



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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

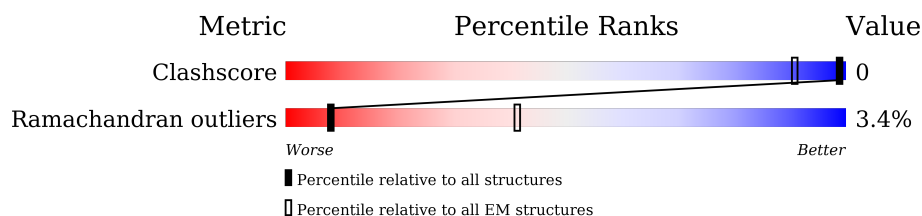
1 Overall quality at a glance

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 ≥ 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⁺-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

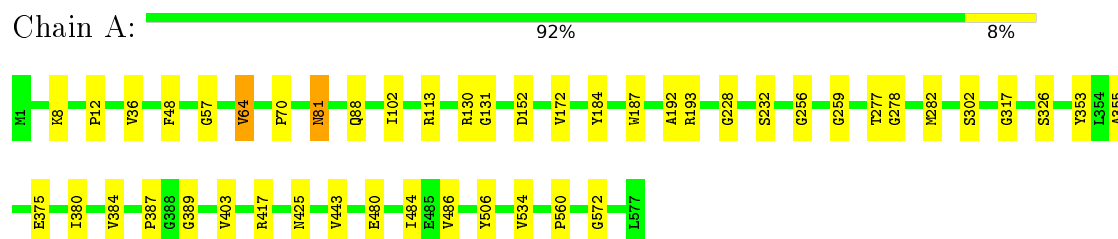
- Molecule 9 is a protein called Vacuolar type ATP synthase subunit.

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

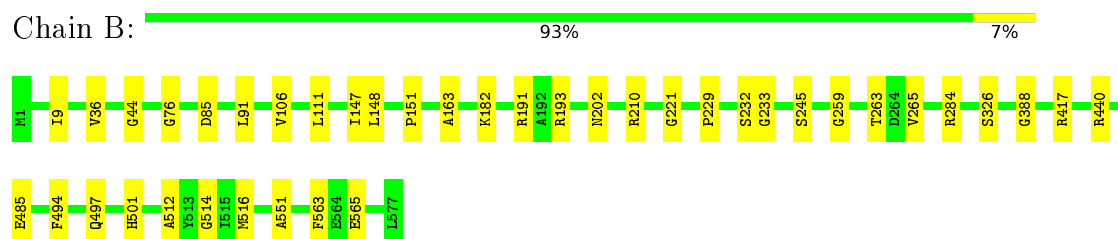
3 Residue-property plots

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.

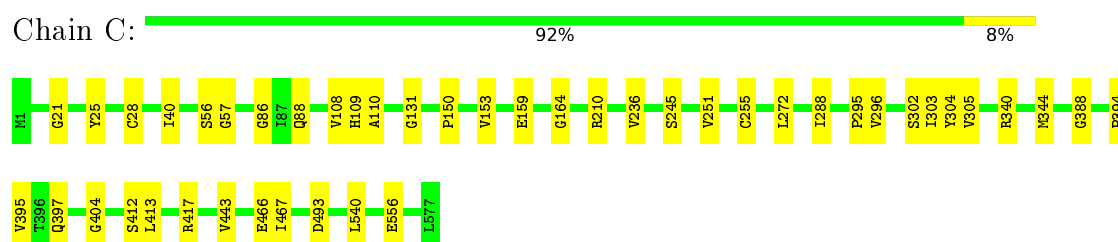
- Molecule 1: V-type ATP synthase alpha chain



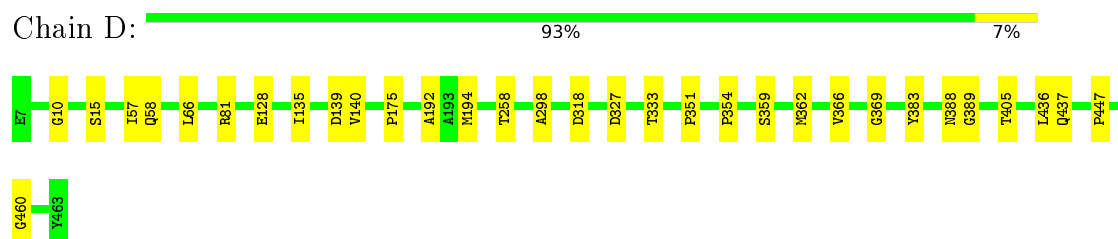
- Molecule 1: V-type ATP synthase alpha chain



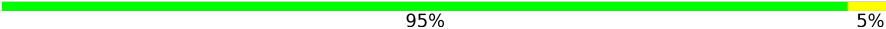
- Molecule 1: V-type ATP synthase alpha chain

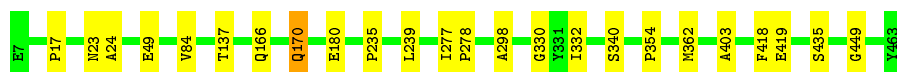


- Molecule 2: V-type ATP synthase beta chain



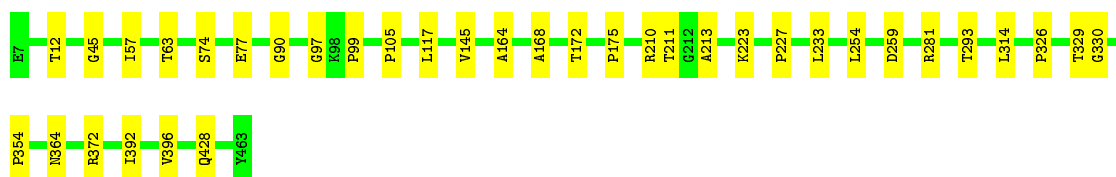
- Molecule 2: V-type ATP synthase beta chain

Chain E:  95% 5%



- Molecule 2: V-type ATP synthase beta chain

Chain F:  92% 8%



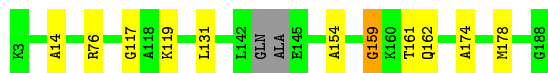
- Molecule 3: V-type ATP synthase subunit E

Chain G:  92% 6% ..




- Molecule 3: V-type ATP synthase subunit E

Chain H:  93% 5% ..



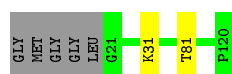
- Molecule 4: V-type ATPase subunit G

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%



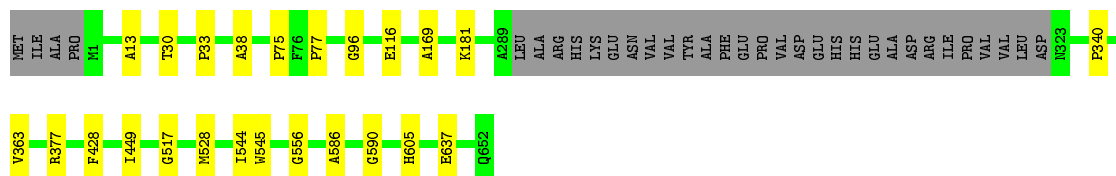
- Molecule 7: V-type ATP synthase subunit C

Chain M:  97% ..




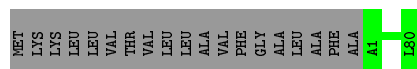
- Molecule 8: Archaeal/vacuolar-type H⁺-ATPase subunit I

Chain N:  91% . 5%



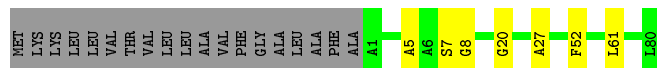
- Molecule 9: Vacuolar type ATP synthase subunit

Chain O:  81% 19%




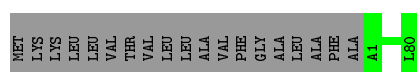
- Molecule 9: Vacuolar type ATP synthase subunit

Chain P:  74% 7% 19%




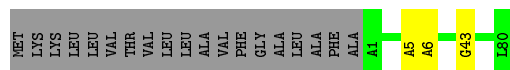
- Molecule 9: Vacuolar type ATP synthase subunit

Chain Q:  81% 19%




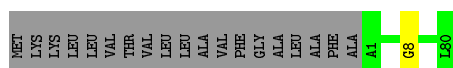
- Molecule 9: Vacuolar type ATP synthase subunit

Chain R:  78% . 19%




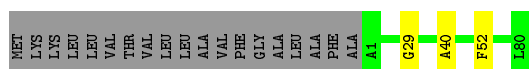
- Molecule 9: Vacuolar type ATP synthase subunit

Chain S:  80% 19%




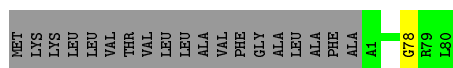
- Molecule 9: Vacuolar type ATP synthase subunit

Chain T:  78% 19%




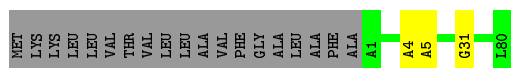
- Molecule 9: Vacuolar type ATP synthase subunit

Chain U:  80% 19%




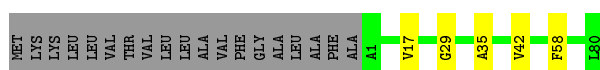
- Molecule 9: Vacuolar type ATP synthase subunit

Chain V:  78% 19%




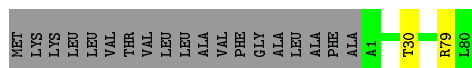
- Molecule 9: Vacuolar type ATP synthase subunit

Chain W:  76% 5% 19%




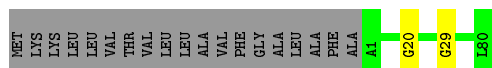
- Molecule 9: Vacuolar type ATP synthase subunit

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

All (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
3	G	127	ASP	N-CA	-6.25	1.33	1.46
9	Y	29	GLY	CA-C	-6.14	1.42	1.51
1	A	259	GLY	CA-C	-6.12	1.42	1.51
3	G	77	GLY	CA-C	6.04	1.61	1.51
1	A	389	GLY	CA-C	-6.02	1.42	1.51
1	B	388	GLY	N-CA	-6.01	1.37	1.46
8	N	77	PRO	N-CA	-5.89	1.37	1.47
1	A	131	GLY	CA-C	-5.80	1.42	1.51
9	P	20	GLY	N-CA	-5.74	1.37	1.46
1	A	81	ASN	C-N	5.71	1.43	1.33
9	T	29	GLY	N-CA	-5.66	1.37	1.46
2	F	281	ARG	C-N	5.59	1.43	1.33
1	A	387	PRO	C-N	5.57	1.43	1.33
1	A	8	LYS	C-N	5.50	1.46	1.34
1	C	131	GLY	CA-C	-5.50	1.43	1.51
9	W	42	VAL	C-N	5.45	1.42	1.33
2	F	211	THR	C-N	5.44	1.42	1.33
2	F	45	GLY	CA-C	-5.42	1.43	1.51
8	N	590	GLY	CA-C	-5.38	1.43	1.51
2	E	449	GLY	N-CA	-5.37	1.38	1.46
1	C	86	GLY	CA-C	-5.30	1.43	1.51
3	H	76	ARG	C-N	5.30	1.42	1.33
1	B	163	ALA	C-N	5.29	1.42	1.33
3	G	188	GLY	CA-C	5.29	1.60	1.51
5	K	170	PRO	N-CA	-5.28	1.38	1.47
9	Z	41	GLY	N-CA	-5.25	1.38	1.46
2	F	254	LEU	N-CA	-5.25	1.35	1.46
1	B	193	ARG	C-N	-5.25	1.24	1.34
3	H	117	GLY	CA-C	-5.23	1.43	1.51
7	M	282	GLY	CA-C	-5.22	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	17	VAL	C-N	5.21	1.42	1.33
1	A	572	GLY	CA-C	-5.21	1.43	1.51
2	D	460	GLY	CA-C	-5.19	1.43	1.51
1	C	493	ASP	C-N	5.19	1.46	1.34
1	C	21	GLY	CA-C	5.18	1.60	1.51
7	M	50	ALA	C-N	5.16	1.42	1.33
5	K	211	GLY	N-CA	-5.16	1.38	1.46
9	V	31	GLY	N-CA	-5.14	1.38	1.46
9	X	30	THR	C-N	5.14	1.42	1.33
1	C	388	GLY	CA-C	-5.13	1.43	1.51
8	N	556	GLY	CA-C	-5.12	1.43	1.51
1	A	375	GLU	C-N	5.09	1.42	1.33
2	D	369	GLY	N-CA	-5.08	1.38	1.46
2	D	447	PRO	C-N	5.08	1.45	1.34
8	N	605	HIS	CA-C	-5.03	1.39	1.52
1	B	245	SER	N-CA	-5.03	1.36	1.46
8	N	528	MET	N-CA	-5.02	1.36	1.46

All (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
1	A	184	TYR	N-CA-C	-6.49	93.48	111.00
7	M	45	TYR	C-N-CA	6.40	135.73	122.30
2	F	329	THR	C-N-CA	6.35	135.64	122.30
1	C	164	GLY	N-CA-C	-6.34	97.24	113.10
1	B	76	GLY	N-CA-C	-6.29	97.39	113.10
2	D	333	THR	O-C-N	6.27	132.73	122.70
1	A	102	ILE	N-CA-C	-6.24	94.16	111.00
3	H	159	GLY	N-CA-C	-6.21	97.56	113.10
1	A	192	ALA	C-N-CA	6.19	137.17	121.70
1	A	380	ILE	O-C-N	6.17	132.56	122.70
8	N	116	GLU	CA-C-O	-6.17	107.15	120.10
2	D	318	ASP	C-N-CA	6.13	137.02	121.70
1	B	501	HIS	N-CA-C	-6.10	94.53	111.00
9	T	52	PHE	C-N-CA	6.09	135.09	122.30
1	A	228	GLY	N-CA-C	-6.03	98.03	113.10
1	A	64	VAL	N-CA-C	-6.01	94.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	314	LEU	O-C-N	-6.00	113.10	122.70
2	D	366	VAL	O-C-N	-5.98	113.04	123.20
1	A	130	ARG	N-CA-C	-5.97	94.88	111.00
1	C	251	VAL	N-CA-C	-5.96	94.90	111.00
2	D	10	GLY	N-CA-C	-5.96	98.21	113.10
4	J	31	LYS	O-C-N	-5.86	113.32	122.70
1	C	540	LEU	O-C-N	-5.79	113.43	122.70
8	N	33	PRO	CA-C-O	-5.75	106.39	120.20
2	F	57	ILE	N-CA-C	-5.75	95.47	111.00
8	N	13	ALA	C-N-CA	5.68	135.90	121.70
2	D	57	ILE	N-CA-C	-5.67	95.69	111.00
2	D	388	ASN	C-N-CA	5.66	134.19	122.30
1	A	353	TYR	N-CA-C	-5.63	95.81	111.00
1	B	182	LYS	O-C-N	-5.62	113.70	122.70
2	F	172	THR	N-CA-C	-5.62	95.84	111.00
9	P	27	ALA	C-N-CA	5.59	135.67	121.70
2	F	233	LEU	C-N-CA	5.57	135.63	121.70
1	C	412	SER	C-N-CA	5.57	135.62	121.70
1	C	153	VAL	N-CA-C	-5.55	96.00	111.00
1	B	191	ARG	N-CA-C	-5.54	96.05	111.00
1	A	355	ALA	O-C-N	5.51	131.52	122.70
2	E	170	GLN	O-C-N	-5.48	113.94	122.70
7	M	122	GLU	O-C-N	-5.46	113.96	122.70
1	A	187	TRP	N-CA-C	-5.42	96.37	111.00
2	D	359	SER	N-CA-C	-5.39	96.46	111.00
9	R	43	GLY	CA-C-O	5.39	130.30	120.60
2	E	330	GLY	C-N-CA	5.38	135.15	121.70
9	W	35	ALA	O-C-N	5.38	131.30	122.70
1	B	516	MET	O-C-N	-5.37	114.10	122.70
3	G	16	ILE	O-C-N	-5.36	114.12	122.70
1	B	44	GLY	C-N-CA	5.35	135.08	121.70
1	A	425	ASN	N-CA-C	-5.34	96.57	111.00
9	W	58	PHE	C-N-CA	5.32	135.00	121.70
9	P	61	LEU	CA-C-N	5.32	131.98	117.10
1	B	111	LEU	N-CA-C	-5.31	96.67	111.00
1	A	534	VAL	N-CA-C	-5.29	96.71	111.00
9	P	61	LEU	CA-C-O	-5.29	108.99	120.10
9	P	52	PHE	C-N-CA	5.28	133.39	122.30
8	N	428	PHE	O-C-N	-5.28	114.23	123.20
2	D	58	GLN	N-CA-C	-5.26	96.80	111.00
1	B	229	PRO	O-C-N	5.25	131.10	122.70
2	F	74	SER	N-CA-C	-5.25	96.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	29	GLY	CA-C-O	-5.23	111.19	120.60
5	K	86	LEU	C-N-CA	5.22	134.75	121.70
8	N	377	ARG	O-C-N	-5.22	114.35	122.70
2	D	81	ARG	O-C-N	-5.16	114.45	122.70
9	T	40	ALA	C-N-CA	5.15	133.12	122.30
1	B	91	LEU	C-N-CA	5.14	134.56	121.70
3	G	139	GLY	N-CA-C	-5.14	100.26	113.10
3	H	154	ALA	N-CA-C	-5.12	97.17	111.00
2	D	194	MET	N-CA-C	-5.10	97.22	111.00
2	F	281	ARG	C-N-CA	5.09	133.00	122.30
2	D	258	THR	N-CA-C	-5.09	97.26	111.00
2	F	428	GLN	C-N-CA	5.09	134.42	121.70
2	E	84	VAL	N-CA-C	-5.08	97.27	111.00
2	F	12	THR	N-CA-C	-5.08	97.27	111.00
2	D	135	ILE	N-CA-C	-5.07	97.31	111.00
1	C	272	LEU	N-CA-C	-5.06	97.33	111.00
1	A	102	ILE	O-C-N	-5.05	114.62	122.70
5	K	97	TRP	C-N-CA	5.05	132.90	122.30
8	N	96	GLY	O-C-N	5.04	130.77	122.70
1	C	404	GLY	O-C-N	-5.04	114.64	122.70
3	H	119	LYS	O-C-N	5.03	130.75	122.70
1	B	148	LEU	C-N-CA	5.03	134.28	121.70
2	E	277	ILE	N-CA-C	-5.03	97.42	111.00
2	F	175	PRO	C-N-CA	5.03	134.28	121.70
5	K	108	PHE	N-CA-C	-5.03	97.43	111.00
1	B	151	PRO	O-C-N	5.01	130.72	122.70
2	E	418	PHE	C-N-CA	5.00	134.20	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 [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2307	0	654	0	0
1	B	2307	0	654	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	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

All (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
1	C	303	ILE
1	C	305	VAL
1	C	466	GLU
1	C	556	GLU
2	D	298	ALA
2	D	327	ASP
2	E	354	PRO
2	E	419	GLU
2	F	354	PRO
6	L	69	PRO
7	M	4	ASP
8	N	637	GLU
9	P	5	ALA
9	R	6	ALA
1	A	64	VAL
1	A	70	PRO
1	A	152	ASP
1	A	302	SER
1	A	326	SER
1	A	480	GLU
1	B	210	ARG
1	B	232	SER
1	B	233	GLY
1	B	512	ALA
1	C	28	CYS
1	C	159	GLU
1	C	340	ARG
1	C	417	ARG
1	C	443	VAL
2	D	15	SER
2	D	139	ASP

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Mol	Chain	Res	Type
2	D	140	VAL
2	D	192	ALA
2	D	389	GLY
2	E	340	SER
2	F	117	LEU
2	F	210	ARG
2	F	227	PRO
2	F	293	THR
2	F	330	GLY
2	F	396	VAL
3	G	14	ALA
3	H	14	ALA
3	H	131	LEU
3	H	162	GLN
3	H	178	MET
5	K	70	PHE
5	K	117	VAL
5	K	168	VAL
6	L	66	ARG
6	L	75	ALA
8	N	38	ALA
8	N	169	ALA
8	N	181	LYS
8	N	544	ILE
9	V	4	ALA
1	A	232	SER
1	A	256	GLY
1	A	278	GLY
1	A	317	GLY
1	B	106	VAL
1	B	284	ARG
1	B	417	ARG
1	B	494	PHE
1	B	551	ALA
1	C	57	GLY
1	C	88	GLN
1	C	255	CYS
1	C	302	SER
1	C	304	TYR
2	D	66	LEU
2	E	17	PRO
2	E	23	ASN

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Mol	Chain	Res	Type
2	E	49	GLU
2	E	137	THR
2	E	239	LEU
2	E	298	ALA
2	E	403	ALA
2	F	90	GLY
2	F	164	ALA
2	F	213	ALA
2	F	259	ASP
2	F	326	PRO
2	F	364	ASN
2	F	372	ARG
3	G	156	GLY
5	K	65	LEU
5	K	180	GLN
5	K	210	GLY
6	L	5	ALA
9	P	7	SER
9	R	5	ALA
9	V	5	ALA
9	Z	8	GLY
1	A	36	VAL
1	A	48	PHE
1	A	57	GLY
1	A	81	ASN
1	A	193	ARG
1	A	282	MET
1	A	403	VAL
1	A	506	TYR
1	B	565	GLU
1	C	110	ALA
1	C	245	SER
1	C	288	ILE
1	C	295	PRO
1	C	344	MET
1	C	397	GLN
1	C	413	LEU
1	C	467	ILE
2	D	128	GLU
2	D	175	PRO
2	D	351	PRO
2	D	405	THR

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Mol	Chain	Res	Type
2	E	24	ALA
2	E	166	GLN
2	F	77	GLU
2	F	97	GLY
3	G	120	ALA
3	G	132	GLU
3	H	161	THR
4	I	81	THR
5	K	116	PRO
5	K	134	ALA
6	L	15	LEU
6	L	55	PRO
8	N	363	VAL
8	N	586	ALA
9	S	8	GLY
1	A	88	GLN
1	A	113	ARG
1	A	277	THR
1	B	36	VAL
1	B	202	ASN
1	B	563	PHE
1	C	25	TYR
1	C	394	PRO
1	C	395	VAL
2	D	362	MET
2	D	383	TYR
2	D	437	GLN
2	E	278	PRO
2	E	362	MET
2	E	435	SER
2	F	63	THR
2	F	168	ALA
2	F	223	LYS
3	G	5	GLU
3	G	13	GLU
3	G	138	ARG
3	H	174	ALA
4	I	119	LEU
4	J	81	THR
5	K	174	ALA
6	L	52	LEU
8	N	75	PRO

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Mol	Chain	Res	Type
9	X	79	ARG
1	A	384	VAL
1	A	484	ILE
1	B	259	GLY
1	B	263	THR
1	B	440	ARG
1	C	56	SER
1	C	150	PRO
2	D	436	LEU
2	E	170	GLN
5	K	153	GLU
8	N	545	TRP
1	A	12	PRO
1	A	172	VAL
2	F	99	PRO
2	F	392	ILE
3	H	159	GLY
9	P	8	GLY
1	A	443	VAL
1	A	486	VAL
2	D	354	PRO
2	E	235	PRO
8	N	340	PRO
1	A	560	PRO
2	F	105	PRO
5	K	179	ILE
1	B	265	VAL
1	B	514	GLY
1	C	40	ILE
1	C	296	VAL
2	E	332	ILE
2	F	145	VAL
8	N	449	ILE
9	U	78	GLY
1	C	236	VAL

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.