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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)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

Overall quality at a glance (i) 1

The following experimental techniques were used to determine the structure: ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 Å.

Clashscore

Ramachandran outliers

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.



158937

154571

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

4023

Mol	Chain	Length	Quality of chain	
1	А	577	8%	8%
1	В	577	93%	7%
1	С	577	92%	8%
2	D	457	93%	7%
2	Е	457	95%	5%
2	F	457	92%	8%
3	G	186	92%	6% ••
3	Н	186	93%	5% ••
4	Ι	105	16% 92%	• 5%



Mol	Chain	Length	Quality of chain	
	-	105	8%	
4	J	105	93%	• 5%
-	V	010	17%	
G	h	210	92%	7%
6	T	100	25%	70/
0		100	93%	1%
7	М	323	97%	••
-			17%	
8	Ν	652	91%	• 5%
			18%	
9	O	99	81%	19%
	- D		26%	
9	Р	99	74% 7%	19%
0		00	14%	
9	Q	99	81%	19%
9	B	99	700/	100/
5	10	55	· · · · · · · · · · · · · · · · · · ·	19%
9	S	99	80%	19%
_			20%	
9	Т	99	78%	19%
			14%	
9	U	99	80%	19%
	• •	00	34%	
9	V	99	78% .	19%
0	117	00	15%	
9	vv	99	/6% 5%	19%
9	X	99	70%	10%
			17%	13/0
9	Y	99	79%	19%
			37%	
9	Z	99	79%	19%



2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	А	577	Total C N O 2307 1154 577 576	0	0
1	В	577	Total C N O 2307 1154 577 576	0	0
1	С	577	Total C N O 2307 1154 577 576	0	0

• Molecule 1 is a protein called V-type ATP synthase alpha chain.

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	457	Total	С	Ν	0	0	0
_	Đ	101	1827	914	457	456	Ŭ	Ŭ
0	Б	457	Total	С	Ν	Ο	0	0
	E	407	1827	914	457	456	0	0
0	Б	457	Total	С	Ν	Ο	0	0
	Г	407	1827	914	457	456	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	184	Total 734	C 368	N 184	O 182	0	0
3	Н	184	Total 734	$\begin{array}{c} \mathrm{C} \\ 368 \end{array}$	N 184	O 182	0	0

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
Н	134	MET	LEU	conflict	UNP P74901
Н	171	MET	LEU	conflict	UNP P74901



Chain	Residue	Modelled	Actual	Comment	Reference
Н	178	MET	LEU	$\operatorname{conflict}$	UNP P74901

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	100	Total	С	Ν	0	0	0
-	4 1	100	399	200	100	99	Ŭ	Ű
4	Т	100	Total	\mathbf{C}	Ν	Ο	0	0
4	J	100	399	200	100	99	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	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	К	210	Total 839	C 420	N 210	O 209	0	0

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

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

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

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

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

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

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		Aton	ns		AltConf	Trace			
0	0	80	Total	С	Ν	0	0	0			
9	0	80	319	160	80	79	0	0			
0	D	80	Total	С	Ν	0	0	0			
9	1	80	319	160	80	79	0	0			
0	0	80	Total	С	Ν	0	0	0			
5	Q	00	319	160	80	79	0	0			
0	В	80	Total	С	Ν	0	0	0			
9	п	80	319	160	80	79	0	0			
9	S	80	Total	С	Ν	Ο	0	0			
3	U U	80	319	160	80	79	0	0			
9	Т	80	Total	\mathbf{C}	Ν	Ο	0	0			
5	T	00	319	160	80	79	0	0			
9	T	80	Total	\mathbf{C}	Ν	Ο	0	0			
5	0	80	319	160	80	79	0	0			
9	V	V 80	Total	\mathbf{C}	Ν	Ο	0	0			
5	v	00	319	160	80	79	0	0			
9	W	W	W	W	80	Total	\mathbf{C}	Ν	Ο	0	0
5	**	00	319	160	80	79	0	0			
9	x	80	Total	\mathbf{C}	Ν	Ο	0	0			
5		00	319	160	80	79	0	0			
9	V	80	Total	\mathbf{C}	Ν	Ο	0	0			
	T	00	319	160	80	79		Ŭ			
9	Z	7 80		\mathbf{C}	Ν	Ο	0	0			
5	L	00	319	160	80	79		U			



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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









A403 1197 F421 1211 F421 212 6428 212 A233 2223 R433 2233 R453 2233 R454 2233 R281 233 R281 233 R281 233 R281 233 R31 233 R31 233 R31 233 R31 234 R31 235 R32 234 R33 234 R33 235 R33 235 R33 235 R33 235 R33 235 R33 235 R34 856

• Molecule 3: V-type ATP synthase subunit E



• Molecule 6: V-type ATP synthase subunit F













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9721	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	35.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0415	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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		Bo	ond lengths	Bond angles			
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	1.50	8/2306~(0.3%)	1.64	13/2881~(0.5%)		
1	В	1.54	5/2306~(0.2%)	1.66	14/2881~(0.5%)		
1	С	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	Е	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	Н	1.52	2/732~(0.3%)	1.56	3/912~(0.3%)		
4	Ι	1.39	0/398	1.34	0/496		
4	J	1.32	0/398	1.48	1/496~(0.2%)		
5	Κ	1.52	3/838~(0.4%)	1.57	3/1046~(0.3%)		
6	L	1.66	0/398	1.66	0/496		
7	М	1.51	3/1278~(0.2%)	1.54	2/1596~(0.1%)		
8	Ν	1.50	5/2472~(0.2%)	1.56	7/3087~(0.2%)		
9	0	1.57	0/318	1.48	0/396		
9	Р	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	Т	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	Х	1.57	1/318~(0.3%)	1.41	0/396		
9	Y	1.64	2/318~(0.6%)	1.45	0/396		
9	Ζ	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	В	0	1
3	G	0	1
7	М	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	В	221	GLY	CA-C	-8.39	1.38	1.51
1	С	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	М	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	А	259	GLY	CA-C	-6.12	1.42	1.51
3	G	77	GLY	CA-C	6.04	1.61	1.51
1	А	389	GLY	CA-C	-6.02	1.42	1.51
1	В	388	GLY	N-CA	-6.01	1.37	1.46
8	Ν	77	PRO	N-CA	-5.89	1.37	1.47
1	А	131	GLY	CA-C	-5.80	1.42	1.51
9	Р	20	GLY	N-CA	-5.74	1.37	1.46
1	А	81	ASN	C-N	5.71	1.43	1.33
9	Т	29	GLY	N-CA	-5.66	1.37	1.46
2	F	281	ARG	C-N	5.59	1.43	1.33
1	А	387	PRO	C-N	5.57	1.43	1.33
1	А	8	LYS	C-N	5.50	1.46	1.34
1	С	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	Е	449	GLY	N-CA	-5.37	1.38	1.46
1	С	86	GLY	CA-C	-5.30	1.43	1.51
3	Н	76	ARG	C-N	5.30	1.42	1.33
1	В	163	ALA	C-N	5.29	1.42	1.33
3	G	188	GLY	CA-C	5.29	1.60	1.51
5	Κ	170	PRO	N-CA	-5.28	1.38	1.47
9	Ζ	41	GLY	N-CA	-5.25	1.38	1.46
2	F	254	LEU	N-CA	-5.25	1.35	1.46
1	В	193	ARG	C-N	-5.25	1.24	1.34
3	Н	117	GLY	CA-C	-5.23	1.43	1.51
7	М	282	GLY	CA-C	-5.22	1.43	1.51



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	17	VAL	C-N	5.21	1.42	1.33
1	А	572	GLY	CA-C	-5.21	1.43	1.51
2	D	460	GLY	CA-C	-5.19	1.43	1.51
1	С	493	ASP	C-N	5.19	1.46	1.34
1	С	21	GLY	CA-C	5.18	1.60	1.51
7	М	50	ALA	C-N	5.16	1.42	1.33
5	Κ	211	GLY	N-CA	-5.16	1.38	1.46
9	V	31	GLY	N-CA	-5.14	1.38	1.46
9	Х	30	THR	C-N	5.14	1.42	1.33
1	С	388	GLY	CA-C	-5.13	1.43	1.51
8	Ν	556	GLY	CA-C	-5.12	1.43	1.51
1	А	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	Ν	605	HIS	CA-C	-5.03	1.39	1.52
1	В	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	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	Е	180	GLU	C-N-CA	6.89	136.76	122.30
1	В	497	GLN	N-CA-C	-6.85	92.51	111.00
1	В	147	ILE	C-N-CA	6.77	138.63	121.70
1	В	9	ILE	N-CA-C	-6.68	92.96	111.00
8	Ν	517	GLY	C-N-CA	6.49	137.93	121.70
1	А	184	TYR	N-CA-C	-6.49	93.48	111.00
7	М	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	С	164	GLY	N-CA-C	-6.34	97.24	113.10
1	В	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	А	102	ILE	N-CA-C	-6.24	94.16	111.00
3	Н	159	GLY	N-CA-C	-6.21	97.56	113.10
1	А	192	ALA	C-N-CA	6.19	137.17	121.70
1	А	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	В	501	HIS	N-CA-C	-6.10	94.53	111.00
9	Т	52	PHE	C-N-CA	6.09	135.09	122.30
1	А	228	GLY	N-CA-C	-6.03	98.03	113.10
1	А	64	VAL	N-CA-C	-6.01	94.77	111.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
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	А	130	ARG	N-CA-C	-5.97	94.88	111.00
1	С	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	С	540	LEU	O-C-N	-5.79	113.43	122.70
8	Ν	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	Ν	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	А	353	TYR	N-CA-C	-5.63	95.81	111.00
1	В	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	Р	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	С	412	SER	C-N-CA	5.57	135.62	121.70
1	С	153	VAL	N-CA-C	-5.55	96.00	111.00
1	В	191	ARG	N-CA-C	-5.54	96.05	111.00
1	А	355	ALA	O-C-N	5.51	131.52	122.70
2	Е	170	GLN	O-C-N	-5.48	113.94	122.70
7	М	122	GLU	O-C-N	-5.46	113.96	122.70
1	А	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	Е	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	В	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	В	44	GLY	C-N-CA	5.35	135.08	121.70
1	А	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	Р	61	LEU	CA-C-N	5.32	131.98	117.10
1	В	111	LEU	N-CA-C	-5.31	96.67	111.00
1	А	534	VAL	N-CA-C	-5.29	96.71	111.00
9	Р	61	LEU	CA-C-O	-5.29	108.99	120.10
9	Р	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	В	229	PRO	O-C-N	5.25	131.10	122.70
2	F	$\overline{74}$	SER	N-CA-C	-5.25	96.83	111.00



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
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	Ν	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	Т	40	ALA	C-N-CA	5.15	133.12	122.30
1	В	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	Н	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	Е	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	С	272	LEU	N-CA-C	-5.06	97.33	111.00
1	А	102	ILE	O-C-N	-5.05	114.62	122.70
5	Κ	97	TRP	C-N-CA	5.05	132.90	122.30
8	Ν	96	GLY	O-C-N	5.04	130.77	122.70
1	С	404	GLY	O-C-N	-5.04	114.64	122.70
3	Н	119	LYS	O-C-N	5.03	130.75	122.70
1	В	148	LEU	C-N-CA	5.03	134.28	121.70
2	Е	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	Κ	108	PHE	N-CA-C	-5.03	97.43	111.00
1	В	151	PRO	O-C-N	5.01	130.72	122.70
2	Е	418	PHE	C-N-CA	5.00	134.20	121.70

Continued from previous page...

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	485	GLU	Mainchain
3	G	139	GLY	Peptide
7	М	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2307	0	654	0	0
1	В	2307	0	654	0	0
1	С	2307	0	654	0	0
2	D	1827	0	510	0	0
2	Е	1827	0	510	0	0
2	F	1827	0	510	0	0
3	G	734	0	191	1	0
3	Н	734	0	191	0	0
4	Ι	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	М	1279	0	357	0	0
8	N	2474	0	691	1	0
9	0	319	0	109	0	0
9	Р	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	Т	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	Х	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 asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 (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	Perce	entiles
1	А	575/577~(100%)	477~(83%)	69~(12%)	29~(5%)	2	20
1	В	575/577~(100%)	491 (85%)	64 (11%)	20~(4%)	3	25
1	С	575/577~(100%)	473 (82%)	70 (12%)	32~(6%)	2	19
2	D	455/457~(100%)	375~(82%)	63 (14%)	17 (4%)	3	24
2	Е	455/457~(100%)	365~(80%)	72 (16%)	18 (4%)	3	23
2	F	455/457~(100%)	361 (79%)	71~(16%)	23~(5%)	2	19
3	G	180/186~(97%)	159 (88%)	14 (8%)	7 (4%)	3	23
3	Н	180/186~(97%)	161 (89%)	12 (7%)	7 (4%)	3	23
4	Ι	98/105~(93%)	96~(98%)	0	2(2%)	7	38
4	J	98/105~(93%)	95~(97%)	2(2%)	1 (1%)	15	55
5	Κ	208/210~(99%)	163 (78%)	34 (16%)	11 (5%)	2	19
6	L	98/100 (98%)	72 (74%)	19 (19%)	7 (7%)	1	14
7	М	318/323~(98%)	306 (96%)	11 (4%)	1 (0%)	41	77
8	Ν	615/652~(94%)	570~(93%)	34~(6%)	11 (2%)	8	40
9	Ο	78/99~(79%)	75~(96%)	3~(4%)	0	100	100
9	Р	78/99~(79%)	73~(94%)	2 (3%)	3~(4%)	3	24
9	Q	78/99~(79%)	72 (92%)	6 (8%)	0	100	100
9	R	78/99~(79%)	75~(96%)	1 (1%)	2(3%)	5	31
9	S	78/99~(79%)	74 (95%)	3~(4%)	1 (1%)	12	48
9	Т	78/99~(79%)	76~(97%)	2 (3%)	0	100	100
9	U	78/99~(79%)	73~(94%)	4(5%)	1 (1%)	12	48
9	V	78/99~(79%)	73 (94%)	3 (4%)	2(3%)	5	31
9	W	78/99~(79%)	74 (95%)	4 (5%)	0	100	100
9	Х	78/99~(79%)	74 (95%)	3 (4%)	1 (1%)	12	48
9	Y	78/99~(79%)	72 (92%)	6 (8%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Per	rce	ntiles
9	Z	78/99~(79%)	72 (92%)	5 (6%)	1 (1%)	1	2	48
All	All	5821/6157~(94%)	5047 (87%)	577 (10%)	197 (3%)	(6	26

All (197) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	417	ARG
1	В	85	ASP
1	В	326	SER
1	С	109	HIS
1	С	210	ARG
1	С	303	ILE
1	С	305	VAL
1	С	466	GLU
1	С	556	GLU
2	D	298	ALA
2	D	327	ASP
2	Е	354	PRO
2	Е	419	GLU
2	F	354	PRO
6	L	69	PRO
7	М	4	ASP
8	Ν	637	GLU
9	Р	5	ALA
9	R	6	ALA
1	А	64	VAL
1	А	70	PRO
1	А	152	ASP
1	А	302	SER
1	А	326	SER
1	А	480	GLU
1	В	210	ARG
1	В	232	SER
1	В	233	GLY
1	В	512	ALA
1	С	28	CYS
1	С	159	GLU
1	С	340	ARG
1	С	417	ARG
1	С	443	VAL
2	D	15	SER
2	D	139	ASP



Mol	Chain	Res	Type
2	D	140	VAL
2	D	192	ALA
2	D	389	GLY
2	Е	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	Н	14	ALA
3	Н	131	LEU
3	Н	162	GLN
3	Н	178	MET
5	К	70	PHE
5	K	117	VAL
5	K	168	VAL
6	L	66	ARG
6	L	75	ALA
8	Ν	38	ALA
8	Ν	169	ALA
8	Ν	181	LYS
8	Ν	544	ILE
9	V	4	ALA
1	А	232	SER
1	А	256	GLY
1	А	278	GLY
1	А	317	GLY
1	В	106	VAL
1	B	284	ARG
1	В	417	ARG
1	B	494	PHE
1	B	551	ALA
1	С	57	GLY
1	С	88	GLN
1	C	255	CYS
1	С	302	SER
1	C	304	TYR
2	D	66	LEU
2	E	17	PRO
2	Е	23	ASN



Mol	Chain	Res	Type
2	Е	49	GLU
2	Е	137	THR
2	Е	239	LEU
2	Е	298	ALA
2	Е	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	Р	7	SER
9	R	5	ALA
9	V	5	ALA
9	Z	8	GLY
1	А	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	В	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



Mol	Chain	Res	Type
2	Е	24	ALA
2	Е	166	GLN
2	F	77	GLU
2	F	97	GLY
3	G	120	ALA
3	G	132	GLU
3	Н	161	THR
4	Ι	81	THR
5	K	116	PRO
5	К	134	ALA
6	L	15	LEU
6	L	55	PRO
8	N	363	VAL
8	Ν	586	ALA
9	S	8	GLY
1	А	88	GLN
1	А	113	ARG
1	А	277	THR
1	В	36	VAL
1	В	202	ASN
1	В	563	PHE
1	С	25	TYR
1	С	394	PRO
1	С	395	VAL
2	D	362	MET
2	D	383	TYR
2	D	437	GLN
2	Е	278	PRO
2	Е	362	MET
2	Ε	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	Ι	119	LEU
4	J	81	THR
5	K	174	ALA
6	L	52	LEU
8	N	75	PRO



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

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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 monosaccharides 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.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8017. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128



The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 128

Y Index: 135

Z Index: 179

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0415. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 510 nm^3 ; this corresponds to an approximate mass of 461 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.105 \AA^{-1}



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8017 and PDB model 5GAS. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0415 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0415).



9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0415) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.1970
А	0.8700	0.2090
В	0.8190	0.2030
С	0.8480	0.2110
D	0.8400	0.2210
Е	0.8130	0.1930
F	0.8520	0.2140
G	0.8470	0.2360
Н	0.8420	0.2400
Ι	0.7970	0.2270
J	0.8670	0.2400
К	0.7790	0.2090
L	0.7190	0.2100
М	0.7220	0.1900
Ν	0.7730	0.1890
0	0.7090	0.1440
Р	0.6080	0.1170
Q	0.7620	0.1520
R	0.7710	0.1670
S	0.7490	0.1570
Т	0.7020	0.1190
U	0.7400	0.1620
V	0.5050	0.0550
W	0.7710	0.2050
Х	0.7210	0.1280
Y	0.7680	0.1890
Z	0.5420	0.1100



