



## wwPDB EM Map/Model Validation Report ⓘ

May 17, 2016 – 05:28 PM EDT

PDB ID : 5GAS  
EMDB ID: : EMD-8017  
Title : Thermus thermophilus V/A-ATPase, conformation 2  
Authors : Schep, D.G.; Zhao, J.; Rubinstein, J.L.  
Deposited on : 2016-02-05  
Resolution : 9.50 Å(reported)  
Based on PDB ID : ?

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

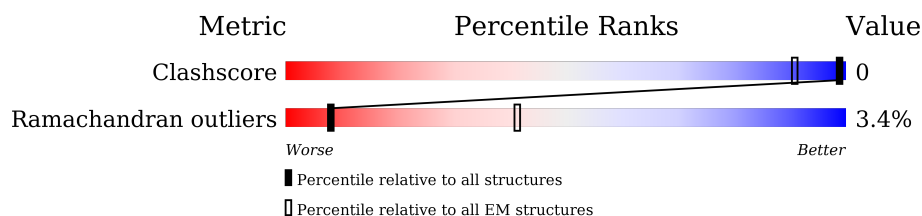
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.50 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	114402	924
Ramachandran outliers	111179	726

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	577	92% 8%
1	B	577	93% 7%
1	C	577	92% 8%
2	D	457	93% 7%
2	E	457	95% 5%
2	F	457	92% 8%
3	G	186	92% 6% ..
3	H	186	93% 5% ..
4	I	105	92% . 5%
4	J	105	93% . 5%
5	K	210	92% 7%

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Mol	Chain	Length	Quality of chain
6	L	100	 93% 7%
7	M	323	 97% ..
8	N	652	 91% • 5%
9	O	99	 81% 19%
9	P	99	 74% 7% 19%
9	Q	99	 81% 19%
9	R	99	 78% • 19%
9	S	99	 80% • 19%
9	T	99	 78% • 19%
9	U	99	 80% • 19%
9	V	99	 78% • 19%
9	W	99	 76% 5% 19%
9	X	99	 79% • 19%
9	Y	99	 79% • 19%
9	Z	99	 79% • 19%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23487 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	B	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	C	577	Total	C	N	O	0	0
			2307	1154	577	576		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	457	Total	C	N	O	0	0
			1827	914	457	456		
2	E	457	Total	C	N	O	0	0
			1827	914	457	456		
2	F	457	Total	C	N	O	0	0
			1827	914	457	456		

- Molecule 3 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	184	Total	C	N	O	0	0
			734	368	184	182		
3	H	184	Total	C	N	O	0	0
			734	368	184	182		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	134	MET	LEU	conflict	UNP P74901
G	171	MET	LEU	conflict	UNP P74901
G	178	MET	LEU	conflict	UNP P74901
H	134	MET	LEU	conflict	UNP P74901
H	171	MET	LEU	conflict	UNP P74901

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Chain	Residue	Modelled	Actual	Comment	Reference
H	178	MET	LEU	conflict	UNP P74901

- Molecule 4 is a protein called V-type ATPase subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	100	Total	C	N	O	0	0
			399	200	100	99		
4	J	100	Total	C	N	O	0	0
			399	200	100	99		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	16	GLY	-	insertion	UNP Q72J66
J	16	GLY	-	insertion	UNP Q72J66

- Molecule 5 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	210	Total	C	N	O	0	0
			839	420	210	209		

- Molecule 6 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	320	Total	C	N	O	0	0
			1279	640	320	319		

- Molecule 8 is a protein called Archaeal/vacuolar-type H<sup>+</sup>-ATPase subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	619	Total	C	N	O	0	0
			2474	1238	619	617		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	154	ARG	LYS	conflict	UNP H9ZQR4
N	164	ALA	VAL	conflict	UNP H9ZQR4
N	173	PRO	ALA	conflict	UNP H9ZQR4

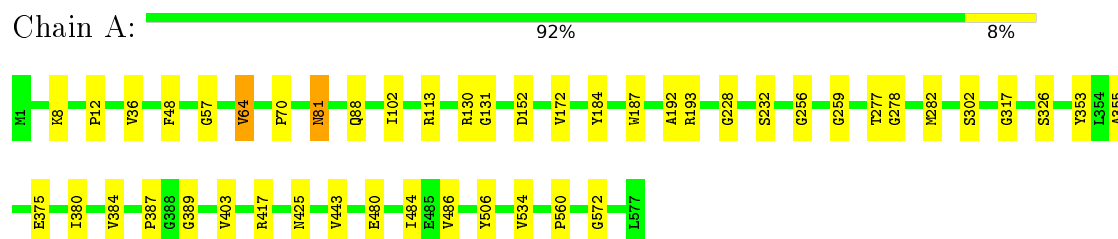
- Molecule 9 is a protein called Vacuolar type ATP synthase subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	80	Total 319	C 160	N 80	O 79	0	0
9	P	80	Total 319	C 160	N 80	O 79	0	0
9	Q	80	Total 319	C 160	N 80	O 79	0	0
9	R	80	Total 319	C 160	N 80	O 79	0	0
9	S	80	Total 319	C 160	N 80	O 79	0	0
9	T	80	Total 319	C 160	N 80	O 79	0	0
9	U	80	Total 319	C 160	N 80	O 79	0	0
9	V	80	Total 319	C 160	N 80	O 79	0	0
9	W	80	Total 319	C 160	N 80	O 79	0	0
9	X	80	Total 319	C 160	N 80	O 79	0	0
9	Y	80	Total 319	C 160	N 80	O 79	0	0
9	Z	80	Total 319	C 160	N 80	O 79	0	0

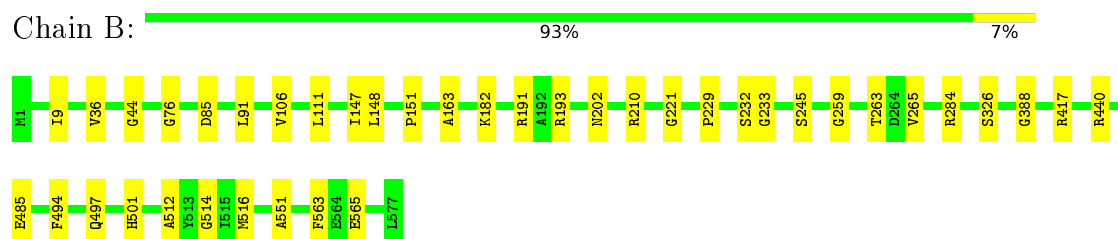
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

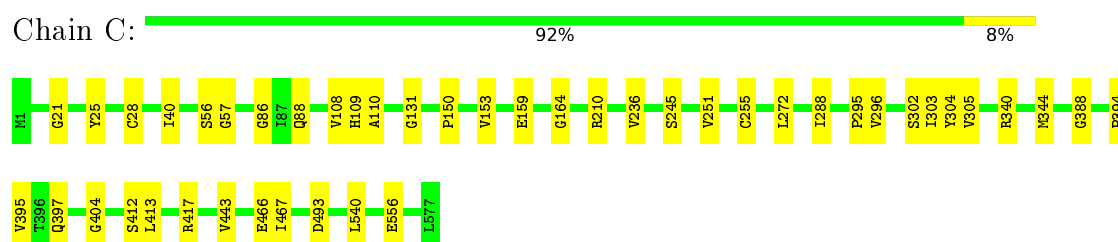
- Molecule 1: V-type ATP synthase alpha chain



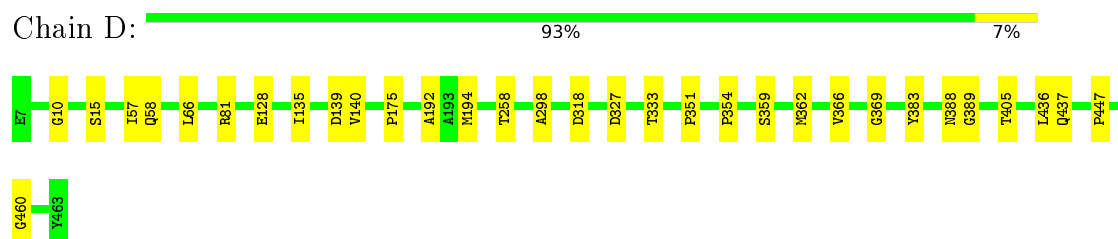
- Molecule 1: V-type ATP synthase alpha chain



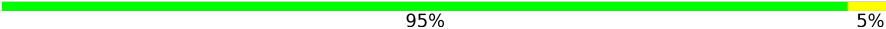
- Molecule 1: V-type ATP synthase alpha chain

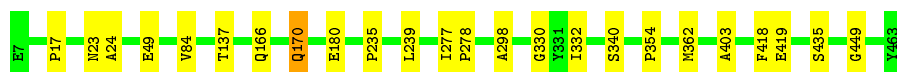


- Molecule 2: V-type ATP synthase beta chain



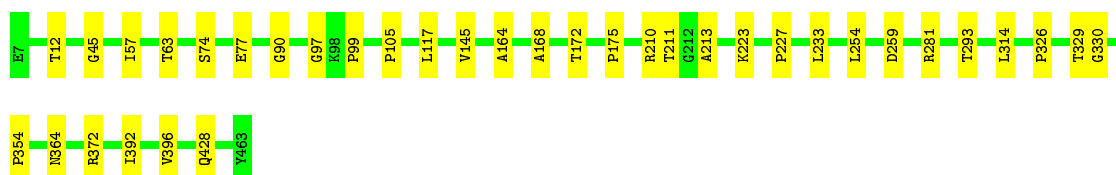
- Molecule 2: V-type ATP synthase beta chain

Chain E:  95% 5%



- Molecule 2: V-type ATP synthase beta chain

Chain F:  92% 8%



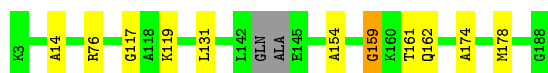
- Molecule 3: V-type ATP synthase subunit E

Chain G:  92% 6% ..




- Molecule 3: V-type ATP synthase subunit E

Chain H:  93% 5% ..



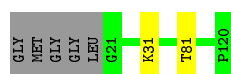
- Molecule 4: V-type ATPase subunit G

Chain I:  92% 5%



- Molecule 4: V-type ATPase subunit G

Chain J:  93% 5%



- Molecule 5: V-type ATP synthase subunit D

Chain K:  92% 7%



- Molecule 6: V-type ATP synthase subunit F



Chain L:  93% 7%



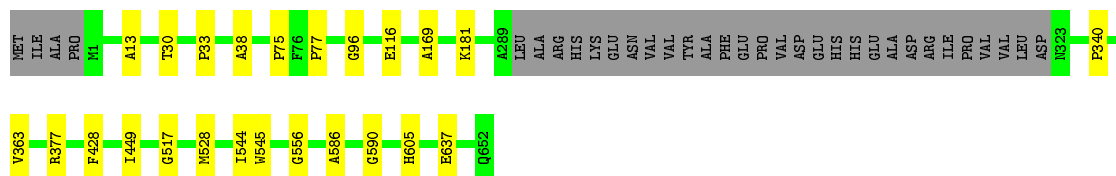
- Molecule 7: V-type ATP synthase subunit C

Chain M:  97% ..




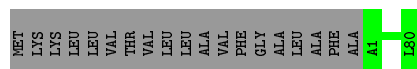
- Molecule 8: Archaeal/vacuolar-type H<sup>+</sup>-ATPase subunit I

Chain N:  91% . 5%



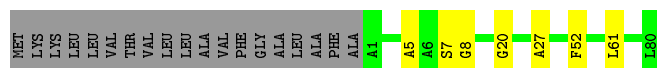
- Molecule 9: Vacuolar type ATP synthase subunit

Chain O:  81% 19%




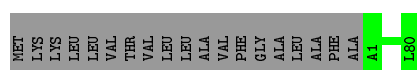
- Molecule 9: Vacuolar type ATP synthase subunit

Chain P:  74% 7% 19%




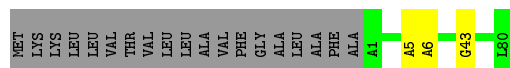
- Molecule 9: Vacuolar type ATP synthase subunit

Chain Q:  81% 19%

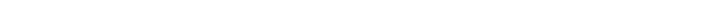


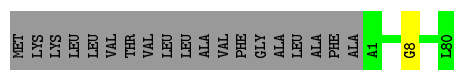
- Molecule 9: Vacuolar type ATP synthase subunit

Chain R:  78% . 19%

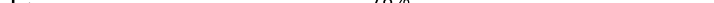


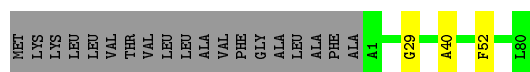
- Molecule 9: Vacuolar type ATP synthase subunit

Chain S:  80% 19%

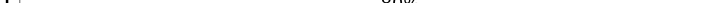


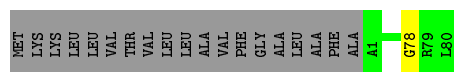
- Molecule 9: Vacuolar type ATP synthase subunit

Chain T:  78% 19%

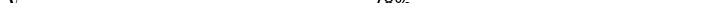


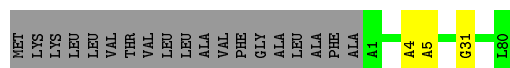
- Molecule 9: Vacuolar type ATP synthase subunit

Chain U:  80% . 19%



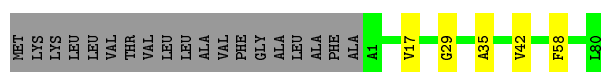
- Molecule 9: Vacuolar type ATP synthase subunit

Chain V:  78% • 19%

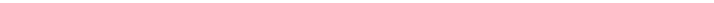


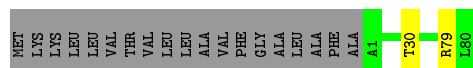
- Molecule 9: Vacuolar type ATP synthase subunit

Chain W:  76% 5% 19%



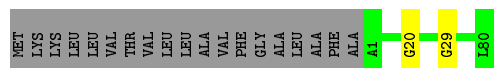
- Molecule 9: Vacuolar type ATP synthase subunit

Chain X:  79% • 19%



- Molecule 9: Vacuolar type ATP synthase subunit

Chain Y:  79% • 19%



- Molecule 9: Vacuolar type ATP synthase subunit

Chain Z:  79% • 19%

MET  
 LYS  
 LYS  
 LEU  
 LEU  
 VAL  
 THR  
 VAL  
 LEU  
 LEU  
 ALA  
 ALA  
 VAL  
 PHE  
 GLY  
 ALA  
 LEU  
 ALA  
 PHE  
 ALA  
 A1  
 G8  
 G41  
 L80

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	9721	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	1.50	8/2306 (0.3%)	1.64	13/2881 (0.5%)
1	B	1.54	5/2306 (0.2%)	1.66	14/2881 (0.5%)
1	C	1.59	6/2306 (0.3%)	1.63	7/2881 (0.2%)
2	D	1.54	3/1826 (0.2%)	1.67	12/2281 (0.5%)
2	E	1.53	1/1826 (0.1%)	1.66	6/2281 (0.3%)
2	F	1.52	4/1826 (0.2%)	1.65	10/2281 (0.4%)
3	G	1.54	3/732 (0.4%)	1.53	2/912 (0.2%)
3	H	1.52	2/732 (0.3%)	1.56	3/912 (0.3%)
4	I	1.39	0/398	1.34	0/496
4	J	1.32	0/398	1.48	1/496 (0.2%)
5	K	1.52	3/838 (0.4%)	1.57	3/1046 (0.3%)
6	L	1.66	0/398	1.66	0/496
7	M	1.51	3/1278 (0.2%)	1.54	2/1596 (0.1%)
8	N	1.50	5/2472 (0.2%)	1.56	7/3087 (0.2%)
9	O	1.57	0/318	1.48	0/396
9	P	1.47	1/318 (0.3%)	1.49	4/396 (1.0%)
9	Q	1.62	0/318	1.51	0/396
9	R	1.51	0/318	1.44	1/396 (0.3%)
9	S	1.57	0/318	1.48	0/396
9	T	1.52	1/318 (0.3%)	1.59	2/396 (0.5%)
9	U	1.59	0/318	1.59	0/396
9	V	1.66	1/318 (0.3%)	1.58	0/396
9	W	1.51	2/318 (0.6%)	1.54	3/396 (0.8%)
9	X	1.57	1/318 (0.3%)	1.41	0/396
9	Y	1.64	2/318 (0.6%)	1.45	0/396
9	Z	1.53	1/318 (0.3%)	1.43	0/396
All	All	1.53	52/23458 (0.2%)	1.59	90/29279 (0.3%)

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	B	0	1
3	G	0	1
7	M	0	1
All	All	0	3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	GLY	CA-C	-8.39	1.38	1.51
1	C	108	VAL	N-CA	-6.66	1.33	1.46
5	K	210	GLY	CA-C	-6.61	1.41	1.51
9	Y	20	GLY	CA-C	-6.51	1.41	1.51
7	M	135	GLY	CA-C	-6.31	1.41	1.51

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	180	GLU	C-N-CA	6.89	136.76	122.30
1	B	497	GLN	N-CA-C	-6.85	92.51	111.00
1	B	147	ILE	C-N-CA	6.77	138.63	121.70
1	B	9	ILE	N-CA-C	-6.68	92.96	111.00
8	N	517	GLY	C-N-CA	6.49	137.93	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	485	GLU	Mainchain
3	G	139	GLY	Peptide
7	M	3	ASP	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	2307	0	654	0	0
1	B	2307	0	654	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2307	0	654	0	0
2	D	1827	0	510	0	0
2	E	1827	0	510	0	0
2	F	1827	0	510	0	0
3	G	734	0	191	1	0
3	H	734	0	191	0	0
4	I	399	0	100	1	0
4	J	399	0	100	0	0
5	K	839	0	230	0	0
6	L	399	0	119	0	0
7	M	1279	0	357	0	0
8	N	2474	0	691	1	0
9	O	319	0	109	0	0
9	P	319	0	109	0	0
9	Q	319	0	109	0	0
9	R	319	0	109	0	0
9	S	319	0	109	0	0
9	T	319	0	109	0	0
9	U	319	0	109	0	0
9	V	319	0	109	0	0
9	W	319	0	109	0	0
9	X	319	0	109	0	0
9	Y	319	0	109	0	0
9	Z	319	0	109	0	0
All	All	23487	0	6779	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)
4:I:21:GLY:HA3	8:N:30:THR:H	1.75	0.52
3:G:121:LEU:H	3:G:139:GLY:HA3	1.85	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	575/577 (100%)	477 (83%)	69 (12%)	29 (5%)	3	31
1	B	575/577 (100%)	491 (85%)	64 (11%)	20 (4%)	4	39
1	C	575/577 (100%)	473 (82%)	70 (12%)	32 (6%)	2	28
2	D	455/457 (100%)	375 (82%)	63 (14%)	17 (4%)	4	38
2	E	455/457 (100%)	365 (80%)	72 (16%)	18 (4%)	4	35
2	F	455/457 (100%)	361 (79%)	71 (16%)	23 (5%)	2	30
3	G	180/186 (97%)	159 (88%)	14 (8%)	7 (4%)	4	36
3	H	180/186 (97%)	161 (89%)	12 (7%)	7 (4%)	4	36
4	I	98/105 (93%)	96 (98%)	0	2 (2%)	9	51
4	J	98/105 (93%)	95 (97%)	2 (2%)	1 (1%)	19	65
5	K	208/210 (99%)	163 (78%)	34 (16%)	11 (5%)	2	29
6	L	98/100 (98%)	72 (74%)	19 (19%)	7 (7%)	1	22
7	M	318/323 (98%)	306 (96%)	11 (4%)	1 (0%)	46	83
8	N	615/652 (94%)	570 (93%)	34 (6%)	11 (2%)	11	53
9	O	78/99 (79%)	75 (96%)	3 (4%)	0	100	100
9	P	78/99 (79%)	73 (94%)	2 (3%)	3 (4%)	4	37
9	Q	78/99 (79%)	72 (92%)	6 (8%)	0	100	100
9	R	78/99 (79%)	75 (96%)	1 (1%)	2 (3%)	7	45
9	S	78/99 (79%)	74 (95%)	3 (4%)	1 (1%)	15	60
9	T	78/99 (79%)	76 (97%)	2 (3%)	0	100	100
9	U	78/99 (79%)	73 (94%)	4 (5%)	1 (1%)	15	60
9	V	78/99 (79%)	73 (94%)	3 (4%)	2 (3%)	7	45
9	W	78/99 (79%)	74 (95%)	4 (5%)	0	100	100
9	X	78/99 (79%)	74 (95%)	3 (4%)	1 (1%)	15	60
9	Y	78/99 (79%)	72 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Z	78/99 (79%)	72 (92%)	5 (6%)	1 (1%)	15	60
All	All	5821/6157 (94%)	5047 (87%)	577 (10%)	197 (3%)	8	40

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	ARG
1	B	85	ASP
1	B	326	SER
1	C	109	HIS
1	C	210	ARG

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

There are no chain breaks in this entry.