



Full wwPDB/EMDatabank EM Map/Model Validation 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 Full wwPDB/EMDatabank EM Map/Model Validation 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

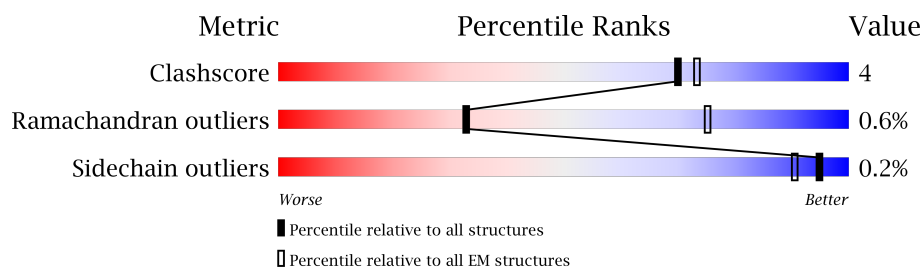
1 Overall quality at a glance

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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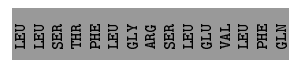
Chain	Residue	Modelled	Actual	Comment	Reference
L	1300	PRO	-	expression tag	UNP W5ZZF5
L	1301	ARG	-	expression tag	UNP W5ZZF5
L	1302	ASP	-	expression tag	UNP W5ZZF5
L	1303	GLY	-	expression tag	UNP W5ZZF5
L	1304	GLN	-	expression tag	UNP W5ZZF5
L	1305	ALA	-	expression tag	UNP W5ZZF5
L	1306	TYR	-	expression 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



Chain D: 33% . 65%

[illegible]

- Molecule 1: Spike glycoprotein

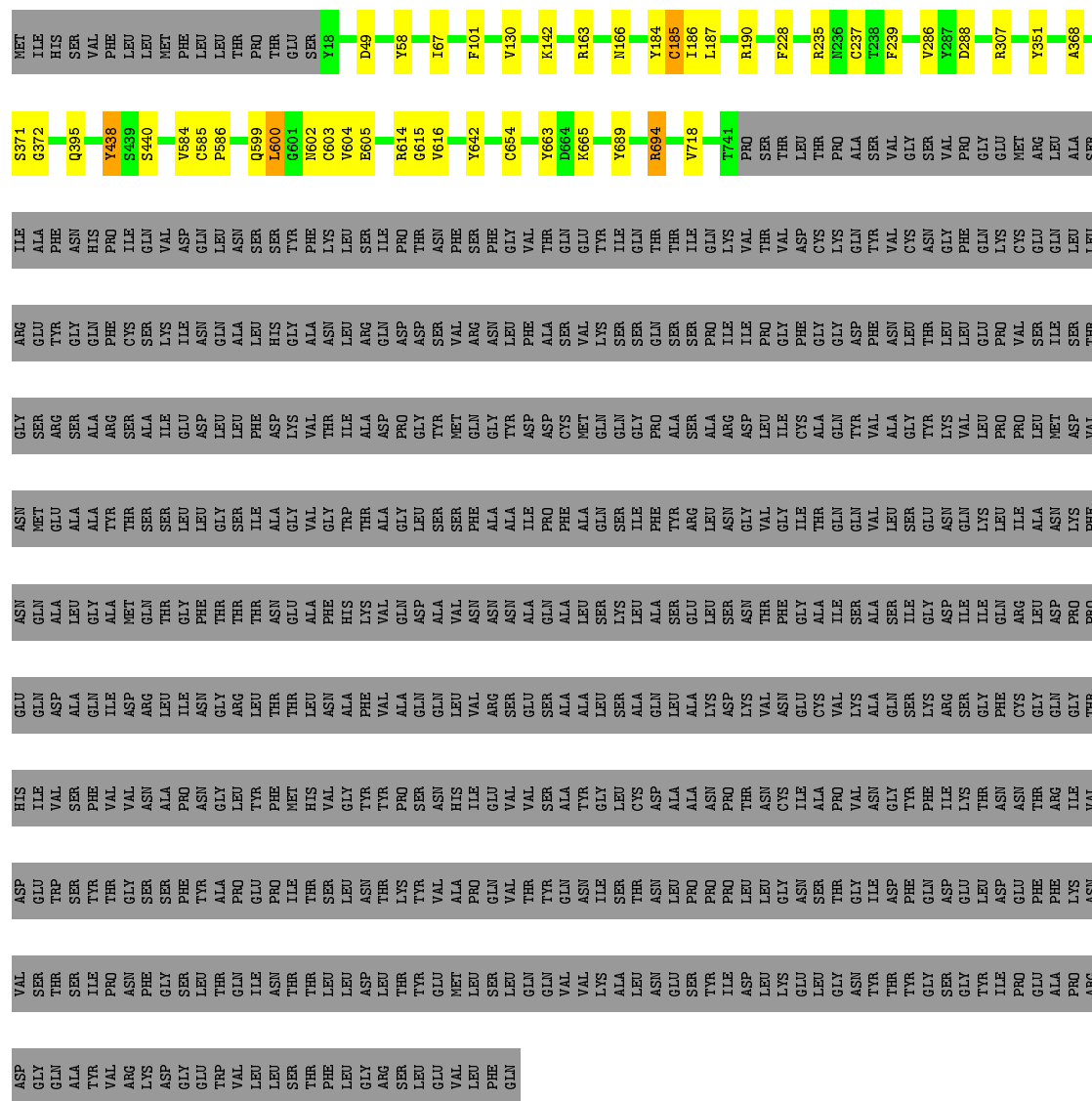
Chain G: 33% 65%

[illegible]

THR
PHE
LEU
GLY
SER
ARG
SER
LEU
LEU
VAL
PHE
GLN

• Molecule 1: Spike glycoprotein

Chain J:  51% 46%





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

- Molecule 2: G4 VH

Chain B: 51% 49%

ALA	VAL	GLN	SER	ASP	LEU	TYR	LEU	THR	LEU	SER	SER	VAL	THR	PRO	VAL	PRO	SER	SER	GLU	VAL	GLY	HIS	THR	PRO	GLN	THR	ASP	CYS	GLY	LYS	GLY	LEU	GLU	VAL	LEU	PHE	GLN
Q1	T110	VAL	SER	ALA	SER	THR	THR	PRO	PRO	SER	SER	THR	THR	PRO	PRO	LEU	ALA	PRO	GLY	SER	ALA	ALA	GLN	THR	ASN	VAL	THR	LEU	GLY	CYS	LEU	VAL	LYS	THR	PHE	PRO	GLU

- Molecule 2: G4 VH

Chain E: 51% 49%

[illegible]

- Molecule 2: G4 VH

Chain H:  51% 49%

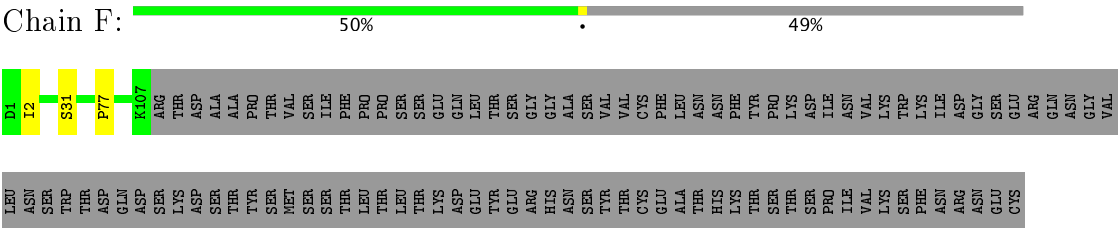
[illegible]

- Molecule 3: G4 VL

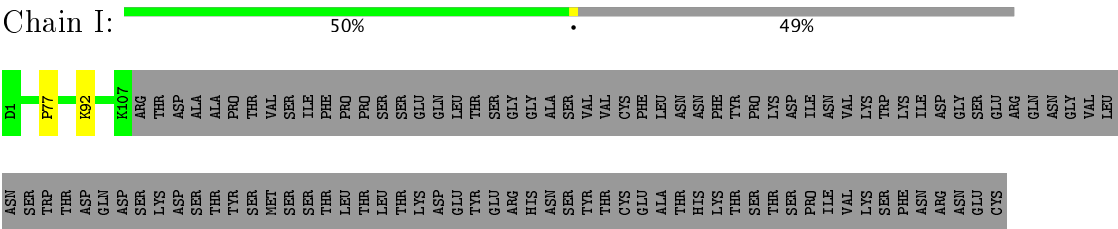
Chain C:  49% 1% 50%

[illegible]

● 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 ⓘ

5.1 Standard geometry ⓘ

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.

All (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
1	K	184	TYR	CB-CG-CD1	-7.19	116.69	121.00
1	L	642	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	L	736	CYS	CA-CB-SG	6.70	126.06	114.00
1	J	694	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	L	694	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	J	307	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	K	307	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	J	190	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	K	323	PHE	CB-CG-CD2	-6.15	116.50	120.80
1	J	694	ARG	NE-CZ-NH2	-6.14	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	735	LEU	C-N-CA	-6.13	106.37	121.70
1	K	185	CYS	O-C-N	5.96	132.23	122.70
1	J	101	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	L	694	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	L	77	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	K	323	PHE	CB-CG-CD1	5.47	124.63	120.80
1	D	909	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	K	378	ALA	C-N-CA	5.40	135.21	121.70
1	J	58	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	K	642	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	J	351	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	J	438	TYR	CB-CG-CD2	-5.31	117.82	121.00
1	J	663	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	G	868	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	868	ASP	CB-CG-OD2	5.23	123.00	118.30
1	L	293	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	868	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	163	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	L	241	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	L	585	CYS	C-N-CD	5.06	139.03	128.40
1	K	738	LEU	C-N-CD	5.06	139.02	128.40
1	J	585	CYS	C-N-CD	5.03	138.96	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

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

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

All (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
1:J:371:SER:HB3	1:J:604:VAL:CG1	1.52	1.34
1:J:371:SER:CB	1:J:604:VAL:CG1	2.01	1.33
1:D:905:TYR:OH	1:D:936:PRO:CA	1.78	1.31
1:L:371:SER:HB3	1:L:604:VAL:CG1	1.60	1.31
1:L:384:ASP:O	1:L:404:PHE:CZ	1.83	1.31
1:L:506:PHE:CD2	1:L:555:VAL:HG21	1.69	1.27
1:L:371:SER:CB	1:L:604:VAL:CG1	2.10	1.26
1:L:506:PHE:CD2	1:L:555:VAL:CG2	2.22	1.21
1:D:905:TYR:OH	1:D:936:PRO:HA	1.47	1.13
1:J:371:SER:OG	1:J:604:VAL:CG1	1.96	1.13
1:K:477:THR:OG1	1:K:573:ILE:O	1.65	1.10
1:J:185:CYS:HB2	1:J:237:CYS:HA	1.34	1.09
1:L:371:SER:OG	1:L:604:VAL:CG1	1.99	1.09
1:K:506:PHE:CE1	1:K:513:GLU:OE2	2.06	1.08
1:D:905:TYR:OH	1:D:936:PRO:N	1.87	1.07
1:J:371:SER:OG	1:J:604:VAL:HG12	1.52	1.02
1:L:371:SER:OG	1:L:604:VAL:HG12	1.55	1.02
1:J:371:SER:CA	1:J:604:VAL:HG12	1.89	1.01
1:A:868:ASP:OD2	1:A:995:LYS:NZ	1.94	0.99
1:J:185:CYS:SG	1:J:186:ILE:N	2.29	0.99
1:J:187:LEU:HD21	1:J:228:PHE:HZ	1.25	0.99
1:L:371:SER:HB3	1:L:604:VAL:HG12	0.99	0.97
1:L:384:ASP:CB	1:L:404:PHE:HE2	1.75	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:384:ASP:O	1:L:404:PHE:CE2	2.18	0.97
1:L:621:THR:O	1:L:648:TYR:HD2	1.45	0.96
1:J:185:CYS:SG	1:J:235:ARG:O	2.23	0.96
1:L:372:GLY:O	1:L:604:VAL:HB	1.66	0.95
1:J:371:SER:HB3	1:J:604:VAL:HG12	0.98	0.95
1:D:905:TYR:CZ	1:D:936:PRO:HB3	2.03	0.92
1:L:506:PHE:CD2	1:L:555:VAL:HG23	2.03	0.92
1:G:912:CYS:HG	1:G:925:CYS:HG	1.09	0.91
1:J:185:CYS:CB	1:J:237:CYS:HA	2.00	0.90
1:L:371:SER:CA	1:L:604:VAL:HG12	2.02	0.90
1:J:185:CYS:HB2	1:J:237:CYS:CA	2.02	0.89
1:J:372:GLY:O	1:J:604:VAL:HB	1.74	0.87
1:J:184:TYR:CE1	1:J:286:VAL:HG11	2.11	0.86
1:J:185:CYS:HG	1:J:237:CYS:HG	1.10	0.84
1:L:425:CYS:SG	1:L:478:CYS:CB	2.66	0.84
1:K:477:THR:HB	1:K:574:THR:HB	1.60	0.83
1:L:506:PHE:HE2	1:L:555:VAL:HG22	1.40	0.83
1:L:621:THR:O	1:L:648:TYR:CD2	2.30	0.83
1:J:371:SER:HB3	1:J:604:VAL:HG13	1.57	0.83
1:K:471:GLN:HG2	1:K:477:THR:HG21	1.61	0.82
1:L:425:CYS:CB	1:L:478:CYS:SG	2.68	0.81
1:L:425:CYS:SG	1:L:478:CYS:HB3	2.19	0.81
1:L:425:CYS:HB3	1:L:478:CYS:SG	2.21	0.81
1:L:384:ASP:O	1:L:404:PHE:HZ	1.58	0.80
1:K:471:GLN:CG	1:K:477:THR:HG21	2.13	0.79
1:K:477:THR:HB	1:K:574:THR:CB	2.11	0.79
1:J:184:TYR:OH	1:J:288:ASP:OD2	2.01	0.79
1:J:184:TYR:CG	1:J:286:VAL:HG21	2.18	0.78
1:L:372:GLY:O	1:L:604:VAL:CB	2.31	0.78
1:D:905:TYR:HH	1:D:936:PRO:HA	1.49	0.77
1:L:477:THR:HB	1:L:574:THR:HG22	1.65	0.77
1:K:506:PHE:CZ	1:K:513:GLU:OE2	2.37	0.76
1:L:602:ASN:O	1:L:616:VAL:HB	1.84	0.76
1:J:187:LEU:HD21	1:J:228:PHE:CZ	2.17	0.75
1:L:384:ASP:CB	1:L:404:PHE:CE2	2.65	0.75
1:L:425:CYS:CB	1:L:478:CYS:HG	2.00	0.74
1:J:371:SER:C	1:J:604:VAL:HG12	2.08	0.74
1:K:477:THR:CB	1:K:573:ILE:O	2.35	0.74
1:K:369:LYS:HG2	1:K:369:LYS:O	1.88	0.74
1:D:905:TYR:OH	1:D:936:PRO:CB	2.36	0.72
1:J:372:GLY:O	1:J:604:VAL:CB	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:381:VAL:HG11	1:L:407:CYS:HA	1.70	0.72
1:L:621:THR:HG22	1:L:622:ALA:N	2.03	0.72
1:D:905:TYR:CZ	1:D:936:PRO:CB	2.73	0.72
1:J:602:ASN:O	1:J:616:VAL:HB	1.90	0.71
1:L:384:ASP:HB2	1:L:404:PHE:HE2	1.54	0.70
1:L:371:SER:HB3	1:L:604:VAL:HG13	1.71	0.70
1:L:477:THR:CG2	1:L:574:THR:HG22	2.21	0.69
1:J:185:CYS:CB	1:J:237:CYS:SG	2.81	0.69
1:J:185:CYS:CB	1:J:237:CYS:HG	2.05	0.69
1:L:506:PHE:HD2	1:L:555:VAL:HG23	1.56	0.68
1:L:406:ASN:HA	1:L:583:SER:HB2	1.76	0.67
1:J:185:CYS:HB2	1:J:237:CYS:CB	2.26	0.66
1:K:506:PHE:CD1	1:K:513:GLU:OE2	2.48	0.66
1:J:371:SER:OG	1:J:604:VAL:HG11	1.92	0.66
1:L:477:THR:CB	1:L:574:THR:HG22	2.26	0.65
1:K:477:THR:HG1	1:K:478:CYS:H	1.45	0.65
1:K:477:THR:HG1	1:K:573:ILE:C	1.92	0.65
1:K:471:GLN:CD	1:K:477:THR:HG21	2.17	0.64
1:L:371:SER:C	1:L:604:VAL:HG12	2.17	0.64
1:J:184:TYR:CD1	1:J:286:VAL:HG21	2.31	0.64
1:K:621:THR:O	1:K:648:TYR:HD2	1.80	0.64
1:K:621:THR:HG22	1:K:622:ALA:N	2.11	0.64
1:L:425:CYS:HG	1:L:478:CYS:CB	2.06	0.64
1:D:905:TYR:CZ	1:D:936:PRO:CA	2.80	0.64
1:J:184:TYR:HB3	1:J:239:PHE:HB2	1.80	0.63
1:K:383:CYS:SG	1:K:409:TYR:HB3	2.38	0.63
1:J:186:ILE:HG22	1:J:187:LEU:N	2.13	0.63
1:L:384:ASP:CA	1:L:404:PHE:HE2	2.12	0.62
1:L:382:GLU:HA	1:L:382:GLU:OE1	1.99	0.62
1:A:897:LYS:HE2	1:A:897:LYS:HA	1.81	0.62
1:J:184:TYR:HD2	1:J:239:PHE:HD1	1.45	0.62
1:J:185:CYS:SG	1:J:237:CYS:HA	2.39	0.61
1:L:384:ASP:HB3	1:L:404:PHE:HE2	1.65	0.61
1:J:184:TYR:CZ	1:J:286:VAL:CG1	2.83	0.61
1:L:384:ASP:HB3	1:L:404:PHE:CE2	2.34	0.61
1:L:477:THR:HG22	1:L:574:THR:HB	1.83	0.61
1:K:738:LEU:HD12	1:K:739:PRO:HD3	1.82	0.60
1:J:184:TYR:CZ	1:J:286:VAL:HG13	2.37	0.60
1:L:621:THR:CG2	1:L:622:ALA:N	2.64	0.59
1:L:371:SER:OG	1:L:604:VAL:HG11	1.97	0.59
1:J:616:VAL:HG13	1:J:616:VAL:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:184:TYR:CD2	1:J:239:PHE:HD1	2.21	0.58
1:L:599:GLN:C	1:L:600:LEU:HG	2.24	0.58
1:L:602:ASN:O	1:L:616:VAL:CB	2.52	0.58
1:J:184:TYR:CD2	1:J:286:VAL:CG2	2.88	0.57
1:L:616:VAL:HG13	1:L:616:VAL:O	2.03	0.57
1:J:371:SER:C	1:J:604:VAL:CG1	2.73	0.56
1:J:599:GLN:C	1:J:600:LEU:HG	2.25	0.56
1:J:184:TYR:CE2	1:J:286:VAL:HG22	2.41	0.56
1:J:187:LEU:CD2	1:J:228:PHE:HZ	2.09	0.56
1:L:506:PHE:CE2	1:L:555:VAL:HG22	2.20	0.56
1:J:372:GLY:O	1:J:604:VAL:CG2	2.54	0.56
1:J:602:ASN:O	1:J:616:VAL:CB	2.54	0.56
1:K:478:CYS:O	1:K:479:LEU:HG	2.06	0.55
1:D:1175:THR:O	1:D:1175:THR:HG23	2.07	0.55
1:D:905:TYR:CZ	1:D:936:PRO:HA	2.40	0.55
1:K:621:THR:CG2	1:K:622:ALA:N	2.70	0.54
1:L:384:ASP:CA	1:L:404:PHE:CE2	2.91	0.54
1:J:184:TYR:CE1	1:J:286:VAL:CG1	2.86	0.53
1:G:1175:THR:HG23	1:G:1175:THR:O	2.07	0.53
1:A:1175:THR:O	1:A:1175:THR:HG23	2.09	0.53
1:J:184:TYR:HD2	1:J:239:PHE:CD1	2.24	0.53
1:L:384:ASP:HB2	1:L:404:PHE:CE2	2.40	0.53
1:L:67:ILE:O	1:L:67:ILE:HG13	2.08	0.53
1:K:172:LEU:HG	1:K:172:LEU:O	2.08	0.53
1:G:875:GLU:OE1	1:G:875:GLU:N	2.35	0.53
1:A:875:GLU:N	1:A:875:GLU:OE1	2.36	0.53
1:K:477:THR:HA	1:K:574:THR:HA	1.91	0.53
1:L:381:VAL:CG1	1:L:407:CYS:HA	2.39	0.52
1:L:621:THR:CG2	1:L:622:ALA:H	2.22	0.52
1:J:185:CYS:SG	1:J:237:CYS:CA	2.98	0.52
1:J:184:TYR:CD2	1:J:286:VAL:HG22	2.45	0.51
1:K:738:LEU:HD12	1:K:739:PRO:CD	2.41	0.51
1:A:875:GLU:O	1:A:875:GLU:HG2	2.09	0.51
1:L:399:PHE:CD1	1:L:399:PHE:O	2.64	0.51
1:G:826:GLN:N	1:G:826:GLN:OE1	2.27	0.50
1:K:477:THR:HG1	1:K:478:CYS:N	2.09	0.50
1:L:240:MET:C	1:L:240:MET:SD	2.89	0.50
1:L:256:ILE:HG23	1:L:256:ILE:O	2.11	0.49
1:J:184:TYR:CD2	1:J:286:VAL:HG21	2.47	0.49
1:L:477:THR:CG2	1:L:574:THR:CG2	2.90	0.49
1:K:477:THR:OG1	1:K:478:CYS:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:912:CYS:SG	1:K:655:VAL:HG12	2.52	0.49
1:L:372:GLY:O	1:L:604:VAL:CG2	2.60	0.49
1:J:166:ASN:O	1:J:186:ILE:HG23	2.11	0.49
1:L:371:SER:HG	1:L:604:VAL:CG1	2.23	0.49
1:L:384:ASP:C	1:L:404:PHE:CE2	2.85	0.48
1:A:1124:VAL:O	1:A:1124:VAL:HG13	2.13	0.48
1:G:897:LYS:HE2	1:G:897:LYS:HA	1.95	0.48
1:J:186:ILE:CG2	1:J:187:LEU:N	2.75	0.48
1:K:471:GLN:HG2	1:K:477:THR:CG2	2.38	0.48
1:L:477:THR:HG22	1:L:574:THR:CB	2.42	0.48
1:J:186:ILE:C	1:J:187:LEU:HD12	2.34	0.48
1:K:477:THR:CA	1:K:573:ILE:O	2.61	0.48
1:G:875:GLU:O	1:G:875:GLU:HG2	2.13	0.48
1:L:371:SER:CB	1:L:604:VAL:HG13	2.29	0.48
1:L:437:CYS:SG	1:L:584:VAL:O	2.72	0.48
1:L:395:GLN:HA	1:L:395:GLN:OE1	2.14	0.47
1:J:694:ARG:NE	1:J:694:ARG:HA	2.29	0.47
1:L:694:ARG:HA	1:L:694:ARG:NE	2.29	0.47
1:J:605:GLU:HA	1:J:614:ARG:HA	1.96	0.47
1:L:382:GLU:O	1:L:407:CYS:HB2	2.15	0.47
1:L:605:GLU:HA	1:L:614:ARG:HA	1.96	0.47
1:L:694:ARG:HA	1:L:694:ARG:HE	1.80	0.47
1:J:372:GLY:O	1:J:604:VAL:HG21	2.14	0.47
1:K:395:GLN:HA	1:K:395:GLN:OE1	2.14	0.47
1:L:342:ASN:OD1	1:L:342:ASN:C	2.53	0.47
1:J:142:LYS:NZ	1:J:142:LYS:HB3	2.29	0.47
1:L:438:TYR:O	1:L:584:VAL:HB	2.14	0.47
1:K:478:CYS:N	1:K:573:ILE:O	2.40	0.46
1:K:439:SER:HA	1:K:582:ASN:HA	1.98	0.46
1:J:130:VAL:HG12	1:J:130:VAL:O	2.16	0.46
1:J:185:CYS:CB	1:J:237:CYS:CA	2.79	0.46
1:K:731:LEU:HB2	1:K:735:LEU:HB3	1.97	0.46
1:A:806:CYS:O	1:A:806:CYS:SG	2.74	0.46
1:J:166:ASN:O	1:J:186:ILE:HG12	2.15	0.46
1:K:606:TYR:C	1:K:606:TYR:CD1	2.88	0.46
1:G:777:TYR:N	1:G:777:TYR:CD2	2.84	0.45
1:D:875:GLU:HB3	1:D:886:ALA:HB3	1.97	0.45
1:K:477:THR:HB	1:K:574:THR:CA	2.45	0.45
1:J:371:SER:CB	1:J:604:VAL:HG13	2.21	0.45
1:K:523:TYR:N	1:K:523:TYR:CD1	2.84	0.45
1:J:665:LYS:HD3	1:J:665:LYS:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:621:THR:O	1:K:648:TYR:CD2	2.65	0.45
1:L:615:GLY:HA2	1:L:654:CYS:SG	2.57	0.45
1:D:806:CYS:SG	1:D:806:CYS:O	2.74	0.45
1:J:184:TYR:CD2	1:J:239:PHE:CD1	3.03	0.45
1:K:130:VAL:HG12	1:K:130:VAL:O	2.17	0.45
3:C:1:ASP:C	3:C:1:ASP:OD1	2.56	0.45
1:D:905:TYR:OH	1:D:935:LEU:C	2.54	0.45
1:D:1036:LEU:HD23	1:D:1036:LEU:HA	1.74	0.44
1:D:905:TYR:CE2	1:D:936:PRO:HB3	2.51	0.44
1:K:378:ALA:HB1	1:K:379:GLU:HA	1.99	0.44
1:L:240:MET:O	1:L:240:MET:SD	2.75	0.44
1:G:1001:PHE:CD2	1:G:1001:PHE:C	2.91	0.44
1:J:615:GLY:HA2	1:J:654:CYS:SG	2.58	0.44
1:L:621:THR:HG22	1:L:622:ALA:H	1.76	0.44
1:L:440:SER:HA	1:L:584:VAL:HG21	2.00	0.44
1:A:1062:GLU:N	1:A:1062:GLU:OE1	2.51	0.44
1:A:1160:ASN:OD1	1:A:1160:ASN:C	2.56	0.44
3:F:2:ILE:N	3:F:2:ILE:HD12	2.32	0.44
1:K:172:LEU:N	1:K:172:LEU:HD23	2.33	0.44
1:J:440:SER:HA	1:J:584:VAL:HG21	2.00	0.43
1:K:590:PHE:CG	1:K:590:PHE:O	2.72	0.43
1:J:438:TYR:O	1:J:584:VAL:HB	2.18	0.43
1:G:932:TYR:HD1	1:G:932:TYR:HA	1.45	0.43
1:A:826:GLN:OE1	1:A:826:GLN:N	2.31	0.43
1:A:965:SER:OG	1:A:966:SER:N	2.52	0.42
1:G:806:CYS:SG	1:G:806:CYS:O	2.77	0.42
1:L:479:LEU:C	1:L:480:ILE:HG13	2.40	0.42
1:L:664:ASP:C	1:L:664:ASP:OD1	2.57	0.42
1:G:1060:PRO:HA	1:G:1063:GLN:HB3	2.00	0.42
1:K:732:GLY:O	1:K:735:LEU:HB2	2.19	0.42
1:K:596:ILE:C	1:K:596:ILE:HD12	2.39	0.42
1:J:49:ASP:OD1	1:J:49:ASP:C	2.58	0.42
1:A:1001:PHE:C	1:A:1001:PHE:CD2	2.93	0.42
1:A:1060:PRO:HA	1:A:1063:GLN:HB3	2.00	0.42
1:A:1120:GLY:O	1:A:1121:THR:OG1	2.31	0.42
1:G:1124:VAL:HG13	1:G:1124:VAL:O	2.19	0.42
1:J:371:SER:C	1:J:604:VAL:HB	2.40	0.42
1:K:633:ASP:OD1	1:K:633:ASP:C	2.58	0.42
3:C:28:TYR:N	3:C:28:TYR:CD1	2.86	0.42
1:G:965:SER:OG	1:G:966:SER:N	2.52	0.42
1:A:872:THR:HG22	1:A:872:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1173:ILE:HG13	1:D:1185:SER:OG	2.20	0.42
1:J:395:GLN:HA	1:J:395:GLN:OE1	2.20	0.42
1:J:371:SER:O	1:J:604:VAL:HB	2.19	0.42
1:L:616:VAL:CG1	1:L:616:VAL:O	2.68	0.42
1:L:185:CYS:SG	1:L:186:ILE:N	2.93	0.41
1:L:506:PHE:CE2	1:L:555:VAL:CB	2.88	0.41
1:K:172:LEU:H	1:K:172:LEU:HD23	1.85	0.41
1:K:326:ASP:C	1:K:326:ASP:OD1	2.56	0.41
1:K:409:TYR:C	1:K:409:TYR:CD1	2.94	0.41
1:D:777:TYR:N	1:D:777:TYR:CD2	2.88	0.41
1:L:371:SER:C	1:L:604:VAL:CG1	2.87	0.41
3:C:92:LYS:C	3:C:92:LYS:HD3	2.41	0.41
1:J:67:ILE:HG23	1:J:67:ILE:O	2.19	0.41
1:L:665:LYS:HD3	1:L:665:LYS:C	2.40	0.41
1:J:689:TYR:C	1:J:689:TYR:CD1	2.94	0.41
1:D:809:TYR:C	1:D:809:TYR:CD2	2.94	0.41
3:I:92:LYS:C	3:I:92:LYS:HD3	2.41	0.41
1:J:184:TYR:CE2	1:J:286:VAL:CG2	3.04	0.41
1:J:603:CYS:O	1:J:603:CYS:SG	2.79	0.41
1:K:130:VAL:CG1	1:K:130:VAL:O	2.69	0.41
1:K:209:THR:HG22	1:K:209:THR:O	2.20	0.41
1:K:621:THR:CG2	1:K:622:ALA:H	2.33	0.41
1:L:130:VAL:O	1:L:130:VAL:HG12	2.20	0.41
1:L:477:THR:O	1:L:478:CYS:SG	2.79	0.41
1:K:677:VAL:O	1:K:677:VAL:HG22	2.20	0.41
1:L:477:THR:C	1:L:478:CYS:SG	3.00	0.41
1:L:719:ASN:OD1	1:L:719:ASN:C	2.59	0.41
1:D:1124:VAL:O	1:D:1124:VAL:HG13	2.21	0.41
1:L:372:GLY:C	1:L:604:VAL:HB	2.39	0.40
1:D:775:SER:OG	1:D:776:SER:N	2.53	0.40
1:L:603:CYS:O	1:L:603:CYS:SG	2.79	0.40
1:J:130:VAL:O	1:J:130:VAL:CG1	2.68	0.40
1:K:427:GLN:HB2	1:K:476:PRO:HB3	2.04	0.40
1:L:604:VAL:O	1:L:604:VAL:HG23	2.21	0.40
1:J:372:GLY:C	1:J:604:VAL:HB	2.39	0.40
1:K:478:CYS:HB3	1:K:479:LEU:H	1.73	0.40
1:K:670:HIS:N	1:K:670:HIS:CD2	2.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (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
1	J	718	VAL
1	K	718	VAL
1	L	718	VAL
3	C	77	PRO
1	D	905	TYR
1	G	961	THR
3	I	77	PRO

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Mol	Chain	Res	Type
1	A	1220	PRO
1	D	1220	PRO
3	F	31	SER
3	F	77	PRO
1	G	1220	PRO
1	K	378	ALA
1	D	956	ALA
1	J	368	ALA
1	K	629	ARG
1	L	368	ALA
1	K	44	TRP
1	L	385	PHE
1	J	586	PRO
1	L	586	PRO

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
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

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	185	CYS
1	J	600	LEU
1	K	477	THR
1	K	670	HIS
1	L	383	CYS
1	L	384	ASP
1	L	600	LEU

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.