



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:47 am GMT

PDB ID : 3JCL
EMDB ID: : EMD-6526
Title : Cryo-electron microscopy structure of a coronavirus spike glycoprotein trimer
Authors : Walls, A.C.; Tortorici, M.A.; Bosch, B.J.; Frenz, B.; Rottier, P.J.M.; DiMaio, F.; Rey, F.A.; Velesler, D.
Deposited on : 2015-12-21
Resolution : 4.00 Å(reported)
Based on PDB ID : 4KQZ, 3R4D, 4H14

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

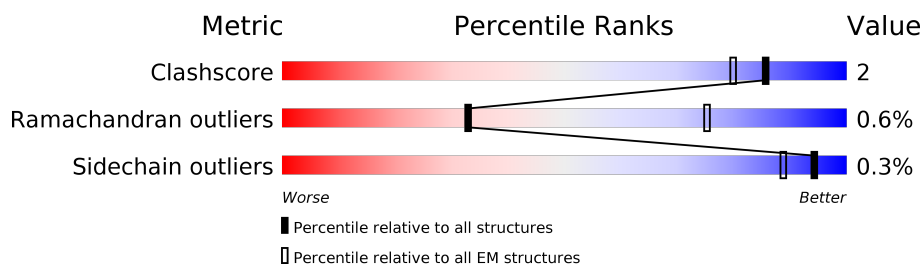
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	1265	
1	B	1265	
1	C	1265	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24822 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	1067	Total	C	N	O	S	0	0
			8274	5234	1406	1586	48		
1	B	1067	Total	C	N	O	S	0	0
			8274	5234	1406	1586	48		
1	C	1067	Total	C	N	O	S	0	0
			8274	5234	1406	1586	48		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	717	SER	ARG	CONFLICT	UNP P11224
A	1232	ILE	-	EXPRESSION TAG	UNP P11224
A	1233	LYS	-	EXPRESSION TAG	UNP P11224
A	1234	ARG	-	EXPRESSION TAG	UNP P11224
A	1235	MET	-	EXPRESSION TAG	UNP P11224
A	1236	LYS	-	EXPRESSION TAG	UNP P11224
A	1237	GLN	-	EXPRESSION TAG	UNP P11224
A	1238	ILE	-	EXPRESSION TAG	UNP P11224
A	1239	GLU	-	EXPRESSION TAG	UNP P11224
A	1240	ASP	-	EXPRESSION TAG	UNP P11224
A	1241	LYS	-	EXPRESSION TAG	UNP P11224
A	1242	ILE	-	EXPRESSION TAG	UNP P11224
A	1243	GLU	-	EXPRESSION TAG	UNP P11224
A	1244	GLU	-	EXPRESSION TAG	UNP P11224
A	1245	ILE	-	EXPRESSION TAG	UNP P11224
A	1246	GLU	-	EXPRESSION TAG	UNP P11224
A	1247	SER	-	EXPRESSION TAG	UNP P11224
A	1248	LYS	-	EXPRESSION TAG	UNP P11224
A	1249	GLN	-	EXPRESSION TAG	UNP P11224
A	1250	LYS	-	EXPRESSION TAG	UNP P11224
A	1251	LYS	-	EXPRESSION TAG	UNP P11224
A	1252	ILE	-	EXPRESSION TAG	UNP P11224
A	1253	GLU	-	EXPRESSION TAG	UNP P11224
A	1254	ASN	-	EXPRESSION TAG	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	GLU	-	EXPRESSION TAG	UNP P11224
A	1256	ILE	-	EXPRESSION TAG	UNP P11224
A	1257	ALA	-	EXPRESSION TAG	UNP P11224
A	1258	ARG	-	EXPRESSION TAG	UNP P11224
A	1259	ILE	-	EXPRESSION TAG	UNP P11224
A	1260	LYS	-	EXPRESSION TAG	UNP P11224
A	1261	LYS	-	EXPRESSION TAG	UNP P11224
A	1262	ILE	-	EXPRESSION TAG	UNP P11224
A	1263	LYS	-	EXPRESSION TAG	UNP P11224
A	1264	LEU	-	EXPRESSION TAG	UNP P11224
A	1265	VAL	-	EXPRESSION TAG	UNP P11224
A	1266	PRO	-	EXPRESSION TAG	UNP P11224
A	1267	ARG	-	EXPRESSION TAG	UNP P11224
A	1268	GLY	-	EXPRESSION TAG	UNP P11224
A	1269	SER	-	EXPRESSION TAG	UNP P11224
A	1270	LEU	-	EXPRESSION TAG	UNP P11224
A	1271	GLU	-	EXPRESSION TAG	UNP P11224
A	1272	TRP	-	EXPRESSION TAG	UNP P11224
A	1273	SER	-	EXPRESSION TAG	UNP P11224
A	1274	HIS	-	EXPRESSION TAG	UNP P11224
A	1275	PRO	-	EXPRESSION TAG	UNP P11224
A	1276	GLN	-	EXPRESSION TAG	UNP P11224
A	1277	PHE	-	EXPRESSION TAG	UNP P11224
A	1278	GLU	-	EXPRESSION TAG	UNP P11224
A	1279	LYS	-	EXPRESSION TAG	UNP P11224
B	717	SER	ARG	CONFLICT	UNP P11224
B	1232	ILE	-	EXPRESSION TAG	UNP P11224
B	1233	LYS	-	EXPRESSION TAG	UNP P11224
B	1234	ARG	-	EXPRESSION TAG	UNP P11224
B	1235	MET	-	EXPRESSION TAG	UNP P11224
B	1236	LYS	-	EXPRESSION TAG	UNP P11224
B	1237	GLN	-	EXPRESSION TAG	UNP P11224
B	1238	ILE	-	EXPRESSION TAG	UNP P11224
B	1239	GLU	-	EXPRESSION TAG	UNP P11224
B	1240	ASP	-	EXPRESSION TAG	UNP P11224
B	1241	LYS	-	EXPRESSION TAG	UNP P11224
B	1242	ILE	-	EXPRESSION TAG	UNP P11224
B	1243	GLU	-	EXPRESSION TAG	UNP P11224
B	1244	GLU	-	EXPRESSION TAG	UNP P11224
B	1245	ILE	-	EXPRESSION TAG	UNP P11224
B	1246	GLU	-	EXPRESSION TAG	UNP P11224
B	1247	SER	-	EXPRESSION TAG	UNP P11224

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1248	LYS	-	EXPRESSION TAG	UNP P11224
B	1249	GLN	-	EXPRESSION TAG	UNP P11224
B	1250	LYS	-	EXPRESSION TAG	UNP P11224
B	1251	LYS	-	EXPRESSION TAG	UNP P11224
B	1252	ILE	-	EXPRESSION TAG	UNP P11224
B	1253	GLU	-	EXPRESSION TAG	UNP P11224
B	1254	ASN	-	EXPRESSION TAG	UNP P11224
B	1255	GLU	-	EXPRESSION TAG	UNP P11224
B	1256	ILE	-	EXPRESSION TAG	UNP P11224
B	1257	ALA	-	EXPRESSION TAG	UNP P11224
B	1258	ARG	-	EXPRESSION TAG	UNP P11224
B	1259	ILE	-	EXPRESSION TAG	UNP P11224
B	1260	LYS	-	EXPRESSION TAG	UNP P11224
B	1261	LYS	-	EXPRESSION TAG	UNP P11224
B	1262	ILE	-	EXPRESSION TAG	UNP P11224
B	1263	LYS	-	EXPRESSION TAG	UNP P11224
B	1264	LEU	-	EXPRESSION TAG	UNP P11224
B	1265	VAL	-	EXPRESSION TAG	UNP P11224
B	1266	PRO	-	EXPRESSION TAG	UNP P11224
B	1267	ARG	-	EXPRESSION TAG	UNP P11224
B	1268	GLY	-	EXPRESSION TAG	UNP P11224
B	1269	SER	-	EXPRESSION TAG	UNP P11224
B	1270	LEU	-	EXPRESSION TAG	UNP P11224
B	1271	GLU	-	EXPRESSION TAG	UNP P11224
B	1272	TRP	-	EXPRESSION TAG	UNP P11224
B	1273	SER	-	EXPRESSION TAG	UNP P11224
B	1274	HIS	-	EXPRESSION TAG	UNP P11224
B	1275	PRO	-	EXPRESSION TAG	UNP P11224
B	1276	GLN	-	EXPRESSION TAG	UNP P11224
B	1277	PHE	-	EXPRESSION TAG	UNP P11224
B	1278	GLU	-	EXPRESSION TAG	UNP P11224
B	1279	LYS	-	EXPRESSION TAG	UNP P11224
C	717	SER	ARG	CONFLICT	UNP P11224
C	1232	ILE	-	EXPRESSION TAG	UNP P11224
C	1233	LYS	-	EXPRESSION TAG	UNP P11224
C	1234	ARG	-	EXPRESSION TAG	UNP P11224
C	1235	MET	-	EXPRESSION TAG	UNP P11224
C	1236	LYS	-	EXPRESSION TAG	UNP P11224
C	1237	GLN	-	EXPRESSION TAG	UNP P11224
C	1238	ILE	-	EXPRESSION TAG	UNP P11224
C	1239	GLU	-	EXPRESSION TAG	UNP P11224
C	1240	ASP	-	EXPRESSION TAG	UNP P11224

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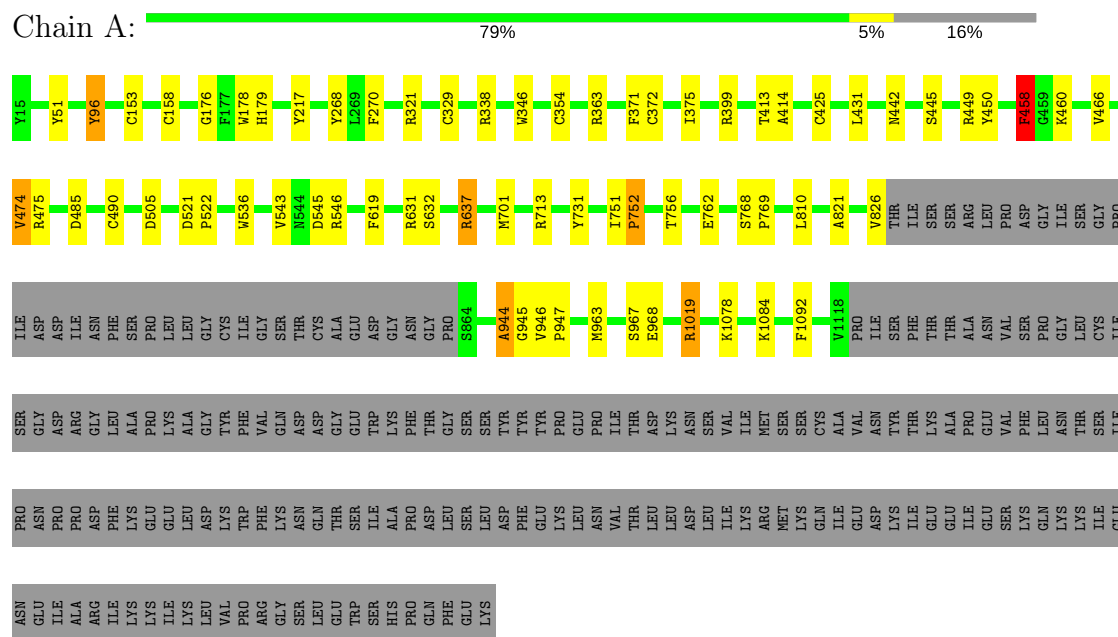
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1241	LYS	-	EXPRESSION TAG	UNP P11224
C	1242	ILE	-	EXPRESSION TAG	UNP P11224
C	1243	GLU	-	EXPRESSION TAG	UNP P11224
C	1244	GLU	-	EXPRESSION TAG	UNP P11224
C	1245	ILE	-	EXPRESSION TAG	UNP P11224
C	1246	GLU	-	EXPRESSION TAG	UNP P11224
C	1247	SER	-	EXPRESSION TAG	UNP P11224
C	1248	LYS	-	EXPRESSION TAG	UNP P11224
C	1249	GLN	-	EXPRESSION TAG	UNP P11224
C	1250	LYS	-	EXPRESSION TAG	UNP P11224
C	1251	LYS	-	EXPRESSION TAG	UNP P11224
C	1252	ILE	-	EXPRESSION TAG	UNP P11224
C	1253	GLU	-	EXPRESSION TAG	UNP P11224
C	1254	ASN	-	EXPRESSION TAG	UNP P11224
C	1255	GLU	-	EXPRESSION TAG	UNP P11224
C	1256	ILE	-	EXPRESSION TAG	UNP P11224
C	1257	ALA	-	EXPRESSION TAG	UNP P11224
C	1258	ARG	-	EXPRESSION TAG	UNP P11224
C	1259	ILE	-	EXPRESSION TAG	UNP P11224
C	1260	LYS	-	EXPRESSION TAG	UNP P11224
C	1261	LYS	-	EXPRESSION TAG	UNP P11224
C	1262	ILE	-	EXPRESSION TAG	UNP P11224
C	1263	LYS	-	EXPRESSION TAG	UNP P11224
C	1264	LEU	-	EXPRESSION TAG	UNP P11224
C	1265	VAL	-	EXPRESSION TAG	UNP P11224
C	1266	PRO	-	EXPRESSION TAG	UNP P11224
C	1267	ARG	-	EXPRESSION TAG	UNP P11224
C	1268	GLY	-	EXPRESSION TAG	UNP P11224
C	1269	SER	-	EXPRESSION TAG	UNP P11224
C	1270	LEU	-	EXPRESSION TAG	UNP P11224
C	1271	GLU	-	EXPRESSION TAG	UNP P11224
C	1272	TRP	-	EXPRESSION TAG	UNP P11224
C	1273	SER	-	EXPRESSION TAG	UNP P11224
C	1274	HIS	-	EXPRESSION TAG	UNP P11224
C	1275	PRO	-	EXPRESSION TAG	UNP P11224
C	1276	GLN	-	EXPRESSION TAG	UNP P11224
C	1277	PHE	-	EXPRESSION TAG	UNP P11224
C	1278	GLU	-	EXPRESSION TAG	UNP P11224
C	1279	LYS	-	EXPRESSION TAG	UNP P11224

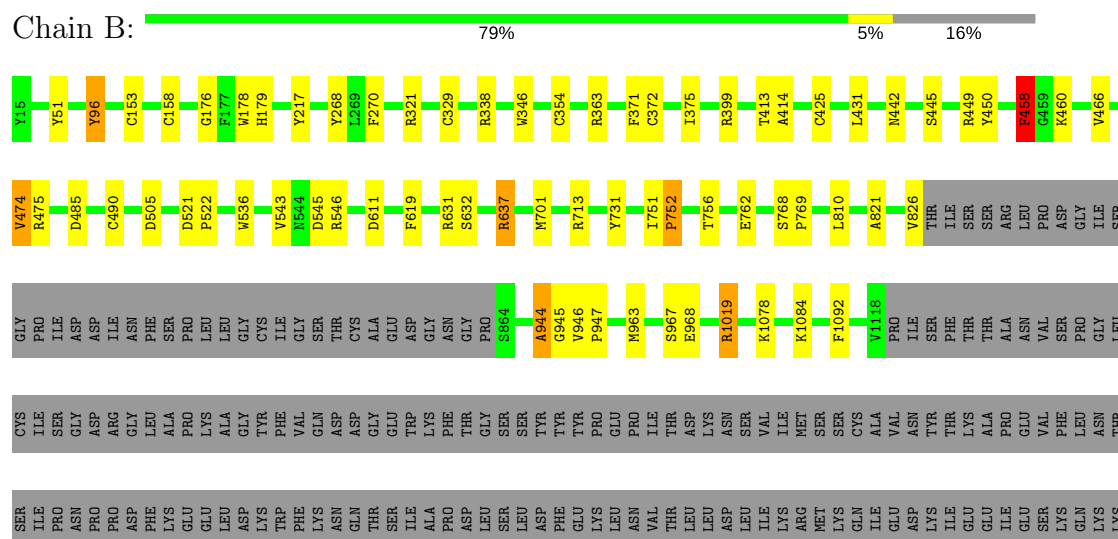
3 Residue-property plots

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.

• Molecule 1: Spike glycoprotein

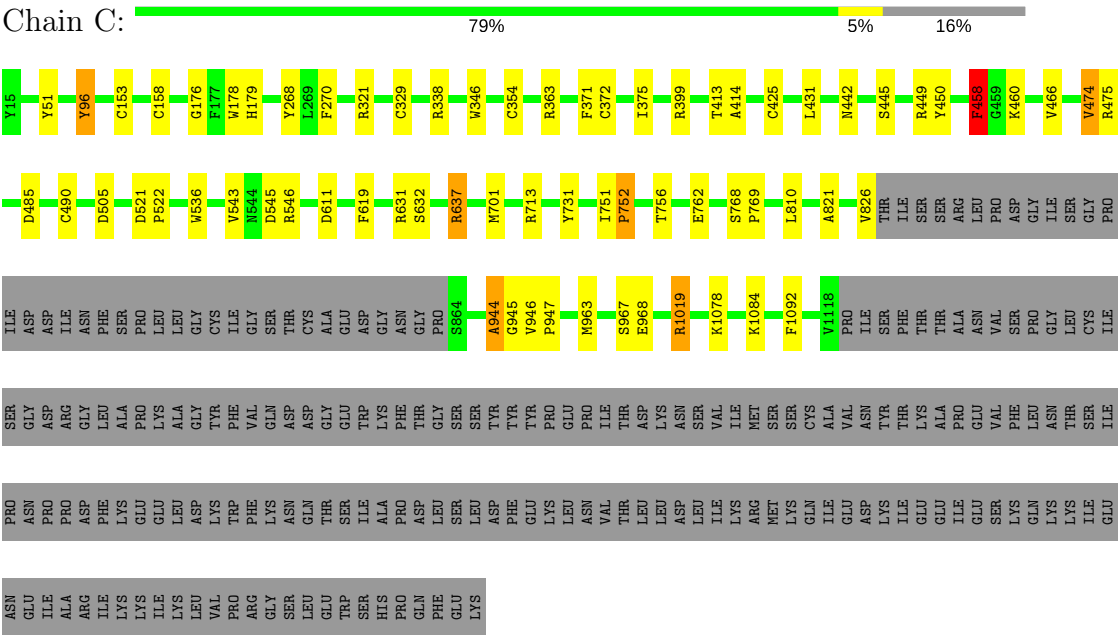


• Molecule 1: Spike glycoprotein



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

● Molecule 1: Spike glycoprotein



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	82000	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	38022	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.93	13/8458 (0.2%)	0.93	15/11523 (0.1%)
1	B	0.93	13/8458 (0.2%)	0.92	15/11523 (0.1%)
1	C	0.93	13/8458 (0.2%)	0.92	15/11523 (0.1%)
All	All	0.93	39/25374 (0.2%)	0.92	45/34569 (0.1%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	PHE	CB-CG	-8.49	1.36	1.51
1	C	270	PHE	CB-CG	-8.48	1.36	1.51
1	B	270	PHE	CB-CG	-8.41	1.37	1.51
1	C	96	TYR	CE2-CZ	-8.19	1.27	1.38
1	A	96	TYR	CE2-CZ	-8.18	1.27	1.38

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	944	ALA	CB-CA-C	-10.98	93.63	110.10
1	C	944	ALA	CB-CA-C	-10.94	93.69	110.10
1	B	944	ALA	CB-CA-C	-10.94	93.70	110.10
1	A	399	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	399	ARG	NE-CZ-NH2	-8.81	115.89	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8274	0	8018	39	0
1	B	8274	0	8018	41	0
1	C	8274	0	8018	40	0
All	All	24822	0	24054	117	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 2.

The worst 5 of 117 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:826:VAL:O	1:C:826:VAL:HG12	1.78	0.83
1:A:826:VAL:HG12	1:A:826:VAL:O	1.78	0.83
1:B:826:VAL:HG12	1:B:826:VAL:O	1.78	0.82
1:A:371:PHE:O	1:A:372:CYS:SG	2.38	0.81
1:B:371:PHE:O	1:B:372:CYS:SG	2.38	0.81

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	1063/1265 (84%)	1002 (94%)	55 (5%)	6 (1%)	28 70
1	B	1063/1265 (84%)	1002 (94%)	55 (5%)	6 (1%)	28 70
1	C	1063/1265 (84%)	1002 (94%)	55 (5%)	6 (1%)	28 70
All	All	3189/3795 (84%)	3006 (94%)	165 (5%)	18 (1%)	33 70

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	PRO

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Mol	Chain	Res	Type
1	B	752	PRO
1	C	752	PRO
1	A	445	SER
1	B	445	SER

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	918/1095 (84%)	915 (100%)	3 (0%)	94	97
1	B	918/1095 (84%)	915 (100%)	3 (0%)	94	97
1	C	918/1095 (84%)	915 (100%)	3 (0%)	94	97
All	All	2754/3285 (84%)	2745 (100%)	9 (0%)	94	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458	PHE
1	C	637	ARG
1	C	179	HIS
1	A	637	ARG
1	B	637	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	ASN
1	C	1061	GLN
1	B	1061	GLN
1	A	1061	GLN
1	C	357	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.