

wwPDB EM Validation Summary Report (i)

Dec 17, 2022 - 10:05 pm GMT

6ZQN PDB ID : EMDB ID EMD-11369 : Title : bovine ATP synthase monomer state 3 (combined) Spikes, T.E.; Montgomery, M.G.; Walker, J.E. Authors : Deposited on 2020-07-10 : 4.00 Å(reported) Resolution : Based on initial models 2V7Q, 2CLY :

This is a wwPDB EM Validation Summary 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. dev 43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	;	Percentile Ranks	Value
Ramachandran outliers			0.0%
Sidechain outliers			0.2%
	Worse		Better
	Percentile relativ	ve to all structures	
	Percentile relativ	ve to all EM structures	
Metric		Whole archive	EM structures

	(# Entries)	(# Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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.

Mol	Chain	Length	Quality of chain	
1	А	510	98%	·
1	В	510	98%	•
1	С	510	95%	5%
2	D	482	97%	•
2	Е	482	97%	•
2	F	482	97%	•
3	G	273	100%	
4	Н	146	90%	10%
5	Ι	50	94%	6%

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Mol	Chain	Length	Quality of chain	
6	J	66	71%	29%
7	K	75	7% 99%	·
7	L	75	99%	•
7	М	75	100%	
7	Ν	75	100%	
7	Ο	75	99%	•
7	Р	75	96%	•••
7	Q	75	99%	
7	R	75	100%	
8	S	190	98%	
9	8	66	6 2%	38%
10	a	226	• 100%	
11	d	160	96%	• •
12	f	87	95%	5%
13	g	102	77%	23%
14	j	60	80%	20%
15	b	214	97%	
16	h	76	80%	• 18%
17	k	57	63%	37%
18	е	70	80%	20%

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2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 81277 atoms, of which 41197 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	$\operatorname{protein}$	called	ATP	synthase	$\operatorname{subunit}$	alpha,	mitochondrial.	

Mol	Chain	Residues			Atom		AltConf	Trace		
1 A	501	Total	С	Η	Ν	Ο	S	0	0	
	501	7741	2405	3923	673	728	12	0	0	
1	р	502	Total	С	Η	Ν	Ο	S	0	0
	302	7760	2408	3935	674	731	12	0	0	
1 C	102	Total	С	Η	Ν	0	S	0	0	
	U	400	7488	2329	3798	652	697	12	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLU	GLN	variant	UNP P19483
А	481	GLY	SER	microheterogeneity	UNP P19483
В	1	GLU	GLN	variant	UNP P19483
В	481	GLY	SER	microheterogeneity	UNP P19483
С	1	GLU	GLN	variant	UNP P19483
С	481	GLY	SER	microheterogeneity	UNP P19483

• Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues		Atoms						Trace
2 D	л	460	Total	С	Η	Ν	0	S	0	0
	409	7163	2254	3605	605	688	11	0	0	
0	F	467	Total	С	Η	Ν	0	S	0	0
	Ľ	407	7132	2243	3593	601	684	11	0	0
0	Б	467	Total	С	Η	Ν	0	S	0	0
2 F	Г	407	7131	2243	3592	601	684	11		U

• Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
3	G	272	Total	С	Н	Ν	0	S	0	0
0	ŭ	G 212	4300	1330	2185	368	409	8	0	Ŭ



• Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
4	Н	131	Total 1940	C 609	Н 970	N 163	O 196	${S \over 2}$	0	0

• Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues		A	AltConf	Trace				
5	Ι	47	Total 764	C 237	Н 395	N 66	O 64	${ m S} { m 2}$	0	0

• Molecule 6 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
6	J	47	Total 731	C 224	Н 361	N 76	O 70	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

• Molecule 7 is a protein called ATP synthase F(0) complex subunit C2, mitochondrial.

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
7	K	74	Total	С	Η	Ν	Ο	S	0	0
1	Γ	14	1079	351	550	82	93	3	0	0
7	т	74	Total	С	Η	Ν	Ο	S	0	0
1		14	1079	351	550	82	93	3	0	0
7	М	75	Total	С	Η	Ν	Ο	S	0	0
1	111	10	1095	356	558	83	94	4	0	0
7	N	75	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
1	11	10	1096	356	559	83	94	4	0	0
7	D	74	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
1	1	14	1079	351	550	82	93	3	0	0
7	В	75	Total	С	Η	N	0	S	0	0
	10	10	1096	356	559	83	94	4	0	0

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Mol	Chain	Residues		A	Atom		AltConf	Trace		
7	0	75	Total	С	Н	Ν	Ο	S	0	0
1	1 0 15	15	1096	356	559	83	94	4	0	
7	0	75	Total	С	Н	Ν	Ο	S	0	0
1	Q	15	1096	356	559	83	94	4	0	0

• Molecule 8 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
8	S	187	Total 2989	C 915	Н 1551	N 248	O 266	S 9	0	0

• Molecule 9 is a protein called ATP synthase protein 8.

Mol	Chain	Residues		A	AltConf	Trace				
9	8	41	Total 696	C 231	Н 352	N 52	O 58	${ m S} { m 3}$	0	0

• Molecule 10 is a protein called ATP synthase subunit a.

Mol	Chain	Residues			AltConf	Trace				
10	a	226	Total 3611	C 1155	Н 1870	N 276	O 298	S 12	0	0

• Molecule 11 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
11	d	155	Total 2549	C 821	Н 1276	N 207	O 242	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
12	f	83	Total 1411	C 456	Н 718	N 120	0 114	${ m S} { m 3}$	0	0

• Molecule 13 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
13	g	79	Total 1291	C 420	H 662	N 100	0 108	S 1	0	0



• Molecule 14 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues		A	AltConf	Trace				
14	j	48	Total 828	C 267	Н 428	N 66	O 65	${ m S} { m 2}$	0	0

• Molecule 15 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
15	b	209	Total 3456	C 1095	H 1755	N 292	O 308	S 6	0	0

• Molecule 16 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
16	h	62	Total 1009	C 326	Н 495	N 87	O 99	${ m S} { m 2}$	0	0

• Molecule 17 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	k	36	Total 596	C 192	Н 307	N 47	O 48	${S \over 2}$	0	0

• Molecule 18 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
18	е	56	Total 951	C 295	Н 487	N 87	O 81	S 1	0	0

• Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues		Atoms					AltConf
10	Λ	1	Total	С	Η	Ν	Ο	Р	0
19	Л	T	43	10	12	5	13	3	0
10	В	1	Total	С	Η	Ν	Ο	Р	0
19	D	T	43	10	12	5	13	3	0
10	С	1	Total	С	Η	Ν	Ο	Р	0
19	U	T	43	10	12	5	13	3	0

• Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
20	А	1	Total Mg 1 1	0
20	В	1	Total Mg 1 1	0
20	С	1	Total Mg 1 1	0
20	D	1	Total Mg 1 1	0
20	F	1	Total Mg 1 1	0

• Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





Mol	Chain	Residues		Atoms					AltConf
91	Л	1	Total	С	Η	Ν	Ο	Р	0
21	D	1	39	10	12	5	10	2	0
91	F	1	Total	С	Η	Ν	Ο	Р	0
21	Ľ	1	39	10	12	5	10	2	0
91	Б	1	Total	С	Η	Ν	Ο	Р	0
21	Г	1	39	10	12	5	10	2	0

- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues		At	oms			AltConf
	f	1	Total	С	Η	Ο	Р	0
	1	1	185	65	101	17	2	0

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Mol	Chain	Residues		Atoms					
- 22	h	1	Total	С	Η	Ο	Р	0	
	D	1	361	123	200	34	4	0	
	h	1	Total	С	Η	Ο	Р	0	
22	D	1	361	123	200	34	4	0	

• Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf	
93	f	1	Total	С	Н	Ο	Р	0
23	1	1	210	66	122	20	2	0
- 12	f	1	Total	С	Η	0	Р	0
20	I	1	210	66	122	20	2	0

• Molecule 24 is water.

Mol	Chain	Residues	Atoms	AltConf
24	А	3	Total O 3 3	0
24	В	3	Total O 3 3	0
24	С	3	Total O 3 3	0
24	D	4	Total O 4 4	0
24	F	4	Total O 4 4	0



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: ATP synthase subunit alpha, mitochondrial



• Molecule 2: ATP synthase subunit beta, mitochondrial Chain F: 97% ALA ALA GLN GLN SER PRO PRO PRO LYS ALA ALA • Molecule 3: ATP synthase subunit gamma, mitochondrial Chain G: 100% • Molecule 4: ATP synthase subunit delta, mitochondrial Chain H: 90% 10% • Molecule 5: ATP synthase subunit epsilon, mitochondrial 8% Chain I: 94% 6% • Molecule 6: ATPase inhibitor, mitochondrial 14% Chain J: 71% 29% GLY SER GLU GLY GLY ASP ASP 20 • Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial Chain K: 99% • Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial Chain L: 99%



D1 A74 MET

• Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial





 \bullet Molecule 15: ATP synthase F(0) complex subunit B1, mitochondrial



Chain b:	97%	••
P1 K1 02 K1 20 K206	4209 GLN VAL MET	
• Molecule	16: ATP synthase-coupling factor 6, mitochondri	al
Chain h:	80%	• 18%
ASN LYS GLU LEU P6 P6 V7	R16 R41 R41 R41 R41 CVAL VAL VAL VAL VAL VAL VAL CVS CIU CVS CIU CVS CIU CVS CIU CVS CIU CVS CIU CVS CIU CVS CIU CVS CVS CVS CVS CVS CVS CVS CVS CVS CVS	
• Molecule	17: ATP synthase membrane subunit DAPIT, m	itochondrial
Chain k:	63%	37%
ALA GLY PRO GLU ALA ALA ALA ALA GLN GLN	HIE PHE 112 140 140 140 140 148 148 148 148 148 148 148 148 148 148	
• Molecule	18: ATP synthase subunit e, mitochondrial	
Chain e:	80%	20%
VAL P2 R50 D51 E52 Q53	R54 R55 B57 A15 A12 A12 A12 A12 A12 A12 A12 A12 A12 A12	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	4.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM $(4k \ge 4k)$	Depositor
Maximum map value	45.029	Depositor
Minimum map value	-26.424	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.103	Depositor
Recommended contour level	7.92	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, ADP, ATP, LHG, MG, M3L

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	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.40	0/3869	0.47	0/5220	
1	В	0.41	0/3874	0.47	0/5225	
1	С	0.41	0/3740	0.47	0/5044	
2	D	0.41	0/3616	0.47	0/4906	
2	Е	0.39	0/3596	0.47	0/4879	
2	F	0.41	0/3596	0.47	0/4879	
3	G	0.38	0/2141	0.46	0/2876	
4	Н	0.41	0/982	0.51	0/1337	
5	Ι	0.44	0/374	0.49	0/501	
6	J	0.38	0/374	0.48	0/495	
7	Κ	0.44	0/526	0.50	0/711	
7	L	0.43	0/526	0.51	0/711	
7	М	0.42	0/534	0.53	0/721	
7	Ν	0.36	0/534	0.53	0/721	
7	0	0.46	0/534	0.62	0/721	
7	Р	0.64	1/526~(0.2%)	0.65	0/711	
7	Q	0.38	0/534	0.66	1/721~(0.1%)	
7	R	0.44	0/534	0.53	0/721	
8	S	0.32	0/1455	0.45	0/1957	
9	8	0.50	0/355	0.53	0/483	
10	а	0.39	0/1779	0.50	0/2433	
11	d	0.31	0/1304	0.42	0/1768	
12	f	0.43	0/711	0.45	0/952	
13	g	0.32	0/646	0.51	0/879	
14	j	0.33	0/410	0.42	0/552	
15	b	0.33	0/1733	0.44	0/2334	
16	h	0.33	0/526	0.49	0/707	
17	k	0.29	0/294	0.41	0/395	
18	е	0.35	0/472	0.52	0/628	
All	All	0.40	1/40095~(0.0%)	0.48	1/54188~(0.0%)	



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Р	47	PHE	C-O	-8.79	1.06	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	Q	50	ALA	N-CA-CB	5.72	118.11	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	ntiles
1	А	499/510~(98%)	450 (90%)	49 (10%)	0	100	100
1	В	498/510~(98%)	453 (91%)	45 (9%)	0	100	100
1	С	479/510~(94%)	423 (88%)	56 (12%)	0	100	100
2	D	467/482~(97%)	430 (92%)	37~(8%)	0	100	100
2	Ε	465/482~(96%)	423 (91%)	42 (9%)	0	100	100
2	F	465/482~(96%)	420 (90%)	45 (10%)	0	100	100
3	G	270/273~(99%)	255~(94%)	15 (6%)	0	100	100
4	Н	129/146~(88%)	115 (89%)	14 (11%)	0	100	100
5	Ι	45/50~(90%)	45 (100%)	0	0	100	100
6	J	45/66~(68%)	41 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
7	Κ	71/75~(95%)	66~(93%)	5 (7%)	0	100	100
7	L	71/75~(95%)	70 (99%)	1 (1%)	0	100	100
7	М	72/75~(96%)	66~(92%)	6 (8%)	0	100	100
7	Ν	72/75~(96%)	67 (93%)	5 (7%)	0	100	100
7	Ο	72/75~(96%)	70 (97%)	2 (3%)	0	100	100
7	Р	71/75~(95%)	67 (94%)	3 (4%)	1 (1%)	11	46
7	Q	72/75~(96%)	69 (96%)	3 (4%)	0	100	100
7	R	72/75~(96%)	66 (92%)	6 (8%)	0	100	100
8	S	185/190~(97%)	173 (94%)	12 (6%)	0	100	100
9	8	39/66~(59%)	33 (85%)	6 (15%)	0	100	100
10	a	224/226~(99%)	195 (87%)	29 (13%)	0	100	100
11	d	153/160~(96%)	136 (89%)	17 (11%)	0	100	100
12	f	81/87~(93%)	71 (88%)	10 (12%)	0	100	100
13	g	77/102~(76%)	70 (91%)	7 (9%)	0	100	100
14	j	46/60~(77%)	44 (96%)	2 (4%)	0	100	100
15	b	207/214~(97%)	197 (95%)	10 (5%)	0	100	100
16	h	60/76~(79%)	53 (88%)	7 (12%)	0	100	100
17	k	34/57~(60%)	34 (100%)	0	0	100	100
18	е	54/70~(77%)	53~(98%)	1 (2%)	0	100	100
All	All	5095/5419~(94%)	4655 (91%)	439 (9%)	1 (0%)	100	100

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All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Р	44	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	406/412~(98%)	405 (100%)	1 (0%)	93	96
1	В	407/412~(99%)	407 (100%)	0	100	100
1	С	391/412~(95%)	391 (100%)	0	100	100
2	D	379/386~(98%)	379~(100%)	0	100	100
2	Е	377/386~(98%)	377 (100%)	0	100	100
2	F	377/386~(98%)	377 (100%)	0	100	100
3	G	230/231~(100%)	230 (100%)	0	100	100
4	Н	104/109~(95%)	104 (100%)	0	100	100
5	Ι	38/41~(93%)	38 (100%)	0	100	100
6	J	34/50~(68%)	34 (100%)	0	100	100
7	К	49/50~(98%)	49 (100%)	0	100	100
7	L	49/50~(98%)	49 (100%)	0	100	100
7	М	50/50~(100%)	50 (100%)	0	100	100
7	Ν	50/50~(100%)	50 (100%)	0	100	100
7	Ο	50/50~(100%)	49 (98%)	1 (2%)	55	73
7	Р	49/50~(98%)	49 (100%)	0	100	100
7	Q	50/50~(100%)	50 (100%)	0	100	100
7	R	50/50~(100%)	50 (100%)	0	100	100
8	S	162/165~(98%)	162 (100%)	0	100	100
9	8	41/66~(62%)	41 (100%)	0	100	100
10	a	200/200~(100%)	199 (100%)	1 (0%)	88	93
11	d	139/142~(98%)	138 (99%)	1 (1%)	84	90
12	f	72/75~(96%)	72 (100%)	0	100	100
13	g	67/83~(81%)	67 (100%)	0	100	100
14	j	42/49~(86%)	42 (100%)	0	100	100
15	b	186/190~(98%)	184 (99%)	2 (1%)	73	85
16	h	56/70~(80%)	55~(98%)	1 (2%)	59	77
17	k	31/46~(67%)	31 (100%)	0	100	100
18	е	47/59~(80%)	47 (100%)	0	100	100
All	All	4183/4370 (96%)	4176 (100%)	7 (0%)	93	96

5 of 7 residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
11	d	47	LYS
15	b	102	LYS
16	h	16	ARG
15	b	120	LYS
10	a	120	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	Ν	44	GLN
8	S	112	HIS
9	8	35	HIS
9	8	36	ASN
13	g	57	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Jol Type Chain		Dec	Tink	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
WIOI	туре	Ullaili	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	M3L	М	43	7	10,11,12	0.55	0	9,14,16	0.48	0
7	M3L	L	43	7	10,11,12	0.45	0	9,14,16	0.74	0
7	M3L	R	43	7	10,11,12	0.48	0	9,14,16	0.62	0
7	M3L	Q	43	7	10,11,12	0.50	0	9,14,16	0.50	0
7	M3L	K	43	7	10,11,12	0.48	0	9,14,16	0.53	0
7	M3L	N	43	7	10,11,12	0.40	0	9,14,16	0.55	0
7	M3L	0	43	7	10,11,12	0.38	0	9,14,16	0.65	0
7	M3L	Р	43	7	10,11,12	0.45	0	9,14,16	0.45	0



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	M3L	М	43	7	-	2/9/10/12	-
7	M3L	L	43	7	-	1/9/10/12	-
7	M3L	R	43	7	-	1/9/10/12	-
7	M3L	Q	43	7	-	1/9/10/12	-
7	M3L	K	43	7	-	1/9/10/12	-
7	M3L	N	43	7	-	1/9/10/12	-
7	M3L	0	43	7	-	3/9/10/12	-
7	M3L	Р	43	7	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	М	43	M3L	N-CA-CB-CG
7	0	43	M3L	N-CA-CB-CG
7	0	43	M3L	O-C-CA-CB
7	R	43	M3L	CG-CD-CE-NZ
7	L	43	M3L	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



Mal	Trung	Chain	Dec	Tinle	Bo	ond leng	ths	Bo	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
22	CDL	b	301	-	77,77,99	1.00	6 (7%)	83,89,111	1.12	4 (4%)
19	ATP	С	600	20	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
22	CDL	f	101	-	83,83,99	0.98	7 (8%)	89,95,111	1.11	4 (4%)
22	CDL	b	302	-	82,82,99	0.98	6 (7%)	88,94,111	1.16	<mark>5 (5%)</mark>
23	LHG	f	103	-	48,48,48	0.62	1 (2%)	51,54,54	1.22	4 (7%)
21	ADP	F	600	20	24,29,29	0.93	1 (4%)	29,45,45	1.57	4 (13%)
19	ATP	В	600	20	26,33,33	0.91	1 (3%)	31,52,52	1.61	4 (12%)
23	LHG	f	102	-	38,38,48	0.70	1 (2%)	41,44,54	1.32	5 (12%)
21	ADP	D	600	20	24,29,29	0.95	1 (4%)	29,45,45	1.61	4 (13%)
19	ATP	А	600	20	26,33,33	0.90	1 (3%)	31,52,52	1.72	5 (16%)
21	ADP	Е	600	-	24,29,29	0.94	1 (4%)	29,45,45	1.55	4 (13%)

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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	b	301	-	-	41/88/88/110	-
19	ATP	С	600	20	-	4/18/38/38	0/3/3/3
22	CDL	f	101	-	-	41/94/94/110	-
22	CDL	b	302	-	-	34/93/93/110	-
23	LHG	f	103	-	-	17/53/53/53	-
21	ADP	F	600	20	-	5/12/32/32	0/3/3/3
19	ATP	В	600	20	-	1/18/38/38	0/3/3/3
23	LHG	f	102	-	-	14/43/43/53	-
21	ADP	D	600	20	-	2/12/32/32	0/3/3/3
19	ATP	A	600	20	-	0/18/38/38	0/3/3/3
21	ADP	Е	600	_	_	5/12/32/32	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
22	b	301	CDL	OA6-CA4	-2.76	1.39	1.46

Continued on next page...



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
22	b	302	CDL	OA6-CA4	-2.75	1.39	1.46
22	f	101	CDL	OB8-CB7	2.70	1.41	1.33
22	f	101	CDL	OA6-CA4	-2.67	1.39	1.46
22	f	101	CDL	OB6-CB4	-2.64	1.40	1.46

Continued from previous page...

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
19	С	600	ATP	PB-O3B-PG	-4.64	116.89	132.83
19	А	600	ATP	PB-O3B-PG	-4.45	117.57	132.83
23	f	102	LHG	O4-P-O5	4.31	133.57	112.24
23	f	103	LHG	O4-P-O5	4.23	133.16	112.24
22	b	302	CDL	OA6-CA5-C11	4.20	120.56	111.50

There are no chirality outliers.

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	С	600	ATP	C5'-O5'-PA-O1A
21	D	600	ADP	C5'-O5'-PA-O3A
21	Е	600	ADP	PB-O3A-PA-O5'
21	Е	600	ADP	C5'-O5'-PA-O1A
21	F	600	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



























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-11369. 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: 250

Y Index: 250





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: 264

Y Index: 253

Z Index: 375

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.92. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 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 281 $\rm nm^3;$ this corresponds to an approximate mass of 254 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 0.250 ${\rm \AA^{-1}}$



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-11369 and PDB model 6ZQN. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 7.92 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 (7.92).



9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 77% 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 (7.92) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7693	0.5020
8	0.8860	0.4780
А	0.7727	0.5470
В	0.7514	0.5480
С	0.7508	0.5460
D	0.7742	0.5570
E	0.7405	0.5470
F	0.7733	0.5560
G	0.7188	0.5290
Н	0.7940	0.5060
Ι	0.7242	0.5290
J	0.5826	0.4990
K	0.7848	0.4510
L	0.8095	0.4640
М	0.8086	0.4660
Ν	0.8161	0.4710
О	0.7899	0.4680
Р	0.8114	0.4750
Q	0.7355	0.4010
R	0.7824	0.4600
S	0.6806	0.4950
a	0.8681	0.4630
b	0.8394	0.3740
d	0.8627	0.3290
е	0.7735	0.3650
f	0.8731	0.4560
g	0.9029	0.3370
h	0.7018	0.2740
j	0.8355	0.3930
k	0.7082	0.3970

0.0

1.0

