



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 05:00 AM EDT

PDB ID : 5A9E  
EMDB ID: : EMD-3101  
Title : Cryo-electron tomography and subtomogram averaging of Rous-Sarcoma-Virus deltaMBD virus-like particles  
Authors : Schur, F.K.M.; Dick, R.A.; Hagen, W.J.H.; Vogt, V.M.; Briggs, J.A.G.  
Deposited on : unknown  
Resolution : 7.70 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](mailto: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.

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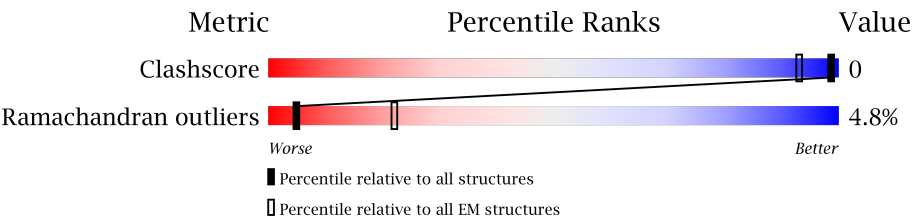
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 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 7.70 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

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  $\geq 3$ , 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	495	<div><div>46%5%•48%</div></div>
1	B	495	<div><div>46%••48%</div></div>
1	C	495	<div><div>47%••48%</div></div>
1	D	495	<div><div>45%6%•48%</div></div>
1	E	495	<div><div>46%••48%</div></div>
1	F	495	<div><div>46%5%48%</div></div>
1	G	495	<div><div>46%5%•48%</div></div>
1	H	495	<div><div>46%5%•48%</div></div>
1	I	495	<div><div>46%5%•48%</div></div>
1	J	495	<div><div>45%6%•48%</div></div>
1	K	495	<div><div>44%6%•48%</div></div>

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Mol	Chain	Length	Quality of chain
1	L	495	<div><div></div><div>45%5%•48%</div></div>
1	M	495	<div><div></div><div>40%•56%</div></div>
1	N	495	<div><div></div><div>40%•56%</div></div>
1	O	495	<div><div></div><div>41%••56%</div></div>
1	P	495	<div><div></div><div>41%••56%</div></div>
1	Q	495	<div><div></div><div>40%•56%</div></div>
1	R	495	<div><div></div><div>40%•56%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17406 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 DELTAMBD GAG PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	255	Total	C	N	O	0	0
			1019	510	255	254		
1	B	255	Total	C	N	O	0	0
			1019	510	255	254		
1	C	255	Total	C	N	O	0	0
			1019	510	255	254		
1	D	255	Total	C	N	O	0	0
			1019	510	255	254		
1	E	255	Total	C	N	O	0	0
			1019	510	255	254		
1	F	255	Total	C	N	O	0	0
			1019	510	255	254		
1	G	255	Total	C	N	O	0	0
			1019	510	255	254		
1	H	255	Total	C	N	O	0	0
			1019	510	255	254		
1	I	255	Total	C	N	O	0	0
			1019	510	255	254		
1	J	255	Total	C	N	O	0	0
			1019	510	255	254		
1	K	255	Total	C	N	O	0	0
			1019	510	255	254		
1	L	255	Total	C	N	O	0	0
			1019	510	255	254		
1	M	216	Total	C	N	O	0	0
			863	432	216	215		
1	N	216	Total	C	N	O	0	0
			863	432	216	215		
1	O	216	Total	C	N	O	0	0
			863	432	216	215		
1	P	216	Total	C	N	O	0	0
			863	432	216	215		
1	Q	216	Total	C	N	O	0	0
			863	432	216	215		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	216	Total	C	N	O	0	0
			863	432	216	215		

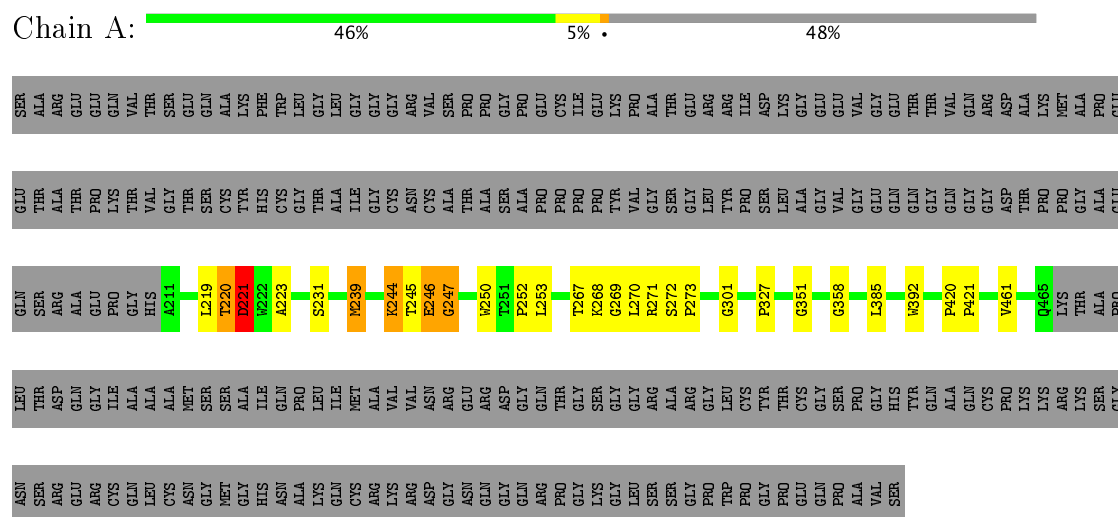
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	SER	-	expression tag	UNP P03322
A	573	GLN	PRO	conflict	UNP P03322
B	83	SER	-	expression tag	UNP P03322
B	573	GLN	PRO	conflict	UNP P03322
C	83	SER	-	expression tag	UNP P03322
C	573	GLN	PRO	conflict	UNP P03322
D	83	SER	-	expression tag	UNP P03322
D	573	GLN	PRO	conflict	UNP P03322
E	83	SER	-	expression tag	UNP P03322
E	573	GLN	PRO	conflict	UNP P03322
F	83	SER	-	expression tag	UNP P03322
F	573	GLN	PRO	conflict	UNP P03322
G	83	SER	-	expression tag	UNP P03322
G	573	GLN	PRO	conflict	UNP P03322
H	83	SER	-	expression tag	UNP P03322
H	573	GLN	PRO	conflict	UNP P03322
I	83	SER	-	expression tag	UNP P03322
I	573	GLN	PRO	conflict	UNP P03322
J	83	SER	-	expression tag	UNP P03322
J	573	GLN	PRO	conflict	UNP P03322
K	83	SER	-	expression tag	UNP P03322
K	573	GLN	PRO	conflict	UNP P03322
L	83	SER	-	expression tag	UNP P03322
L	573	GLN	PRO	conflict	UNP P03322
M	83	SER	-	expression tag	UNP P03322
M	573	GLN	PRO	conflict	UNP P03322
N	83	SER	-	expression tag	UNP P03322
N	573	GLN	PRO	conflict	UNP P03322
O	83	SER	-	expression tag	UNP P03322
O	573	GLN	PRO	conflict	UNP P03322
P	83	SER	-	expression tag	UNP P03322
P	573	GLN	PRO	conflict	UNP P03322
Q	83	SER	-	expression tag	UNP P03322
Q	573	GLN	PRO	conflict	UNP P03322
R	83	SER	-	expression tag	UNP P03322
R	573	GLN	PRO	conflict	UNP P03322

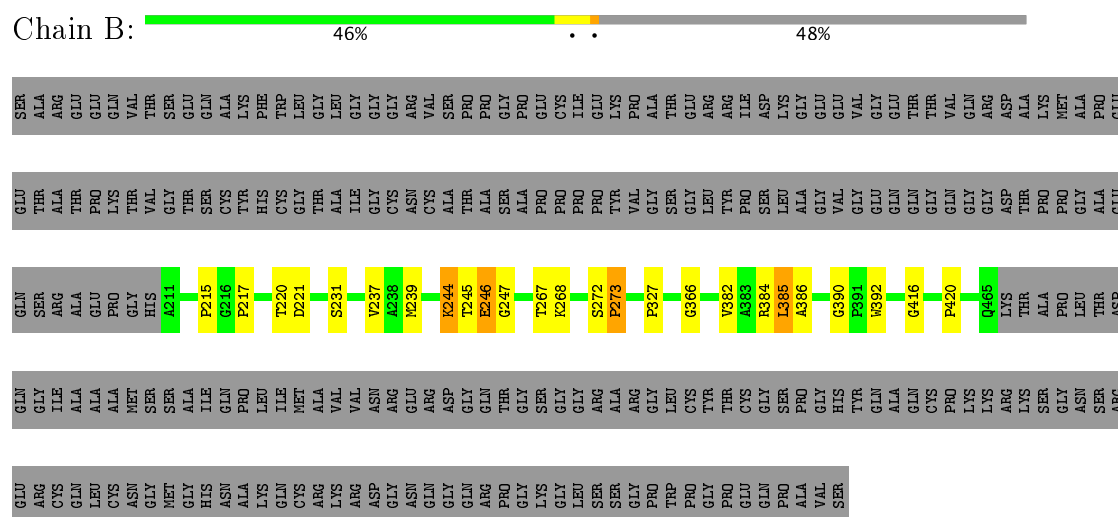
### 3 Residue-property plots

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: DELTAMBD GAG PROTEIN

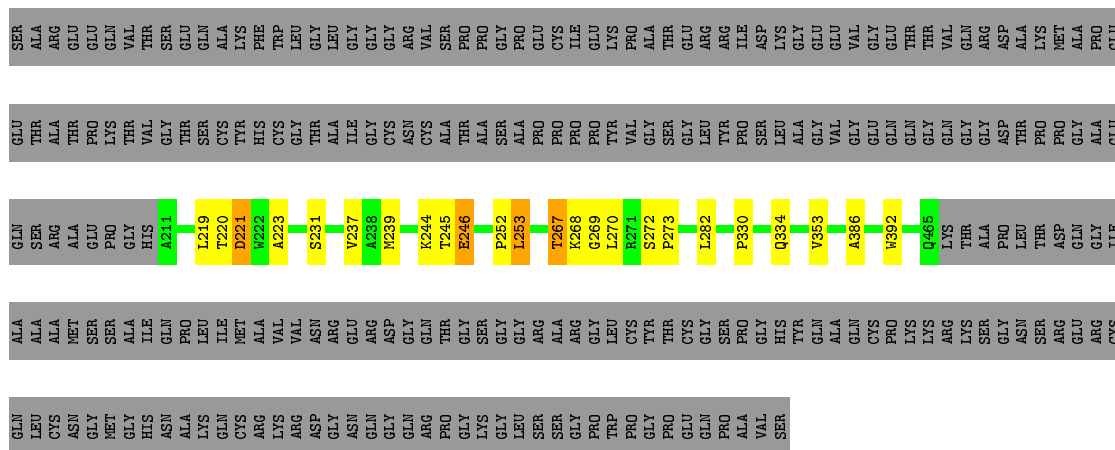


#### • Molecule 1: DELTAMBD GAG PROTEIN



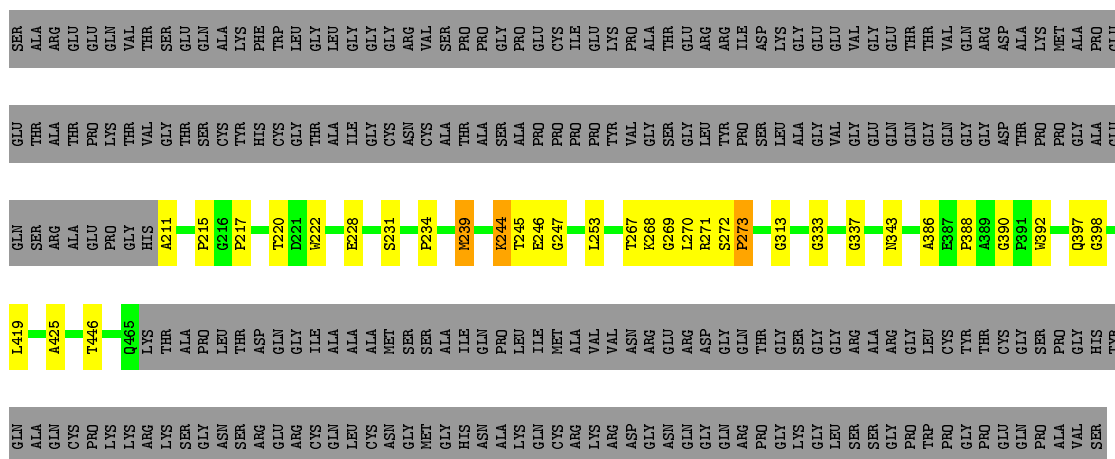
#### • Molecule 1: DELTAMBD GAG PROTEIN





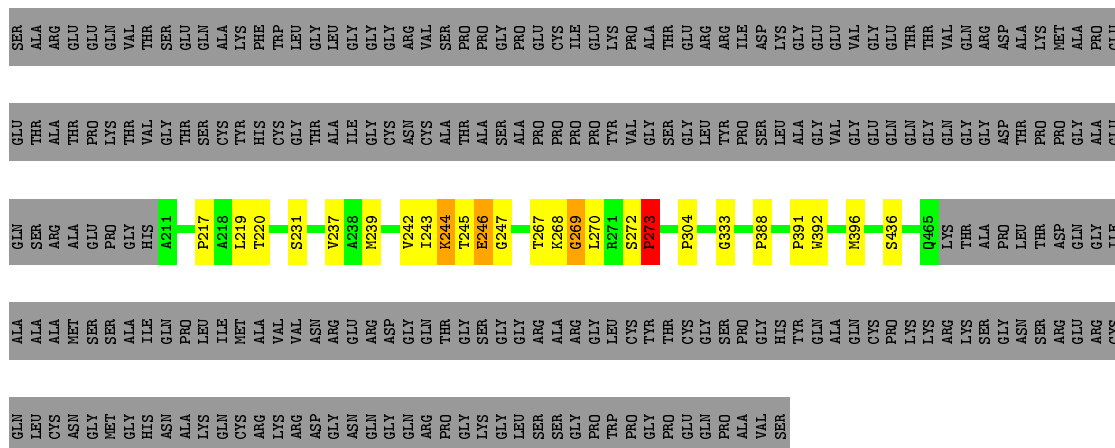
### • Molecule 1: DELTAMBD GAG PROTEIN

Chain D: 45% 6% 48%



### • Molecule 1: DELTAMBD GAG PROTEIN

Chain E: 46% 2% 48%



### • Molecule 1: DELTAMBD GAG PROTEIN

48%

48%

48%

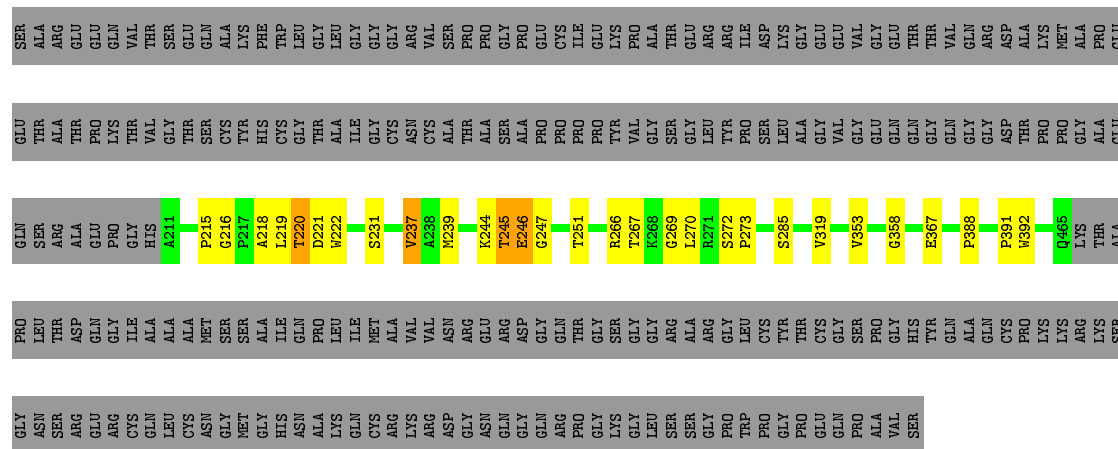
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM



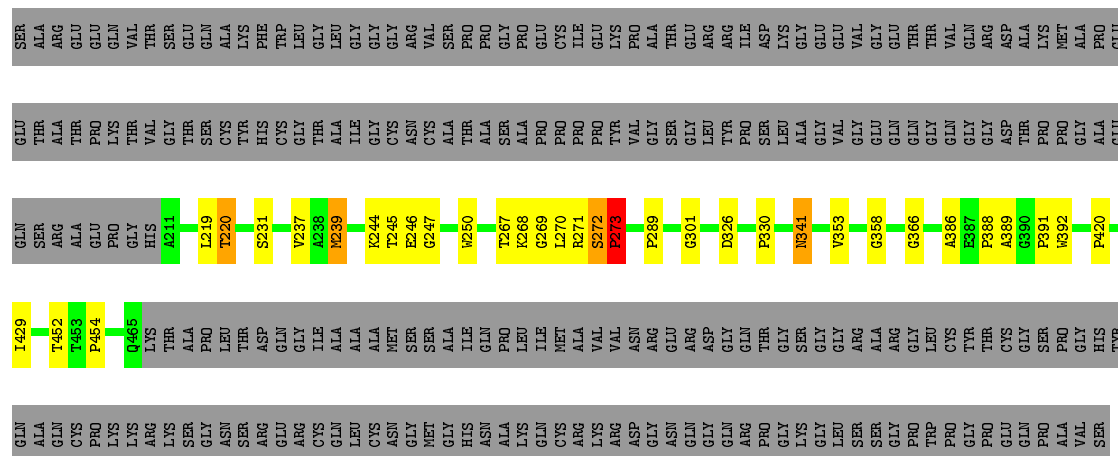
- Molecule 1: DELTAMBD GAG PROTEIN

Chain I:  46% 5% 48%



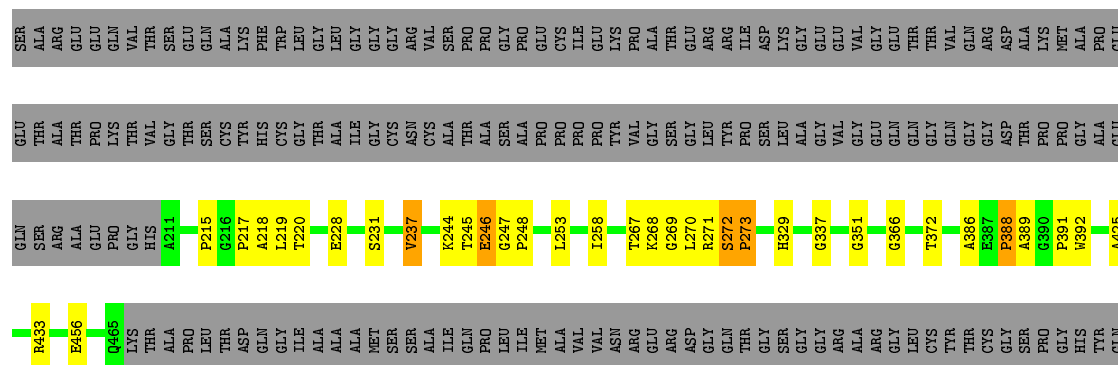
- Molecule 1: DELTAMBD GAG PROTEIN

Chain J:  45% 6% 48%



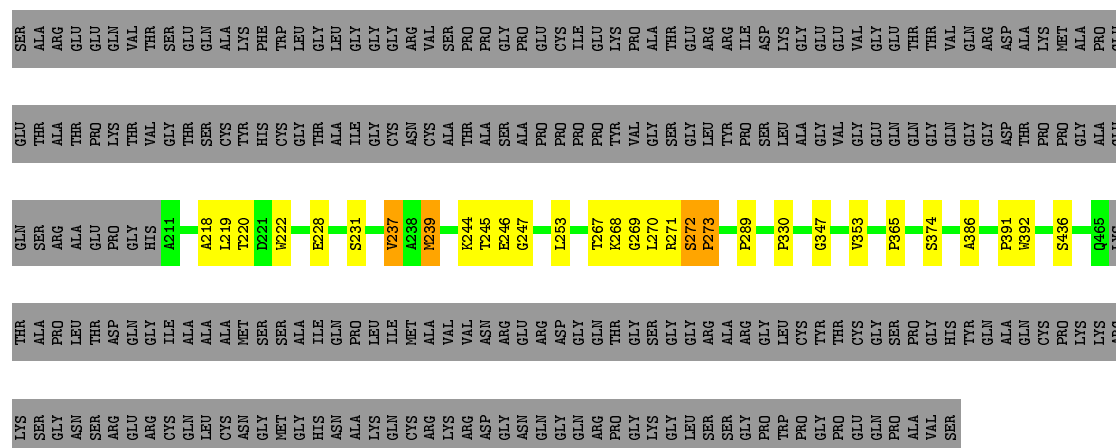
- Molecule 1: DELTAMBD GAG PROTEIN

Chain K:  44% 6% 48%



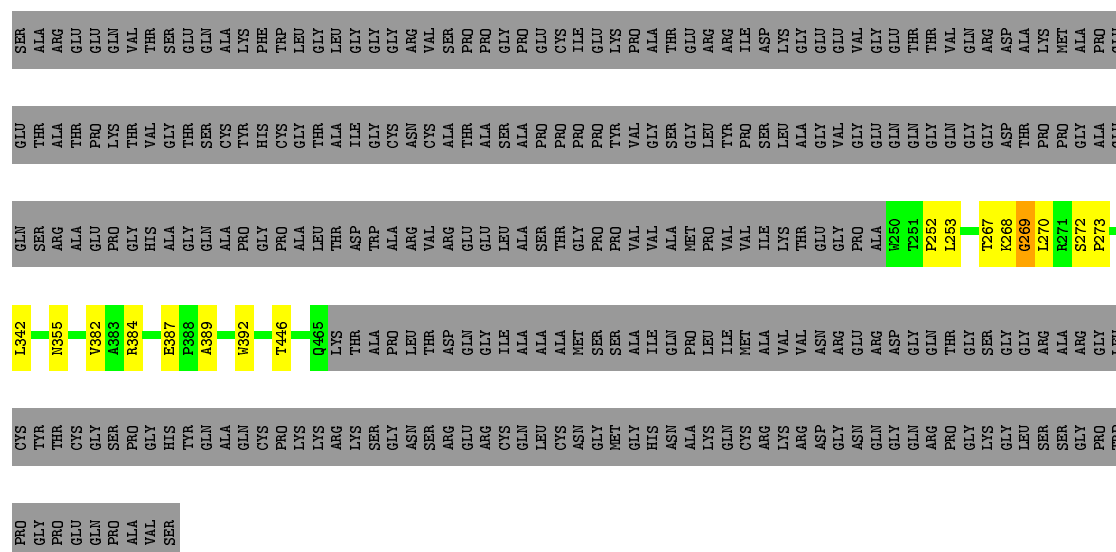
- Molecule 1: DELTAMBD GAG PROTEIN

Chain L:  45% 5% 48%



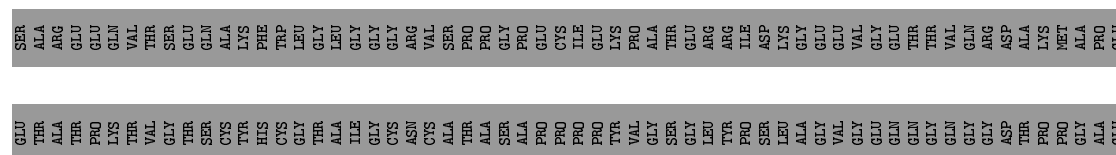
- Molecule 1: DELTAMBD GAG PROTEIN

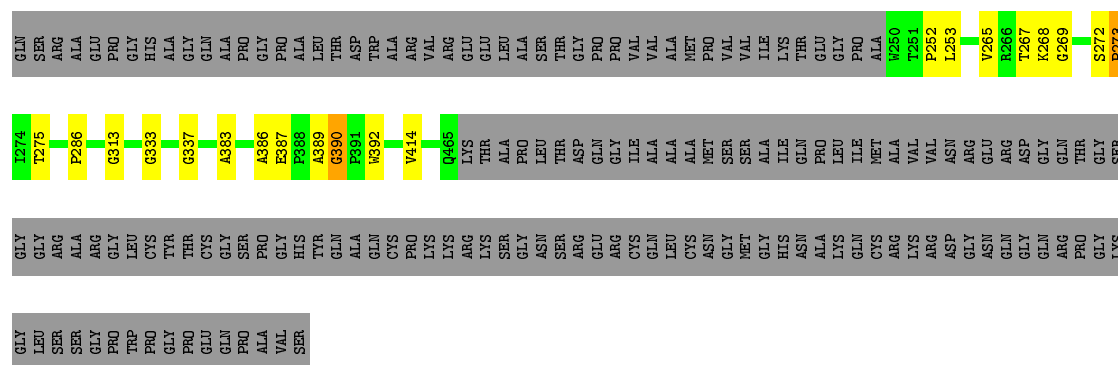
Chain M:  40% 0% 56%



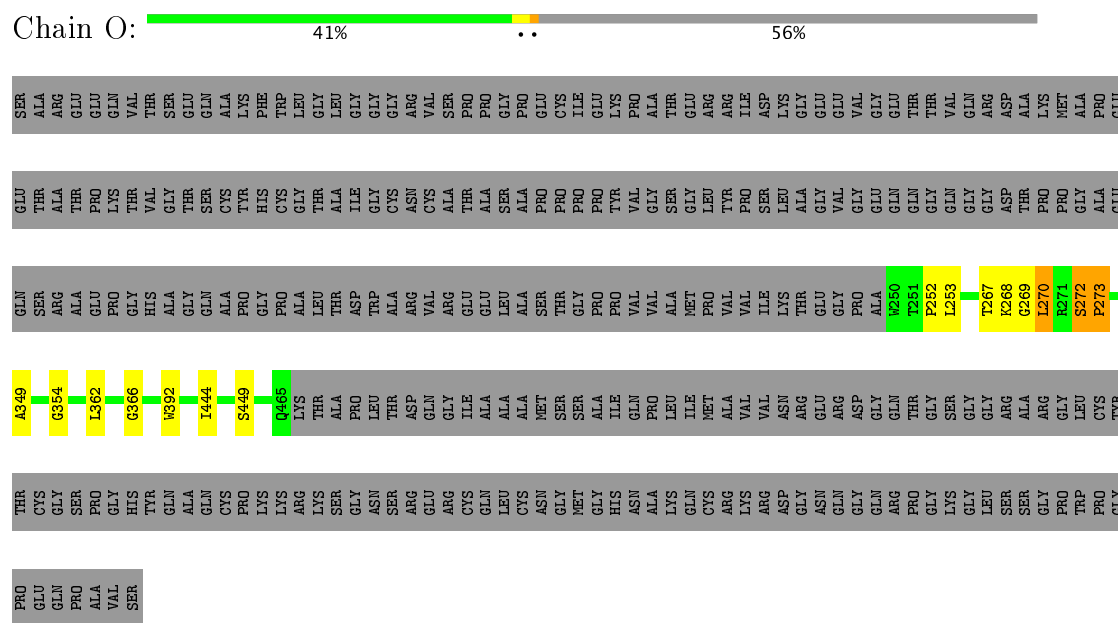
- Molecule 1: DELTAMBD GAG PROTEIN

Chain N:  40% 1% 56%

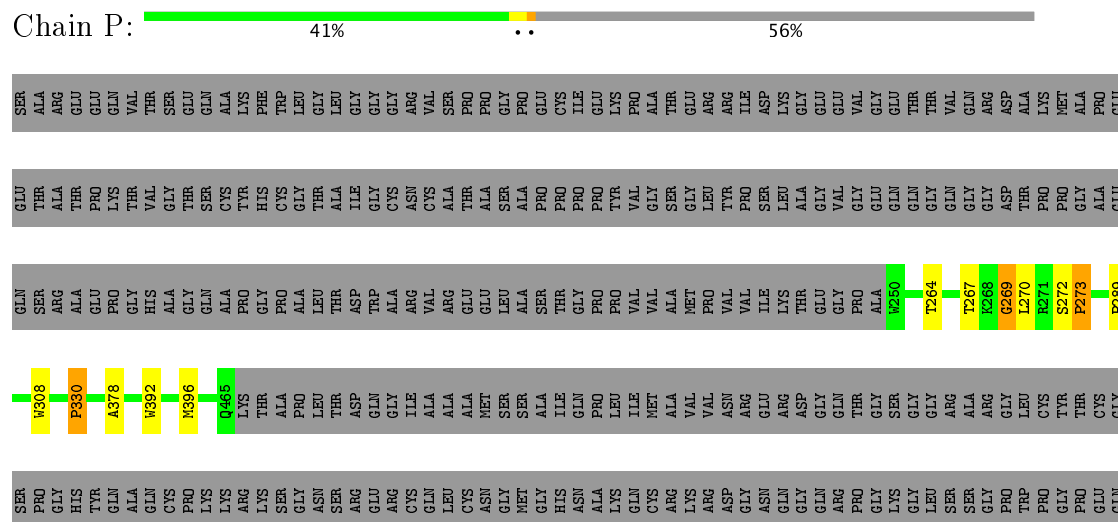




- Molecule 1: DELTAMBD GAG PROTEIN



- Molecule 1: DELTAMBD GAG PROTEIN





## 4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of tilted images used	8375	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPING OF INDIVIDUAL MICROGRAPHS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN MULTISCAN	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	1.43	1/1018 (0.1%)	1.70	8/1271 (0.6%)
1	B	1.40	2/1018 (0.2%)	1.62	3/1271 (0.2%)
1	C	1.45	0/1018	1.64	3/1271 (0.2%)
1	D	1.44	4/1018 (0.4%)	1.73	14/1271 (1.1%)
1	E	1.44	3/1018 (0.3%)	1.60	4/1271 (0.3%)
1	F	1.46	1/1018 (0.1%)	1.70	9/1271 (0.7%)
1	G	1.44	0/1018	1.72	6/1271 (0.5%)
1	H	1.51	1/1018 (0.1%)	1.63	5/1271 (0.4%)
1	I	1.49	2/1018 (0.2%)	1.68	7/1271 (0.6%)
1	J	1.50	5/1018 (0.5%)	1.70	7/1271 (0.6%)
1	K	1.47	4/1018 (0.4%)	1.69	14/1271 (1.1%)
1	L	1.49	2/1018 (0.2%)	1.67	4/1271 (0.3%)
1	M	1.47	1/862 (0.1%)	1.65	6/1076 (0.6%)
1	N	1.42	2/862 (0.2%)	1.66	7/1076 (0.7%)
1	O	1.47	3/862 (0.3%)	1.63	2/1076 (0.2%)
1	P	1.39	0/862	1.62	6/1076 (0.6%)
1	Q	1.49	3/862 (0.3%)	1.65	5/1076 (0.5%)
1	R	1.42	2/862 (0.2%)	1.57	2/1076 (0.2%)
All	All	1.46	36/17388 (0.2%)	1.66	112/21708 (0.5%)

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	11
1	B	0	10
1	C	0	10
1	D	0	9
1	E	0	12
1	F	0	11
1	G	0	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	11
1	I	0	9
1	J	0	13
1	K	0	11
1	L	0	11
1	M	0	3
1	N	0	4
1	O	0	5
1	P	0	4
1	Q	0	6
1	R	0	5
All	All	0	158

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	GLY	CA-C	-6.71	1.41	1.51
1	R	437	GLN	C-N	6.15	1.46	1.34
1	A	301	GLY	C-N	-6.07	1.22	1.34
1	J	326	ASP	C-N	-6.00	1.22	1.34
1	Q	333	GLY	CA-C	-5.99	1.42	1.51
1	E	333	GLY	N-CA	5.98	1.55	1.46
1	M	355	ASN	N-CA	-5.93	1.34	1.46
1	K	337	GLY	CA-C	-5.90	1.42	1.51
1	O	354	GLY	CA-C	-5.89	1.42	1.51
1	J	454	PRO	N-CA	-5.84	1.37	1.47
1	E	304	PRO	CA-C	-5.59	1.41	1.52
1	H	252	PRO	CA-C	5.58	1.64	1.52
1	I	215	PRO	C-N	5.58	1.43	1.33
1	J	452	THR	N-CA	5.56	1.57	1.46
1	D	313	GLY	CA-C	-5.56	1.43	1.51
1	B	366	GLY	CA-C	-5.51	1.43	1.51
1	D	397	GLN	CA-C	-5.48	1.38	1.52
1	J	429	ILE	N-CA	-5.43	1.35	1.46
1	I	358	GLY	CA-C	-5.42	1.43	1.51
1	J	366	GLY	N-CA	-5.40	1.38	1.46
1	O	366	GLY	CA-C	-5.40	1.43	1.51
1	L	365	PRO	CA-C	-5.36	1.42	1.52
1	O	362	LEU	N-CA	-5.35	1.35	1.46
1	E	269	GLY	N-CA	-5.32	1.38	1.46
1	D	343	ASN	N-CA	-5.30	1.35	1.46
1	K	389	ALA	N-CA	-5.30	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	313	GLY	N-CA	5.29	1.53	1.46
1	K	433	ARG	N-CA	-5.28	1.35	1.46
1	F	359	GLN	CA-C	5.25	1.66	1.52
1	L	347	GLY	CA-C	-5.25	1.43	1.51
1	R	398	GLY	CA-C	-5.22	1.43	1.51
1	Q	347	GLY	CA-C	-5.20	1.43	1.51
1	N	337	GLY	CA-C	-5.08	1.43	1.51
1	D	333	GLY	CA-C	-5.07	1.43	1.51
1	Q	416	GLY	CA-C	-5.04	1.43	1.51
1	K	366	GLY	N-CA	-5.02	1.38	1.46

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	389	ALA	C-N-CA	7.78	138.63	122.30
1	H	217	PRO	C-N-CA	7.34	140.04	121.70
1	N	414	VAL	O-C-N	-7.06	111.41	122.70
1	P	330	PRO	N-CA-C	6.85	129.91	112.10
1	D	337	GLY	O-C-N	-6.65	112.06	122.70
1	K	329	HIS	N-CA-C	6.64	128.94	111.00
1	B	385	LEU	N-CA-C	6.64	128.93	111.00
1	O	444	ILE	O-C-N	-6.46	112.36	122.70
1	H	212	GLY	C-N-CA	6.42	137.76	121.70
1	D	217	PRO	O-C-N	-6.41	112.44	122.70
1	J	239	MET	CA-C-N	6.33	134.84	117.10
1	K	215	PRO	C-N-CA	6.27	135.46	122.30
1	E	217	PRO	C-N-CA	6.25	137.34	121.70
1	B	217	PRO	C-N-CA	6.25	137.32	121.70
1	J	358	GLY	O-C-N	-6.23	112.72	122.70
1	G	284	SER	O-C-N	-6.22	112.75	122.70
1	M	384	ARG	O-C-N	-6.18	112.81	122.70
1	K	217	PRO	O-C-N	-6.17	112.82	122.70
1	D	273	PRO	N-CA-C	6.17	128.14	112.10
1	D	239	MET	CA-C-N	6.16	134.35	117.10
1	G	399	PRO	C-N-CA	6.13	137.03	121.70
1	G	253	LEU	N-CA-C	6.11	127.50	111.00
1	K	258	ILE	O-C-N	-6.11	112.93	122.70
1	F	463	ASP	O-C-N	-6.03	113.05	122.70
1	G	374	SER	O-C-N	-6.03	113.06	122.70
1	F	220	THR	C-N-CA	6.01	136.73	121.70
1	M	382	VAL	O-C-N	-5.93	113.22	122.70
1	I	319	VAL	O-C-N	-5.89	113.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	396	MET	O-C-N	-5.88	113.29	122.70
1	N	390	GLY	CA-C-N	5.80	133.35	117.10
1	P	396	MET	N-CA-C	-5.80	95.34	111.00
1	B	416	GLY	O-C-N	-5.78	113.45	122.70
1	H	289	PRO	N-CA-C	5.78	127.13	112.10
1	L	289	PRO	N-CA-C	5.78	127.11	112.10
1	Q	261	LEU	O-C-N	-5.76	113.48	122.70
1	K	237	VAL	N-CA-C	5.76	126.55	111.00
1	A	220	THR	C-N-CA	5.74	136.06	121.70
1	K	351	GLY	O-C-N	-5.73	113.53	122.70
1	D	211	ALA	CA-C-N	5.72	127.64	116.20
1	M	342	LEU	O-C-N	-5.71	113.56	122.70
1	M	387	GLU	CA-C-N	5.68	133.00	117.10
1	A	239	MET	O-C-N	-5.67	110.32	121.10
1	C	253	LEU	N-CA-C	5.65	126.26	111.00
1	Q	271	ARG	N-CA-C	-5.64	95.76	111.00
1	Q	434	GLN	O-C-N	-5.63	113.69	122.70
1	J	341	ASN	N-CA-C	5.62	126.17	111.00
1	G	311	ALA	O-C-N	-5.61	113.73	122.70
1	D	390	GLY	N-CA-C	-5.59	99.12	113.10
1	A	461	VAL	C-N-CA	5.55	135.59	121.70
1	K	388	PRO	N-CA-C	5.55	126.53	112.10
1	D	398	GLY	N-CA-C	-5.54	99.25	113.10
1	I	367	GLU	O-C-N	-5.54	113.84	122.70
1	D	215	PRO	O-C-N	-5.51	113.83	123.20
1	I	216	GLY	CA-C-O	-5.51	110.69	120.60
1	I	237	VAL	N-CA-C	5.50	125.86	111.00
1	N	383	ALA	N-CA-C	5.50	125.86	111.00
1	K	425	ALA	CA-C-N	5.46	132.39	117.10
1	F	390	GLY	N-CA-C	-5.46	99.46	113.10
1	F	234	PRO	CA-C-N	5.41	132.25	117.10
1	F	246	GLU	O-C-N	-5.40	114.02	123.20
1	I	251	THR	O-C-N	-5.39	110.86	121.10
1	K	372	THR	O-C-N	-5.38	114.08	122.70
1	N	265	VAL	C-N-CA	5.36	135.10	121.70
1	C	282	LEU	O-C-N	-5.36	114.13	122.70
1	I	220	THR	C-N-CA	5.36	135.09	121.70
1	M	446	THR	O-C-N	-5.35	114.14	122.70
1	L	237	VAL	N-CA-C	5.32	125.36	111.00
1	A	221	ASP	N-CA-C	5.32	125.35	111.00
1	R	275	THR	CA-C-O	5.30	131.24	120.10
1	N	333	GLY	N-CA-C	5.29	126.33	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	402	SER	O-C-N	-5.29	114.24	122.70
1	K	456	GLU	O-C-N	-5.27	114.26	122.70
1	A	239	MET	CA-C-N	5.27	131.86	117.10
1	D	211	ALA	O-C-N	-5.25	114.28	123.20
1	D	222	TRP	N-CA-C	5.25	125.17	111.00
1	L	239	MET	CA-C-N	5.24	131.76	117.10
1	I	266	ARG	C-N-CA	5.22	134.76	121.70
1	J	220	THR	O-C-N	-5.20	114.38	122.70
1	Q	350	ASP	C-N-CA	5.19	133.20	122.30
1	R	425	ALA	CA-C-N	5.19	131.63	117.10
1	J	289	PRO	CA-C-N	5.19	128.61	117.20
1	K	215	PRO	CA-C-N	5.19	126.58	116.20
1	P	378	ALA	O-C-N	-5.18	114.41	122.70
1	N	275	THR	O-C-N	5.17	130.97	122.70
1	A	421	PRO	C-N-CA	5.16	134.61	121.70
1	L	374	SER	O-C-N	-5.16	114.44	122.70
1	J	273	PRO	N-CA-C	5.16	125.51	112.10
1	P	264	THR	O-C-N	-5.16	114.45	122.70
1	C	267	THR	O-C-N	-5.15	114.47	122.70
1	A	244	LYS	O-C-N	-5.14	114.47	122.70
1	E	243	ILE	C-N-CA	5.14	134.54	121.70
1	P	289	PRO	O-C-N	-5.13	114.48	122.70
1	H	413	ALA	O-C-N	-5.13	114.49	122.70
1	E	273	PRO	N-CA-C	5.12	125.42	112.10
1	K	246	GLU	O-C-N	-5.12	114.49	123.20
1	K	218	ALA	N-CA-C	5.12	124.82	111.00
1	D	446	THR	O-C-N	-5.10	114.54	122.70
1	J	389	ALA	CA-C-N	5.09	126.39	116.20
1	D	425	ALA	CA-C-N	5.09	131.34	117.10
1	H	411	ILE	O-C-N	-5.08	114.58	122.70
1	A	247	GLY	CA-C-N	5.07	131.29	117.10
1	O	349	ALA	O-C-N	-5.07	114.59	122.70
1	F	246	GLU	CA-C-N	5.06	126.33	116.20
1	F	460	TYR	O-C-N	-5.06	114.61	122.70
1	F	323	ALA	O-C-N	-5.05	114.62	122.70
1	D	419	LEU	O-C-N	-5.05	111.51	121.10
1	K	389	ALA	N-CA-C	-5.03	97.43	111.00
1	G	274	ILE	O-C-N	-5.02	114.67	122.70
1	F	389	ALA	O-C-N	-5.02	114.67	123.20
1	M	389	ALA	N-CA-C	-5.02	97.45	111.00
1	P	308	TRP	O-C-N	-5.02	114.67	122.70
1	D	234	PRO	CA-C-O	-5.01	108.17	120.20

There are no chirality outliers.

All (158) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	LEU	Peptide
1	A	220	THR	Peptide
1	A	221	ASP	Peptide
1	A	244	LYS	Peptide
1	A	245	THR	Peptide
1	A	246	GLU	Peptide
1	A	247	GLY	Peptide
1	A	268	LYS	Peptide
1	A	269	GLY	Peptide
1	A	270	LEU	Peptide
1	A	272	SER	Peptide
1	B	220	THR	Peptide
1	B	221	ASP	Peptide
1	B	244	LYS	Peptide
1	B	245	THR	Peptide
1	B	246	GLU	Peptide
1	B	247	GLY	Peptide
1	B	268	LYS	Peptide
1	B	272	SER	Peptide
1	B	273	PRO	Peptide
1	B	386	ALA	Peptide
1	C	219	LEU	Peptide
1	C	220	THR	Peptide
1	C	221	ASP	Peptide
1	C	244	LYS	Peptide
1	C	245	THR	Peptide
1	C	246	GLU	Peptide
1	C	268	LYS	Peptide
1	C	269	GLY	Peptide
1	C	270	LEU	Peptide
1	C	272	SER	Peptide
1	D	220	THR	Peptide
1	D	244	LYS	Peptide
1	D	245	THR	Peptide
1	D	246	GLU	Peptide
1	D	247	GLY	Peptide
1	D	268	LYS	Peptide
1	D	269	GLY	Peptide
1	D	270	LEU	Peptide
1	D	272	SER	Peptide

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Mol	Chain	Res	Type	Group
1	E	219	LEU	Peptide
1	E	220	THR	Peptide
1	E	242	VAL	Peptide
1	E	244	LYS	Peptide
1	E	245	THR	Peptide
1	E	246	GLU	Peptide
1	E	247	GLY	Peptide
1	E	268	LYS	Peptide
1	E	269	GLY	Peptide
1	E	270	LEU	Peptide
1	E	272	SER	Peptide
1	E	273	PRO	Peptide
1	F	219	LEU	Peptide
1	F	220	THR	Peptide
1	F	244	LYS	Peptide
1	F	245	THR	Peptide
1	F	246	GLU	Peptide
1	F	247	GLY	Peptide
1	F	268	LYS	Peptide
1	F	269	GLY	Peptide
1	F	270	LEU	Peptide
1	F	272	SER	Peptide
1	F	283	MET	Mainchain
1	G	220	THR	Peptide
1	G	244	LYS	Peptide
1	G	245	THR	Peptide
1	G	246	GLU	Peptide
1	G	247	GLY	Peptide
1	G	268	LYS	Peptide
1	G	269	GLY	Mainchain
1	G	270	LEU	Peptide
1	G	272	SER	Peptide
1	G	273	PRO	Peptide
1	G	386	ALA	Peptide
1	G	388	PRO	Mainchain
1	G	464	ARG	Mainchain
1	H	220	THR	Peptide
1	H	244	LYS	Peptide
1	H	245	THR	Mainchain,Peptide
1	H	246	GLU	Peptide
1	H	247	GLY	Peptide
1	H	268	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	H	269	GLY	Peptide
1	H	270	LEU	Peptide
1	H	272	SER	Peptide
1	H	273	PRO	Peptide
1	I	220	THR	Peptide
1	I	244	LYS	Peptide
1	I	245	THR	Peptide
1	I	246	GLU	Peptide
1	I	247	GLY	Peptide
1	I	269	GLY	Peptide
1	I	270	LEU	Peptide
1	I	272	SER	Peptide
1	I	285	SER	Mainchain
1	J	219	LEU	Mainchain
1	J	220	THR	Mainchain,Peptide
1	J	244	LYS	Peptide
1	J	245	THR	Peptide
1	J	246	GLU	Peptide
1	J	247	GLY	Peptide
1	J	268	LYS	Peptide
1	J	269	GLY	Mainchain
1	J	270	LEU	Peptide
1	J	272	SER	Peptide
1	J	273	PRO	Peptide
1	J	301	GLY	Mainchain
1	K	219	LEU	Peptide
1	K	220	THR	Peptide
1	K	244	LYS	Peptide
1	K	245	THR	Peptide
1	K	246	GLU	Peptide
1	K	247	GLY	Peptide
1	K	268	LYS	Peptide
1	K	269	GLY	Peptide
1	K	270	LEU	Peptide
1	K	272	SER	Peptide
1	K	273	PRO	Peptide
1	L	219	LEU	Peptide
1	L	220	THR	Peptide
1	L	244	LYS	Peptide
1	L	245	THR	Peptide
1	L	246	GLU	Peptide
1	L	247	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	L	268	LYS	Peptide
1	L	269	GLY	Peptide
1	L	270	LEU	Peptide
1	L	272	SER	Peptide
1	L	273	PRO	Peptide
1	M	269	GLY	Peptide
1	M	270	LEU	Peptide
1	M	272	SER	Peptide
1	N	268	LYS	Peptide
1	N	269	GLY	Peptide
1	N	272	SER	Peptide
1	N	273	PRO	Peptide
1	O	268	LYS	Peptide
1	O	269	GLY	Peptide
1	O	270	LEU	Peptide
1	O	272	SER	Peptide
1	O	273	PRO	Peptide
1	P	269	GLY	Peptide
1	P	270	LEU	Peptide
1	P	272	SER	Peptide
1	P	273	PRO	Peptide
1	Q	268	LYS	Peptide
1	Q	269	GLY	Mainchain
1	Q	270	LEU	Peptide
1	Q	272	SER	Peptide
1	Q	273	PRO	Peptide
1	Q	386	ALA	Peptide
1	R	269	GLY	Peptide
1	R	270	LEU	Peptide
1	R	272	SER	Peptide
1	R	288	LEU	Mainchain
1	R	386	ALA	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	1019	0	266	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1019	0	266	1	0
1	C	1019	0	266	0	0
1	D	1019	0	266	0	0
1	E	1019	0	266	0	0
1	F	1019	0	266	0	0
1	G	1019	0	266	0	0
1	H	1019	0	266	0	0
1	I	1019	0	266	0	0
1	J	1019	0	266	0	0
1	K	1019	0	266	0	0
1	L	1019	0	266	0	0
1	M	863	0	225	0	0
1	N	863	0	225	0	0
1	O	863	0	225	0	0
1	P	863	0	225	0	0
1	Q	863	0	225	0	0
1	R	863	0	225	0	0
All	All	17406	0	4542	2	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 0.

All (2) 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:382:VAL:C	1:B:384:ARG:H	2.21	0.43
1:A:351:GLY:O	1:A:358:GLY:HA3	2.20	0.42

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	253/495 (51%)	210 (83%)	28 (11%)	15 (6%)	2	23
1	B	253/495 (51%)	216 (85%)	25 (10%)	12 (5%)	3	28
1	C	253/495 (51%)	218 (86%)	20 (8%)	15 (6%)	2	23
1	D	253/495 (51%)	220 (87%)	22 (9%)	11 (4%)	3	29
1	E	253/495 (51%)	224 (88%)	18 (7%)	11 (4%)	3	29
1	F	253/495 (51%)	222 (88%)	20 (8%)	11 (4%)	3	29
1	G	253/495 (51%)	221 (87%)	17 (7%)	15 (6%)	2	23
1	H	253/495 (51%)	212 (84%)	27 (11%)	14 (6%)	2	25
1	I	253/495 (51%)	218 (86%)	20 (8%)	15 (6%)	2	23
1	J	253/495 (51%)	218 (86%)	19 (8%)	16 (6%)	1	22
1	K	253/495 (51%)	224 (88%)	16 (6%)	13 (5%)	2	26
1	L	253/495 (51%)	214 (85%)	22 (9%)	17 (7%)	1	21
1	M	214/495 (43%)	190 (89%)	17 (8%)	7 (3%)	4	35
1	N	214/495 (43%)	188 (88%)	17 (8%)	9 (4%)	3	30
1	O	214/495 (43%)	195 (91%)	11 (5%)	8 (4%)	4	33
1	P	214/495 (43%)	191 (89%)	18 (8%)	5 (2%)	7	43
1	Q	214/495 (43%)	188 (88%)	19 (9%)	7 (3%)	4	35
1	R	214/495 (43%)	191 (89%)	15 (7%)	8 (4%)	4	33
All	All	4320/8910 (48%)	3760 (87%)	351 (8%)	209 (5%)	5	28

All (209) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLU
1	A	267	THR
1	A	271	ARG
1	A	273	PRO
1	A	327	PRO
1	A	392	TRP
1	B	246	GLU
1	B	267	THR
1	B	273	PRO
1	B	385	LEU
1	C	253	LEU
1	C	267	THR
1	C	386	ALA
1	C	392	TRP

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Mol	Chain	Res	Type
1	D	273	PRO
1	D	386	ALA
1	E	267	THR
1	E	273	PRO
1	F	246	GLU
1	F	273	PRO
1	F	392	TRP
1	G	221	ASP
1	G	245	THR
1	G	253	LEU
1	G	273	PRO
1	H	246	GLU
1	H	273	PRO
1	I	237	VAL
1	I	245	THR
1	I	273	PRO
1	I	353	VAL
1	I	388	PRO
1	I	392	TRP
1	J	237	VAL
1	J	273	PRO
1	J	353	VAL
1	J	388	PRO
1	K	237	VAL
1	K	267	THR
1	K	392	TRP
1	L	237	VAL
1	L	267	THR
1	L	273	PRO
1	L	386	ALA
1	M	273	PRO
1	M	392	TRP
1	N	273	PRO
1	N	392	TRP
1	O	273	PRO
1	O	392	TRP
1	P	267	THR
1	P	273	PRO
1	P	392	TRP
1	Q	386	ALA
1	Q	392	TRP
1	R	253	LEU

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Mol	Chain	Res	Type
1	R	267	THR
1	R	273	PRO
1	R	392	TRP
1	R	419	LEU
1	A	221	ASP
1	A	250	TRP
1	A	253	LEU
1	A	420	PRO
1	B	215	PRO
1	B	237	VAL
1	B	392	TRP
1	C	221	ASP
1	C	223	ALA
1	C	237	VAL
1	C	273	PRO
1	C	334	GLN
1	C	353	VAL
1	D	267	THR
1	D	392	TRP
1	E	237	VAL
1	E	392	TRP
1	E	436	SER
1	F	267	THR
1	F	271	ARG
1	F	327	PRO
1	F	388	PRO
1	G	267	THR
1	G	271	ARG
1	G	272	SER
1	G	392	TRP
1	H	267	THR
1	H	353	VAL
1	H	388	PRO
1	H	392	TRP
1	H	418	ASP
1	I	218	ALA
1	I	221	ASP
1	I	222	TRP
1	I	231	SER
1	J	267	THR
1	J	271	ARG
1	J	272	SER

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Mol	Chain	Res	Type
1	J	341	ASN
1	J	392	TRP
1	J	420	PRO
1	L	218	ALA
1	L	271	ARG
1	L	272	SER
1	M	253	LEU
1	M	267	THR
1	M	269	GLY
1	N	253	LEU
1	N	267	THR
1	O	252	PRO
1	O	267	THR
1	P	269	GLY
1	Q	267	THR
1	R	386	ALA
1	R	449	SER
1	A	231	SER
1	A	252	PRO
1	A	385	LEU
1	B	244	LYS
1	B	327	PRO
1	B	420	PRO
1	C	252	PRO
1	D	228	GLU
1	D	244	LYS
1	E	244	LYS
1	F	387	GLU
1	G	388	PRO
1	H	231	SER
1	I	267	THR
1	J	250	TRP
1	K	271	ARG
1	K	272	SER
1	K	391	PRO
1	L	222	TRP
1	L	231	SER
1	L	253	LEU
1	L	391	PRO
1	L	392	TRP
1	L	436	SER
1	M	252	PRO

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Mol	Chain	Res	Type
1	N	252	PRO
1	N	387	GLU
1	N	390	GLY
1	O	253	LEU
1	O	270	LEU
1	O	272	SER
1	P	330	PRO
1	Q	387	GLU
1	Q	390	GLY
1	B	231	SER
1	D	271	ARG
1	D	388	PRO
1	E	231	SER
1	E	246	GLU
1	F	231	SER
1	G	222	TRP
1	G	451	LEU
1	H	228	GLU
1	H	248	PRO
1	H	272	SER
1	I	246	GLU
1	J	231	SER
1	K	228	GLU
1	K	231	SER
1	K	273	PRO
1	K	386	ALA
1	L	228	GLU
1	L	353	VAL
1	M	268	LYS
1	Q	449	SER
1	A	223	ALA
1	C	246	GLU
1	C	330	PRO
1	D	253	LEU
1	F	239	MET
1	G	228	GLU
1	G	231	SER
1	G	353	VAL
1	H	213	GLN
1	H	330	PRO
1	J	386	ALA
1	K	248	PRO

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Mol	Chain	Res	Type
1	K	253	LEU
1	K	388	PRO
1	N	386	ALA
1	O	449	SER
1	R	452	THR
1	A	239	MET
1	C	231	SER
1	D	231	SER
1	E	239	MET
1	E	388	PRO
1	E	391	PRO
1	F	228	GLU
1	H	218	ALA
1	I	219	LEU
1	J	330	PRO
1	L	330	PRO
1	N	286	PRO
1	D	239	MET
1	G	391	PRO
1	Q	333	GLY
1	B	239	MET
1	I	391	PRO
1	J	239	MET
1	C	239	MET
1	J	391	PRO
1	L	239	MET
1	I	239	MET

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 [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.