE	ALA	PHE	LYS	SER	TYR	ASN	GLN	GLY	ASN	GLN	GLY	ASN	ALA	ALA	ALA	GLY	LYS	LYS
PRO	PRO	ASN	THR	THR	SER	SER	TYR	SER	PRO	VAL	VAL	ASP	ALA	ALA	ALA	ANG	ANG	THR
LYS	ARG	VAL	VAL	TYR	GLY	VAL	VAL	VAL	ILE	SER	ILE	ILE	THR	THR	THR	THR	THR	THR
ASP	THR	THR	THR	THR	THR	CYS	PRO	THR	CYS	PRO	GLN	GLN	GLN	THR	THR	THR	THR	THR
GLY	GLY	GLY	GLY	PRO	GLY	PRO	CYS	GLY	PRO	CYS	ASN	GLN	GLN	VAL	VAL	GLN	GLN	GLN
THR	THR	THR	THR	LEU	ASN	LYS	VAL	PHE	THR	THR	PHE	THR	THR	THR	THR	THR	THR	THR
ALA	ALA	THR	GLN	GLN	THR	GLU	SER	THR	ASN	SER	ASN	ASN	THR	THR	THR	THR	THR	THR
ILE	ILE	THR	THR	THR	TYR	GLU	ILE	THR	TYR	ILE	ASN	ASN	THR	THR	THR	THR	THR	THR
VAL	VAL	THR	THR	PRO	TYR	PHE	PRO	VAL	CYS	VAL	VAL	VAL	GLU	GLU	VAL	VAL	VAL	VAL
ARG	ARG	ARG	VAL	VAL	LEU	ALA	VAL	ALA	ASN	GLN	GLN	GLN	THR	THR	THR	THR	THR	THR
LYS	LYS	THR	GLY	GLY	ASN	ASN	THR	SER	SER	SER	SER	SER	GLU	THR	PHE	PHE	LYS	LYS
ASP																		

ASN	TYR	ASN	GLY	VAL	LYS	SER
TYR	THR	ASP	ILE	ASN	ALA	ALA
TYR	TYR	PHE	GLN	THR	SER	GLN
GLY	GLY	ASP	ILE	PHE	LYS	ILE
SER	SER	ASP	GLY	ILE	ARG	ASP
GLY	TYR	LEU	LEU	LYS	SER	ILE
TYR	TYR	LEU	THR	ASN	GLY	ILE
ILE	ASP	ASP	ASN	ASN	PHE	GLN
PRO	PRO	GLU	GLU	THR	CYS	ARG
GLU	GLU	PHE	PHE	ARG	GLY	LEU
ALA	ALA	LYS	ILE	ILE	GLN	ASP
PRO	PRO	ASN	VAL	GLY	PRO	PRO
ARG	ASP	ASN	VAL	THR	THR	PRO
ASP	ASP	VAL	ASP	GLU	HIS	GLU
GLN	GLN	SER	SER	ILE	ILE	GLN
ALA	ALA	THR	THR	TRP	VAL	ASP
TYR	TYR	SER	SER	SER	SER	ALA
VAL	VAL	ILE	PRO	TYR	PHE	GLN
THR	THR	PRO	PRO	THR	VAL	ILE
ARG	ARG	ASN	ASN	GLY	VAL	ASN
LYS	LYS	PHE	ASN	SER	ASN	ARG
ASP	ASP	GLY	GLY	SER	ALA	LEU
GLY	GLY	SER	SER	PHE	PRO	ILE
GLU	GLU	LEU	LEU	TYR	ASN	ASN
TRP	TRP	THR	THR	ALA	GLY	GLY
VAL	VAL	GLN	GLN	PRO	LEU	ARG
ILE	ILE	ILE	ILE	GLU	TYR	LEU
ASN	ASN	THR	ASN	PRO	PHE	THR
LEU	LEU	THR	THR	ILE	MET	THR
SER	SER	THR	THR	THR	HIS	LEU
PHE	PHE	LEU	LEU	SER	VAL	ASN
GLY	GLY	LEU	LEU	SER	GLY	ALA
ARG	ARG	ASP	ASP	ASN	TYR	PHE
SER	SER	LEU	LEU	THR	TYR	VAL
LEU	LEU	THR	THR	LYS	PRO	ALA
LEU	LEU	TYR	TYR	TYR	SER	GLN
GLU	GLU	GLU	GLU	VAL	ASN	GLN
VAL	VAL	MET	MET	ALA	HIS	LEU
LEU	LEU	LEU	LEU	PRO	ILE	VAL
PHE	PHE	SER	SER	GLN	GLU	ARG
GLN	GLN	LEU	LEU	VAL	VAL	SER
		GLN	GLN	THR	VAL	GLU
				TYR	VAL	SER
				TYR	ALA	ALA
				ASN	GLY	LEU
				THR	LEU	SER
				SER	CYS	ALA
				ASN	ASP	GLN
				LEU	ALA	ALA
				PRO	ALA	ALA
				PRO	ASN	LYS
				PRO	PRO	ASP
				LEU	THR	LYS
				LEU	ASN	VAL
				GLY	CYS	ASN
				ASN	ILE	GLU
				SER	ALA	CYS
				THR	TYR	TYR

- Molecule 2: G4 VH

Chain B:  51% 49%

[illegible]

- Molecule 2: G4 VH

Chain E:  51% 49%

[illegible]

- Molecule 2: G4 VH

Chain H: 

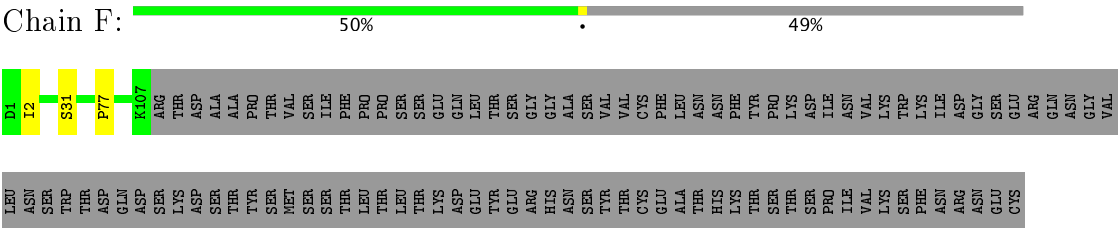
[illegible]

- Molecule 3: G4 VL

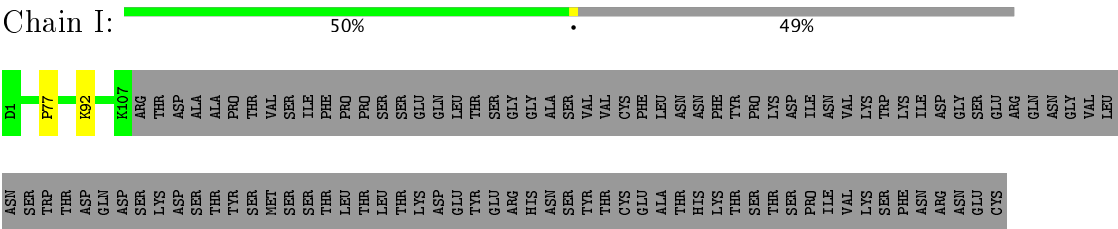
Chain C:  49% 1% 50%

D1	Y28	P77	K92	K107	ARG	THR	THR	ASP	ALA	PRO	THR	THR	VAL	SER	ILE	PHE	PRO	PRO	SER	SER	GLN	LEU	THR	THR	SER	GLY	GLY	ALA	SER	VAL	VAL	CYS	PHE	PHE	LEU	ASN	ASN	PHE	THR	THR	PRO	LYS	ASP	ILE	ASN	VAL	LYS	LYS	TRP	LYS	LYS	VAL	GLU	GLU	SER	GLY	ASP	ILE	ARG	GLN	ASN
VAL	LEU	ASN	SER	TRP	THR	ASP	GLN	ASP	LYS	ASP	ASP	THR	TYR	THR	MET	SER	SER	SER	THR	LEU	LEU	THR	THR	THR	THR	LYS	ASP	GLU	GLU	TYR	GLU	ARG	HIS	ASN	SER	TYR	THR	THR	CYS	GLU	GLU	ALA	THR	HIS	LYS	THR	SER	THR	PRO	ILE	VAL	VAL	LYS	SER	PHE	ASN	ARG	ASN	GLU	CYS	

● Molecule 3: G4 VL



● Molecule 3: G4 VL



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10544	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 ($e^-/\text{\AA}^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.75	0/3603	0.82	2/4899 (0.0%)
1	D	0.76	0/3611	0.81	2/4910 (0.0%)
1	G	0.77	0/3599	0.84	2/4894 (0.0%)
1	J	0.72	0/5789	0.89	12/7881 (0.2%)
1	K	0.73	0/5789	0.89	8/7881 (0.1%)
1	L	0.71	0/5782	0.89	11/7871 (0.1%)
2	B	0.71	0/972	0.82	0/1317
2	E	0.72	0/972	0.80	0/1317
2	H	0.70	0/972	0.81	0/1317
3	C	0.72	0/852	0.77	0/1153
3	F	0.76	0/852	0.84	0/1153
3	I	0.72	0/852	0.78	0/1153
All	All	0.73	0/33645	0.86	37/45746 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	932	TYR	CB-CG-CD1	-9.33	115.40	121.00
1	A	932	TYR	CB-CG-CD1	-8.11	116.13	121.00
1	J	642	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	L	185	CYS	O-C-N	-7.32	110.99	122.70
1	L	736	CYS	N-CA-C	-7.31	91.27	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3531	0	3454	15	0
1	D	3538	0	3463	20	0
1	G	3527	0	3453	14	0
1	J	5645	0	5413	74	0
1	K	5645	0	5413	52	0
1	L	5638	0	5408	91	0
2	B	948	0	904	0	0
2	E	948	0	904	0	0
2	H	948	0	904	0	0
3	C	835	0	816	3	0
3	F	835	0	816	1	0
3	I	835	0	816	1	0
All	All	32873	0	31764	270	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 4.

The worst 5 of 270 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:L:371:SER:CB	1:L:604:VAL:HG12	1.25	1.63
1:J:371:SER:CB	1:J:604:VAL:HG12	1.17	1.59
1:L:506:PHE:CE2	1:L:555:VAL:CG2	1.77	1.54
1:L:506:PHE:CE2	1:L:555:VAL:HG21	0.85	1.37
1:L:506:PHE:HE2	1:L:555:VAL:CG2	1.20	1.36

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	A	457/1329 (34%)	439 (96%)	15 (3%)	3 (1%)	25	68
1	D	458/1329 (34%)	441 (96%)	12 (3%)	5 (1%)	17	60
1	G	456/1329 (34%)	438 (96%)	15 (3%)	3 (1%)	25	68
1	J	722/1329 (54%)	685 (95%)	34 (5%)	3 (0%)	38	77
1	K	722/1329 (54%)	688 (95%)	30 (4%)	4 (1%)	28	71
1	L	721/1329 (54%)	685 (95%)	32 (4%)	4 (1%)	28	71
2	B	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	E	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	H	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
3	C	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	20	63
3	F	109/218 (50%)	105 (96%)	2 (2%)	2 (2%)	10	50
3	I	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	20	63
All	All	4214/9327 (45%)	4034 (96%)	154 (4%)	26 (1%)	33	71

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	940	ASP
1	A	961	THR
1	D	961	THR
1	D	965	SER
1	G	940	ASP

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	386/1148 (34%)	386 (100%)	0	100	100
1	D	387/1148 (34%)	387 (100%)	0	100	100
1	G	386/1148 (34%)	386 (100%)	0	100	100
1	J	633/1148 (55%)	631 (100%)	2 (0%)	94	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	633/1148 (55%)	631 (100%)	2 (0%)	94	96
1	L	632/1148 (55%)	629 (100%)	3 (0%)	91	95
2	B	102/202 (50%)	102 (100%)	0	100	100
2	E	102/202 (50%)	102 (100%)	0	100	100
2	H	102/202 (50%)	102 (100%)	0	100	100
3	C	93/192 (48%)	93 (100%)	0	100	100
3	F	93/192 (48%)	93 (100%)	0	100	100
3	I	93/192 (48%)	93 (100%)	0	100	100
All	All	3642/8070 (45%)	3635 (100%)	7 (0%)	95	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	670	HIS
1	L	600	LEU
1	L	383	CYS
1	J	600	LEU
1	L	384	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	808	GLN
1	D	812	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.