Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 03:10 pm GMT

PDB ID	:	9FJK
EMDB ID	:	EMD-50503
Title	:	Omicron BA.1 Spike protein with neutralizing NTD specific mAb K501SP6
Authors	:	Bjoernsson, K.H.; Walker, M.R.; Raghavan, S.S.R.; Ward, A.B.; Barfod, L.K.
Deposited on	:	2024-05-31
Resolution	:	2.84 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

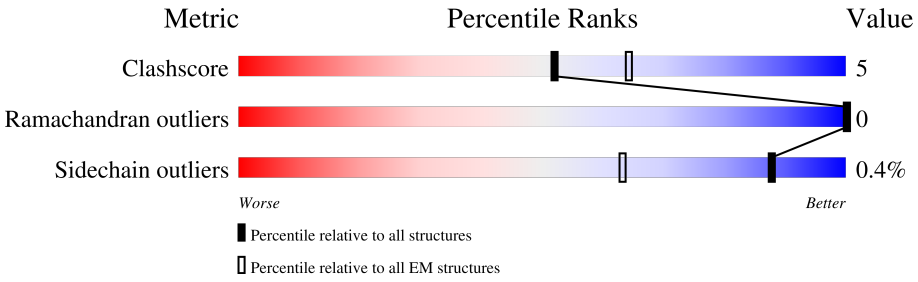
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1277	72% 9% · 19%
1	B	1277	72% 10% 18%
1	C	1277	74% 8% 17%
2	H	129	82% 17% ·
3	L	134	72% 10% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26529 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1040	Total	C	N	O	S	0	0
			8185	5244	1361	1543	37		
1	B	1047	Total	C	N	O	S	0	0
			8226	5265	1369	1555	37		
1	C	1055	Total	C	N	O	S	0	0
			8288	5307	1379	1565	37		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	206	LEU	ASN	variant	UNP P0DTC2
A	207	VAL	LEU	variant	UNP P0DTC2
A	208	ARG	VAL	variant	UNP P0DTC2
A	209	GLU	ARG	variant	UNP P0DTC2
A	210	PRO	-	insertion	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	680	SER	ARG	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	889	PRO	ALA	engineered mutation	UNP P0DTC2
A	896	PRO	ALA	engineered mutation	UNP P0DTC2
A	939	PRO	ALA	engineered mutation	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
A	1205	GLN	-	linker	UNP P0DTC2
A	1206	GLY	-	linker	UNP P0DTC2
A	1207	SER	-	linker	UNP P0DTC2
A	1229	LEU	PHE	engineered mutation	UNP P10104
A	1235	GLY	-	expression tag	UNP P10104
A	1236	ARG	-	expression tag	UNP P10104
A	1237	SER	-	expression tag	UNP P10104
A	1238	LEU	-	expression tag	UNP P10104
A	1239	GLU	-	expression tag	UNP P10104
A	1240	VAL	-	expression tag	UNP P10104
A	1241	LEU	-	expression tag	UNP P10104
A	1242	PHE	-	expression tag	UNP P10104
A	1243	GLN	-	expression tag	UNP P10104
A	1244	GLY	-	expression tag	UNP P10104
A	1245	PRO	-	expression tag	UNP P10104
A	1246	GLY	-	expression tag	UNP P10104
A	1247	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1248	ALA	-	expression tag	UNP P10104
A	1249	TRP	-	expression tag	UNP P10104
A	1250	SER	-	expression tag	UNP P10104
A	1251	HIS	-	expression tag	UNP P10104
A	1252	PRO	-	expression tag	UNP P10104
A	1253	GLN	-	expression tag	UNP P10104
A	1254	PHE	-	expression tag	UNP P10104
A	1255	GLU	-	expression tag	UNP P10104
A	1256	LYS	-	expression tag	UNP P10104
A	1257	GLY	-	expression tag	UNP P10104
A	1258	GLY	-	expression tag	UNP P10104
A	1259	GLY	-	expression tag	UNP P10104
A	1260	SER	-	expression tag	UNP P10104
A	1261	GLY	-	expression tag	UNP P10104
A	1262	GLY	-	expression tag	UNP P10104
A	1263	GLY	-	expression tag	UNP P10104
A	1264	GLY	-	expression tag	UNP P10104
A	1265	SER	-	expression tag	UNP P10104
A	1266	GLY	-	expression tag	UNP P10104
A	1267	GLY	-	expression tag	UNP P10104
A	1268	SER	-	expression tag	UNP P10104
A	1269	ALA	-	expression tag	UNP P10104
A	1270	TRP	-	expression tag	UNP P10104
A	1271	SER	-	expression tag	UNP P10104
A	1272	HIS	-	expression tag	UNP P10104
A	1273	PRO	-	expression tag	UNP P10104
A	1274	GLN	-	expression tag	UNP P10104
A	1275	PHE	-	expression tag	UNP P10104
A	1276	GLU	-	expression tag	UNP P10104
A	1277	LYS	-	expression tag	UNP P10104
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	variant	UNP P0DTC2
B	140	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	206	LEU	ASN	variant	UNP P0DTC2
B	207	VAL	LEU	variant	UNP P0DTC2
B	208	ARG	VAL	variant	UNP P0DTC2
B	209	GLU	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	210	PRO	-	insertion	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	ARG	GLN	variant	UNP P0DTC2
B	493	SER	GLY	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	544	LYS	THR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	engineered mutation	UNP P0DTC2
B	680	SER	ARG	engineered mutation	UNP P0DTC2
B	682	SER	ARG	engineered mutation	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	conflict	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	889	PRO	ALA	engineered mutation	UNP P0DTC2
B	896	PRO	ALA	engineered mutation	UNP P0DTC2
B	939	PRO	ALA	engineered mutation	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	1205	GLN	-	linker	UNP P0DTC2
B	1206	GLY	-	linker	UNP P0DTC2
B	1207	SER	-	linker	UNP P0DTC2
B	1229	LEU	PHE	engineered mutation	UNP P10104
B	1235	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1236	ARG	-	expression tag	UNP P10104
B	1237	SER	-	expression tag	UNP P10104
B	1238	LEU	-	expression tag	UNP P10104
B	1239	GLU	-	expression tag	UNP P10104
B	1240	VAL	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	PHE	-	expression tag	UNP P10104
B	1243	GLN	-	expression tag	UNP P10104
B	1244	GLY	-	expression tag	UNP P10104
B	1245	PRO	-	expression tag	UNP P10104
B	1246	GLY	-	expression tag	UNP P10104
B	1247	SER	-	expression tag	UNP P10104
B	1248	ALA	-	expression tag	UNP P10104
B	1249	TRP	-	expression tag	UNP P10104
B	1250	SER	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	PRO	-	expression tag	UNP P10104
B	1253	GLN	-	expression tag	UNP P10104
B	1254	PHE	-	expression tag	UNP P10104
B	1255	GLU	-	expression tag	UNP P10104
B	1256	LYS	-	expression tag	UNP P10104
B	1257	GLY	-	expression tag	UNP P10104
B	1258	GLY	-	expression tag	UNP P10104
B	1259	GLY	-	expression tag	UNP P10104
B	1260	SER	-	expression tag	UNP P10104
B	1261	GLY	-	expression tag	UNP P10104
B	1262	GLY	-	expression tag	UNP P10104
B	1263	GLY	-	expression tag	UNP P10104
B	1264	GLY	-	expression tag	UNP P10104
B	1265	SER	-	expression tag	UNP P10104
B	1266	GLY	-	expression tag	UNP P10104
B	1267	GLY	-	expression tag	UNP P10104
B	1268	SER	-	expression tag	UNP P10104
B	1269	ALA	-	expression tag	UNP P10104
B	1270	TRP	-	expression tag	UNP P10104
B	1271	SER	-	expression tag	UNP P10104
B	1272	HIS	-	expression tag	UNP P10104
B	1273	PRO	-	expression tag	UNP P10104
B	1274	GLN	-	expression tag	UNP P10104
B	1275	PHE	-	expression tag	UNP P10104
B	1276	GLU	-	expression tag	UNP P10104
B	1277	LYS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	variant	UNP P0DTC2
C	140	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	206	LEU	ASN	variant	UNP P0DTC2
C	207	VAL	LEU	variant	UNP P0DTC2
C	208	ARG	VAL	variant	UNP P0DTC2
C	209	GLU	ARG	variant	UNP P0DTC2
C	210	PRO	-	insertion	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	336	ASP	GLY	variant	UNP P0DTC2
C	368	LEU	SER	variant	UNP P0DTC2
C	370	PRO	SER	variant	UNP P0DTC2
C	372	PHE	SER	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	variant	UNP P0DTC2
C	443	SER	GLY	variant	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	variant	UNP P0DTC2
C	490	ARG	GLN	variant	UNP P0DTC2
C	493	SER	GLY	variant	UNP P0DTC2
C	495	ARG	GLN	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	variant	UNP P0DTC2
C	544	LYS	THR	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	engineered mutation	UNP P0DTC2
C	680	SER	ARG	engineered mutation	UNP P0DTC2
C	682	SER	ARG	engineered mutation	UNP P0DTC2
C	761	LYS	ASN	variant	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2
C	814	PRO	PHE	conflict	UNP P0DTC2
C	853	LYS	ASN	variant	UNP P0DTC2
C	889	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	896	PRO	ALA	engineered mutation	UNP P0DTC2
C	939	PRO	ALA	engineered mutation	UNP P0DTC2
C	951	HIS	GLN	variant	UNP P0DTC2
C	966	LYS	ASN	variant	UNP P0DTC2
C	978	PHE	LEU	variant	UNP P0DTC2
C	983	PRO	LYS	engineered mutation	UNP P0DTC2
C	984	PRO	VAL	engineered mutation	UNP P0DTC2
C	1205	GLN	-	linker	UNP P0DTC2
C	1206	GLY	-	linker	UNP P0DTC2
C	1207	SER	-	linker	UNP P0DTC2
C	1229	LEU	PHE	engineered mutation	UNP P10104
C	1235	GLY	-	expression tag	UNP P10104
C	1236	ARG	-	expression tag	UNP P10104
C	1237	SER	-	expression tag	UNP P10104
C	1238	LEU	-	expression tag	UNP P10104
C	1239	GLU	-	expression tag	UNP P10104
C	1240	VAL	-	expression tag	UNP P10104
C	1241	LEU	-	expression tag	UNP P10104
C	1242	PHE	-	expression tag	UNP P10104
C	1243	GLN	-	expression tag	UNP P10104
C	1244	GLY	-	expression tag	UNP P10104
C	1245	PRO	-	expression tag	UNP P10104
C	1246	GLY	-	expression tag	UNP P10104
C	1247	SER	-	expression tag	UNP P10104
C	1248	ALA	-	expression tag	UNP P10104
C	1249	TRP	-	expression tag	UNP P10104
C	1250	SER	-	expression tag	UNP P10104
C	1251	HIS	-	expression tag	UNP P10104
C	1252	PRO	-	expression tag	UNP P10104
C	1253	GLN	-	expression tag	UNP P10104
C	1254	PHE	-	expression tag	UNP P10104
C	1255	GLU	-	expression tag	UNP P10104
C	1256	LYS	-	expression tag	UNP P10104
C	1257	GLY	-	expression tag	UNP P10104
C	1258	GLY	-	expression tag	UNP P10104
C	1259	GLY	-	expression tag	UNP P10104
C	1260	SER	-	expression tag	UNP P10104
C	1261	GLY	-	expression tag	UNP P10104
C	1262	GLY	-	expression tag	UNP P10104
C	1263	GLY	-	expression tag	UNP P10104
C	1264	GLY	-	expression tag	UNP P10104
C	1265	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1266	GLY	-	expression tag	UNP P10104
C	1267	GLY	-	expression tag	UNP P10104
C	1268	SER	-	expression tag	UNP P10104
C	1269	ALA	-	expression tag	UNP P10104
C	1270	TRP	-	expression tag	UNP P10104
C	1271	SER	-	expression tag	UNP P10104
C	1272	HIS	-	expression tag	UNP P10104
C	1273	PRO	-	expression tag	UNP P10104
C	1274	GLN	-	expression tag	UNP P10104
C	1275	PHE	-	expression tag	UNP P10104
C	1276	GLU	-	expression tag	UNP P10104
C	1277	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called K501SP6 Fv Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	129	Total	C	N	O	S	0	0
			1014	646	162	202	4		

- Molecule 3 is a protein called K501SP6 Fv Light Chain.

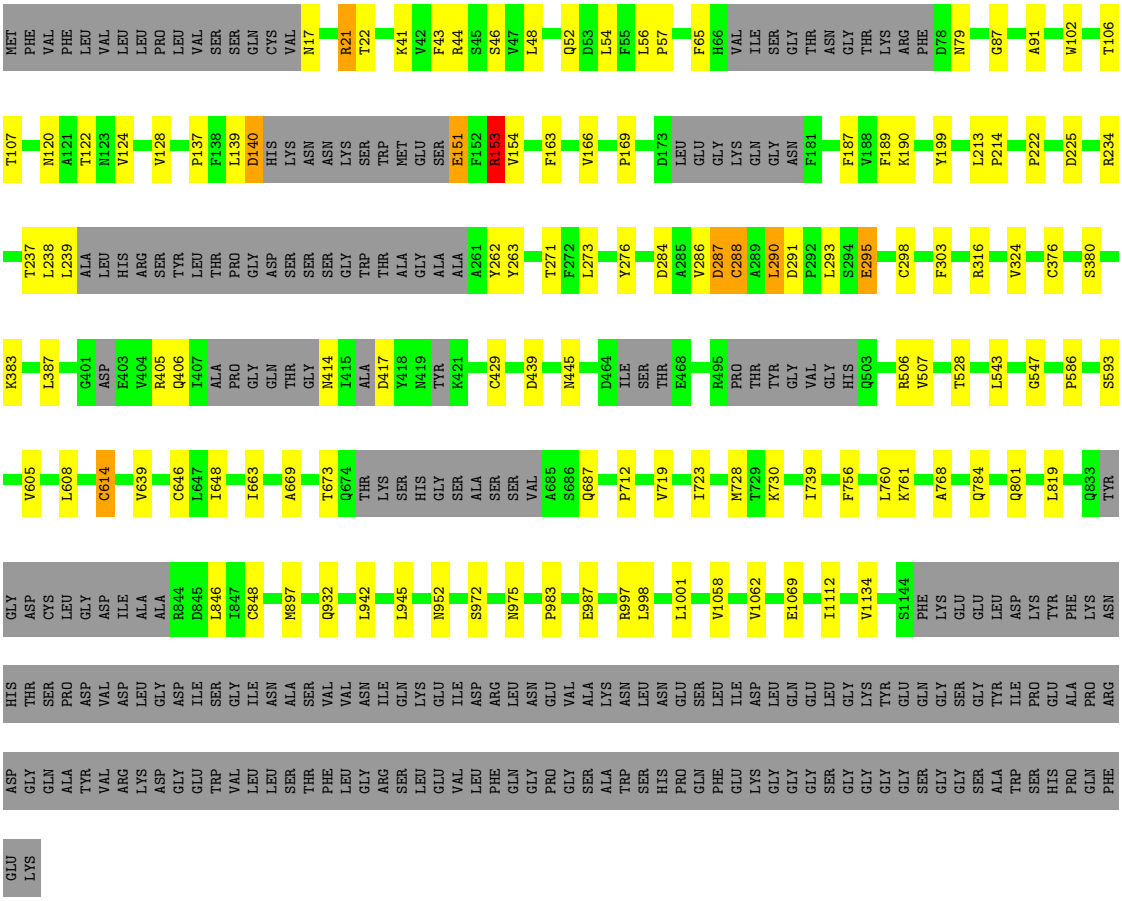
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			816	505	140	169	2		

3 Residue-property plots (i)

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

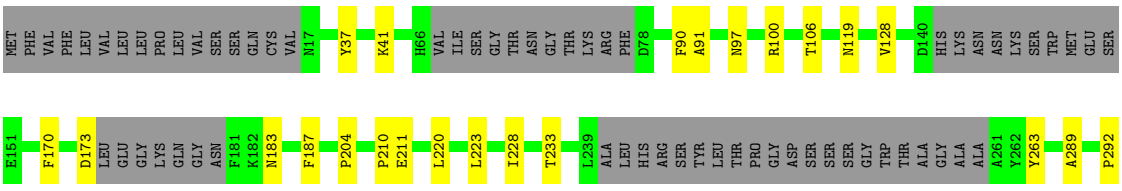
- Molecule 1: Spike glycoprotein,Fibritin

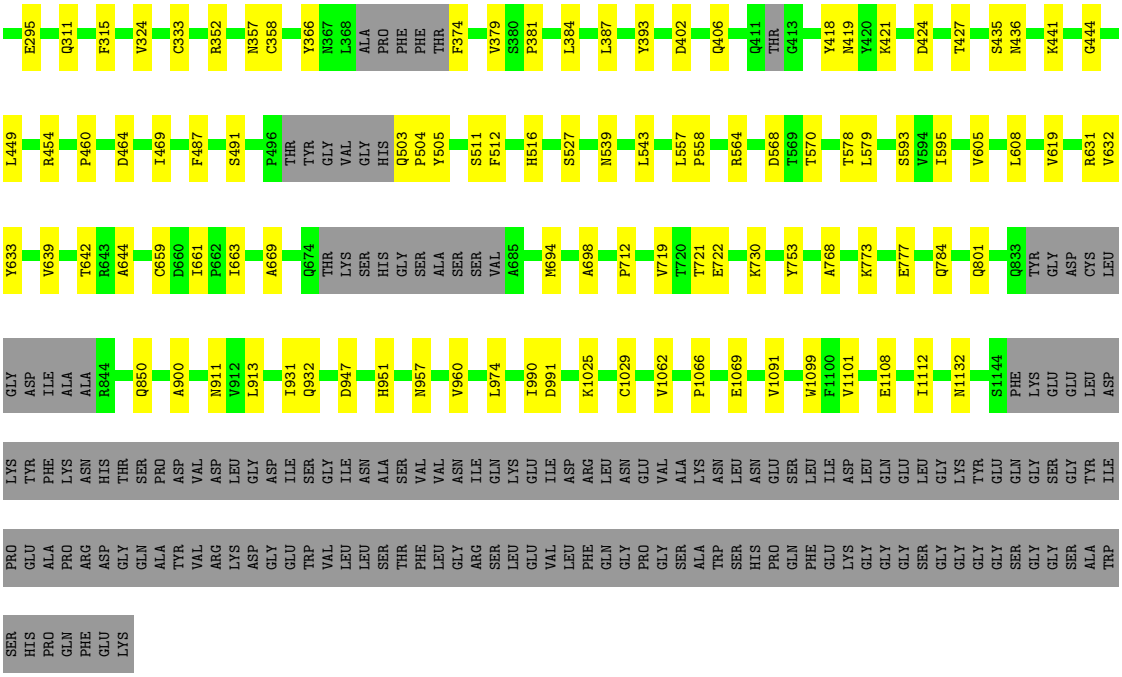
Chain A:



- Molecule 1: Spike glycoprotein,Fibritin

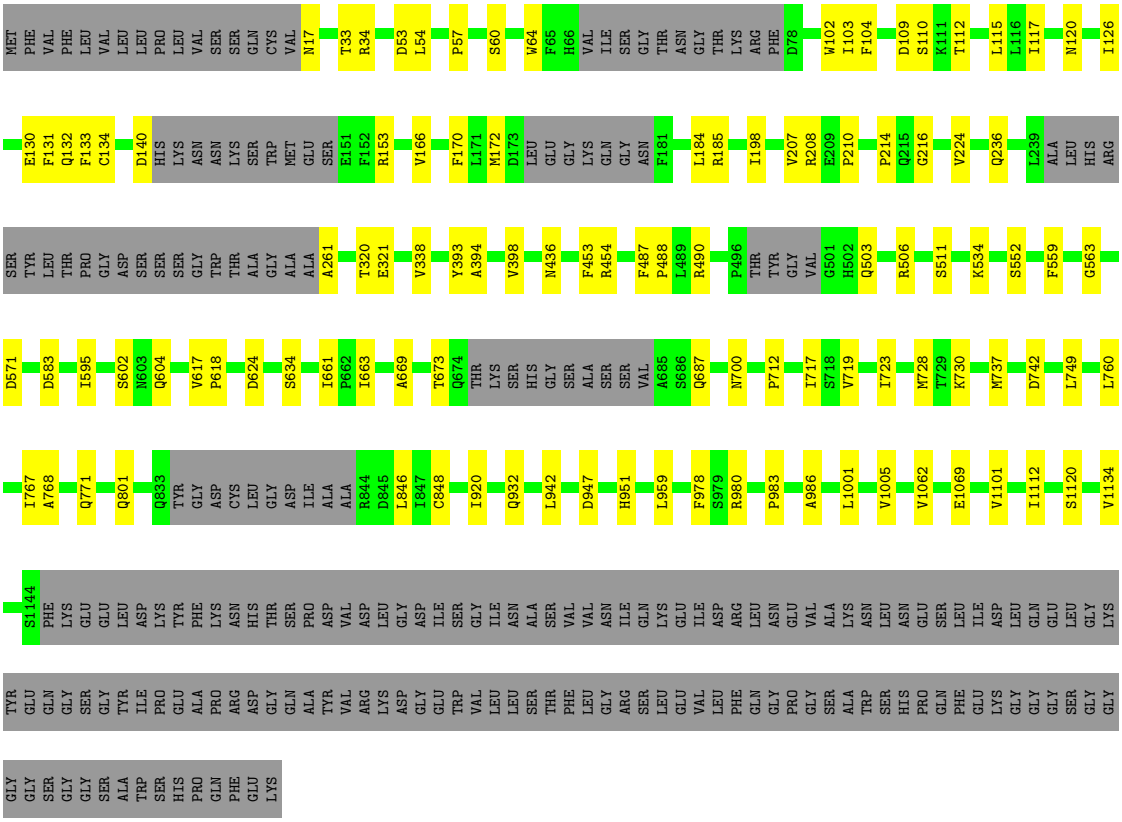
Chain B:





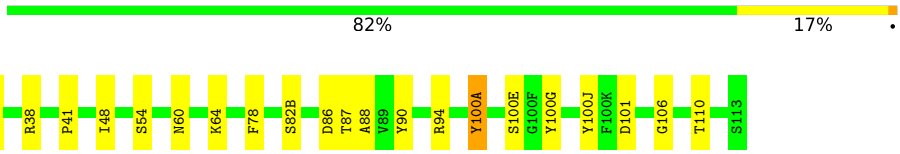
• Molecule 1: Spike glycoprotein,Fibritin

Chain C:



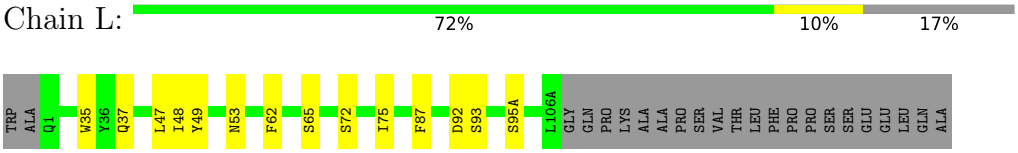
• Molecule 2: K501SP6 Fv Heavy Chain

Chain H:



• Molecule 3: K501SP6 Fv Light Chain

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87875	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	195000	Depositor
Image detector	FEI FALCON IV (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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/8372	0.60	4/11383 (0.0%)
1	B	0.29	0/8416	0.58	0/11449
1	C	0.30	0/8484	0.59	1/11546 (0.0%)
2	H	0.34	0/1042	0.78	2/1417 (0.1%)
3	L	0.30	0/834	0.61	0/1139
All	All	0.30	0/27148	0.60	7/36934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	H	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	101	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	998	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	756	PHE	CB-CG-CD1	5.35	124.55	120.80
1	C	184	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	756	PHE	CB-CG-CD2	-5.16	117.19	120.80
2	H	100(A)	TYR	CA-CB-CG	5.06	123.02	113.40
1	A	543	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	ARG	Sidechain
1	A	614	CYS	Peptide
2	H	100(J)	TYR	Peptide

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	8185	0	8036	107	0
1	B	8226	0	8074	120	0
1	C	8288	0	8131	64	0
2	H	1014	0	964	37	0
3	L	816	0	780	11	0
All	All	26529	0	25985	274	0

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

All (274) 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:B:579:LEU:HB2	2:H:64:LYS:CE	1.23	1.64
1:A:44:ARG:HH22	1:B:564:ARG:CA	1.18	1.52
1:A:48:LEU:CD1	1:A:303:PHE:HE1	1.21	1.50
1:A:48:LEU:HD11	1:A:303:PHE:CE1	1.51	1.45
1:A:44:ARG:HH22	1:B:564:ARG:N	1.09	1.44
1:A:44:ARG:NH2	1:B:564:ARG:H	1.10	1.43
1:B:579:LEU:CB	2:H:64:LYS:HE3	1.49	1.39
1:A:48:LEU:CD1	1:A:303:PHE:CE1	2.03	1.38
1:A:44:ARG:NH2	1:B:564:ARG:N	1.65	1.38
1:A:284:ASP:OD2	1:A:303:PHE:CE2	1.76	1.38
1:B:579:LEU:CB	2:H:64:LYS:CE	2.02	1.35
1:B:352:ARG:NH2	2:H:100(A):TYR:HE1	1.28	1.29
1:B:579:LEU:HB2	2:H:64:LYS:NZ	1.47	1.26
1:A:44:ARG:NH2	1:B:564:ARG:CA	1.97	1.25
1:B:558:PRO:HD3	3:L:93:SER:O	1.36	1.23
1:A:273:LEU:HD11	1:A:298:CYS:CA	1.70	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:NH2	2:H:100(A):TYR:CE1	2.12	1.16
1:A:48:LEU:HD12	1:A:303:PHE:HE1	1.05	1.15
1:A:273:LEU:HD11	1:A:298:CYS:HA	1.14	1.13
1:B:579:LEU:CG	2:H:64:LYS:HE3	1.81	1.11
1:A:273:LEU:HG	1:A:298:CYS:SG	1.92	1.09
1:A:284:ASP:OD2	1:A:303:PHE:HE2	1.12	1.08
1:A:48:LEU:HD11	1:A:303:PHE:CD1	1.91	1.04
1:B:579:LEU:CB	2:H:64:LYS:NZ	2.15	1.04
1:A:44:ARG:NH2	1:B:564:ARG:CB	2.19	1.03
1:A:44:ARG:NH2	1:B:564:ARG:HB2	1.72	1.03
1:B:579:LEU:CA	2:H:64:LYS:NZ	2.25	0.99
1:A:273:LEU:CD1	1:A:298:CYS:HA	1.93	0.98
1:A:43:PHE:HE1	1:B:557:LEU:HD12	1.30	0.96
1:A:284:ASP:OD2	1:A:303:PHE:CD2	2.18	0.95
1:A:273:LEU:CG	1:A:298:CYS:SG	2.54	0.95
1:A:44:ARG:HH21	1:B:564:ARG:H	1.16	0.94
1:A:43:PHE:CZ	1:B:557:LEU:HB2	2.04	0.92
1:A:273:LEU:CD1	1:A:298:CYS:SG	2.59	0.91
1:A:43:PHE:CE1	1:B:557:LEU:HB2	2.08	0.89
1:B:579:LEU:CD1	2:H:64:LYS:HE3	2.04	0.88
1:A:43:PHE:CE1	1:B:557:LEU:HD12	2.09	0.87
1:B:579:LEU:HB2	2:H:64:LYS:HE3	0.89	0.87
1:B:579:LEU:HB2	2:H:64:LYS:HZ1	1.41	0.85
1:A:273:LEU:HD11	1:A:298:CYS:SG	2.16	0.84
1:A:44:ARG:HH22	1:B:564:ARG:C	1.76	0.83
1:B:558:PRO:CD	3:L:93:SER:O	2.26	0.80
1:A:44:ARG:CZ	1:B:564:ARG:HB2	2.12	0.79
1:C:17:ASN:N	1:C:134:CYS:HG	1.82	0.78
1:A:48:LEU:HD12	1:A:303:PHE:CE1	1.91	0.77
1:B:579:LEU:CG	2:H:64:LYS:CE	2.53	0.77
1:A:273:LEU:HD11	1:A:298:CYS:CB	2.16	0.76
1:B:579:LEU:HD12	2:H:64:LYS:HE3	1.67	0.76
1:B:579:LEU:C	2:H:64:LYS:NZ	2.43	0.72
1:A:293:LEU:HB2	1:A:605:VAL:HG11	1.73	0.70
1:C:110:SER:H	1:C:132:GLN:HE22	1.39	0.70
1:C:801:GLN:NE2	1:C:932:GLN:OE1	2.26	0.66
1:A:151:GLU:HB2	1:A:153:ARG:HE	1.62	0.65
1:A:761:LYS:HE3	1:B:311:GLN:HB3	1.79	0.65
1:B:579:LEU:CA	2:H:64:LYS:CE	2.75	0.63
1:A:41:LYS:NZ	1:B:516:HIS:O	2.32	0.63
1:B:436:ASN:HB3	1:B:505:TYR:HE1	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:MET:O	1:C:185:ARG:NH2	2.33	0.61
1:C:947:ASP:O	1:C:951:HIS:ND1	2.29	0.61
1:B:579:LEU:CB	2:H:64:LYS:HZ1	2.02	0.61
1:A:137:PRO:HB3	1:A:154:VAL:HA	1.83	0.60
1:B:170:PHE:HA	1:B:223:LEU:HD21	1.83	0.60
1:A:846:LEU:HG	1:A:848:CYS:H	1.66	0.60
1:C:624:ASP:HB3	1:C:634:SER:HB2	1.84	0.60
1:B:333:CYS:HA	1:B:358:CYS:HB3	1.84	0.60
1:A:43:PHE:CE1	1:B:557:LEU:CB	2.85	0.59
1:A:52:GLN:HG2	1:A:271:THR:HG22	1.85	0.59
1:C:109:ASP:OD1	1:C:132:GLN:NE2	2.36	0.58
2:H:22:CYS:HB3	2:H:78:PHE:HB3	1.84	0.58
1:B:947:ASP:O	1:B:951:HIS:ND1	2.31	0.58
1:C:104:PHE:HB2	1:C:115:LEU:HB3	1.85	0.58
1:B:564:ARG:NH2	1:B:568:ASP:OD1	2.35	0.58
1:C:198:ILE:HB	1:C:224:VAL:HB	1.85	0.58
1:A:222:PRO:HB2	2:H:100(G):TYR:HE2	1.68	0.57
1:A:293:LEU:HB2	1:A:605:VAL:CG1	2.35	0.57
1:B:441:LYS:O	1:B:503:GLN:N	2.38	0.57
1:B:379:VAL:HG21	1:B:387:LEU:HD11	1.87	0.57
1:C:393:TYR:HB2	1:C:511:SER:HB3	1.86	0.57
1:B:578:THR:O	2:H:64:LYS:HG2	2.05	0.57
1:B:289:ALA:HB1	1:B:632:VAL:HG11	1.87	0.56
1:A:760:LEU:HD21	1:A:1001:LEU:HB3	1.86	0.56
1:A:187:PHE:HA	1:A:199:TYR:O	2.06	0.56
1:A:784:GLN:HG2	1:B:698:ALA:HB3	1.85	0.56
1:A:719:VAL:HG22	1:A:1062:VAL:HG22	1.88	0.56
1:C:34:ARG:NH1	1:C:216:GLY:O	2.38	0.56
1:C:1112:ILE:HG22	1:C:1134:VAL:HG13	1.89	0.55
1:B:712:PRO:HG3	1:B:1066:PRO:HB3	1.88	0.55
1:B:381:PRO:HA	1:B:384:LEU:HD23	1.89	0.55
1:B:631:ARG:NH2	1:B:633:TYR:OH	2.40	0.55
1:A:380:SER:N	1:C:980:ARG:O	2.39	0.55
1:C:338:VAL:HG21	1:C:394:ALA:HB1	1.89	0.55
1:C:846:LEU:HG	1:C:848:CYS:H	1.71	0.54
1:B:557:LEU:HD22	3:L:93:SER:HB2	1.89	0.54
1:C:120:ASN:HB2	1:C:166:VAL:HG11	1.90	0.54
1:B:900:ALA:HB2	1:B:913:LEU:HD22	1.88	0.54
1:A:43:PHE:HE1	1:B:557:LEU:CD1	2.12	0.54
1:C:320:THR:OG1	1:C:534:LYS:NZ	2.38	0.54
1:A:43:PHE:CE1	1:B:557:LEU:CD1	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:O	1:B:119:ASN:ND2	2.39	0.54
1:C:53:ASP:OD1	1:C:54:LEU:N	2.41	0.54
1:B:850:GLN:HG2	1:B:960:VAL:HG21	1.90	0.53
1:C:1101:VAL:HG23	1:C:1112:ILE:HG12	1.91	0.53
1:B:558:PRO:HG2	3:L:95(A):SER:OG	2.08	0.53
1:C:321:GLU:HG2	1:C:534:LYS:HZ2	1.72	0.53
1:B:441:LYS:HE3	1:B:444:GLY:HA2	1.89	0.53
1:A:44:ARG:HH21	1:B:564:ARG:N	1.80	0.53
1:A:225:ASP:HB2	2:H:100(E):SER:HB3	1.91	0.53
1:C:760:LEU:HD21	1:C:1001:LEU:HB3	1.91	0.53
1:B:579:LEU:N	2:H:64:LYS:CE	2.66	0.52
1:B:722:GLU:OE2	1:B:1025:LYS:NZ	2.34	0.52
1:C:115:LEU:HD12	1:C:126:ILE:HD13	1.92	0.52
1:A:46:SER:HA	1:A:276:TYR:O	2.09	0.52
2:H:38:ARG:NH1	2:H:86:ASP:OD1	2.42	0.52
1:B:357:ASN:ND2	2:H:54:SER:HB2	2.25	0.52
1:B:324:VAL:HG13	1:B:527:SER:HA	1.92	0.52
1:A:723:ILE:HG12	1:A:1058:VAL:HG22	1.91	0.52
1:C:617:VAL:HG22	1:C:618:PRO:HD2	1.92	0.52
1:A:287:ASP:HB2	1:A:290:LEU:HB3	1.92	0.51
1:B:1099:TRP:HB2	1:B:1132:ASN:HD22	1.75	0.51
1:B:619:VAL:HG13	1:B:639:VAL:HG21	1.92	0.51
1:B:974:LEU:HD13	1:B:990:ILE:HD12	1.93	0.51
1:A:44:ARG:CZ	1:B:564:ARG:CB	2.81	0.51
1:A:273:LEU:HD11	1:A:298:CYS:N	2.24	0.51
1:B:659:CYS:HB2	1:B:694:MET:HE3	1.92	0.51
2:H:87:THR:HG23	2:H:110:THR:HA	1.92	0.51
1:C:602:SER:OG	1:C:604:GLN:OE1	2.25	0.51
1:A:21:ARG:HD3	1:A:22:THR:H	1.76	0.50
1:B:753:TYR:OH	1:B:991:ASP:OD1	2.29	0.50
1:A:124:VAL:HB	1:A:169:PRO:HA	1.93	0.50
1:A:739:ILE:O	1:A:997:ARG:NH1	2.45	0.50
1:A:439:ASP:OD1	1:A:445:ASN:ND2	2.41	0.50
1:A:897:MET:HE1	1:B:1091:VAL:HG23	1.94	0.50
1:A:1112:ILE:HG22	1:A:1134:VAL:HG13	1.93	0.50
1:A:639:VAL:HG22	1:A:648:ILE:HG12	1.93	0.50
1:C:103:ILE:HB	1:C:236:GLN:HB2	1.93	0.50
1:B:850:GLN:NE2	1:B:957:ASN:OD1	2.45	0.50
1:C:983:PRO:HA	1:C:986:ALA:HB3	1.94	0.50
2:H:41:PRO:HD3	2:H:88:ALA:HA	1.92	0.50
1:A:213:LEU:HD12	1:A:214:PRO:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:THR:O	2:H:64:LYS:CG	2.60	0.49
1:B:419:ASN:ND2	1:B:464:ASP:O	2.41	0.49
1:C:208:ARG:HB3	1:C:210:PRO:HD2	1.93	0.49
1:A:288:CYS:HB3	1:A:295:GLU:HA	1.94	0.49
1:B:210:PRO:HG2	1:B:211:GLU:HG3	1.94	0.49
1:C:552:SER:HA	1:C:583:ASP:HB2	1.93	0.49
1:A:124:VAL:O	1:A:166:VAL:HA	2.12	0.49
1:B:90:PHE:HB3	1:B:187:PHE:HB2	1.95	0.49
1:C:719:VAL:HG22	1:C:1062:VAL:HG22	1.95	0.49
1:A:65:PHE:O	1:A:262:TYR:HB3	2.13	0.49
1:A:286:VAL:HG23	1:A:303:PHE:CE2	2.48	0.49
1:B:719:VAL:HG22	1:B:1062:VAL:HG22	1.95	0.49
1:C:33:THR:OG1	1:C:216:GLY:O	2.30	0.49
1:B:1101:VAL:HG23	1:B:1112:ILE:HG12	1.95	0.48
1:C:487:PHE:O	1:C:490:ARG:NH1	2.38	0.48
3:L:37:GLN:HB2	3:L:47:LEU:HD22	1.94	0.48
1:A:801:GLN:NE2	1:A:932:GLN:OE1	2.36	0.48
1:B:393:TYR:HB3	1:B:511:SER:HB2	1.95	0.48
1:C:207:VAL:HG12	1:C:208:ARG:HG2	1.96	0.48
1:B:366:TYR:HH	1:B:374:PHE:N	2.12	0.48
1:A:712:PRO:HA	1:A:1069:GLU:HA	1.96	0.48
1:C:140:ASP:OD2	1:C:153:ARG:NH2	2.40	0.48
3:L:65:SER:HG	3:L:72:SER:HG	1.61	0.48
1:A:128:VAL:HB	1:A:163:PHE:HB3	1.96	0.47
3:L:35:TRP:HA	3:L:87:PHE:O	2.14	0.47
1:A:46:SER:CA	1:A:276:TYR:O	2.63	0.47
1:A:54:LEU:HD12	1:A:190:LYS:HE3	1.96	0.47
1:A:739:ILE:HG12	1:A:997:ARG:HB3	1.96	0.47
1:B:91:ALA:HB3	1:B:263:TYR:HB2	1.96	0.47
1:B:579:LEU:HG	2:H:64:LYS:CE	2.40	0.47
1:B:784:GLN:OE1	1:C:700:ASN:ND2	2.43	0.47
1:A:79:ASN:HB3	1:A:239:LEU:HD23	1.97	0.47
1:A:983:PRO:O	1:A:987:GLU:HB2	2.14	0.47
1:C:728:MET:H	1:C:771:GLN:HG2	1.80	0.47
1:A:376:CYS:HA	1:A:429:CYS:HA	1.96	0.47
1:C:64:TRP:HE1	1:C:261:ALA:HA	1.80	0.47
1:C:742:ASP:OD1	1:C:742:ASP:N	2.48	0.47
1:A:43:PHE:CE1	1:B:557:LEU:CG	2.97	0.47
1:A:972:SER:OG	1:B:568:ASP:OD2	2.33	0.47
1:B:801:GLN:OE1	1:B:932:GLN:NE2	2.42	0.47
1:A:316:ARG:HH21	1:C:737:MET:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ALA:HB3	1:A:263:TYR:HB2	1.97	0.46
1:A:324:VAL:H	1:A:528:THR:HB	1.79	0.46
1:B:578:THR:HA	2:H:64:LYS:HG3	1.98	0.46
1:B:402:ASP:O	1:B:406:GLN:NE2	2.48	0.46
1:B:642:THR:HG22	1:B:644:ALA:H	1.81	0.46
1:C:57:PRO:HB2	1:C:60:SER:HB2	1.97	0.46
1:C:453:PHE:HB2	1:C:488:PRO:HB3	1.98	0.46
2:H:15:SER:HA	2:H:82(B):SER:HA	1.96	0.46
1:A:405:ARG:HG3	1:A:406:GLN:HG3	1.98	0.46
1:B:418:TYR:HB3	1:B:454:ARG:HD3	1.98	0.46
1:A:673:THR:HG22	1:A:687:GLN:HG2	1.97	0.46
1:A:287:ASP:OD1	1:A:287:ASP:N	2.49	0.46
1:B:324:VAL:HG23	1:B:539:ASN:HB3	1.97	0.45
2:H:48:ILE:HA	2:H:60:ASN:HB2	1.97	0.45
1:A:506:ARG:NH1	1:A:507:VAL:O	2.50	0.45
1:C:563:GLY:O	1:C:571:ASP:N	2.47	0.45
2:H:90:TYR:O	2:H:106:GLY:HA2	2.16	0.45
1:C:170:PHE:HE1	1:C:198:ILE:HG21	1.82	0.45
1:A:380:SER:HB3	1:A:383:LYS:HB2	1.98	0.45
1:B:579:LEU:C	2:H:64:LYS:HZ1	2.18	0.45
1:C:712:PRO:HA	1:C:1069:GLU:HA	1.98	0.45
1:C:102:TRP:HB2	1:C:117:ILE:HB	1.98	0.45
1:B:315:PHE:HA	1:B:631:ARG:HD3	1.99	0.45
1:B:37:TYR:HA	1:B:220:LEU:H	1.81	0.45
2:H:30:SER:OG	2:H:94:ARG:NE	2.41	0.45
1:B:543:LEU:HD11	1:B:570:THR:HG21	1.97	0.45
1:C:959:LEU:HD11	1:C:1001:LEU:HD23	1.98	0.45
1:A:87:GLY:HA2	1:A:189:PHE:O	2.17	0.44
1:C:436:ASN:HD21	1:C:503:GLN:HG2	1.82	0.44
1:A:728:MET:HG3	1:A:952:ASN:HD21	1.82	0.44
1:B:41:LYS:HG2	1:C:559:PHE:HD2	1.82	0.44
1:B:579:LEU:HD12	2:H:64:LYS:CE	2.44	0.44
1:B:579:LEU:N	2:H:64:LYS:HE2	2.23	0.44
1:A:106:THR:O	1:A:234:ARG:NH2	2.51	0.44
1:A:593:SER:HB2	1:A:608:LEU:HB3	2.00	0.44
1:A:723:ILE:HD13	1:A:942:LEU:HD13	1.99	0.44
1:C:730:LYS:HD2	1:C:768:ALA:HB1	2.00	0.44
1:C:398:VAL:HG22	1:C:506:ARG:HG2	2.00	0.44
3:L:35:TRP:HB2	3:L:48:ILE:HG22	2.00	0.44
1:B:595:ILE:HG23	1:B:661:ILE:HG21	2.00	0.44
1:B:97:ASN:ND2	1:B:173:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD11	1:C:980:ARG:HA	2.00	0.43
1:A:730:LYS:HD2	1:A:768:ALA:HB1	2.01	0.43
1:B:712:PRO:HA	1:B:1069:GLU:HA	2.00	0.43
1:B:721:THR:HG23	1:B:931:ILE:HD12	2.00	0.43
1:B:911:ASN:ND2	1:B:1108:GLU:OE2	2.47	0.43
3:L:49:TYR:O	3:L:53:ASN:N	2.49	0.43
1:A:614:CYS:HB3	1:A:646:CYS:HB3	1.88	0.43
1:B:579:LEU:HG	2:H:64:LYS:HE2	1.99	0.43
1:C:767:ILE:O	1:C:771:GLN:OE1	2.37	0.43
1:A:120:ASN:O	1:A:122:THR:N	2.51	0.43
1:A:663:ILE:HD11	1:A:669:ALA:HB2	2.01	0.43
1:B:730:LYS:HD2	1:B:768:ALA:HB1	2.00	0.43
1:B:593:SER:HB2	1:B:608:LEU:HB3	1.99	0.43
1:C:673:THR:HG22	1:C:687:GLN:HG2	1.99	0.43
1:A:46:SER:N	1:A:276:TYR:O	2.52	0.43
1:B:773:LYS:NZ	1:B:777:GLU:OE2	2.43	0.43
1:B:469:ILE:HG12	1:B:487:PHE:HB2	1.99	0.42
1:A:140:ASP:OD2	1:A:140:ASP:N	2.52	0.42
1:A:106:THR:OG1	1:A:107:THR:N	2.52	0.42
1:B:295:GLU:OE1	1:B:633:TYR:OH	2.31	0.42
1:C:112:THR:HA	1:C:130:GLU:HA	2.00	0.42
1:A:102:TRP:CD1	1:A:237:THR:HG22	2.55	0.42
1:A:139:LEU:HD23	1:A:238:LEU:HB3	2.02	0.42
1:A:383:LYS:NZ	1:C:978:PHE:O	2.43	0.42
1:B:128:VAL:HG21	1:B:228:ILE:HG21	2.02	0.42
1:B:608:LEU:HD22	1:B:663:ILE:HG23	2.02	0.42
1:B:435:SER:OG	1:B:504:PRO:O	2.31	0.41
1:C:760:LEU:HG	1:C:1005:VAL:HG21	2.02	0.41
1:C:595:ILE:HG23	1:C:661:ILE:HG21	2.02	0.41
1:C:723:ILE:HD13	1:C:942:LEU:HD23	2.01	0.41
1:A:56:LEU:HD12	1:A:57:PRO:HD2	2.02	0.41
1:B:424:ASP:OD1	1:B:424:ASP:N	2.53	0.41
1:A:414:ASN:O	1:A:417:ASP:N	2.53	0.41
1:B:292:PRO:HG2	1:B:605:VAL:HG21	2.02	0.41
1:C:131:PHE:HB3	1:C:133:PHE:CZ	2.55	0.41
1:C:749:LEU:HD11	1:C:978:PHE:HZ	1.86	0.41
3:L:92:ASP:OD2	3:L:95(A):SER:N	2.53	0.41
1:B:106:THR:HA	1:B:233:THR:H	1.86	0.41
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.56	0.41
1:A:942:LEU:HD12	1:A:945:LEU:HD12	2.02	0.41
1:B:421:LYS:HB3	1:B:460:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:GLY:HA2	1:A:586:PRO:HA	2.03	0.41
1:A:819:LEU:HD22	1:A:942:LEU:HD11	2.02	0.41
1:B:183:ASN:HA	1:B:204:PRO:HA	2.02	0.41
1:B:1025:LYS:O	1:B:1029:CYS:HB2	2.21	0.41
1:C:17:ASN:N	1:C:134:CYS:SG	2.91	0.41
1:C:663:ILE:HD11	1:C:669:ALA:HB2	2.03	0.41
1:B:427:THR:OG1	1:B:512:PHE:O	2.34	0.40
1:B:449:LEU:HA	1:B:491:SER:HA	2.03	0.40
1:C:717:ILE:HG13	1:C:920:ILE:HG23	2.03	0.40
1:B:911:ASN:ND2	1:C:1120:SER:OG	2.54	0.40
1:C:34:ARG:HH21	1:C:214:PRO:HG2	1.87	0.40
1:B:663:ILE:HD11	1:B:669:ALA:HB2	2.03	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	1014/1277 (79%)	976 (96%)	38 (4%)	0	100	100
1	B	1027/1277 (80%)	986 (96%)	41 (4%)	0	100	100
1	C	1039/1277 (81%)	989 (95%)	50 (5%)	0	100	100
2	H	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
3	L	109/134 (81%)	99 (91%)	10 (9%)	0	100	100
All	All	3316/4094 (81%)	3164 (95%)	152 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	919/1108 (83%)	908 (99%)	11 (1%)	67 85
1	B	923/1108 (83%)	923 (100%)	0	100 100
1	C	929/1108 (84%)	928 (100%)	1 (0%)	92 98
2	H	112/112 (100%)	112 (100%)	0	100 100
3	L	91/109 (84%)	91 (100%)	0	100 100
All	All	2974/3545 (84%)	2962 (100%)	12 (0%)	88 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	21	ARG
1	A	140	ASP
1	A	151	GLU
1	A	153	ARG
1	A	287	ASP
1	A	288	CYS
1	A	290	LEU
1	A	291	ASP
1	A	295	GLU
1	A	975	ASN
1	C	454	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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.