



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 9, 2020 – 11:47 AM EST

PDB ID : 6T63
EMDB ID: : EMD-10383
Title : A model of the EIAV CA-SP hexamer (C2) from Gag-deltaMA tubes assembled at pH6
Authors : Dick, R.A.; Xu, C.; Morado, D.R.; Kravchuk, V.; Ricana, C.L.; Lyddon, T.D.; Broad, A.M.; Feathers, J.R.; Johnson, M.C.; Vogt, V.M.; Perilla, J.R.; Briggs, J.A.G.; Schur, F.K.M.
Deposited on : 2019-10-17
Resolution : 3.80 Å(reported)
Based on PDB ID : 2EIA

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

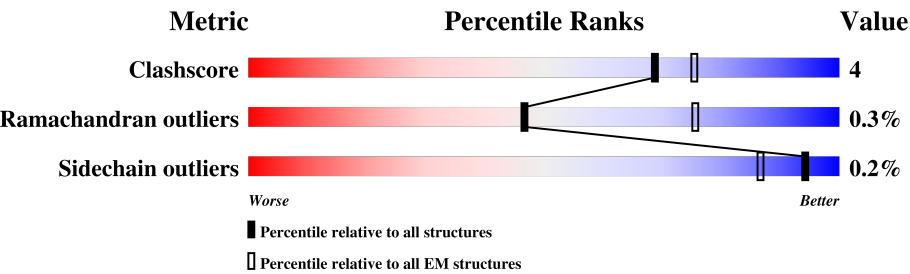
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

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 3.80 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. 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	486	39% 5% 55%
1	B	486	40% . 55%
1	C	486	42% . 55%
1	D	486	40% 5% 55%
1	E	486	40% 5% 55%
1	F	486	40% . 55%
1	G	486	42% . 55%
1	H	486	41% . 55%
1	I	486	41% . 55%

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Mol	Chain	Length	Quality of chain
1	J	486	 39% 5% 55%
1	K	486	 40% 5% 55%
1	L	486	 42% 5% 55%
1	M	486	 40% 5% 55%
1	N	486	 40% 5% 55%
1	O	486	 40% 5% 55%
1	P	486	 41% 5% 55%
1	Q	486	 41% 5% 55%
1	R	486	 41% 5% 55%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30978 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 Gag polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	B	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	C	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	F	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	D	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	H	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	I	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	E	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	G	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	J	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	K	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	L	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	O	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	M	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	Q	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	R	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		
1	N	217	Total	C	N	O	S	0	0
			1721	1081	304	324	12		

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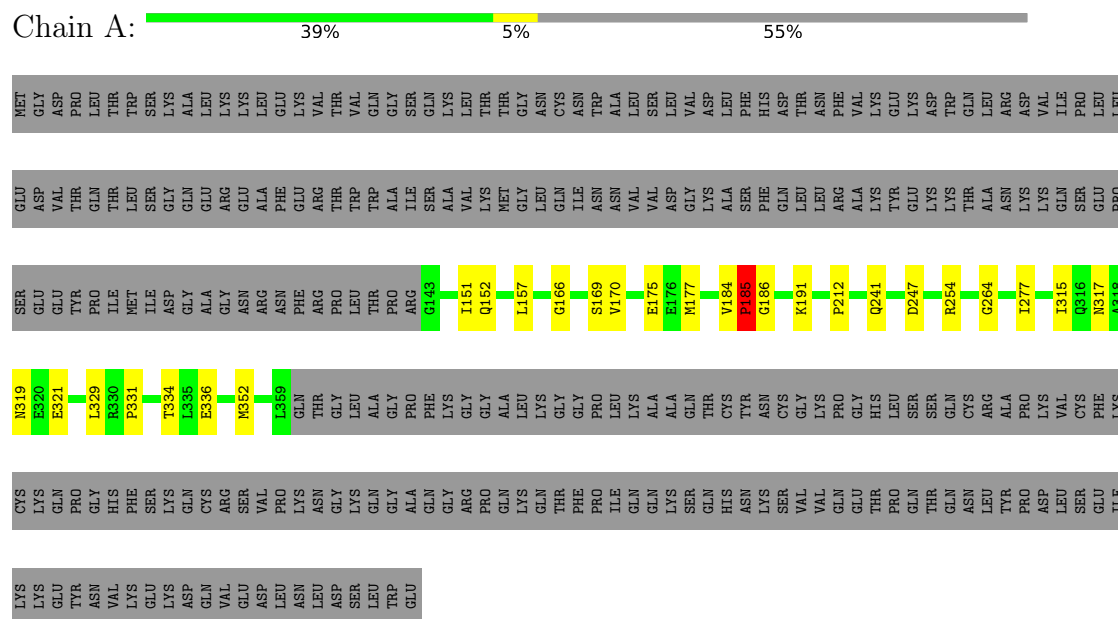
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	P	217	1721	1081	304	324	12	0	0

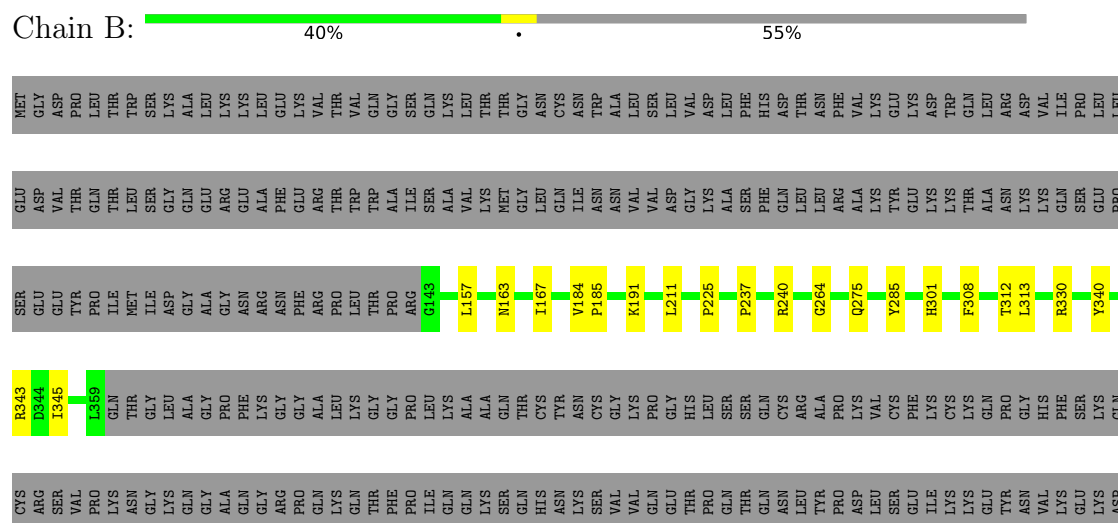
3 Residue-property plots

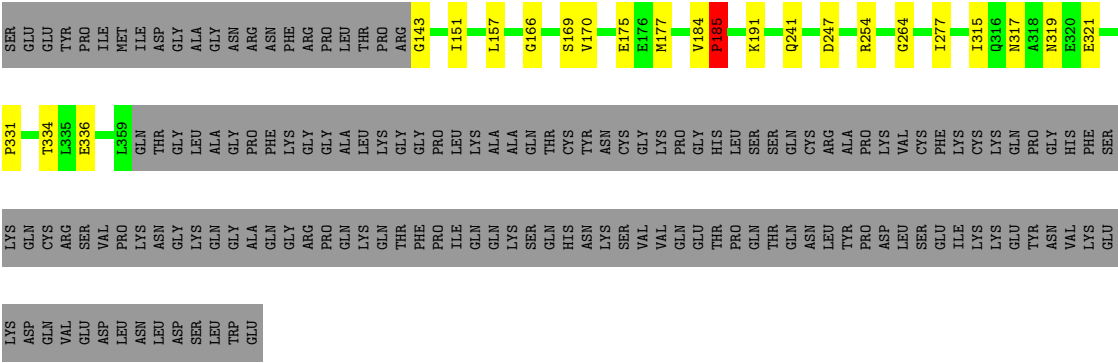
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Gag polyprotein



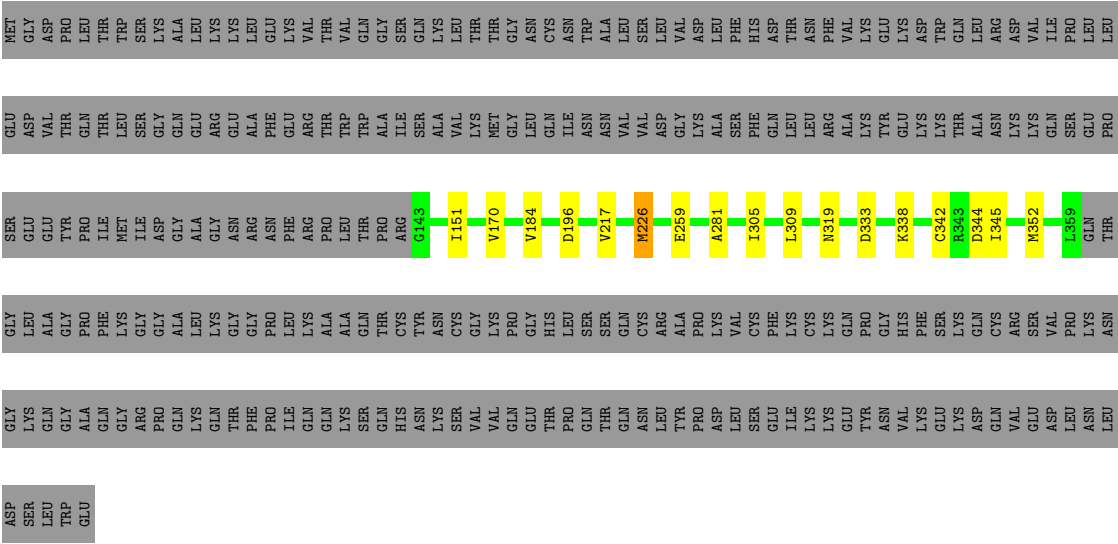
• Molecule 1: Gag polyprotein





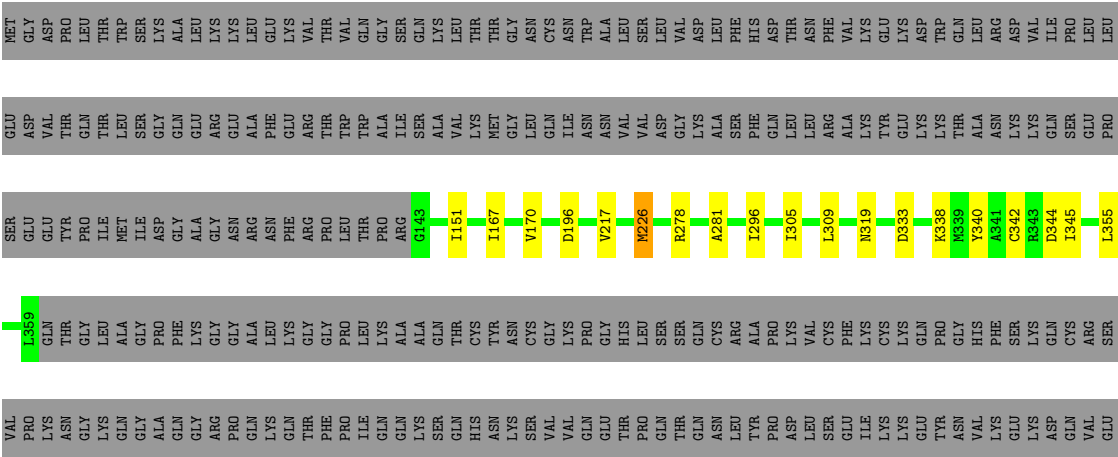
• Molecule 1: Gag polyprotein

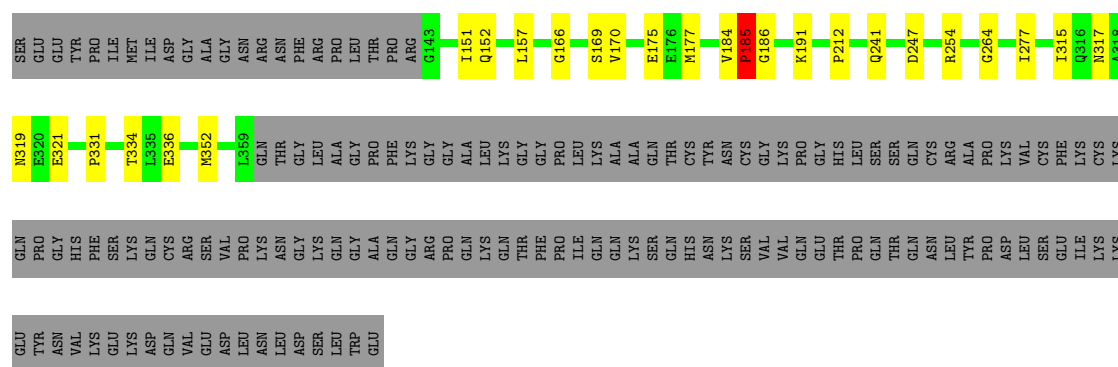
Chain H: 41% 55%



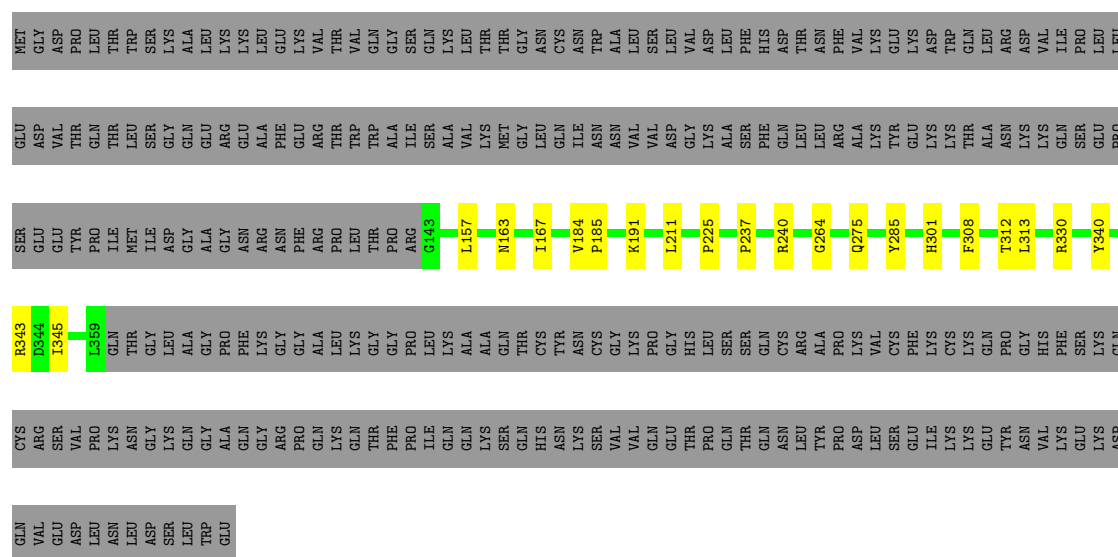
• Molecule 1: Gag polyprotein

Chain I: 41% 55%

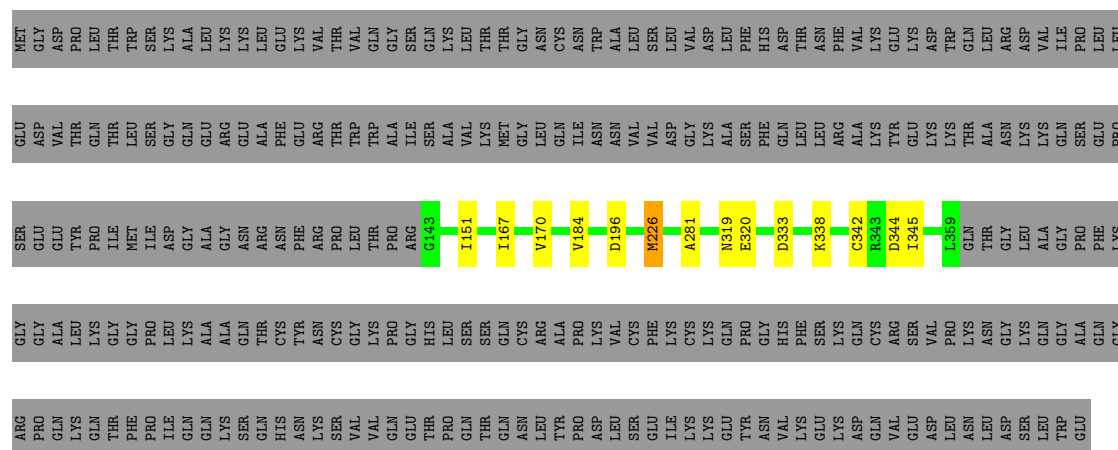




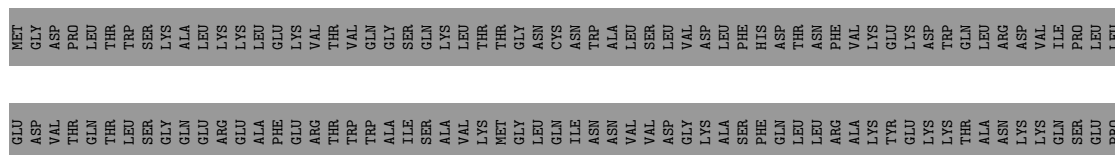
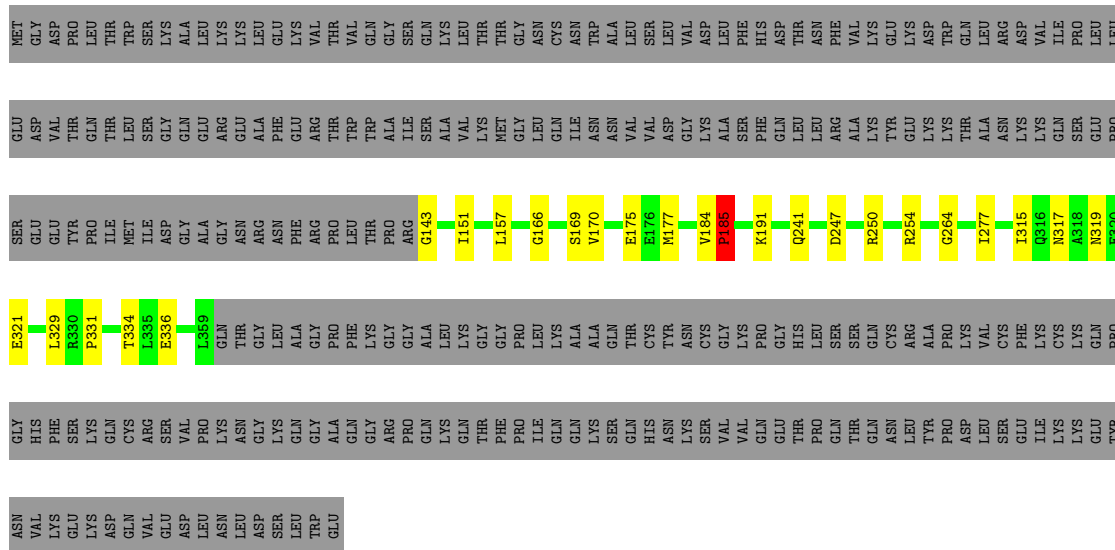
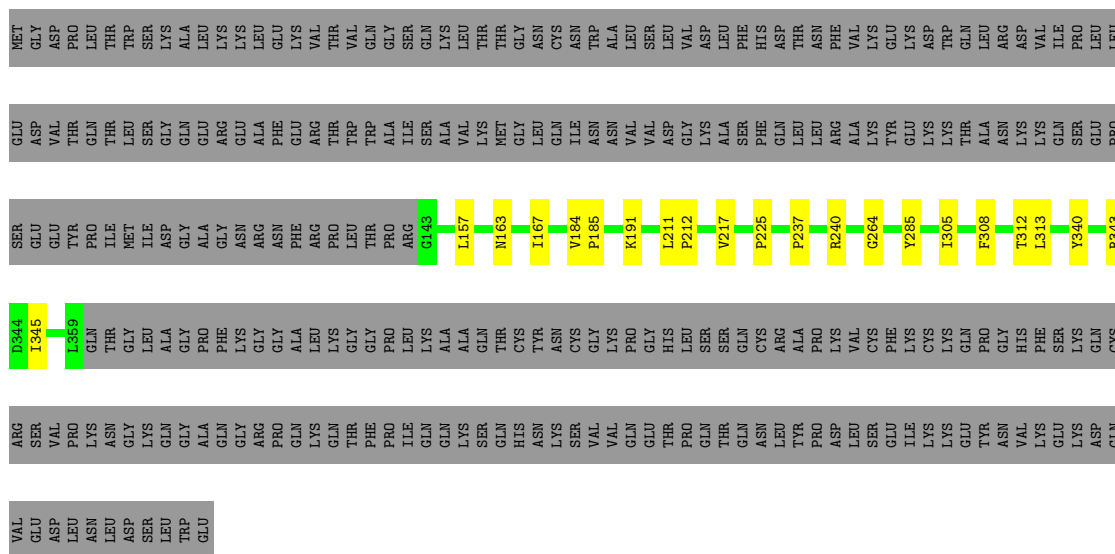
- Molecule 1: Gag polyprotein



- Molecule 1: Gag polyprotein



- Molecule 1: Gag polypprotein





ASN VAL LYS GLU LYS ASP GLN VAL GLU ASP LEU ASN LEU ASP SER LEU TRP GLU

- Molecule 1: Gag polyprotein

Chain P:  41% 1% 55%

MET	GLY	ASP	GLY	ASP	PRO	LEU	THR	TRP	SER	LYS	ALA	ALA	LEU	LYS	LYS	GLU	LEU	LEU	LYS	VAL	THR	VAL	GLN	GLY	SER	SER	GLN	LYS	LYS	GLY	GLY	ASN	CYS	ASN	TRP	TRP	LEU	LEU	LEU	SER	LEU	VAL	VAL	ASN	THR	HIS	PHE	PHE	VAL	VAL	LYS	LYS	ASP	ASP	GLU	LEU	GLN	TRP	TRP	TRP	THR	ASP	ARG	LEU	LEU	VAL	ASP	VAL	ILE	PRO	PRO	LEU	LEU
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[illegible][illegible]

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

4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	112929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF-correction was performed using NOVACTF	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	3.4	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.31	0/1755	0.52	0/2375
1	B	0.31	0/1755	0.51	0/2375
1	C	0.30	0/1755	0.53	1/2375 (0.0%)
1	D	0.31	0/1755	0.52	0/2375
1	E	0.31	0/1755	0.52	0/2375
1	F	0.31	0/1755	0.51	0/2375
1	G	0.31	0/1755	0.51	0/2375
1	H	0.31	0/1755	0.53	1/2375 (0.0%)
1	I	0.30	0/1755	0.53	1/2375 (0.0%)
1	J	0.31	0/1755	0.52	0/2375
1	K	0.31	0/1755	0.51	0/2375
1	L	0.30	0/1755	0.53	1/2375 (0.0%)
1	M	0.31	0/1755	0.52	0/2375
1	N	0.31	0/1755	0.52	0/2375
1	O	0.31	0/1755	0.51	0/2375
1	P	0.31	0/1755	0.51	0/2375
1	Q	0.30	0/1755	0.53	1/2375 (0.0%)
1	R	0.30	0/1755	0.53	1/2375 (0.0%)
All	All	0.31	0/31590	0.52	6/42750 (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	1
1	D	0	1
1	E	0	1
1	J	0	1
1	M	0	1
1	N	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	196	ASP	CB-CG-OD2	6.26	123.93	118.30
1	R	196	ASP	CB-CG-OD2	6.24	123.92	118.30
1	I	196	ASP	CB-CG-OD2	6.23	123.91	118.30
1	L	196	ASP	CB-CG-OD2	6.18	123.86	118.30
1	C	196	ASP	CB-CG-OD2	6.18	123.86	118.30
1	Q	196	ASP	CB-CG-OD2	6.15	123.83	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	PRO	Peptide
1	D	185	PRO	Peptide
1	E	185	PRO	Peptide
1	J	185	PRO	Peptide
1	M	185	PRO	Peptide
1	N	185	PRO	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	1721	0	1718	35	0
1	B	1721	0	1716	18	0
1	C	1721	0	1717	11	0
1	D	1721	0	1718	18	0
1	E	1721	0	1718	31	0
1	F	1721	0	1718	17	0
1	G	1721	0	1718	12	0
1	H	1721	0	1716	14	0
1	I	1721	0	1718	20	0
1	J	1721	0	1718	35	0
1	K	1721	0	1716	18	0
1	L	1721	0	1717	12	0
1	M	1721	0	1718	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1721	0	1718	31	0
1	O	1721	0	1718	17	0
1	P	1721	0	1718	13	0
1	Q	1721	0	1716	16	0
1	R	1721	0	1718	21	0
All	All	30978	0	30914	255	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 (255) 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:A:170:VAL:HG11	1:C:170:VAL:HG13	1.31	1.11
1:K:330:ARG:NH1	1:R:340:TYR:CD1	1.91	1.10
1:J:170:VAL:HG11	1:L:170:VAL:HG13	1.30	1.04
1:B:330:ARG:NH1	1:I:340:TYR:CD1	1.91	1.03
1:I:170:VAL:HG13	1:E:170:VAL:HG11	1.44	0.98
1:R:170:VAL:HG13	1:N:170:VAL:HG11	1.44	0.96
1:D:170:VAL:HG11	1:H:170:VAL:HG13	1.51	0.91
1:M:170:VAL:HG11	1:Q:170:VAL:HG13	1.51	0.90
1:B:330:ARG:HH12	1:I:340:TYR:HD1	1.19	0.85
1:K:330:ARG:HH12	1:R:340:TYR:HD1	1.19	0.83
1:A:186:GLY:CA	1:N:152:GLN:HE22	1.96	0.78
1:J:170:VAL:HG11	1:L:170:VAL:CG1	2.12	0.78
1:E:152:GLN:HE22	1:J:186:GLY:CA	1.96	0.78
1:A:152:GLN:HE22	1:N:186:GLY:CA	1.98	0.76
1:E:186:GLY:CA	1:J:152:GLN:HE22	1.98	0.76
1:K:312:THR:HG21	1:O:312:THR:HG21	1.68	0.75
1:A:170:VAL:HG11	1:C:170:VAL:CG1	2.13	0.75
1:B:312:THR:HG21	1:F:312:THR:HG21	1.68	0.75
1:A:186:GLY:HA2	1:N:152:GLN:HE22	1.51	0.75
1:E:152:GLN:HE22	1:J:186:GLY:HA2	1.51	0.73
1:E:254:ARG:NH2	1:G:167:ILE:O	2.21	0.72
1:N:254:ARG:NH2	1:P:167:ILE:O	2.21	0.72
1:N:166:GLY:HA3	1:P:167:ILE:HD12	1.71	0.72
1:K:330:ARG:NH1	1:R:340:TYR:CE1	2.58	0.72
1:E:186:GLY:HA2	1:J:152:GLN:HE22	1.55	0.71
1:B:330:ARG:NH1	1:I:340:TYR:CE1	2.58	0.71
1:E:166:GLY:HA3	1:G:167:ILE:HD12	1.71	0.70
1:A:152:GLN:HE22	1:N:186:GLY:HA2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLY:CA	1:N:152:GLN:NE2	2.55	0.69
1:E:152:GLN:NE2	1:J:186:GLY:CA	2.55	0.69
1:F:167:ILE:O	1:D:254:ARG:NH2	2.25	0.68
1:E:152:GLN:NE2	1:J:186:GLY:HA2	2.08	0.68
1:A:186:GLY:HA2	1:N:152:GLN:NE2	2.08	0.68
1:A:152:GLN:NE2	1:N:186:GLY:CA	2.58	0.67
1:E:186:GLY:CA	1:J:152:GLN:NE2	2.58	0.67
1:O:167:ILE:HD12	1:M:166:GLY:HA3	1.76	0.66
1:R:170:VAL:CG1	1:N:170:VAL:HG11	2.24	0.66
1:I:355:LEU:HD13	1:J:352:MET:CE	2.26	0.66
1:F:167:ILE:HD12	1:D:166:GLY:HA3	1.77	0.66
1:J:170:VAL:CG1	1:L:170:VAL:HG13	2.20	0.66
1:M:170:VAL:CG1	1:Q:170:VAL:HG13	2.26	0.65
1:A:352:MET:CE	1:R:355:LEU:HD13	2.26	0.65
1:J:166:GLY:HA3	1:K:167:ILE:HD12	1.79	0.65
1:E:186:GLY:HA2	1:J:152:GLN:NE2	2.13	0.63
1:A:152:GLN:NE2	1:N:186:GLY:HA2	2.13	0.63
1:A:166:GLY:HA3	1:B:167:ILE:HD12	1.79	0.63
1:A:254:ARG:NH2	1:B:167:ILE:O	2.30	0.63
1:B:308:PHE:CZ	1:F:313:LEU:HD21	2.34	0.63
1:K:308:PHE:CZ	1:O:313:LEU:HD21	2.34	0.62
1:J:254:ARG:NH2	1:K:167:ILE:O	2.30	0.61
1:I:170:VAL:CG1	1:E:170:VAL:HG11	2.24	0.61
1:H:352:MET:HB3	1:G:358:ALA:HB2	1.82	0.61
1:I:278:ARG:NH2	1:J:336:GLU:OE2	2.31	0.61
1:D:170:VAL:CG1	1:H:170:VAL:HG13	2.26	0.61
1:O:167:ILE:O	1:M:254:ARG:NH2	2.25	0.60
1:Q:352:MET:HB3	1:P:358:ALA:HB2	1.82	0.59
1:A:336:GLU:OE2	1:R:278:ARG:NH2	2.31	0.58
1:I:170:VAL:HG13	1:E:170:VAL:CG1	2.28	0.58
1:R:170:VAL:HG13	1:N:170:VAL:CG1	2.28	0.57
1:O:340:TYR:O	1:O:343:ARG:NH1	2.38	0.57
1:P:340:TYR:O	1:P:343:ARG:NH1	2.38	0.56
1:A:170:VAL:CG1	1:C:170:VAL:HG13	2.20	0.56
1:K:340:TYR:O	1:K:343:ARG:NH1	2.38	0.56
1:F:340:TYR:O	1:F:343:ARG:NH1	2.38	0.56
1:G:340:TYR:O	1:G:343:ARG:NH1	2.38	0.56
1:E:152:GLN:HE22	1:J:186:GLY:HA3	1.71	0.56
1:B:340:TYR:O	1:B:343:ARG:NH1	2.38	0.55
1:A:152:GLN:HE22	1:N:186:GLY:HA3	1.71	0.55
1:L:344:ASP:N	1:L:344:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:ASP:N	1:H:344:ASP:OD1	2.40	0.54
1:Q:344:ASP:OD1	1:Q:344:ASP:N	2.40	0.54
1:C:344:ASP:OD1	1:C:344:ASP:N	2.40	0.54
1:K:313:LEU:HD21	1:O:308:PHE:CZ	2.43	0.54
1:B:313:LEU:HD21	1:F:308:PHE:CZ	2.43	0.53
1:E:186:GLY:HA3	1:J:152:GLN:HE22	1.71	0.53
1:M:170:VAL:HG11	1:Q:170:VAL:CG1	2.32	0.53
1:R:344:ASP:N	1:R:344:ASP:OD1	2.41	0.53
1:A:186:GLY:HA3	1:N:152:GLN:HE22	1.71	0.53
1:D:170:VAL:HG11	1:H:170:VAL:CG1	2.32	0.53
1:I:344:ASP:OD1	1:I:344:ASP:N	2.40	0.52
1:I:226:MET:SD	1:I:226:MET:N	2.83	0.51
1:L:226:MET:SD	1:L:226:MET:N	2.83	0.51
1:K:285:TYR:HB2	1:K:345:ILE:HD11	1.93	0.51
1:F:285:TYR:HB2	1:F:345:ILE:HD11	1.93	0.51
1:H:226:MET:N	1:H:226:MET:SD	2.83	0.51
1:P:285:TYR:HB2	1:P:345:ILE:HD11	1.93	0.51
1:Q:226:MET:SD	1:Q:226:MET:N	2.83	0.51
1:E:185:PRO:HB3	1:J:185:PRO:O	2.11	0.51
1:A:185:PRO:HB3	1:N:185:PRO:O	2.12	0.50
1:O:285:TYR:HB2	1:O:345:ILE:HD11	1.93	0.50
1:B:285:TYR:HB2	1:B:345:ILE:HD11	1.93	0.50
1:E:185:PRO:O	1:J:185:PRO:HB3	2.12	0.50
1:H:333:ASP:O	1:H:338:LYS:NZ	2.45	0.50
1:C:333:ASP:O	1:C:338:LYS:NZ	2.45	0.50
1:A:185:PRO:O	1:N:185:PRO:HB3	2.11	0.50
1:M:143:GLY:HA2	1:Q:259:GLU:OE2	2.12	0.50
1:C:226:MET:N	1:C:226:MET:SD	2.83	0.50
1:R:226:MET:N	1:R:226:MET:SD	2.83	0.50
1:R:333:ASP:O	1:R:338:LYS:NZ	2.45	0.49
1:G:285:TYR:HB2	1:G:345:ILE:HD11	1.93	0.49
1:L:333:ASP:O	1:L:338:LYS:NZ	2.45	0.49
1:D:334:THR:HG22	1:D:336:GLU:H	1.78	0.49
1:I:333:ASP:O	1:I:338:LYS:NZ	2.45	0.49
1:K:301:HIS:CE1	1:O:305:ILE:HD11	2.47	0.49
1:Q:333:ASP:O	1:Q:338:LYS:NZ	2.45	0.49
1:D:143:GLY:HA2	1:H:259:GLU:OE2	2.12	0.49
1:N:334:THR:HG22	1:N:336:GLU:H	1.78	0.49
1:J:334:THR:HG22	1:J:336:GLU:H	1.78	0.49
1:I:342:CYS:HB2	1:I:345:ILE:HD11	1.95	0.49
1:M:334:THR:HG22	1:M:336:GLU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:342:CYS:HB2	1:Q:345:ILE:HD11	1.95	0.48
1:E:334:THR:HG22	1:E:336:GLU:H	1.78	0.48
1:B:301:HIS:CE1	1:F:305:ILE:HD11	2.47	0.48
1:N:169:SER:OG	1:N:177:MET:SD	2.72	0.48
1:C:342:CYS:HB2	1:C:345:ILE:HD11	1.95	0.48
1:M:169:SER:OG	1:M:177:MET:SD	2.72	0.48
1:A:334:THR:HG22	1:A:336:GLU:H	1.78	0.48
1:J:169:SER:OG	1:J:177:MET:SD	2.71	0.48
1:P:184:VAL:HB	1:P:191:LYS:HE2	1.96	0.48
1:Q:281:ALA:HA	1:Q:319:ASN:HD21	1.79	0.48
1:R:342:CYS:HB2	1:R:345:ILE:HD11	1.95	0.48
1:D:247:ASP:N	1:D:247:ASP:OD2	2.47	0.48
1:O:184:VAL:HB	1:O:191:LYS:HE2	1.96	0.48
1:G:184:VAL:HB	1:G:191:LYS:HE2	1.96	0.48
1:M:247:ASP:OD2	1:M:247:ASP:N	2.47	0.48
1:J:247:ASP:OD2	1:J:247:ASP:N	2.47	0.48
1:R:281:ALA:HA	1:R:319:ASN:HD21	1.79	0.48
1:B:184:VAL:HB	1:B:191:LYS:HE2	1.96	0.47
1:C:281:ALA:HA	1:C:319:ASN:HD21	1.79	0.47
1:E:169:SER:OG	1:E:177:MET:SD	2.72	0.47
1:N:247:ASP:N	1:N:247:ASP:OD2	2.47	0.47
1:K:184:VAL:HB	1:K:191:LYS:HE2	1.96	0.47
1:A:352:MET:HE3	1:R:355:LEU:HD13	1.96	0.47
1:I:355:LEU:HD13	1:J:352:MET:HE3	1.96	0.47
1:I:281:ALA:HA	1:I:319:ASN:HD21	1.79	0.47
1:A:169:SER:OG	1:A:177:MET:SD	2.72	0.47
1:F:184:VAL:HB	1:F:191:LYS:HE2	1.96	0.47
1:H:342:CYS:HB2	1:H:345:ILE:HD11	1.95	0.47
1:L:281:ALA:HA	1:L:319:ASN:HD21	1.79	0.47
1:N:166:GLY:CA	1:P:167:ILE:HD12	2.44	0.47
1:A:151:ILE:HG21	1:A:185:PRO:HD2	1.97	0.47
1:D:169:SER:OG	1:D:177:MET:SD	2.72	0.47
1:E:175:GLU:HG2	1:E:241:GLN:HE22	1.80	0.47
1:L:342:CYS:HB2	1:L:345:ILE:HD11	1.95	0.47
1:M:175:GLU:HG2	1:M:241:GLN:HE22	1.80	0.47
1:N:250:ARG:HE	1:N:250:ARG:HB2	1.58	0.47
1:O:237:PRO:HG2	1:O:240:ARG:HB2	1.97	0.47
1:A:247:ASP:OD2	1:A:247:ASP:N	2.47	0.46
1:P:237:PRO:HG2	1:P:240:ARG:HB2	1.97	0.46
1:F:237:PRO:HG2	1:F:240:ARG:HB2	1.97	0.46
1:J:151:ILE:HG21	1:J:185:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:PRO:HG2	1:G:240:ARG:HB2	1.97	0.46
1:E:247:ASP:OD2	1:E:247:ASP:N	2.47	0.46
1:H:281:ALA:HA	1:H:319:ASN:HD21	1.79	0.46
1:B:275:GLN:OE1	1:F:308:PHE:CD1	2.69	0.46
1:D:175:GLU:HG2	1:D:241:GLN:HE22	1.80	0.46
1:J:170:VAL:CG1	1:L:170:VAL:CG1	2.90	0.46
1:A:175:GLU:HG2	1:A:241:GLN:HE22	1.80	0.46
1:E:319:ASN:ND2	1:E:321:GLU:OE1	2.49	0.46
1:J:319:ASN:ND2	1:J:321:GLU:OE1	2.49	0.46
1:K:237:PRO:HG2	1:K:240:ARG:HB2	1.97	0.46
1:M:151:ILE:HG21	1:M:185:PRO:HD2	1.97	0.46
1:N:175:GLU:HG2	1:N:241:GLN:HE22	1.80	0.46
1:D:319:ASN:ND2	1:D:321:GLU:OE1	2.49	0.46
1:B:237:PRO:HG2	1:B:240:ARG:HB2	1.97	0.45
1:D:151:ILE:HG21	1:D:185:PRO:HD2	1.97	0.45
1:O:212:PRO:HD3	1:R:217:VAL:HG21	1.98	0.45
1:E:166:GLY:CA	1:G:167:ILE:HD12	2.44	0.45
1:M:319:ASN:ND2	1:M:321:GLU:OE1	2.49	0.45
1:J:175:GLU:HG2	1:J:241:GLN:HE22	1.80	0.45
1:H:217:VAL:HG22	1:G:210:PRO:HG2	1.99	0.45
1:N:151:ILE:HG21	1:N:185:PRO:HD2	1.97	0.45
1:A:319:ASN:ND2	1:A:321:GLU:OE1	2.49	0.45
1:K:275:GLN:OE1	1:O:308:PHE:CD1	2.69	0.45
1:E:151:ILE:HG21	1:E:185:PRO:HD2	1.97	0.45
1:M:143:GLY:CA	1:Q:255:GLN:CG	2.91	0.45
1:N:319:ASN:ND2	1:N:321:GLU:OE1	2.49	0.45
1:F:167:ILE:HD12	1:D:166:GLY:CA	2.47	0.45
1:Q:217:VAL:HG22	1:P:210:PRO:HG2	1.98	0.45
1:D:277:ILE:O	1:D:317:ASN:ND2	2.50	0.44
1:E:329:LEU:HA	1:E:329:LEU:HD12	1.87	0.44
1:J:277:ILE:O	1:J:317:ASN:ND2	2.50	0.44
1:M:277:ILE:O	1:M:317:ASN:ND2	2.50	0.44
1:N:277:ILE:O	1:N:317:ASN:ND2	2.50	0.44
1:A:170:VAL:CG1	1:C:170:VAL:CG1	2.90	0.44
1:E:277:ILE:O	1:E:317:ASN:ND2	2.50	0.44
1:F:212:PRO:HD3	1:I:217:VAL:HG21	1.98	0.44
1:A:277:ILE:O	1:A:317:ASN:ND2	2.50	0.44
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.87	0.44
1:H:305:ILE:HD12	1:I:309:LEU:HD11	2.00	0.44
1:A:315:ILE:HG21	1:A:331:PRO:HB3	2.00	0.43
1:N:315:ILE:HG21	1:N:331:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:HA	1:C:167:ILE:HD11	2.00	0.43
1:J:184:VAL:HG11	1:J:191:LYS:HB3	2.01	0.43
1:M:184:VAL:HG11	1:M:191:LYS:HB3	2.01	0.43
1:Q:305:ILE:HD12	1:R:309:LEU:HD11	2.00	0.43
1:D:184:VAL:HG11	1:D:191:LYS:HB3	2.01	0.43
1:N:184:VAL:HG11	1:N:191:LYS:HB3	2.01	0.43
1:C:320:GLU:HG3	1:C:320:GLU:H	1.66	0.43
1:E:315:ILE:HG21	1:E:331:PRO:HB3	2.00	0.43
1:F:211:LEU:HD13	1:F:225:PRO:HB2	2.01	0.42
1:J:315:ILE:HG21	1:J:331:PRO:HB3	2.00	0.42
1:K:211:LEU:HD13	1:K:225:PRO:HB2	2.01	0.42
1:M:191:LYS:HE3	1:M:191:LYS:HB2	1.93	0.42
1:D:157:LEU:HD22	1:D:264:GLY:HA3	2.02	0.42
1:D:315:ILE:HG21	1:D:331:PRO:HB3	2.00	0.42
1:A:212:PRO:HD3	1:F:217:VAL:HG21	2.02	0.42
1:I:296:ILE:HD13	1:I:296:ILE:HA	1.94	0.42
1:K:163:ASN:HA	1:L:167:ILE:HD11	2.00	0.42
1:N:157:LEU:HD22	1:N:264:GLY:HA3	2.02	0.42
1:R:167:ILE:HD11	1:P:163:ASN:HA	2.02	0.42
1:L:320:GLU:H	1:L:320:GLU:HG3	1.66	0.42
1:E:157:LEU:HD22	1:E:264:GLY:HA3	2.02	0.42
1:E:184:VAL:HG11	1:E:191:LYS:HB3	2.01	0.42
1:O:167:ILE:HD12	1:M:166:GLY:CA	2.47	0.42
1:M:315:ILE:HG21	1:M:331:PRO:HB3	2.00	0.42
1:A:184:VAL:HG11	1:A:191:LYS:HB3	2.01	0.41
1:A:185:PRO:HB3	1:N:185:PRO:C	2.41	0.41
1:G:163:ASN:O	1:G:167:ILE:HG12	2.20	0.41
1:G:211:LEU:HD13	1:G:225:PRO:HB2	2.01	0.41
1:I:151:ILE:HA	1:I:151:ILE:HD13	1.87	0.41
1:O:163:ASN:O	1:O:167:ILE:HG12	2.20	0.41
1:R:320:GLU:HG3	1:R:320:GLU:H	1.66	0.41
1:R:296:ILE:HA	1:R:296:ILE:HD13	1.94	0.41
1:J:157:LEU:HD22	1:J:264:GLY:HA3	2.02	0.41
1:B:211:LEU:HD13	1:B:225:PRO:HB2	2.02	0.41
1:E:185:PRO:C	1:J:185:PRO:HB3	2.41	0.41
1:B:163:ASN:O	1:B:167:ILE:HG12	2.20	0.41
1:F:157:LEU:HD22	1:F:264:GLY:HA3	2.03	0.41
1:E:185:PRO:HB3	1:J:185:PRO:C	2.41	0.41
1:O:211:LEU:HD13	1:O:225:PRO:HB2	2.01	0.41
1:J:212:PRO:HD3	1:O:217:VAL:HG21	2.02	0.41
1:Q:320:GLU:HG3	1:Q:320:GLU:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD22	1:B:264:GLY:HA3	2.03	0.41
1:I:167:ILE:HD11	1:G:163:ASN:HA	2.02	0.41
1:M:329:LEU:HD12	1:M:329:LEU:HA	1.87	0.41
1:P:157:LEU:HD22	1:P:264:GLY:HA3	2.03	0.41
1:Q:151:ILE:HA	1:Q:151:ILE:HD13	1.88	0.41
1:A:157:LEU:HD22	1:A:264:GLY:HA3	2.02	0.41
1:M:250:ARG:HE	1:M:250:ARG:HB2	1.58	0.41
1:O:157:LEU:HD22	1:O:264:GLY:HA3	2.03	0.41
1:P:211:LEU:HD13	1:P:225:PRO:HB2	2.01	0.41
1:K:163:ASN:O	1:K:167:ILE:HG12	2.20	0.41
1:M:157:LEU:HD22	1:M:264:GLY:HA3	2.02	0.41
1:P:163:ASN:O	1:P:167:ILE:HG12	2.20	0.41
1:J:191:LYS:HB2	1:J:191:LYS:HE3	1.93	0.40
1:K:157:LEU:HD22	1:K:264:GLY:HA3	2.03	0.40
1:H:151:ILE:HG21	1:H:184:VAL:HG23	2.04	0.40
1:L:151:ILE:HG21	1:L:184:VAL:HG23	2.04	0.40
1:R:151:ILE:HA	1:R:151:ILE:HD13	1.88	0.40
1:A:185:PRO:C	1:N:185:PRO:HB3	2.41	0.40
1:D:191:LYS:HE3	1:D:191:LYS:HB2	1.93	0.40
1:F:163:ASN:O	1:F:167:ILE:HG12	2.20	0.40
1:H:309:LEU:HD11	1:I:305:ILE:HD12	2.04	0.40
1:Q:309:LEU:HD11	1:R:305:ILE:HD12	2.04	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	215/486 (44%)	199 (93%)	15 (7%)	1 (0%)	31	71
1	B	215/486 (44%)	201 (94%)	13 (6%)	1 (0%)	31	71
1	C	215/486 (44%)	197 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	215/486 (44%)	199 (93%)	15 (7%)	1 (0%)	31	71
1	E	215/486 (44%)	200 (93%)	14 (6%)	1 (0%)	31	71
1	F	215/486 (44%)	201 (94%)	13 (6%)	1 (0%)	31	71
1	G	215/486 (44%)	201 (94%)	13 (6%)	1 (0%)	31	71
1	H	215/486 (44%)	197 (92%)	18 (8%)	0	100	100
1	I	215/486 (44%)	197 (92%)	18 (8%)	0	100	100
1	J	215/486 (44%)	199 (93%)	15 (7%)	1 (0%)	31	71
1	K	215/486 (44%)	201 (94%)	13 (6%)	1 (0%)	31	71
1	L	215/486 (44%)	197 (92%)	18 (8%)	0	100	100
1	M	215/486 (44%)	200 (93%)	14 (6%)	1 (0%)	31	71
1	N	215/486 (44%)	200 (93%)	14 (6%)	1 (0%)	31	71
1	O	215/486 (44%)	201 (94%)	13 (6%)	1 (0%)	31	71
1	P	215/486 (44%)	201 (94%)	13 (6%)	1 (0%)	31	71
1	Q	215/486 (44%)	197 (92%)	18 (8%)	0	100	100
1	R	215/486 (44%)	197 (92%)	18 (8%)	0	100	100
All	All	3870/8748 (44%)	3585 (93%)	273 (7%)	12 (0%)	47	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	PRO
1	D	185	PRO
1	E	185	PRO
1	J	185	PRO
1	M	185	PRO
1	N	185	PRO
1	B	185	PRO
1	F	185	PRO
1	G	185	PRO
1	K	185	PRO
1	O	185	PRO
1	P	185	PRO

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	187/421 (44%)	187 (100%)	0	100	100
1	B	187/421 (44%)	187 (100%)	0	100	100
1	C	187/421 (44%)	186 (100%)	1 (0%)	90	96
1	D	187/421 (44%)	187 (100%)	0	100	100
1	E	187/421 (44%)	187 (100%)	0	100	100
1	F	187/421 (44%)	187 (100%)	0	100	100
1	G	187/421 (44%)	187 (100%)	0	100	100
1	H	187/421 (44%)	186 (100%)	1 (0%)	90	96
1	I	187/421 (44%)	186 (100%)	1 (0%)	90	96
1	J	187/421 (44%)	187 (100%)	0	100	100
1	K	187/421 (44%)	187 (100%)	0	100	100
1	L	187/421 (44%)	186 (100%)	1 (0%)	90	96
1	M	187/421 (44%)	187 (100%)	0	100	100
1	N	187/421 (44%)	187 (100%)	0	100	100
1	O	187/421 (44%)	187 (100%)	0	100	100
1	P	187/421 (44%)	187 (100%)	0	100	100
1	Q	187/421 (44%)	186 (100%)	1 (0%)	90	96
1	R	187/421 (44%)	186 (100%)	1 (0%)	90	96
All	All	3366/7578 (44%)	3360 (100%)	6 (0%)	94	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	226	MET
1	H	226	MET
1	I	226	MET
1	L	226	MET
1	Q	226	MET
1	R	226	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	163	ASN
1	A	241	GLN
1	B	154	ASN
1	B	158	ASN
1	B	178	ASN
1	B	190	GLN
1	B	279	GLN
1	B	301	HIS
1	C	154	ASN
1	C	207	ASN
1	C	248	GLN
1	C	279	GLN
1	F	154	ASN
1	F	158	ASN
1	F	178	ASN
1	F	190	GLN
1	F	279	GLN
1	D	163	ASN
1	D	241	GLN
1	H	154	ASN
1	H	207	ASN
1	H	248	GLN
1	H	279	GLN
1	I	154	ASN
1	I	207	ASN
1	I	248	GLN
1	I	255	GLN
1	I	279	GLN
1	E	152	GLN
1	E	163	ASN
1	E	241	GLN
1	G	154	ASN
1	G	158	ASN
1	G	178	ASN
1	G	190	GLN
1	G	279	GLN
1	J	152	GLN
1	J	163	ASN
1	J	241	GLN
1	K	154	ASN

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Mol	Chain	Res	Type
1	K	158	ASN
1	K	178	ASN
1	K	190	GLN
1	K	279	GLN
1	K	301	HIS
1	L	154	ASN
1	L	207	ASN
1	L	241	GLN
1	L	248	GLN
1	L	279	GLN
1	O	154	ASN
1	O	158	ASN
1	O	178	ASN
1	O	190	GLN
1	O	279	GLN
1	M	163	ASN
1	M	241	GLN
1	Q	154	ASN
1	Q	207	ASN
1	Q	248	GLN
1	Q	279	GLN
1	R	154	ASN
1	R	207	ASN
1	R	241	GLN
1	R	248	GLN
1	R	255	GLN
1	R	279	GLN
1	N	152	GLN
1	N	163	ASN
1	N	241	GLN
1	P	154	ASN
1	P	158	ASN
1	P	178	ASN
1	P	190	GLN
1	P	279	GLN

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.