



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 2, 2017 – 06:36 AM EDT

PDB ID : 5W9M
EMDB ID: : EMD-8788
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : unknown
Resolution : 4.70 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

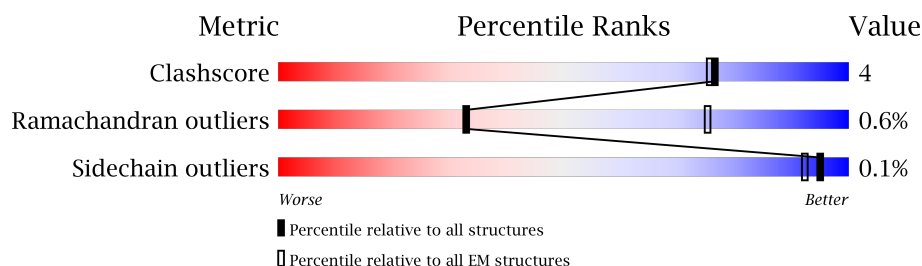
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	
1	D	1329	
1	E	1329	
1	F	1329	
1	G	1329	
1	J	1329	
2	B	233	
2	H	233	
3	C	218	

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31126 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	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	D	457	Total	C	N	O	S	0	0
			3496	2214	590	675	17		
1	G	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	E	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	F	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	J	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	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	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	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	engineered mutation	UNP W5ZZF5
D	1061	PRO	LEU	engineered mutation	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	engineered mutation	UNP W5ZZF5
G	1061	PRO	LEU	engineered mutation	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
E	506	PHE	LEU	conflict	UNP W5ZZF5
E	748	ALA	ARG	conflict	UNP W5ZZF5
E	751	GLY	ARG	conflict	UNP W5ZZF5
E	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
E	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
E	1292	GLY	-	expression tag	UNP W5ZZF5
E	1293	SER	-	expression tag	UNP W5ZZF5
E	1294	GLY	-	expression tag	UNP W5ZZF5
E	1295	TYR	-	expression tag	UNP W5ZZF5
E	1296	ILE	-	expression tag	UNP W5ZZF5
E	1297	PRO	-	expression tag	UNP W5ZZF5
E	1298	GLU	-	expression tag	UNP W5ZZF5
E	1299	ALA	-	expression tag	UNP W5ZZF5
E	1300	PRO	-	expression tag	UNP W5ZZF5
E	1301	ARG	-	expression tag	UNP W5ZZF5

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1301	ARG	-	expression tag	UNP W5ZZF5
F	1302	ASP	-	expression tag	UNP W5ZZF5
F	1303	GLY	-	expression tag	UNP W5ZZF5
F	1304	GLN	-	expression tag	UNP W5ZZF5
F	1305	ALA	-	expression tag	UNP W5ZZF5
F	1306	TYR	-	expression tag	UNP W5ZZF5
F	1307	VAL	-	expression tag	UNP W5ZZF5
F	1308	ARG	-	expression tag	UNP W5ZZF5
F	1309	LYS	-	expression tag	UNP W5ZZF5
F	1310	ASP	-	expression tag	UNP W5ZZF5
F	1311	GLY	-	expression tag	UNP W5ZZF5
F	1312	GLU	-	expression tag	UNP W5ZZF5
F	1313	TRP	-	expression tag	UNP W5ZZF5
F	1314	VAL	-	expression tag	UNP W5ZZF5
F	1315	LEU	-	expression tag	UNP W5ZZF5
F	1316	LEU	-	expression tag	UNP W5ZZF5
F	1317	SER	-	expression tag	UNP W5ZZF5
F	1318	THR	-	expression tag	UNP W5ZZF5
F	1319	PHE	-	expression tag	UNP W5ZZF5
F	1320	LEU	-	expression tag	UNP W5ZZF5
F	1321	GLY	-	expression tag	UNP W5ZZF5
F	1322	ARG	-	expression tag	UNP W5ZZF5
F	1323	SER	-	expression tag	UNP W5ZZF5
F	1324	LEU	-	expression tag	UNP W5ZZF5
F	1325	GLU	-	expression tag	UNP W5ZZF5
F	1326	VAL	-	expression tag	UNP W5ZZF5
F	1327	LEU	-	expression tag	UNP W5ZZF5
F	1328	PHE	-	expression tag	UNP W5ZZF5
F	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	engineered mutation	UNP W5ZZF5
J	1061	PRO	LEU	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5
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

- 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	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	I	111	Total 835	C 522	N 143	O 166	S 4	0	0

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

[illegible]

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

- Molecule 1: Spike glycoprotein

Chain G:  33% . 65%

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

Tyr	Ser	Val	Ser	Ser	Phe	Glu	Ala	Lys	Pro	Ser	Gly	Ser	Val	Glu	Gln	Ala	Gly	Glu	Val	Glu	Cys	Asp	Phe	Ser	Ser	Pro	Pro	Pro	Gln	Gln	Val	Tyr	Asn	Phe	Lys	Arg	Leu	Val	Phe	Thr	Thr	Asn	Cys	Asn	Tyr	Leu	Leu	Thr	Lys	Leu	Ser	Leu	Phe	Ser	Val
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ASN	ASP	PHE	THR	CYS	GLN	ILE	PRO	ALA	ILE	ALA	ASN	CYS	TYR	SER	SER	LEU	LEU	ASP	TYR	PHE	SER	SER	PRO	LEU	SER	SER	LYS	NET	LYS	SER	SER	ASP	LEU	SER	VAL	ALA	GLY	PRO	ILE	SER	GLN	PHE	ASN	TYR	LYS	GLN	SER	PHE	SER	PRO	THR	CYS	LEU
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GLY	ASN	CYS	VAL	GLU	TYR	SER	GLY	LEU	TYR	GLY	VAL	SER	GLY	ARG	ALA	THR	ALA	VAL	GLN	ASN	CYS	GLN	GLN	ASP	ASP	ASP	GLY	TYR	TYR	ASN	GLN	LEU	VAL	GLY	TYR	TYR	SER	ASP	ASP	GLY	ASN	ARG	ALA	CYS	VAL	SER	SER	PRO	VAL
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VAL	ILE	TYR	ASP	LYS	GLU	THR	LYS	THR	HIS	ALA	THR	LEU	PHE	GLY	GLY	SER	VAL	VAL	ALA	CYS	GLU	HIS	ILE	ILE	SER	SER	THR	THR	MET	SER	GLN	SER	SER	ARG	ARG	THR	ARG	SER	MET	THR	LEU	LYS	ARG	ARG	GLN	LEU	THR	THR	ASP	SER	SER	TYR	GLY	PRO	PRO	VAL	VAL	GLY	CYS	VAL	LEU	LEU	LEU	VAL	ASN
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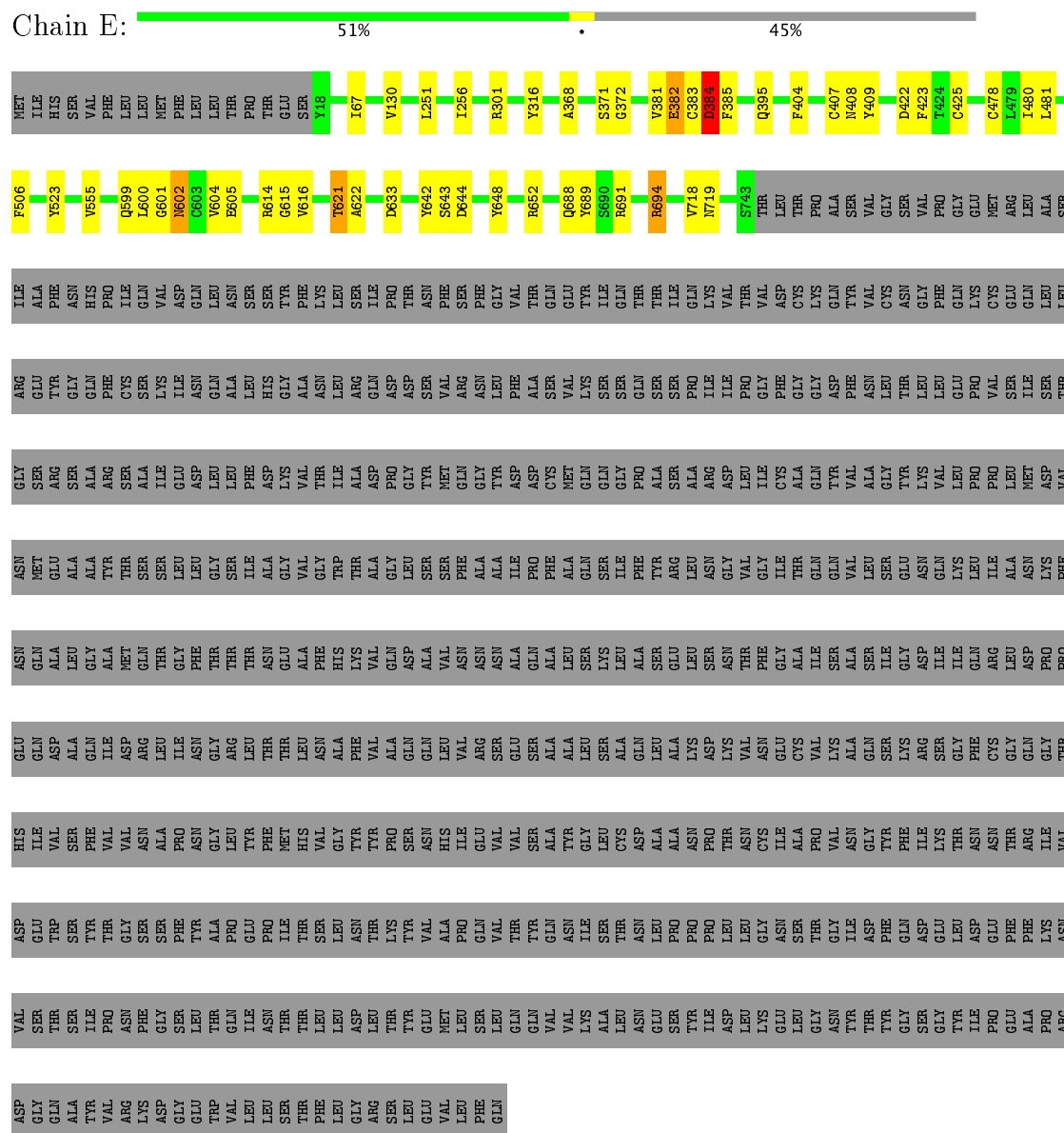
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Year	Number of cases	Gender
2013	34	Y
2014	38	N
2015	56	R
2016	62	R
2017	60	R
2018	63	Y
2019	124	E
2020	141	P
2021	160	P
2022	173	U
2023	185	U
2024	220	P
2025	223	U
2026		U
2027		U
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2030		U
2031		U
2032		U
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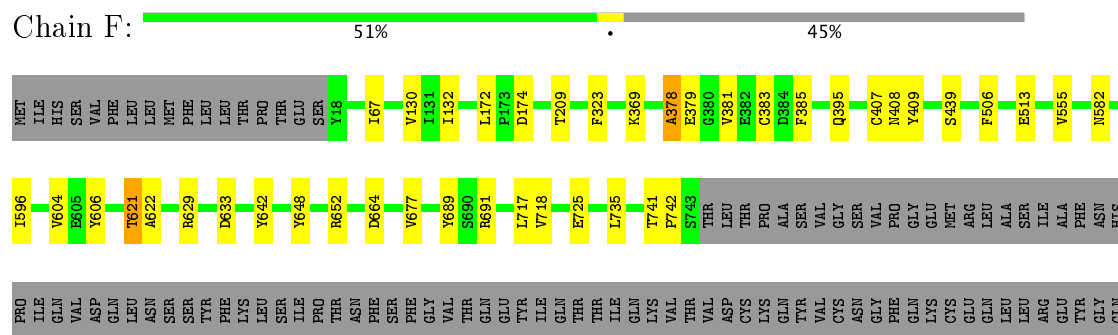
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REUY GRUULUEN

- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



[illegible]

- Molecule 1: Spike glycoprotein

Chain J:  52% . 45%

VAL	ARG	ASN	PHE	GLN	ARG	SER	Y595	MET
ARG	ASN	ASN	ALA	GLY	ASN	PHE	1596	ILE
GLU	ALA	ALA	ILE	TYR	PHE	GLY		HIS
SER	GLN	ALA	PRO	ASP	ALA	THR	Y602	VAL
ALA	ALA	ALA	PHE	CYS	SER	GLN	Y629	PHE
ALA	LEU	LEU	ALA	MET	VAL	TYR		LEU
SER	LEU	LYS	GLN	MET	LYS	TYR	Y670	LEU
ALA	LEU	LYS	ILE	GLN	SER	GLN		MET
GLN	ALA	ALA	PHE	PRO	GLN	THR	Y691	PHE
LEU	GLU	LEU	ARG	ALA	SER	THR		LEU
ALA	LEU	LYS	THR	ALA	SER	ILE	Y718	THR
ASP	ASN	LYS	LEU	ALA	PRO	GLN	Y719	PRO
LYS	ASN	GLY	ILE	ARG	ILE	VAL		THR
VAL	THR	VAL	VAL	ASP	ILE	VAL	Y735	GLU
ASN	PHE	THR	GLY	ILE	PRO	VAL	Y743	SER
GLN	GLY	ILE	ILE	CYS	PHE	ASP	THR	Y148
CYS	THR	ALA	THR	ALA	GLY	THR		I67
VAL	ILE	GLN	GLN	GLY	GLY	PRO		Y130
LYS	SER	LYS	VAL	THR	ASP	ALA		VAL
ALA	ALA	ALA	VAL	VAL	PHE	SER		L172
GLN	SER	SER	LEU	ALA	ASN	VAL		Y184
SER	ILE	ILE	SER	ALA	CYS	GLY		
LYS	GLY	ASP	GLU	LYS	THR	SER		T209
ARG	GLY	ILE	ASN	VAL	LEU	VAL		
ILE	ILE	ILE	GLN	VAL	GLN	PRO		Y240
GLY	ILE	ILE	LYS	LEU	ILE	GLY		Y241
PHE	ANG	GLN	LEU	PRO	VAL	LYS		Y293
CYS	LEU	LEU	ILE	PRO	VAL	GLU		
GLY	LEU	ANG	ILE	VAL	SER	MET		Y307
GLN	ASP	ASN	ASN	MET	THR	ARG		Y369
GLY	ASP	ALA	ALA	THR	GLU	ALA		Y378
PHE	LEU	LEU	SER	ARG	ARG	ASN		Q395
VAL	PHE	GLY	GLY	ALA	ALA	HIS		
VAL	ILE	ILE	ALA	TYR	ARG	PRO		F399
VAL	ASP	ASP	MET	THR	SER	ILE		
ASN	ANG	ANG	GLN	THR	SER	GLN		C425
ALA	LEU	LEU	THR	SER	ALA	VAL		S426
PRO	ILE	ILE	GLY	LEU	ILE	ASP		Q427
GLY	ASN	ASN	PHE	GLY	ASN	GLN		
LEU	GLY	GLY	THR	THR	LEU	LEU		Y430
TYR	ARG	ARG	THR	SER	ALA	ASN		
PHE	THR	THR	GLN	ILE	PHE	SER		Y439
MET	THR	GLU	ASN	ALA	LYS	THR		F506
HIS	LEU	ALA	ALA	VAL	THR	LYS		
VAL	ASN	ALA	HIS	GLY	ILE	LEU		Y555
GLY	ALA	VAL	VAL	TAP	ILE	SER		N582
TYR	PHE	VAL	VAL	THR	ALA	GLN		
PRO	VAL	VAL	VAL	THR	ASP	ILE		
SER	ALA	GLN	GLN	GLY	GLY	PRO		Y593
ASN	ASN	ASN	ASP	LEU	THR	THR		Y594
VAL	LEU	LEU	VAL	SER	VAL	ASN		
THR	THR	THR	THR	SER	MET	PHE		

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

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9333	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	0.76	0/3618	0.82	2/4921 (0.0%)
1	D	0.76	0/3568	0.82	4/4851 (0.1%)
1	E	0.71	0/5803	0.88	6/7901 (0.1%)
1	F	0.72	0/5803	0.88	6/7901 (0.1%)
1	G	0.76	0/3618	0.84	3/4921 (0.1%)
1	J	0.73	0/5803	0.90	6/7901 (0.1%)
2	B	0.74	0/972	0.87	1/1317 (0.1%)
2	H	0.77	0/972	0.85	0/1317
3	C	0.76	0/852	0.83	1/1153 (0.1%)
3	I	0.77	0/852	0.87	0/1153
All	All	0.74	0/31861	0.86	29/43336 (0.1%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	691	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	D	932	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	J	184	TYR	CB-CG-CD1	-7.62	116.43	121.00
1	J	691	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	F	642	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	F	652	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	932	TYR	CB-CG-CD2	-6.29	117.22	121.00
1	E	523	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	E	642	TYR	CB-CG-CD1	-5.96	117.42	121.00
3	C	96	ARG	NE-CZ-NH2	5.94	123.27	120.30
2	B	97	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	J	307	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	J	399	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	E	694	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	J	241	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	F	378	ALA	C-N-CA	5.59	135.68	121.70
1	E	652	ARG	NE-CZ-NH2	-5.53	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	323	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	F	691	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	F	323	PHE	CB-CG-CD1	5.44	124.61	120.80
1	G	1141	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	E	316	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	D	868	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	868	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	868	ASP	CB-CG-OD2	5.14	122.92	118.30
1	D	909	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	D	1156	CYS	O-C-N	-5.09	114.56	122.70
1	J	293	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	G	1220	PRO	N-CA-C	5.00	125.11	112.10

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	3545	0	3470	9	0
1	D	3496	0	3420	22	0
1	E	5658	0	5423	85	0
1	F	5658	0	5423	49	0
1	G	3545	0	3471	14	0
1	J	5658	0	5425	26	0
2	B	948	0	904	2	0
2	H	948	0	904	0	0
3	C	835	0	816	4	0
3	I	835	0	816	2	0
All	All	31126	0	30072	212	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 (212) 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:F:506:PHE:HE2	1:F:555:VAL:CG2	0.99	1.62
1:J:506:PHE:CE2	1:J:555:VAL:HG21	1.13	1.60
1:E:506:PHE:CE2	1:E:555:VAL:CG2	1.76	1.58
1:J:506:PHE:CE2	1:J:555:VAL:CG2	1.94	1.51
1:F:506:PHE:CE2	1:F:555:VAL:CG2	1.74	1.43
1:E:371:SER:CB	1:E:604:VAL:HG12	1.48	1.40
1:E:506:PHE:CD2	1:E:555:VAL:HG21	1.55	1.39
1:F:506:PHE:CE2	1:F:555:VAL:HG21	0.86	1.37
1:E:506:PHE:CE2	1:E:555:VAL:HG21	0.83	1.36
1:E:506:PHE:CD2	1:E:555:VAL:CG2	2.10	1.34
1:E:371:SER:CB	1:E:604:VAL:CG1	2.05	1.30
1:D:905:TYR:OH	1:D:936:PRO:N	1.70	1.24
1:E:371:SER:HB3	1:E:604:VAL:CG1	1.66	1.20
1:G:905:TYR:OH	1:G:934:VAL:O	1.60	1.18
1:E:506:PHE:HE2	1:E:555:VAL:CG2	1.26	1.18
1:E:384:ASP:O	1:E:404:PHE:CZ	1.98	1.16
1:E:371:SER:C	1:E:604:VAL:HG12	1.64	1.15
1:E:372:GLY:O	1:E:604:VAL:HB	1.44	1.15
1:E:371:SER:CA	1:E:604:VAL:HG12	1.77	1.14
1:E:384:ASP:O	1:E:404:PHE:HZ	1.27	1.14
1:F:506:PHE:CE1	1:F:513:GLU:OE2	2.01	1.13
1:F:506:PHE:CD2	1:F:555:VAL:CG2	2.31	1.12
1:E:371:SER:OG	1:E:604:VAL:CG1	1.96	1.12
1:F:506:PHE:CD2	1:F:555:VAL:HG21	1.85	1.09
1:J:506:PHE:HE2	1:J:555:VAL:CG2	1.41	1.08
1:J:506:PHE:CD2	1:J:555:VAL:HG21	1.89	1.05
1:E:371:SER:HB3	1:E:604:VAL:HG13	1.39	1.03
1:D:905:TYR:OH	1:D:936:PRO:CA	2.07	1.02
1:J:506:PHE:CD2	1:J:555:VAL:CG2	2.41	1.02
1:E:372:GLY:O	1:E:604:VAL:CB	2.07	1.02
1:F:506:PHE:CD2	1:F:555:VAL:HG23	1.99	0.96
1:E:506:PHE:CD2	1:E:555:VAL:HG23	1.99	0.94
1:E:371:SER:CB	1:E:604:VAL:HG13	1.92	0.93
1:E:383:CYS:HG	1:E:407:CYS:HG	1.09	0.93
1:J:506:PHE:HE2	1:J:555:VAL:HG22	1.36	0.89
1:F:506:PHE:CE2	1:F:555:VAL:HG23	2.05	0.87
1:F:506:PHE:CZ	1:F:513:GLU:OE2	2.28	0.85
1:F:621:THR:HG22	1:F:622:ALA:H	1.42	0.83
1:E:371:SER:C	1:E:604:VAL:CG1	2.47	0.81
1:E:602:ASN:HB3	1:E:604:VAL:HG13	1.64	0.80
1:E:506:PHE:HE2	1:E:555:VAL:HG22	1.41	0.80
1:F:506:PHE:HE2	1:F:555:VAL:CB	1.94	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ARG:HG2	1:E:301:ARG:O	1.81	0.78
1:E:506:PHE:CE2	1:E:555:VAL:HG22	2.13	0.77
1:D:905:TYR:OH	1:D:936:PRO:CD	2.32	0.77
1:E:600:LEU:N	1:E:601:GLY:HA2	1.99	0.76
1:F:506:PHE:CE2	1:F:555:VAL:CB	2.69	0.74
1:J:506:PHE:CD2	1:J:555:VAL:HG23	2.23	0.73
1:E:381:VAL:H	1:E:408:ASN:HD22	1.37	0.73
1:F:383:CYS:HB2	1:F:385:PHE:CE2	2.24	0.72
1:E:384:ASP:O	1:E:404:PHE:CE1	2.42	0.71
1:E:372:GLY:N	1:E:604:VAL:HG12	2.05	0.71
1:F:506:PHE:CD1	1:F:513:GLU:OE2	2.44	0.70
1:J:240:MET:O	1:J:240:MET:SD	2.50	0.70
1:E:371:SER:OG	1:E:604:VAL:HG13	1.85	0.70
1:E:372:GLY:C	1:E:604:VAL:HB	2.13	0.69
1:D:905:TYR:OH	1:D:935:LEU:C	2.32	0.68
1:F:369:LYS:O	1:F:369:LYS:HG2	1.94	0.68
1:E:506:PHE:HD2	1:E:555:VAL:HG23	1.50	0.67
1:D:905:TYR:CZ	1:D:936:PRO:HB3	2.28	0.67
1:E:506:PHE:HD2	1:E:555:VAL:CG2	1.93	0.67
1:F:506:PHE:HD2	1:F:555:VAL:HG23	1.54	0.66
1:E:371:SER:OG	1:E:604:VAL:HG12	1.73	0.66
1:E:381:VAL:HG12	1:E:407:CYS:HB2	1.78	0.66
1:J:426:SER:O	1:J:427:GLN:HB2	1.96	0.66
1:E:621:THR:O	1:E:648:TYR:HD2	1.80	0.65
1:J:691:ARG:NE	1:J:691:ARG:HA	2.10	0.65
1:E:616:VAL:O	1:E:616:VAL:HG13	1.95	0.64
1:E:422:ASP:HB3	1:E:481:LEU:HB2	1.79	0.64
1:E:371:SER:HB3	1:E:604:VAL:HG12	1.41	0.63
1:J:172:LEU:HD12	1:J:172:LEU:O	1.98	0.63
1:E:372:GLY:N	1:E:604:VAL:CG1	2.62	0.63
1:E:372:GLY:O	1:E:604:VAL:CG2	2.47	0.62
1:E:621:THR:HG22	1:E:622:ALA:N	2.16	0.60
1:D:905:TYR:OH	1:D:936:PRO:HA	1.99	0.60
1:E:384:ASP:CB	1:E:404:PHE:HE1	2.14	0.60
1:J:506:PHE:CZ	1:J:555:VAL:HG21	2.13	0.59
1:D:905:TYR:HH	1:D:936:PRO:N	1.95	0.59
1:E:600:LEU:N	1:E:601:GLY:CA	2.66	0.58
1:F:621:THR:O	1:F:648:TYR:HD2	1.86	0.58
1:J:691:ARG:HE	1:J:691:ARG:HA	1.67	0.58
1:J:240:MET:SD	1:J:240:MET:C	2.82	0.58
1:E:383:CYS:SG	1:E:409:TYR:HB3	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:875:GLU:N	1:G:875:GLU:OE1	2.35	0.56
1:F:621:THR:O	1:F:648:TYR:HB3	2.06	0.56
1:D:826:GLN:N	1:D:826:GLN:OE1	2.27	0.56
1:D:905:TYR:CE2	1:D:936:PRO:HB3	2.41	0.56
1:J:425:CYS:SG	1:J:430:PRO:HA	2.46	0.56
1:G:875:GLU:HG2	1:G:875:GLU:O	2.05	0.55
1:E:372:GLY:O	1:E:604:VAL:CG1	2.55	0.55
1:E:256:ILE:HG23	1:E:256:ILE:O	2.07	0.54
1:E:383:CYS:O	1:E:385:PHE:N	2.40	0.54
1:J:67:ILE:O	1:J:67:ILE:HG13	2.08	0.54
1:E:67:ILE:O	1:E:67:ILE:HG13	2.08	0.54
2:B:85:GLU:N	2:B:85:GLU:OE1	2.35	0.54
1:E:602:ASN:O	1:E:615:GLY:O	2.26	0.53
1:E:383:CYS:HB3	1:E:385:PHE:CD2	2.43	0.53
1:F:621:THR:HG22	1:F:622:ALA:N	2.19	0.53
1:E:384:ASP:CA	1:E:404:PHE:HE1	2.22	0.53
1:G:823:GLU:N	1:G:823:GLU:OE1	2.37	0.53
1:D:905:TYR:HH	1:D:936:PRO:CA	2.20	0.52
1:E:381:VAL:N	1:E:408:ASN:HD22	2.07	0.52
1:A:826:GLN:OE1	1:A:826:GLN:N	2.27	0.51
1:D:905:TYR:CZ	1:D:936:PRO:CB	2.92	0.51
1:D:905:TYR:OH	1:D:936:PRO:CB	2.57	0.50
1:F:172:LEU:N	1:F:172:LEU:HD23	2.26	0.50
1:A:1001:PHE:C	1:A:1001:PHE:CD1	2.83	0.50
1:A:934:VAL:O	1:A:934:VAL:HG13	2.12	0.50
1:G:826:GLN:OE1	1:G:826:GLN:N	2.27	0.50
1:E:382:GLU:O	1:E:407:CYS:HB2	2.11	0.50
1:J:395:GLN:HA	1:J:395:GLN:OE1	2.12	0.50
1:E:422:ASP:CB	1:E:481:LEU:HB2	2.41	0.50
1:E:130:VAL:HG12	1:E:130:VAL:O	2.12	0.50
1:E:506:PHE:CE2	1:E:555:VAL:CB	2.83	0.49
1:G:1160:ASN:OD1	1:G:1160:ASN:C	2.51	0.49
2:B:72:ASP:OD1	2:B:72:ASP:C	2.51	0.49
1:A:815:GLN:OE1	1:A:815:GLN:N	2.33	0.48
1:F:381:VAL:O	1:F:407:CYS:HB2	2.13	0.48
1:F:381:VAL:O	1:F:407:CYS:HA	2.12	0.48
1:F:172:LEU:HD23	1:F:172:LEU:H	1.79	0.48
3:C:80:GLU:OE1	3:C:80:GLU:N	2.36	0.47
1:E:383:CYS:HB3	1:E:385:PHE:CE2	2.50	0.47
1:G:906:MET:N	1:G:907:GLN:HA	2.30	0.47
1:A:777:TYR:CD1	1:A:777:TYR:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:606:TYR:C	1:F:606:TYR:CD1	2.88	0.47
1:D:905:TYR:HH	1:D:935:LEU:C	2.17	0.47
1:E:251:LEU:C	1:E:251:LEU:HD23	2.36	0.47
1:G:938:LEU:HG	1:G:938:LEU:O	2.16	0.46
1:F:725:GLU:N	1:F:725:GLU:OE1	2.32	0.46
1:F:735:LEU:N	1:F:735:LEU:HD12	2.31	0.46
1:E:616:VAL:CG1	1:E:616:VAL:O	2.62	0.46
1:F:67:ILE:O	1:F:67:ILE:HG13	2.15	0.46
1:E:689:TYR:CD1	1:E:689:TYR:C	2.89	0.46
1:E:601:GLY:O	1:E:602:ASN:HB2	2.16	0.46
1:A:905:TYR:CE2	1:A:936:PRO:HB3	2.30	0.45
1:E:621:THR:CG2	1:E:622:ALA:N	2.78	0.45
1:F:395:GLN:HA	1:F:395:GLN:OE1	2.15	0.45
1:F:596:ILE:HD12	1:F:596:ILE:C	2.36	0.45
1:E:371:SER:HB3	1:E:604:VAL:N	2.32	0.45
1:F:381:VAL:O	1:F:407:CYS:CA	2.64	0.45
1:E:372:GLY:O	1:E:604:VAL:HG21	2.16	0.45
1:G:1173:ILE:HG13	1:G:1185:SER:OG	2.16	0.45
3:C:65:SER:OG	3:C:72:SER:OG	2.32	0.45
1:E:425:CYS:HA	1:E:478:CYS:HA	1.98	0.45
1:F:689:TYR:CD1	1:F:689:TYR:C	2.91	0.45
1:E:621:THR:O	1:E:648:TYR:CD2	2.65	0.44
1:F:383:CYS:CB	1:F:385:PHE:CE2	2.98	0.44
1:F:439:SER:HA	1:F:582:ASN:HA	1.99	0.44
1:J:735:LEU:HD22	1:J:735:LEU:N	2.32	0.44
1:E:371:SER:CB	1:E:602:ASN:OD1	2.65	0.44
1:J:369:LYS:O	1:J:369:LYS:HG2	2.18	0.44
3:C:1:ASP:C	3:C:1:ASP:OD1	2.55	0.44
1:J:439:SER:HA	1:J:582:ASN:HA	1.98	0.44
1:E:130:VAL:O	1:E:130:VAL:CG1	2.66	0.44
1:F:677:VAL:HG22	1:F:677:VAL:O	2.17	0.44
1:J:130:VAL:HG12	1:J:130:VAL:O	2.17	0.44
1:F:381:VAL:O	1:F:408:ASN:N	2.46	0.44
1:A:875:GLU:O	1:A:875:GLU:HG2	2.18	0.43
1:D:801:LYS:HE2	1:D:801:LYS:HB2	1.87	0.43
1:F:633:ASP:C	1:F:633:ASP:OD1	2.57	0.43
1:E:422:ASP:O	1:E:480:ILE:HA	2.17	0.43
1:J:735:LEU:HA	1:J:735:LEU:HD13	1.80	0.43
1:A:965:SER:OG	1:A:966:SER:N	2.51	0.43
1:D:905:TYR:CZ	1:D:936:PRO:CA	2.98	0.43
1:F:664:ASP:C	1:F:664:ASP:OD1	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1124:VAL:HG13	1:G:1124:VAL:O	2.18	0.43
1:D:1183:GLU:HG3	1:D:1183:GLU:O	2.19	0.43
1:E:371:SER:OG	1:E:602:ASN:OD1	2.29	0.43
3:C:28:TYR:CD1	3:C:28:TYR:N	2.85	0.43
1:F:383:CYS:CB	1:F:385:PHE:CZ	3.02	0.42
1:J:719:ASN:OD1	1:J:719:ASN:C	2.57	0.42
1:E:422:ASP:HB3	1:E:481:LEU:CB	2.47	0.42
1:E:605:GLU:HB2	1:E:614:ARG:HG2	2.00	0.42
1:E:719:ASN:OD1	1:E:719:ASN:C	2.57	0.42
1:F:130:VAL:HG12	1:F:130:VAL:O	2.18	0.42
1:F:409:TYR:CD1	1:F:409:TYR:C	2.93	0.42
3:I:43:PRO:HA	3:I:44:PRO:HD3	1.93	0.42
1:E:688:GLN:HA	1:E:688:GLN:OE1	2.19	0.42
1:J:593:ASP:N	1:J:594:THR:HA	2.35	0.42
1:F:741:THR:HA	1:F:742:PRO:HD3	1.87	0.42
1:D:988:GLN:HB3	1:D:1195:GLU:OE2	2.20	0.42
1:D:806:CYS:O	1:D:806:CYS:SG	2.78	0.42
1:G:906:MET:HG3	1:G:906:MET:O	2.20	0.42
1:E:381:VAL:HG13	1:E:407:CYS:HA	1.25	0.41
1:D:759:LEU:N	1:F:717:LEU:O	2.53	0.41
1:E:371:SER:HB2	1:E:602:ASN:OD1	2.20	0.41
1:F:369:LYS:CG	1:F:369:LYS:O	2.60	0.41
1:G:801:LYS:HE2	1:G:801:LYS:HB2	1.93	0.41
1:E:371:SER:HB3	1:E:604:VAL:CA	2.50	0.41
1:J:670:HIS:N	1:J:670:HIS:CD2	2.86	0.41
1:A:756:GLU:N	1:A:756:GLU:OE1	2.49	0.41
1:F:689:TYR:CD1	1:F:689:TYR:O	2.74	0.41
1:E:395:GLN:OE1	1:E:395:GLN:HA	2.21	0.41
1:E:384:ASP:C	1:E:404:PHE:CE1	2.94	0.41
1:F:378:ALA:HB1	1:F:379:GLU:HA	2.03	0.41
1:F:604:VAL:HG13	1:F:604:VAL:O	2.21	0.41
1:J:209:THR:O	1:J:209:THR:HG22	2.20	0.41
1:F:132:ILE:HD12	1:F:132:ILE:HA	1.83	0.41
1:E:371:SER:OG	1:E:604:VAL:HG11	2.04	0.41
1:E:384:ASP:N	1:E:404:PHE:CE1	2.89	0.41
1:G:1060:PRO:HA	1:G:1063:GLN:HB3	2.03	0.41
1:G:774:ASN:OD1	1:G:774:ASN:C	2.59	0.41
1:D:905:TYR:OH	1:D:936:PRO:HD3	2.18	0.40
1:E:599:GLN:C	1:E:601:GLY:HA2	2.42	0.40
1:E:643:SER:OG	1:E:644:ASP:N	2.54	0.40
1:F:209:THR:O	1:F:209:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:70:ASP:OD1	3:I:70:ASP:C	2.58	0.40
1:D:927:GLN:HB2	1:D:932:TYR:HB2	2.03	0.40
1:E:633:ASP:C	1:E:633:ASP:OD1	2.60	0.40
1:F:174:ASP:OD1	1:F:174:ASP:C	2.59	0.40
1:D:775:SER:OG	1:D:776:SER:N	2.53	0.40
1:E:384:ASP:N	1:E:404:PHE:HE1	2.19	0.40

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	459/1329 (34%)	443 (96%)	15 (3%)	1 (0%)	51	85
1	D	451/1329 (34%)	435 (96%)	12 (3%)	4 (1%)	20	63
1	E	724/1329 (54%)	691 (95%)	28 (4%)	5 (1%)	25	68
1	F	724/1329 (54%)	693 (96%)	28 (4%)	3 (0%)	38	77
1	G	459/1329 (34%)	442 (96%)	15 (3%)	2 (0%)	38	77
1	J	724/1329 (54%)	700 (97%)	19 (3%)	5 (1%)	25	68
2	B	117/233 (50%)	114 (97%)	3 (3%)	0	100	100
2	H	117/233 (50%)	112 (96%)	5 (4%)	0	100	100
3	C	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	20	63
3	I	109/218 (50%)	103 (94%)	5 (5%)	1 (1%)	20	63
All	All	3993/8876 (45%)	3837 (96%)	134 (3%)	22 (1%)	33	71

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	962	ALA

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Mol	Chain	Res	Type
1	E	384	ASP
1	J	378	ALA
1	D	961	THR
1	D	965	SER
1	E	718	VAL
1	F	718	VAL
1	J	602	ASN
1	J	718	VAL
3	C	77	PRO
3	I	77	PRO
1	A	1220	PRO
1	D	1220	PRO
1	E	368	ALA
1	E	382	GLU
1	E	621	THR
1	F	621	THR
1	J	596	ILE
1	D	956	ALA
1	G	956	ALA
1	F	629	ARG
1	J	629	ARG

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	388/1148 (34%)	388 (100%)	0	100	100
1	D	382/1148 (33%)	382 (100%)	0	100	100
1	E	635/1148 (55%)	631 (99%)	4 (1%)	89	94
1	F	635/1148 (55%)	635 (100%)	0	100	100
1	G	388/1148 (34%)	388 (100%)	0	100	100
1	J	635/1148 (55%)	634 (100%)	1 (0%)	94	96
2	B	102/202 (50%)	102 (100%)	0	100	100
2	H	102/202 (50%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	93/192 (48%)	93 (100%)	0	100	100
3	I	93/192 (48%)	93 (100%)	0	100	100
All	All	3453/7676 (45%)	3448 (100%)	5 (0%)	95	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	384	ASP
1	E	423	PHE
1	E	602	ASN
1	E	694	ARG
1	J	670	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.