



Full wwPDB EM Model Validation Report ⓘ

May 21, 2020 – 03:41 PM EDT

PDB ID : 6X2C
EMDB ID : EMD-22001
Title : SARS-CoV-2 u1S2q All Down RBD State Spike Protein Trimer
Authors : Henderson, R.; Acharya, P.
Deposited on : 2020-05-20
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

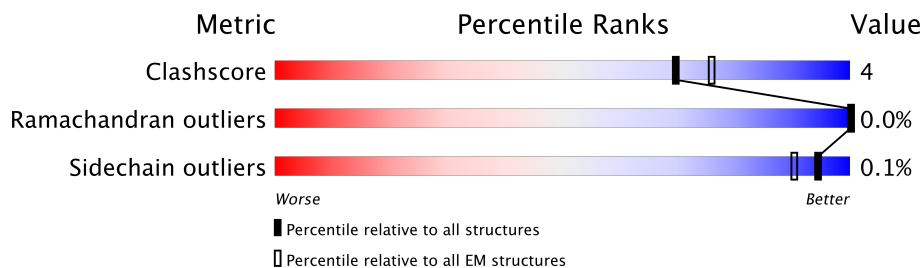
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1273	68% 8% 24%
1	B	1273	68% 8% 24%
1	C	1273	67% 9% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22827 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	972	Total	C	N	O	S	0	0
			7609	4868	1261	1447	33		
1	B	972	Total	C	N	O	S	0	0
			7609	4868	1261	1447	33		
1	C	972	Total	C	N	O	S	0	0
			7609	4868	1261	1447	33		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	570	LEU	ALA	engineered mutation	UNP P0DTC2
A	572	ILE	THR	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	855	TYR	PHE	engineered mutation	UNP P0DTC2
A	856	ILE	ASN	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	570	LEU	ALA	engineered mutation	UNP P0DTC2
B	572	ILE	THR	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	855	TYR	PHE	engineered mutation	UNP P0DTC2
B	856	ILE	ASN	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	570	LEU	ALA	engineered mutation	UNP P0DTC2
C	572	ILE	THR	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	855	TYR	PHE	engineered mutation	UNP P0DTC2
C	856	ILE	ASN	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

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

TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	192430	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 ($e^-/\text{\AA}^2$)	68.82	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K3 (6k 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	0/7777	0.54	3/10579 (0.0%)
1	B	0.32	2/7777 (0.0%)	0.53	1/10579 (0.0%)
1	C	0.32	2/7777 (0.0%)	0.53	1/10579 (0.0%)
All	All	0.32	4/23331 (0.0%)	0.54	5/31737 (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
1	B	0	2
1	C	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	569	ILE	C-N	5.61	1.47	1.34
1	C	569	ILE	C-N	5.59	1.47	1.34
1	B	570	LEU	C-O	5.24	1.33	1.23
1	C	570	LEU	C-O	5.23	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	LEU	CA-CB-CG	-8.11	96.64	115.30
1	B	570	LEU	C-N-CA	6.99	139.17	121.70
1	C	570	LEU	C-N-CA	6.97	139.14	121.70
1	A	570	LEU	CB-CA-C	5.15	119.99	110.20
1	A	570	LEU	C-N-CA	5.10	134.46	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	570	LEU	Peptide
1	A	86	PHE	Peptide
1	B	570	LEU	Peptide
1	B	86	PHE	Peptide
1	C	570	LEU	Peptide
1	C	86	PHE	Peptide

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	7609	0	7444	69	0
1	B	7609	0	7445	61	0
1	C	7609	0	7445	69	0
All	All	22827	0	22334	179	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 (179) 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:C:856:ILE:HG21	1:C:966:LEU:HD11	1.46	0.97
1:A:856:ILE:HG21	1:A:966:LEU:HD11	1.48	0.95
1:C:856:ILE:HG21	1:C:966:LEU:CD1	2.14	0.77
1:A:856:ILE:HG21	1:A:966:LEU:CD1	2.15	0.76
1:C:856:ILE:HG22	1:C:856:ILE:O	1.91	0.71
1:A:856:ILE:HG22	1:A:856:ILE:O	1.91	0.71
1:A:355:ARG:NH2	1:B:200:TYR:OH	2.30	0.62
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.83	0.60
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.83	0.60
1:C:448:ASN:HB3	1:C:497:PHE:HB2	1.83	0.59
1:A:738:CYS:SG	1:A:764:ASN:ND2	2.78	0.57
1:B:738:CYS:SG	1:B:764:ASN:ND2	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.87	0.57
1:C:738:CYS:SG	1:C:764:ASN:ND2	2.78	0.57
1:B:564:GLN:OE1	1:B:577:ARG:NH1	2.39	0.56
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.39	0.56
1:A:564:GLN:OE1	1:A:577:ARG:NH1	2.39	0.56
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	1.88	0.55
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.88	0.55
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.89	0.55
1:A:894:LEU:HD21	1:C:1072:GLU:HG2	1.88	0.55
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.89	0.55
1:A:980:ILE:HG23	1:A:984:LEU:HD12	1.88	0.55
1:C:564:GLN:OE1	1:C:577:ARG:NH1	2.39	0.55
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.89	0.55
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	1.88	0.54
1:B:454:ARG:NH1	1:B:468:ILE:O	2.41	0.54
1:C:340:GLU:OE1	1:C:356:LYS:NZ	2.40	0.54
1:C:454:ARG:NH1	1:C:468:ILE:O	2.41	0.54
1:B:980:ILE:HG23	1:B:984:LEU:HD12	1.88	0.54
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.90	0.54
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.39	0.54
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.89	0.54
1:A:720:ILE:HG13	1:A:923:ILE:HG23	1.89	0.54
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.39	0.54
1:C:277:LEU:HD22	1:C:285:ILE:HD11	1.90	0.54
1:A:895:GLN:NE2	1:C:1074:ASN:OD1	2.38	0.53
1:B:277:LEU:HD22	1:B:285:ILE:HD11	1.90	0.53
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.90	0.53
1:A:355:ARG:HH21	1:B:200:TYR:HH	1.56	0.53
1:C:980:ILE:HG23	1:C:984:LEU:HD12	1.88	0.53
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.89	0.53
1:A:1030:SER:HB3	1:C:1041:ASP:HB2	1.90	0.53
1:C:815:ARG:HD2	1:C:823:PHE:HE2	1.73	0.53
1:A:277:LEU:HD22	1:A:285:ILE:HD11	1.90	0.53
1:B:340:GLU:OE1	1:B:356:LYS:NZ	2.40	0.53
1:A:340:GLU:OE1	1:A:356:LYS:NZ	2.40	0.53
1:A:815:ARG:HD2	1:A:823:PHE:HE2	1.73	0.53
1:A:206:LYS:HB2	1:A:223:LEU:HA	1.91	0.53
1:A:454:ARG:NH1	1:A:468:ILE:O	2.41	0.52
1:B:1041:ASP:HB2	1:C:1030:SER:HB3	1.91	0.52
1:A:389:ASP:OD1	1:A:528:LYS:NZ	2.35	0.52
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:HB2	1:C:223:LEU:HA	1.91	0.52
1:B:815:ARG:HD2	1:B:823:PHE:HE2	1.73	0.52
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.92	0.51
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.92	0.51
1:B:303:LEU:HD12	1:B:308:VAL:HG22	1.93	0.51
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.44	0.51
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.92	0.51
1:C:389:ASP:OD1	1:C:528:LYS:NZ	2.35	0.51
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.44	0.51
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.93	0.51
1:B:206:LYS:HB2	1:B:223:LEU:HA	1.91	0.51
1:A:390:LEU:HD21	1:B:983:ARG:HG2	1.92	0.51
1:C:303:LEU:HD12	1:C:308:VAL:HG22	1.93	0.51
1:B:451:TYR:HB2	1:B:497:PHE:HE2	1.76	0.51
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.93	0.51
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.93	0.51
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.44	0.51
1:B:389:ASP:OD1	1:B:528:LYS:NZ	2.35	0.51
1:A:901:GLN:HE21	1:A:905:ARG:HH21	1.59	0.50
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.94	0.50
1:A:451:TYR:HB2	1:A:497:PHE:HE2	1.76	0.50
1:C:856:ILE:CG2	1:C:856:ILE:O	2.59	0.50
1:C:451:TYR:HB2	1:C:497:PHE:HE2	1.76	0.50
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.94	0.50
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.45	0.49
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.93	0.49
1:C:366:SER:O	1:C:370:ASN:ND2	2.46	0.49
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.94	0.49
1:B:901:GLN:HE21	1:B:905:ARG:HH21	1.59	0.49
1:C:358:ILE:HB	1:C:395:VAL:HB	1.95	0.49
1:A:358:ILE:HB	1:A:395:VAL:HB	1.95	0.49
1:B:366:SER:O	1:B:370:ASN:ND2	2.46	0.49
1:C:901:GLN:HE21	1:C:905:ARG:HH21	1.59	0.49
1:A:366:SER:O	1:A:370:ASN:ND2	2.46	0.48
1:C:596:SER:HB2	1:C:611:LEU:HB3	1.95	0.48
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.45	0.48
1:B:596:SER:HB2	1:B:611:LEU:HB3	1.95	0.48
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.96	0.47
1:B:358:ILE:HB	1:B:395:VAL:HB	1.95	0.47
1:A:37:TYR:HB3	1:A:223:LEU:HB2	1.97	0.47
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:SER:HB2	1:A:611:LEU:HB3	1.95	0.47
1:A:727:LEU:HD11	1:A:1028:LYS:HD2	1.96	0.47
1:B:120:VAL:HB	1:B:127:VAL:HB	1.97	0.46
1:C:120:VAL:HB	1:C:127:VAL:HB	1.97	0.46
1:B:736:VAL:HG22	1:B:858:LEU:HG	1.98	0.46
1:A:752:LEU:HD11	1:A:990:GLU:HG2	1.97	0.46
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.97	0.46
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	1.96	0.46
1:A:856:ILE:O	1:A:856:ILE:CG2	2.59	0.46
1:B:34:ARG:HH21	1:B:217:PRO:HB2	1.81	0.46
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.97	0.46
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.97	0.46
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.97	0.46
1:C:736:VAL:HG22	1:C:858:LEU:HG	1.98	0.46
1:A:726:ILE:HD13	1:A:945:LEU:HD13	1.98	0.45
1:A:120:VAL:HB	1:A:127:VAL:HB	1.97	0.45
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.97	0.45
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.81	0.45
1:B:752:LEU:HD11	1:B:990:GLU:HG2	1.97	0.45
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.45	0.45
1:B:726:ILE:HD13	1:B:945:LEU:HD13	1.98	0.45
1:C:196:ASN:HD21	1:C:235:ILE:HD12	1.82	0.45
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.81	0.45
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.81	0.45
1:A:736:VAL:HG22	1:A:858:LEU:HG	1.98	0.45
1:C:34:ARG:HH21	1:C:217:PRO:HB2	1.81	0.45
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.82	0.45
1:A:95:THR:OG1	1:A:264:ALA:O	2.36	0.44
1:A:563:GLN:HG3	1:B:43:PHE:HB2	1.99	0.44
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.99	0.44
1:C:752:LEU:HD11	1:C:990:GLU:HG2	1.97	0.44
1:C:985:ASP:O	1:C:989:ALA:N	2.49	0.44
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.99	0.44
1:B:95:THR:OG1	1:B:264:ALA:O	2.36	0.44
1:B:196:ASN:HD21	1:B:235:ILE:HD12	1.82	0.44
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.82	0.44
1:A:34:ARG:HH21	1:A:217:PRO:HB2	1.81	0.44
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.99	0.44
1:A:196:ASN:HD21	1:A:235:ILE:HD12	1.82	0.44
1:A:985:ASP:O	1:A:989:ALA:N	2.49	0.44
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TYR:HB2	1:B:270:LEU:HG	2.00	0.44
1:C:726:ILE:HD13	1:C:945:LEU:HD13	1.98	0.44
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	2.00	0.43
1:B:656:VAL:HG12	1:B:658:ASN:H	1.83	0.43
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.82	0.43
1:A:894:LEU:HD13	1:C:715:PRO:HD3	2.01	0.43
1:A:656:VAL:HG12	1:A:658:ASN:H	1.83	0.42
1:C:656:VAL:HG12	1:C:658:ASN:H	1.83	0.42
1:C:91:TYR:HB2	1:C:270:LEU:HG	2.00	0.42
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.89	0.42
1:B:985:ASP:O	1:B:989:ALA:N	2.49	0.42
1:A:900:MET:HG2	1:C:1079:PRO:HB3	2.01	0.42
1:A:91:TYR:HB2	1:A:270:LEU:HG	2.00	0.42
1:A:395:VAL:HG13	1:A:515:PHE:HE1	1.85	0.42
1:C:95:THR:OG1	1:C:264:ALA:O	2.36	0.42
1:A:603:ASN:HD22	1:A:603:ASN:HA	1.64	0.42
1:B:287:ASP:HB3	1:B:306:PHE:HE2	1.85	0.42
1:B:395:VAL:HG13	1:B:515:PHE:HE1	1.85	0.42
1:C:395:VAL:HG13	1:C:515:PHE:HE1	1.85	0.42
1:A:970:PHE:HA	1:B:756:TYR:HD1	1.86	0.41
1:C:1086:LYS:HB3	1:C:1122:VAL:HG13	2.03	0.41
1:B:1123:SER:OG	1:C:918:GLU:OE2	2.26	0.41
1:C:287:ASP:HB3	1:C:306:PHE:HE2	1.85	0.41
1:A:790:LYS:HE2	1:C:704:SER:HB3	2.02	0.41
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.89	0.41
1:A:1086:LYS:HB3	1:A:1122:VAL:HG13	2.03	0.41
1:A:913:GLN:HE22	1:C:1090:PRO:HD2	1.85	0.41
1:A:357:ARG:HH12	1:B:228:ASP:HB3	1.86	0.41
1:A:789:TYR:HA	1:C:703:ASN:O	2.21	0.41
1:B:498:GLN:H	1:B:501:ASN:HD21	1.69	0.41
1:A:498:GLN:H	1:A:501:ASN:HD21	1.69	0.41
1:B:1086:LYS:HB3	1:B:1122:VAL:HG13	2.03	0.41
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.85	0.41
1:B:326:ILE:HB	1:B:541:PHE:HA	2.03	0.41
1:C:201:PHE:HB3	1:C:229:LEU:HB2	2.03	0.41
1:C:726:ILE:HG22	1:C:948:LEU:HD13	2.03	0.41
1:A:726:ILE:HG22	1:A:948:LEU:HD13	2.03	0.40
1:B:201:PHE:HB3	1:B:229:LEU:HB2	2.03	0.40
1:B:726:ILE:HG22	1:B:948:LEU:HD13	2.03	0.40
1:C:1126:CYS:HA	1:C:1132:ILE:HD13	2.03	0.40
1:B:716:THR:N	1:B:1071:GLN:O	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:CYS:HA	1:B:1132:ILE:HD13	2.03	0.40
1:C:498:GLN:H	1:C:501:ASN:HD21	1.69	0.40
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.55	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	948/1273 (74%)	907 (96%)	40 (4%)	1 (0%)	53	87
1	B	948/1273 (74%)	906 (96%)	42 (4%)	0	100	100
1	C	948/1273 (74%)	907 (96%)	41 (4%)	0	100	100
All	All	2844/3819 (74%)	2720 (96%)	123 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	LEU

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	853/1099 (78%)	852 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	853/1099 (78%)	852 (100%)	1 (0%)	94	98
1	C	853/1099 (78%)	852 (100%)	1 (0%)	94	98
All	All	2559/3297 (78%)	2556 (100%)	3 (0%)	94	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	603	ASN
1	B	603	ASN
1	C	603	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	245	HIS
1	A	370	ASN
1	A	450	ASN
1	A	501	ASN
1	A	603	ASN
1	A	1119	ASN
1	B	196	ASN
1	B	370	ASN
1	B	450	ASN
1	B	501	ASN
1	B	603	ASN
1	B	1119	ASN
1	C	196	ASN
1	C	370	ASN
1	C	450	ASN
1	C	501	ASN
1	C	603	ASN
1	C	1119	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.