



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 7, 2016 – 06:43 PM EST

PDB ID : 5LQX
EMDB ID: : EMD-4100
Title : Structure of F-ATPase from Pichia angusta, state3
Authors : Vinothkumar, K.R.; Montgomery, M.G.; Liu, S.; Walker, J.E.
Deposited on : 2016-08-17
Resolution : 7.90 Å(reported)

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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

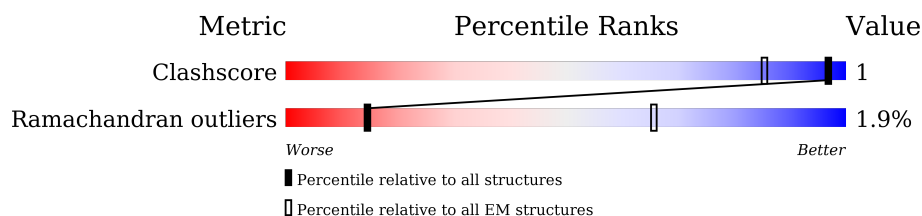
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 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.











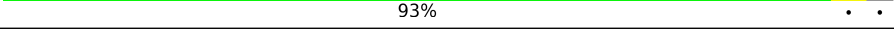


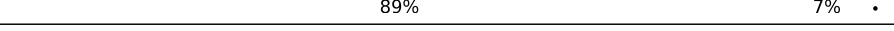



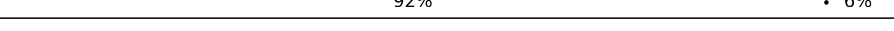
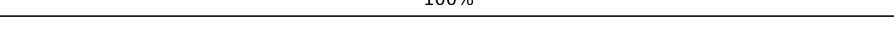


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726

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	1	31	97% .
2	2	25	100%
3	3	17	100%
4	4	27	100%
5	A	510	97% ..
5	B	510	96% ..
5	C	510	95% ..
6	D	476	97% ..
6	E	476	97% ..
6	F	476	97% ..
7	G	269	98% ..

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Mol	Chain	Length	Quality of chain
8	H	138	 86% 7% 7%
9	I	63	 90% 10%
10	J	66	 65% 35%
11	K	76	 92% . . .
11	L	76	 87% 7% 7%
11	M	76	 86% 9% 5%
11	N	76	 89% 5% 5%
11	O	76	 91% . . .
11	P	76	 93% . .
11	Q	76	 91% . . .
11	R	76	 89% 7% .
11	S	76	 89% 7% .
11	T	76	 89% . . 5%
12	U	194	 78% 6% 16%
13	V	204	 74% . 25%
14	W	155	 92% . 6%
15	X	21	 100%
16	Y	252	 46% . 52%
17	Z	44	 86% 14%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 24174 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 ATP synthase subunit f.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 2 is a protein called ATP synthase AAP1 subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 3 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 4 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	27	Total	C	N	O	0	0
			135	81	27	27		

- Molecule 5 is a protein called ATP synthase alpha subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	503	Total	C	N	O	0	0
			2469	1463	503	503		
5	B	500	Total	C	N	O	1	0
			2458	1458	500	500		
5	C	498	Total	C	N	O	0	0
			2444	1448	498	498		

- Molecule 6 is a protein called ATP synthase beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	471	Total	C	N	O	0	0
			2306	1364	471	471		
6	E	469	Total	C	N	O	0	0
			2297	1359	469	469		
6	F	470	Total	C	N	O	1	0
			2303	1363	470	470		

- Molecule 7 is a protein called ATP synthase gamma subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	267	Total	C	N	O	0	0
			1323	789	267	267		

- Molecule 8 is a protein called ATP synthase delta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	128	Total	C	N	O	0	0
			633	377	128	128		

- Molecule 9 is a protein called ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	57	Total	C	N	O	0	0
			284	170	57	57		

- Molecule 10 is a protein called ATP synthase inhibitor protein IF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	43	Total	C	N	O	0	0
			211	125	43	43		

- Molecule 11 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	73	Total	C	N	O	0	0
			356	210	73	73		
11	L	71	Total	C	N	O	0	0
			347	205	71	71		
11	M	72	Total	C	N	O	0	0
			352	208	72	72		
11	N	72	Total	C	N	O	0	0
			352	208	72	72		

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	73	Total	C	N	O	0	0
			357	211	73	73		
11	P	74	Total	C	N	O	0	0
			362	214	74	74		
11	Q	74	Total	C	N	O	0	0
			362	214	74	74		
11	R	73	Total	C	N	O	0	0
			357	211	73	73		
11	S	73	Total	C	N	O	0	0
			357	211	73	73		
11	T	72	Total	C	N	O	0	0
			352	208	72	72		

- Molecule 12 is a protein called ATP synthase OSCP subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	163	Total	C	N	O	0	0
			810	484	163	163		

- Molecule 13 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	V	154	Total	C	N	O	0	0
			767	459	154	154		

- Molecule 14 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	W	145	Total	C	N	O	0	0
			723	433	145	145		

- Molecule 15 is a protein called ATP synthase subunit h.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	21	Total	C	N	O	0	0
			105	63	21	21		

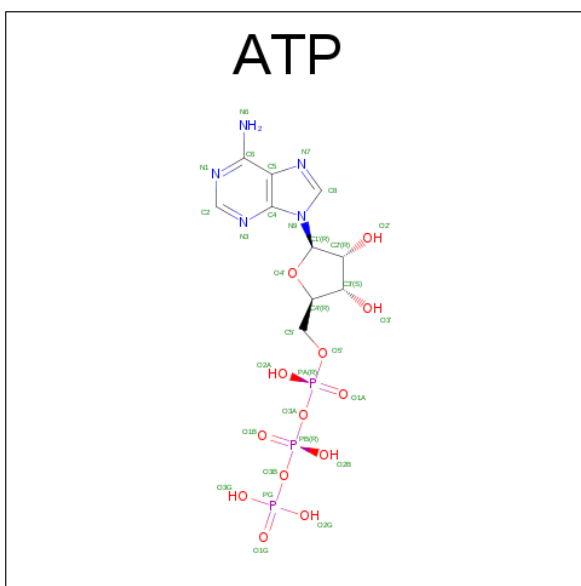
- Molecule 16 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	122	Total	C	N	O	0	0
			601	357	122	122		

- Molecule 17 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Z	44	Total	C	N	O	0	0
			220	132	44	44		

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

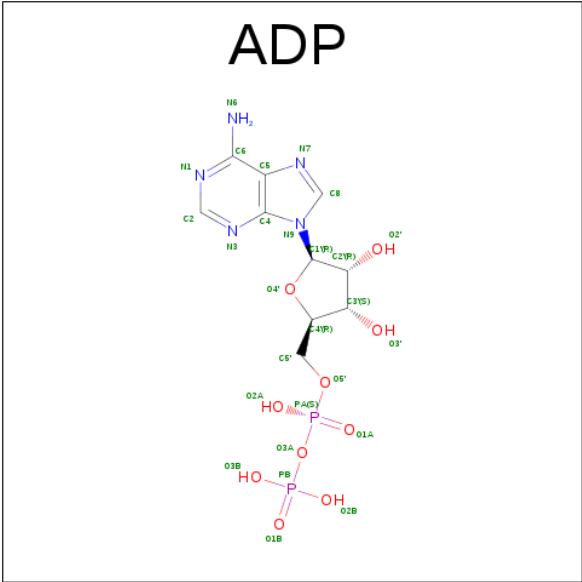


Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Mg	0
			1	1	
19	A	1	Total	Mg	0
			1	1	
19	D	1	Total	Mg	0
			1	1	
19	C	1	Total	Mg	0
			1	1	
19	F	1	Total	Mg	0
			1	1	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots [i](#)

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: ATP synthase subunit f

Chain 1:  97%



- Molecule 2: ATP synthase AAP1 subunit

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: ATP synthase subunit a

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: ATP synthase subunit b

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: ATP synthase alpha subunit

Chain A:  97%



- Molecule 5: ATP synthase alpha subunit

Chain B:  96%



- Molecule 5: ATP synthase alpha subunit

Chain C:  95%



- Molecule 6: ATP synthase beta subunit

Chain D:  97%



- Molecule 6: ATP synthase beta subunit

Chain E:  97%



- Molecule 6: ATP synthase beta subunit

Chain F:  97%




- Molecule 7: ATP synthase gamma subunit

Chain G:  98%




- Molecule 8: ATP synthase delta subunit

Chain H:  86% 7% 7%



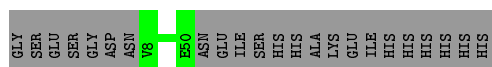
- Molecule 9: ATP synthase epsilon subunit

Chain I:  90% 10%



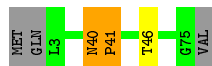
- Molecule 10: ATP synthase inhibitor protein IF1

Chain J:  65% 35%



- Molecule 11: ATP synthase subunit c

Chain K: 92%



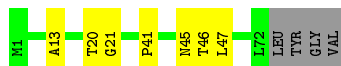
- Molecule 11: ATP synthase subunit c

Chain L: 87%



- Molecule 11: ATP synthase subunit c

Chain M: 86%



- Molecule 11: ATP synthase subunit c

Chain N: 89%



- Molecule 11: ATP synthase subunit c

Chain O: 91%



- Molecule 11: ATP synthase subunit c

Chain P: 93%



- Molecule 11: ATP synthase subunit c

Chain Q: 91%




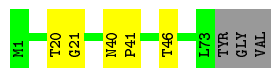
- Molecule 11: ATP synthase subunit c

Chain R:  89% 7%




- Molecule 11: ATP synthase subunit c

Chain S:  89% 7%




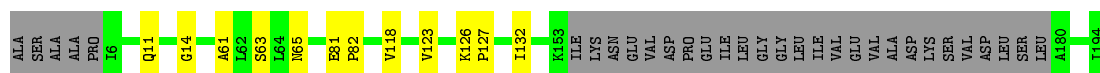
- Molecule 11: ATP synthase subunit c

Chain T:  89% 5%



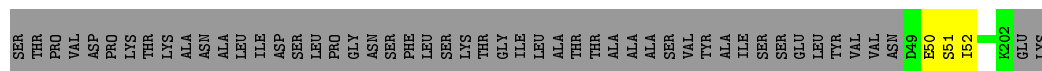
- Molecule 12: ATP synthase OSCP subunit

Chain U:  78% 6% 16%



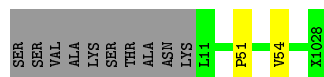
- Molecule 13: ATP synthase subunit b

Chain V:  74% 25%



- Molecule 14: ATP synthase subunit d

Chain W:  92% 6%



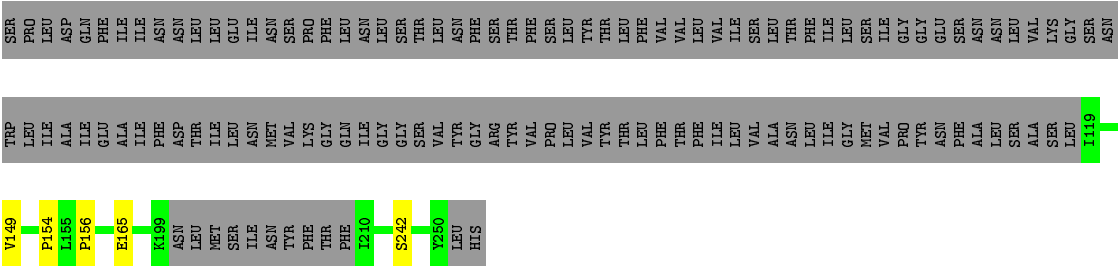
- Molecule 15: ATP synthase subunit h

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: ATP synthase subunit a

Chain Y:  46% 52%



- Molecule 17: ATP synthase subunit a

Chain Z:

86%

14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	17590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81395	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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
10	J	0.23	0/210	0.37	0/290
11	K	0.23	0/355	0.41	0/490
11	L	0.23	0/346	0.39	0/478
11	M	0.23	0/351	0.39	0/485
11	N	0.22	0/351	0.37	0/485
11	O	0.23	0/356	0.39	0/492
11	P	0.23	0/361	0.38	0/499
11	Q	0.23	0/361	0.39	0/499
11	R	0.23	0/356	0.39	0/492
11	S	0.23	0/356	0.39	0/492
11	T	0.23	0/351	0.38	0/485
12	U	0.23	0/808	0.39	0/1125
13	V	0.22	0/766	0.32	0/1069
14	W	0.22	0/581	0.38	0/809
16	Y	0.23	0/599	0.37	0/830
5	A	0.24	0/2468	0.42	0/3426
5	B	0.24	0/2459	0.43	0/3413
5	C	0.24	0/2443	0.43	0/3391
6	D	0.24	0/2305	0.43	0/3196
6	E	0.24	0/2296	0.43	0/3184
6	F	0.25	0/2305	0.43	0/3196
7	G	0.23	0/1322	0.38	0/1842
8	H	0.27	0/632	0.45	0/879
9	I	0.24	0/282	0.41	0/391
All	All	0.24	0/23020	0.41	0/31938

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	150	0	32	0	0
2	2	125	0	27	0	0
3	3	85	0	19	0	0
4	4	135	0	29	0	0
5	A	2469	0	1189	3	0
5	B	2458	0	1187	2	0
5	C	2444	0	1179	2	0
6	D	2306	0	1110	2	0
6	E	2297	0	1103	1	0
6	F	2303	0	1107	3	0
7	G	1323	0	630	0	0
8	H	633	0	316	3	0
9	I	284	0	140	0	0
10	J	211	0	116	0	0
11	K	356	0	188	1	0
11	L	347	0	183	2	0
11	M	352	0	188	4	0
11	N	352	0	188	1	0
11	O	357	0	190	2	0
11	P	362	0	192	0	0
11	Q	362	0	192	2	0
11	R	357	0	190	2	0
11	S	357	0	190	2	0
11	T	352	0	185	2	0
12	U	810	0	362	1	0
13	V	767	0	369	1	0
14	W	723	0	296	0	0
15	X	105	0	23	0	0
16	Y	601	0	279	1	0
17	Z	220	0	48	5	0
18	A	31	0	12	0	0
19	A	1	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	1	0	0	0	0
19	F	1	0	0	0	0
20	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	27	0	12	0	0
20	D	27	0	12	0	0
20	E	27	0	12	0	0
20	F	27	0	12	0	0
All	All	24174	0	11519	34	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 1.

All (34) 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)
16:Y:242:SER:CB	17:Z:1020:UNK:CB	2.64	0.76
17:Z:1025:UNK:O	17:Z:1027:UNK:N	2.39	0.56
17:Z:1025:UNK:C	17:Z:1027:UNK:N	2.69	0.55
12:U:63:SER:O	12:U:65:ASN:N	2.42	0.52
8:H:30:VAL:HA	8:H:59:VAL:HA	1.92	0.52
17:Z:1017:UNK:O	17:Z:1021:UNK:CB	2.60	0.50
17:Z:1025:UNK:O	17:Z:1026:UNK:C	2.59	0.50
5:B:53:GLU:HA	5:B:96:ILE:HA	1.94	0.48
5:C:271:ASP:HA	5:C:272:ASP:HA	1.54	0.47
6:F:257:ASP:HA	6:F:258:ASN:HA	1.57	0.47
5:B:271:ASP:HA	5:B:272:ASP:HA	1.53	0.46
6:D:257:ASP:HA	6:D:258:ASN:HA	1.53	0.45
5:A:364:ARG:HA	5:A:365:PRO:HA	1.82	0.44
11:R:21:GLY:HA3	11:S:20:THR:HA	2.00	0.44
11:L:21:GLY:HA3	11:M:20:THR:HA	2.00	0.43
5:A:271:ASP:HA	5:A:272:ASP:HA	1.54	0.43
5:A:292:GLY:N	5:A:296:TYR:O	2.52	0.43
11:Q:21:GLY:HA3	11:R:20:THR:HA	2.01	0.43
6:E:257:ASP:HA	6:E:258:ASN:HA	1.52	0.43
13:V:50:GLU:O	13:V:52:ILE:N	2.52	0.43
6:F:49:LEU:HA	6:F:64:ALA:HA	1.99	0.43
8:H:34:ALA:HA	8:H:52:LEU:HA	2.01	0.42
11:K:40:ASN:HA	11:K:41:PRO:HA	1.90	0.42
11:Q:40:ASN:HA	11:Q:41:PRO:HA	1.85	0.42
11:O:40:ASN:HA	11:O:41:PRO:HA	1.75	0.42
11:S:21:GLY:HA3	11:T:20:THR:HA	2.02	0.42
11:L:15:ALA:HB2	11:M:13:ALA:HA	2.02	0.41
11:T:40:ASN:HA	11:T:41:PRO:HA	1.82	0.41
5:C:53:GLU:HA	5:C:96:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:346:TYR:HA	6:D:347:PRO:HA	1.81	0.41
11:M:45:ASN:O	11:M:47:LEU:N	2.53	0.41
8:H:40:GLY:N	11:O:39:ARG:O	2.47	0.40
6:F:346:TYR:HA	6:F:347:PRO:HA	1.83	0.40
11:M:21:GLY:HA3	11:N:20:THR:HA	2.03	0.40

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	Percentiles	
5	A	501/510 (98%)	446 (89%)	51 (10%)	4 (1%)	24	69
5	B	497/510 (98%)	444 (89%)	49 (10%)	4 (1%)	24	69
5	C	496/510 (97%)	446 (90%)	43 (9%)	7 (1%)	14	58
6	D	469/476 (98%)	432 (92%)	31 (7%)	6 (1%)	15	60
6	E	467/476 (98%)	425 (91%)	35 (8%)	7 (2%)	13	57
6	F	469/476 (98%)	426 (91%)	39 (8%)	4 (1%)	21	67
7	G	265/269 (98%)	240 (91%)	21 (8%)	4 (2%)	13	57
8	H	126/138 (91%)	104 (82%)	18 (14%)	4 (3%)	5	41
9	I	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
10	J	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
11	K	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	3	34
11	L	69/76 (91%)	63 (91%)	3 (4%)	3 (4%)	3	34
11	M	70/76 (92%)	66 (94%)	2 (3%)	2 (3%)	6	43
11	N	70/76 (92%)	66 (94%)	1 (1%)	3 (4%)	3	34
11	O	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	3	34
11	P	72/76 (95%)	66 (92%)	3 (4%)	3 (4%)	3	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Q	72/76 (95%)	65 (90%)	3 (4%)	4 (6%)	2	28
11	R	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	3	34
11	S	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	3	34
11	T	70/76 (92%)	64 (91%)	3 (4%)	3 (4%)	3	34
12	U	159/194 (82%)	116 (73%)	33 (21%)	10 (6%)	2	25
13	V	152/204 (74%)	146 (96%)	5 (3%)	1 (1%)	26	71
14	W	113/155 (73%)	108 (96%)	3 (3%)	2 (2%)	11	53
16	Y	118/252 (47%)	104 (88%)	10 (8%)	4 (3%)	5	40
All	All	4633/5059 (92%)	4175 (90%)	371 (8%)	87 (2%)	14	52

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	60	PRO
11	K	41	PRO
11	L	41	PRO
11	M	41	PRO
11	Q	41	PRO
11	R	41	PRO
11	S	41	PRO
11	T	41	PRO
12	U	81	GLU
12	U	126	LYS
12	U	127	PRO
14	W	51	PRO
16	Y	149	VAL
16	Y	154	PRO
16	Y	156	PRO
5	B	8	PRO
5	C	147	PRO
6	D	323	PRO
6	E	340	ILE
6	F	42	GLY
6	F	323	PRO
11	M	46	THR
12	U	82	PRO
12	U	118	VAL
12	U	132	ILE
13	V	51	SER

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Mol	Chain	Res	Type
5	A	70	PRO
5	B	12	SER
5	B	24	GLU
5	C	21	VAL
5	C	24	GLU
6	E	323	PRO
6	E	341	SER
6	F	163	GLY
8	H	23	THR
8	H	62	SER
11	L	46	THR
11	N	46	THR
11	O	41	PRO
11	O	46	THR
11	Q	2	GLN
11	Q	46	THR
11	R	46	THR
11	S	46	THR
11	T	46	THR
12	U	11	GLN
12	U	14	GLY
12	U	123	VAL
16	Y	165	GLU
5	A	159	VAL
6	E	145	LEU
11	K	40	ASN
11	K	46	THR
11	L	40	ASN
11	N	41	PRO
11	O	40	ASN
11	P	40	ASN
11	P	41	PRO
11	P	46	THR
11	Q	40	ASN
11	R	40	ASN
11	S	40	ASN
11	T	40	ASN
12	U	61	ALA
5	C	69	GLU
6	D	82	ALA
6	D	225	GLU
6	E	82	ALA

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Mol	Chain	Res	Type
6	E	225	GLU
6	F	221	GLY
7	G	183	PRO
7	G	196	ILE
11	N	40	ASN
5	A	69	GLU
5	C	70	PRO
5	C	204	VAL
6	D	221	GLY
8	H	16	ALA
5	A	204	VAL
5	C	140	PRO
6	D	163	GLY
7	G	164	VAL
8	H	17	PRO
5	B	263	GLY
6	D	83	PRO
6	E	16	VAL
14	W	54	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](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
18	ATP	A	600	19	26,33,33	0.97	1 (3%)	26,52,52	1.62	1 (3%)
20	ADP	B	600	19	24,29,29	0.99	1 (4%)	23,45,45	1.69	1 (4%)
20	ADP	C	600	19	24,29,29	0.99	1 (4%)	23,45,45	1.69	1 (4%)
20	ADP	D	600	19	24,29,29	0.99	1 (4%)	23,45,45	1.68	1 (4%)
20	ADP	E	600	-	24,29,29	0.98	1 (4%)	23,45,45	1.70	1 (4%)
20	ADP	F	600	19	24,29,29	0.98	1 (4%)	23,45,45	1.68	1 (4%)

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
18	ATP	A	600	19	-	0/18/38/38	0/3/3/3
20	ADP	B	600	19	-	0/12/32/32	0/3/3/3
20	ADP	C	600	19	-	0/12/32/32	0/3/3/3
20	ADP	D	600	19	-	0/12/32/32	0/3/3/3
20	ADP	E	600	-	-	0/12/32/32	0/3/3/3
20	ADP	F	600	19	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	600	ADP	C5-C4	3.10	1.47	1.40
20	E	600	ADP	C5-C4	3.12	1.47	1.40
20	C	600	ADP	C5-C4	3.12	1.47	1.40
20	B	600	ADP	C5-C4	3.13	1.47	1.40
20	D	600	ADP	C5-C4	3.13	1.47	1.40
18	A	600	ATP	C5-C4	3.13	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	600	ADP	N3-C2-N1	-6.59	123.69	128.87
20	E	600	ADP	N3-C2-N1	-6.58	123.70	128.87
20	B	600	ADP	N3-C2-N1	-6.55	123.72	128.87
20	F	600	ADP	N3-C2-N1	-6.55	123.72	128.87
20	D	600	ADP	N3-C2-N1	-6.52	123.75	128.87
18	A	600	ATP	N3-C2-N1	-6.52	123.75	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	W	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	127:SER	C	1001:UNK	N	4.70
1	W	12:ASP	C	13:TRP	N	4.53