



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:31 pm GMT

PDB ID : 5GAR
EMDB ID: : EMD-8016
Title : Thermus thermophilus V/A-ATPase, conformation 1
Authors : Schep, D.G.; Zhao, J.; Rubinstein, J.L.
Deposited on : 2016-02-05
Resolution : 6.40 Å(reported)
Based on PDB ID : ?

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

<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

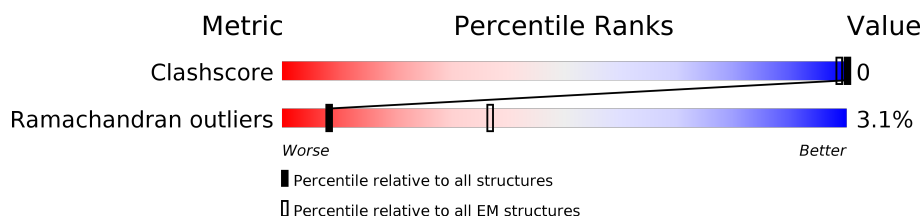
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.40 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 ≥ 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	 95% 5%
1	B	577	 93% 6%
1	C	577	 95% 5%
2	D	457	 93% 7%
2	E	457	 93% 7%
2	F	457	 95% 5%
3	G	186	 93% 6% .
3	H	186	 95% . .
4	I	105	 94% . 5%
4	J	105	 93% . 5%
5	K	210	 91% 9%

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Mol	Chain	Length	Quality of chain
6	L	100	<div><div></div><div>90%10%</div></div>
7	M	323	<div><div></div><div>95%<div><div></div><div></div></div></div></div>
8	N	652	<div><div></div><div>91%<div><div></div><div></div></div></div><div>5%</div></div>
9	O	99	<div><div></div><div>78%<div><div></div><div></div></div></div><div>19%</div></div>
9	P	99	<div><div></div><div>78%<div><div></div><div></div></div></div><div>19%</div></div>
9	Q	99	<div><div></div><div>78%<div><div></div><div></div></div></div><div>19%</div></div>
9	R	99	<div><div></div><div>80%<div><div></div><div></div></div></div><div>19%</div></div>
9	S	99	<div><div></div><div>79%<div><div></div><div></div></div></div><div>19%</div></div>
9	T	99	<div><div></div><div>79%<div><div></div><div></div></div></div><div>19%</div></div>
9	U	99	<div><div></div><div>80%<div><div></div><div></div></div></div><div>19%</div></div>
9	V	99	<div><div></div><div>80%<div><div></div><div></div></div></div><div>19%</div></div>
9	W	99	<div><div></div><div>76%5%19%</div></div>
9	X	99	<div><div></div><div>78%<div><div></div><div></div></div></div><div>19%</div></div>
9	Y	99	<div><div></div><div>80%<div><div></div><div></div></div></div><div>19%</div></div>
9	Z	99	<div><div></div><div>79%<div><div></div><div></div></div></div><div>19%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23483 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	576	Total	C	N	O	0	0
			2303	1152	576	575		
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⁺-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

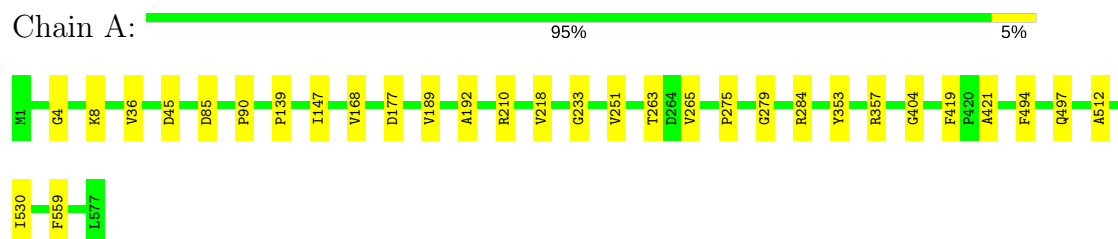
- Molecule 9 is a protein called Vacuolar type ATP synthase subunit.

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

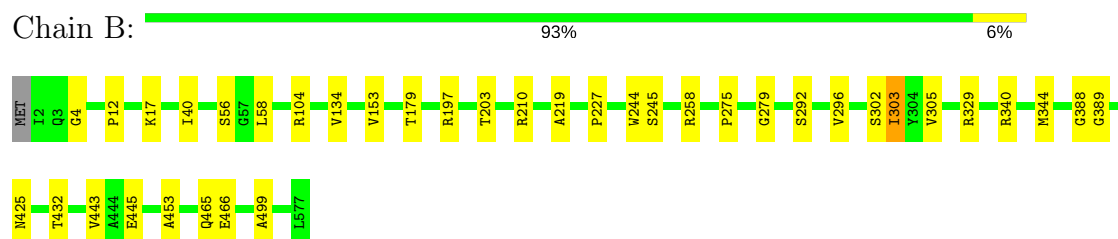
3 Residue-property plots

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

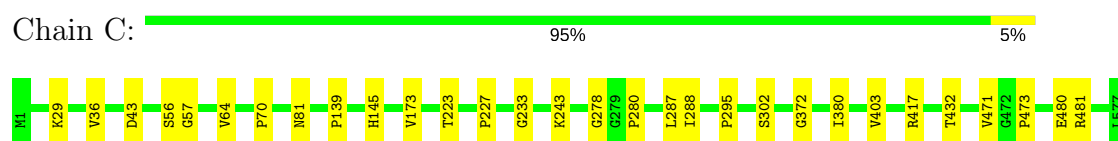
- Molecule 1: V-type ATP synthase alpha chain



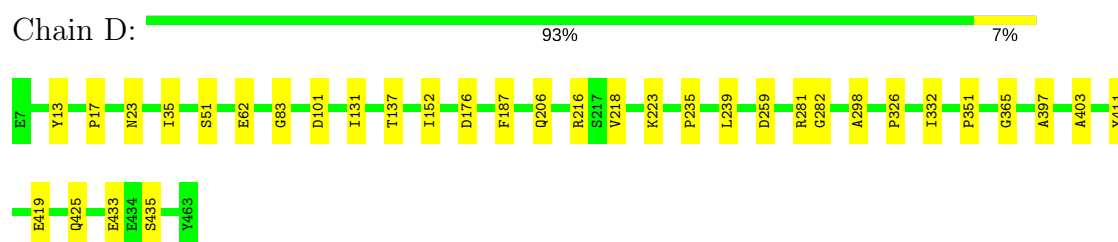
- Molecule 1: V-type ATP synthase alpha chain



- Molecule 1: V-type ATP synthase alpha chain

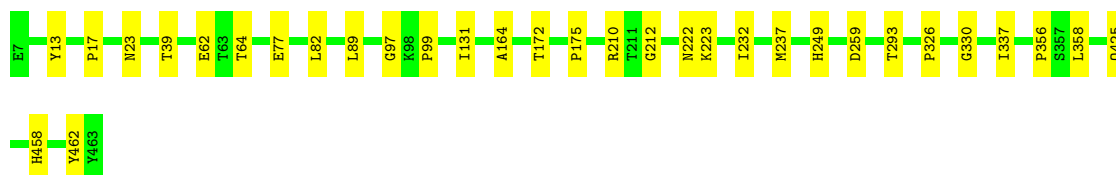


- Molecule 2: V-type ATP synthase beta chain



- Molecule 2: V-type ATP synthase beta chain





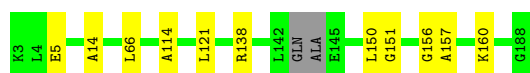
- Molecule 2: V-type ATP synthase beta chain

Chain F: 95% 5%



- Molecule 3: V-type ATP synthase subunit E

Chain G: 93% 6%



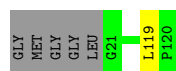
- Molecule 3: V-type ATP synthase subunit E

Chain H: 95% 5%



- Molecule 4: V-type ATPase subunit G

Chain I: 94% 5%



- Molecule 4: V-type ATPase subunit G

Chain J: 93% 5%



- Molecule 5: V-type ATP synthase subunit D

Chain K: 91% 9%



- Molecule 6: V-type ATP synthase subunit F

Chain L: 90% 10%



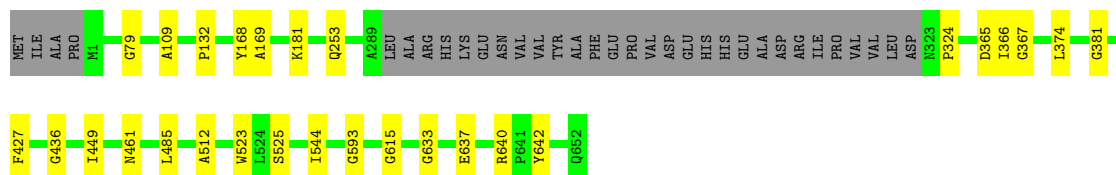
- Molecule 7: V-type ATP synthase subunit C

Chain M: 95%



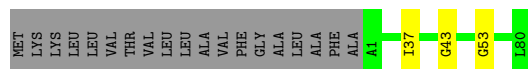
- Molecule 8: Archaeal/vacuolar-type H⁺-ATPase subunit I

Chain N: 91%



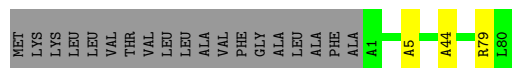
- Molecule 9: Vacuolar type ATP synthase subunit

Chain O: 78%



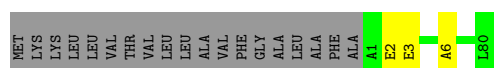
- Molecule 9: Vacuolar type ATP synthase subunit

Chain P: 78%



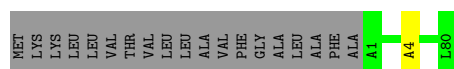
- Molecule 9: Vacuolar type ATP synthase subunit

Chain Q: 78%



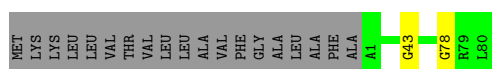
- Molecule 9: Vacuolar type ATP synthase subunit

Chain R: 80%

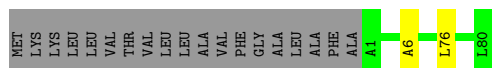
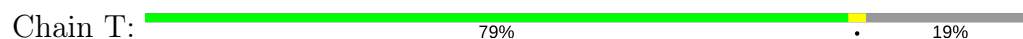


- Molecule 9: Vacuolar type ATP synthase subunit

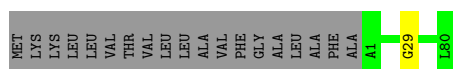
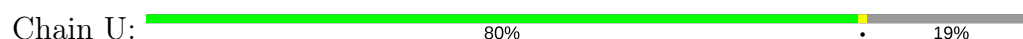
Chain S: 79%



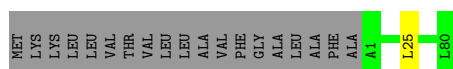
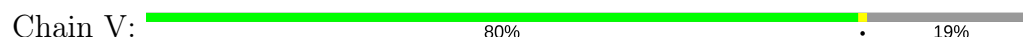
- Molecule 9: Vacuolar type ATP synthase subunit



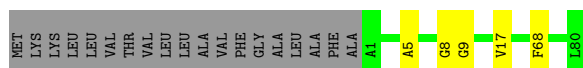
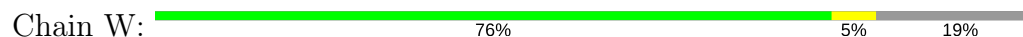
- Molecule 9: Vacuolar type ATP synthase subunit



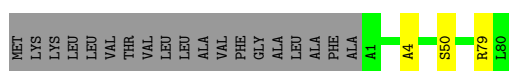
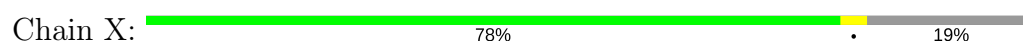
- Molecule 9: Vacuolar type ATP synthase subunit



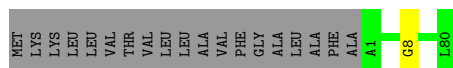
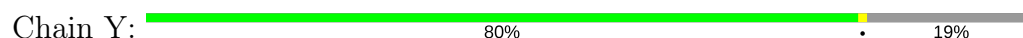
- Molecule 9: Vacuolar type ATP synthase subunit



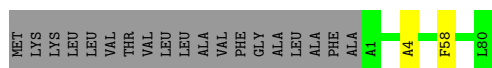
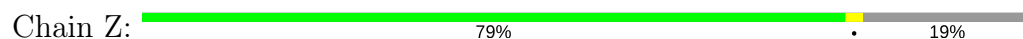
- Molecule 9: Vacuolar type ATP synthase subunit



- Molecule 9: Vacuolar type ATP synthase subunit



- Molecule 9: Vacuolar type ATP synthase subunit



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	197178	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	34483	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	1.51	4/2306 (0.2%)	1.64	12/2881 (0.4%)
1	B	1.54	5/2302 (0.2%)	1.62	10/2876 (0.3%)
1	C	1.53	2/2306 (0.1%)	1.65	8/2881 (0.3%)
2	D	1.56	4/1826 (0.2%)	1.66	10/2281 (0.4%)
2	E	1.53	2/1826 (0.1%)	1.67	10/2281 (0.4%)
2	F	1.51	2/1826 (0.1%)	1.66	4/2281 (0.2%)
3	G	1.50	1/732 (0.1%)	1.54	2/912 (0.2%)
3	H	1.49	2/732 (0.3%)	1.52	1/912 (0.1%)
4	I	1.44	0/398	1.47	0/496
4	J	1.46	0/398	1.47	1/496 (0.2%)
5	K	1.48	2/838 (0.2%)	1.60	6/1046 (0.6%)
6	L	1.53	2/398 (0.5%)	1.66	3/496 (0.6%)
7	M	1.50	2/1278 (0.2%)	1.55	7/1596 (0.4%)
8	N	1.54	7/2472 (0.3%)	1.55	8/3087 (0.3%)
9	O	1.59	3/318 (0.9%)	1.56	0/396
9	P	1.53	0/318	1.55	2/396 (0.5%)
9	Q	1.55	0/318	1.54	1/396 (0.3%)
9	R	1.55	0/318	1.54	0/396
9	S	1.61	2/318 (0.6%)	1.43	0/396
9	T	1.57	0/318	1.51	1/396 (0.3%)
9	U	1.60	1/318 (0.3%)	1.56	0/396
9	V	1.59	0/318	1.51	1/396 (0.3%)
9	W	1.59	1/318 (0.3%)	1.56	1/396 (0.3%)
9	X	1.50	0/318	1.53	0/396
9	Y	1.50	0/318	1.58	0/396
9	Z	1.58	0/318	1.67	1/396 (0.3%)
All	All	1.53	42/23454 (0.2%)	1.60	89/29274 (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
7	M	0	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	151	GLY	N-CA	-6.96	1.35	1.46
3	H	156	GLY	CA-C	-6.65	1.41	1.51
7	M	117	GLY	CA-C	-6.52	1.41	1.51
1	C	372	GLY	N-CA	-6.33	1.36	1.46
8	N	374	LEU	C-N	6.32	1.48	1.34
2	E	64	THR	C-N	6.16	1.44	1.33
1	C	278	GLY	CA-C	-6.10	1.42	1.51
8	N	633	GLY	N-CA	-5.93	1.37	1.46
5	K	78	GLY	CA-C	-5.85	1.42	1.51
9	S	43	GLY	N-CA	-5.77	1.37	1.46
9	O	37	ILE	C-N	5.71	1.43	1.33
8	N	615	GLY	N-CA	-5.68	1.37	1.46
1	B	4	GLY	CA-C	-5.66	1.42	1.51
5	K	111	GLY	CA-C	-5.64	1.42	1.51
9	U	29	GLY	CA-C	5.45	1.60	1.51
1	A	353	TYR	N-CA	-5.43	1.35	1.46
8	N	79	GLY	CA-C	-5.42	1.43	1.51
1	B	227	PRO	N-CA	-5.41	1.38	1.47
8	N	485	LEU	C-N	5.36	1.42	1.33
1	B	17	LYS	C-N	5.35	1.42	1.33
9	W	68	PHE	C-N	5.34	1.42	1.33
2	F	400	GLY	N-CA	-5.33	1.38	1.46
2	E	39	THR	C-N	5.31	1.42	1.33
1	B	12	PRO	N-CA	-5.30	1.38	1.47
3	H	155	VAL	C-N	5.29	1.42	1.33
1	A	357	ARG	CA-C	-5.28	1.39	1.52
2	D	282	GLY	CA-C	-5.26	1.43	1.51
2	D	51	SER	N-CA	-5.25	1.35	1.46
1	A	192	ALA	CA-C	-5.23	1.39	1.52
9	O	43	GLY	N-CA	-5.22	1.38	1.46
2	D	83	GLY	CA-C	-5.21	1.43	1.51
7	M	17	GLY	N-CA	-5.20	1.38	1.46
2	F	298	ALA	C-N	5.20	1.42	1.33
6	L	20	GLY	CA-C	-5.18	1.43	1.51
9	O	53	GLY	N-CA	-5.10	1.38	1.46
1	B	425	ASN	C-N	5.08	1.42	1.33
8	N	461	ASN	C-N	5.07	1.45	1.34
1	A	279	GLY	CA-C	-5.04	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	298	ALA	C-N	5.04	1.42	1.33
8	N	593	GLY	N-CA	5.04	1.53	1.46
6	L	22	GLY	N-CA	-5.03	1.38	1.46
9	S	78	GLY	CA-C	-5.02	1.43	1.51

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	139	ASP	O-C-N	-6.91	111.64	122.70
2	D	35	ILE	O-C-N	6.67	133.37	122.70
2	E	462	TYR	N-CA-C	-6.56	93.29	111.00
1	B	303	ILE	C-N-CA	6.28	137.40	121.70
7	M	78	GLY	C-N-CA	6.21	137.24	121.70
2	E	337	ILE	N-CA-C	-6.20	94.26	111.00
1	C	473	PRO	C-N-CA	6.16	137.10	121.70
1	C	43	ASP	N-CA-C	-6.13	94.46	111.00
1	A	218	VAL	N-CA-C	-6.04	94.68	111.00
1	C	173	VAL	N-CA-C	-6.02	94.74	111.00
2	F	111	ARG	N-CA-C	-6.00	94.80	111.00
1	A	404	GLY	N-CA-C	-5.92	98.30	113.10
7	M	23	SER	O-C-N	-5.82	113.39	122.70
8	N	427	PHE	C-N-CA	5.82	136.24	121.70
9	P	44	ALA	O-C-N	5.79	131.96	122.70
2	F	54	TYR	O-C-N	5.75	131.90	122.70
2	E	212	GLY	O-C-N	-5.72	113.55	122.70
9	T	76	LEU	O-C-N	5.71	131.83	122.70
8	N	253	GLN	O-C-N	-5.70	113.58	122.70
2	F	195	GLY	N-CA-C	-5.69	98.88	113.10
8	N	109	ALA	O-C-N	-5.67	113.63	122.70
1	B	58	LEU	O-C-N	5.67	131.76	122.70
1	B	279	GLY	N-CA-C	-5.65	98.98	113.10
1	B	153	VAL	N-CA-C	-5.64	95.78	111.00
9	Z	58	PHE	O-C-N	5.59	131.65	122.70
6	L	85	ASP	C-N-CA	5.55	135.57	121.70
1	A	419	PHE	N-CA-C	-5.53	96.06	111.00
1	B	244	TRP	C-N-CA	5.51	135.47	121.70
5	K	108	PHE	N-CA-C	-5.49	96.17	111.00
2	D	206	GLN	C-N-CA	5.47	135.37	121.70
5	K	86	LEU	N-CA-C	-5.47	96.24	111.00
1	B	465	GLN	C-N-CA	5.43	135.28	121.70
3	H	136	ARG	O-C-N	-5.43	114.01	122.70
2	D	397	ALA	O-C-N	5.43	131.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	172	THR	N-CA-C	-5.42	96.36	111.00
3	G	66	LEU	O-C-N	-5.41	114.04	122.70
8	N	381	GLY	N-CA-C	-5.38	99.64	113.10
7	M	142	VAL	CA-C-N	5.38	132.17	117.10
1	A	8	LYS	O-C-N	5.37	131.30	122.70
7	M	9	ASN	C-N-CA	5.37	135.13	121.70
9	V	25	LEU	O-C-N	-5.37	114.11	122.70
3	G	121	LEU	N-CA-C	-5.37	96.51	111.00
8	N	324	PRO	CA-C-O	-5.36	107.33	120.20
1	B	453	ALA	C-N-CA	5.36	135.10	121.70
8	N	132	PRO	O-C-N	5.36	131.27	122.70
1	A	251	VAL	N-CA-C	-5.35	96.56	111.00
2	D	433	GLU	C-N-CA	5.32	135.00	121.70
2	E	232	ILE	O-C-N	-5.31	114.21	122.70
2	E	222	ASN	C-N-CA	5.30	134.95	121.70
1	B	197	ARG	N-CA-C	-5.29	96.70	111.00
1	C	29	LYS	N-CA-C	-5.29	96.71	111.00
1	A	4	GLY	N-CA-C	-5.28	99.89	113.10
1	A	559	PHE	CA-C-N	5.27	131.87	117.10
1	A	497	GLN	N-CA-C	-5.27	96.77	111.00
1	A	189	VAL	O-C-N	-5.27	114.27	122.70
5	K	102	PRO	C-N-CA	5.26	134.86	121.70
2	D	131	ILE	C-N-CA	5.19	134.67	121.70
1	A	530	ILE	O-C-N	-5.18	114.41	122.70
2	E	249	HIS	C-N-CA	5.17	134.61	121.70
9	W	17	VAL	C-N-CA	5.16	133.14	122.30
1	C	223	THR	N-CA-C	-5.16	97.07	111.00
1	C	481	ARG	O-C-N	-5.16	114.45	122.70
2	E	131	ILE	O-C-N	-5.13	114.50	122.70
5	K	61	TYR	C-N-CA	5.12	134.51	121.70
1	C	145	HIS	N-CA-C	-5.12	97.19	111.00
7	M	78	GLY	CA-C-O	-5.12	111.39	120.60
1	C	380	ILE	N-CA-C	-5.11	97.21	111.00
2	D	411	TYR	C-N-CA	5.11	134.47	121.70
1	A	147	ILE	C-N-CA	5.10	134.46	121.70
8	N	512	ALA	C-N-CA	5.10	134.46	121.70
9	P	44	ALA	CA-C-O	-5.09	109.40	120.10
1	B	329	ARG	C-N-CA	5.09	134.43	121.70
2	D	365	GLY	O-C-N	-5.09	114.56	122.70
5	K	86	LEU	CA-C-N	-5.09	106.00	117.20
1	A	421	ALA	N-CA-C	-5.09	97.26	111.00
6	L	74	ILE	N-CA-C	-5.09	97.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	218	VAL	N-CA-C	-5.08	97.29	111.00
2	E	458	HIS	CA-C-O	-5.07	109.46	120.10
5	K	2	SER	N-CA-C	-5.06	97.33	111.00
2	D	187	PHE	O-C-N	5.05	130.78	122.70
4	J	82	GLU	O-C-N	5.05	130.78	122.70
7	M	283	VAL	C-N-CA	5.03	132.87	122.30
6	L	51	LEU	N-CA-C	-5.03	97.41	111.00
9	Q	2	GLU	C-N-CA	5.03	134.28	121.70
2	D	152	ILE	N-CA-C	-5.02	97.44	111.00
8	N	523	TRP	C-N-CA	5.02	134.25	121.70
1	B	203	THR	N-CA-C	-5.02	97.45	111.00
7	M	243	GLU	N-CA-C	-5.02	97.45	111.00
2	E	356	PRO	O-C-N	5.00	130.71	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2303	0	650	0	0
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	0	0
3	H	734	0	191	0	0
4	I	399	0	100	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	2474	0	691	0	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	23483	0	6775	0	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.

There are no clashes within the asymmetric unit.

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%)	504 (88%)	56 (10%)	15 (3%)	6	40
1	B	574/577 (100%)	477 (83%)	73 (13%)	24 (4%)	3	30
1	C	575/577 (100%)	499 (87%)	56 (10%)	20 (4%)	4	34
2	D	455/457 (100%)	370 (81%)	65 (14%)	20 (4%)	3	29
2	E	455/457 (100%)	369 (81%)	66 (14%)	20 (4%)	3	29
2	F	455/457 (100%)	377 (83%)	57 (12%)	21 (5%)	3	28
3	G	180/186 (97%)	162 (90%)	10 (6%)	8 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	180/186 (97%)	167 (93%)	9 (5%)	4 (2%)	8	44
4	I	98/105 (93%)	93 (95%)	4 (4%)	1 (1%)	18	61
4	J	98/105 (93%)	94 (96%)	3 (3%)	1 (1%)	18	61
5	K	208/210 (99%)	172 (83%)	25 (12%)	11 (5%)	2	25
6	L	98/100 (98%)	78 (80%)	15 (15%)	5 (5%)	2	26
7	M	318/323 (98%)	307 (96%)	7 (2%)	4 (1%)	14	56
8	N	615/652 (94%)	559 (91%)	43 (7%)	13 (2%)	8	45
9	O	78/99 (79%)	76 (97%)	2 (3%)	0	100	100
9	P	78/99 (79%)	74 (95%)	2 (3%)	2 (3%)	6	40
9	Q	78/99 (79%)	72 (92%)	4 (5%)	2 (3%)	6	40
9	R	78/99 (79%)	73 (94%)	4 (5%)	1 (1%)	14	56
9	S	78/99 (79%)	74 (95%)	4 (5%)	0	100	100
9	T	78/99 (79%)	75 (96%)	2 (3%)	1 (1%)	14	56
9	U	78/99 (79%)	75 (96%)	3 (4%)	0	100	100
9	V	78/99 (79%)	72 (92%)	6 (8%)	0	100	100
9	W	78/99 (79%)	74 (95%)	1 (1%)	3 (4%)	4	32
9	X	78/99 (79%)	74 (95%)	1 (1%)	3 (4%)	4	32
9	Y	78/99 (79%)	74 (95%)	3 (4%)	1 (1%)	14	56
9	Z	78/99 (79%)	74 (95%)	3 (4%)	1 (1%)	14	56
All	All	5820/6157 (94%)	5115 (88%)	524 (9%)	181 (3%)	8	36

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	VAL
1	B	258	ARG
1	B	303	ILE
1	B	305	VAL
1	B	466	GLU
1	C	227	PRO
1	C	480	GLU
2	D	259	ASP
2	D	419	GLU
2	E	62	GLU
2	E	175	PRO

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Mol	Chain	Res	Type
2	F	25	LYS
2	F	139	ASP
2	F	176	ASP
2	F	298	ALA
5	K	117	VAL
7	M	4	ASP
8	N	169	ALA
8	N	365	ASP
8	N	642	TYR
9	Q	3	GLU
1	A	85	ASP
1	A	210	ARG
1	A	233	GLY
1	A	512	ALA
1	B	210	ARG
1	B	292	SER
1	B	443	VAL
1	B	445	GLU
1	C	64	VAL
1	C	70	PRO
1	C	302	SER
1	C	403	VAL
1	C	417	ARG
1	C	471	VAL
2	D	17	PRO
2	D	176	ASP
2	D	239	LEU
2	D	332	ILE
2	D	425	GLN
2	E	82	LEU
2	E	97	GLY
2	E	210	ARG
2	E	330	GLY
2	F	15	SER
2	F	140	VAL
2	F	192	ALA
2	F	327	ASP
3	G	14	ALA
3	G	150	LEU
3	G	157	ALA
3	H	14	ALA
5	K	168	VAL

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Mol	Chain	Res	Type
6	L	64	ARG
8	N	544	ILE
9	R	4	ALA
9	T	6	ALA
9	Z	4	ALA
1	A	177	ASP
1	A	494	PHE
1	B	104	ARG
1	B	219	ALA
1	B	296	VAL
1	B	302	SER
1	B	340	ARG
1	C	233	GLY
1	C	295	PRO
1	C	432	THR
2	D	23	ASN
2	D	101	ASP
2	E	17	PRO
2	E	23	ASN
2	E	77	GLU
2	E	164	ALA
2	E	293	THR
2	E	425	GLN
2	F	88	MET
2	F	128	GLU
2	F	351	PRO
2	F	415	ALA
3	G	114	ALA
3	G	156	GLY
3	G	160	LYS
3	H	162	GLN
3	H	178	MET
5	K	69	ALA
5	K	70	PHE
5	K	82	GLY
5	K	110	ASP
6	L	23	ALA
7	M	185	GLN
8	N	367	GLY
8	N	449	ILE
8	N	525	SER
8	N	637	GLU

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Mol	Chain	Res	Type
9	Q	6	ALA
9	W	8	GLY
9	X	4	ALA
9	Y	8	GLY
1	A	90	PRO
1	B	432	THR
1	B	499	ALA
1	C	36	VAL
1	C	56	SER
1	C	57	GLY
1	C	81	ASN
2	D	137	THR
2	D	281	ARG
2	D	435	SER
2	E	89	LEU
2	E	223	LYS
2	E	358	LEU
2	F	137	THR
2	F	214	LEU
2	F	389	GLY
3	H	114	ALA
6	L	52	LEU
7	M	224	PHE
8	N	181	LYS
8	N	436	GLY
8	N	640	ARG
9	P	5	ALA
9	X	79	ARG
1	A	36	VAL
1	A	45	ASP
1	A	263	THR
1	A	284	ARG
1	B	56	SER
1	B	245	SER
1	C	243	LYS
1	C	287	LEU
2	D	62	GLU
2	D	216	ARG
2	D	403	ALA
2	E	13	TYR
2	E	326	PRO
2	F	259	ASP

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Mol	Chain	Res	Type
2	F	402	ASP
2	F	421	PHE
2	F	437	GLN
3	G	138	ARG
5	K	99	SER
5	K	134	ALA
5	K	180	GLN
6	L	55	PRO
6	L	79	GLU
8	N	366	ILE
9	P	79	ARG
9	W	5	ALA
9	W	9	GLY
9	X	50	SER
1	A	139	PRO
1	B	179	THR
2	D	13	TYR
2	D	223	LYS
2	E	237	MET
2	E	259	ASP
2	F	436	LEU
3	G	5	GLU
4	J	81	THR
5	K	174	ALA
7	M	184	ASP
8	N	168	TYR
1	A	168	VAL
1	A	275	PRO
2	E	99	PRO
1	B	40	ILE
1	B	388	GLY
1	B	389	GLY
2	D	326	PRO
2	D	351	PRO
1	C	280	PRO
1	C	288	ILE
4	I	119	LEU
5	K	179	ILE
1	A	265	VAL
1	B	275	PRO
1	C	139	PRO
2	D	235	PRO

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Mol	Chain	Res	Type
1	B	344	MET
2	F	390	VAL

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 [i](#)

There are no chain breaks in this entry.