



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 08:36 AM EDT

PDB ID : 5LQZ  
EMDB ID: : EMD-4102  
Title : Structure of F-ATPase from Pichia angusta, state1  
Authors : Vinothkumar, K.R.; Montgomery, M.G.; Liu, S.; Walker, J.E.  
Deposited on : unknown  
Resolution : 7.00 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](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

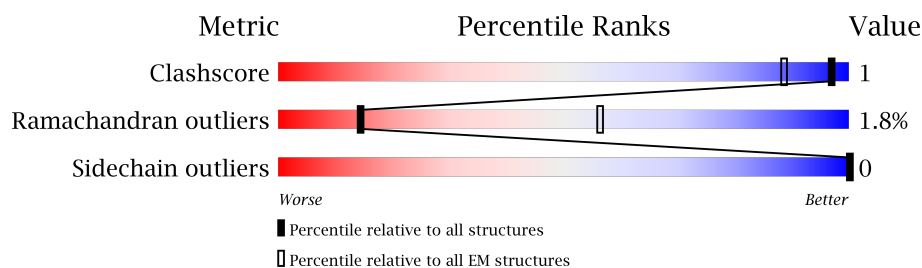
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.00 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.



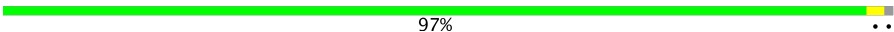
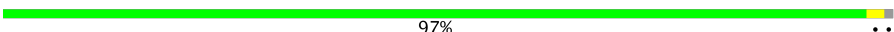














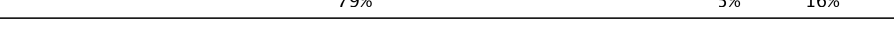
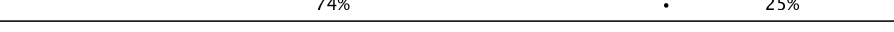

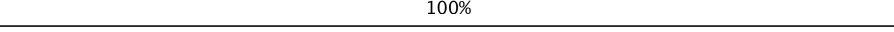

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	30	100%
2	2	25	100%
3	3	17	100%
4	4	27	100%
5	A	510	97% ..
5	B	510	95% . .
5	C	510	97% ..
6	D	476	97% ..
6	E	476	96% ..

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Mol	Chain	Length	Quality of chain
6	F	476	 97% ..
7	G	269	 97% ..
8	H	138	 88% 5% 7% ..
9	I	63	 90% 10% ..
10	J	66	 65% 35% ..
11	K	76	 92% . .
11	L	76	 88% 5% 7% ..
11	M	76	 86% 9% 5% ..
11	N	76	 89% 5% 5% ..
11	O	76	 92% . . .
11	P	76	 93% . .
11	Q	76	 92% 5% .
11	R	76	 92% . .
11	S	76	 92% . . .
11	T	76	 91% . . 5% ..
12	U	194	 79% 5% 16% ..
13	V	204	 74% . 25% ..
14	W	155	 92% . 6% ..
15	X	21	 100%
16	Y	252	 46% . 52% ..
17	Z	44	 84% 16%

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 24199 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 subunit AAP1.

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	506	Total	C	N	O	0	0
			2484	1472	506	506		
5	B	492	Total	C	N	O	0	0
			2415	1431	492	492		
5	C	503	Total	C	N	O	0	0
			2469	1463	503	503		

- 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	0	0
			2301	1361	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
			359	213	73	73		
11	L	71	Total	C	N	O	0	0
			350	208	71	71		
11	M	72	Total	C	N	O	0	0
			355	211	72	72		
11	N	72	Total	C	N	O	0	0
			355	211	72	72		

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	73	Total	C	N	O	0	0
			360	214	73	73		
11	P	74	Total	C	N	O	0	0
			365	217	74	74		
11	Q	74	Total	C	N	O	0	0
			365	217	74	74		
11	R	73	Total	C	N	O	0	0
			360	214	73	73		
11	S	73	Total	C	N	O	0	0
			360	214	73	73		
11	T	72	Total	C	N	O	0	0
			355	211	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		

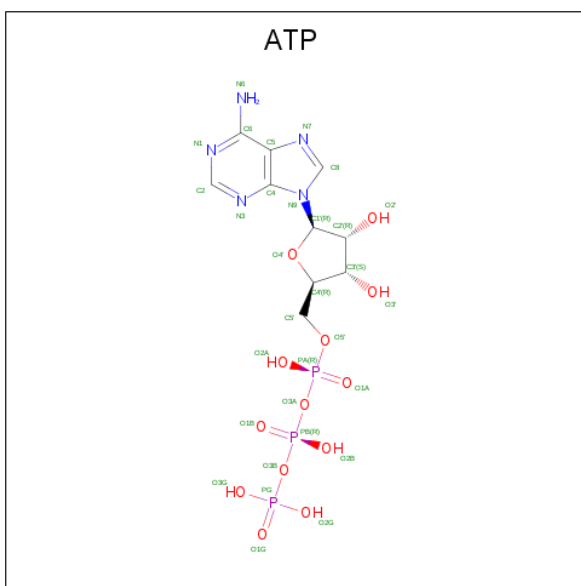
- Molecule 16 is a protein called ATP synthase subunit a.

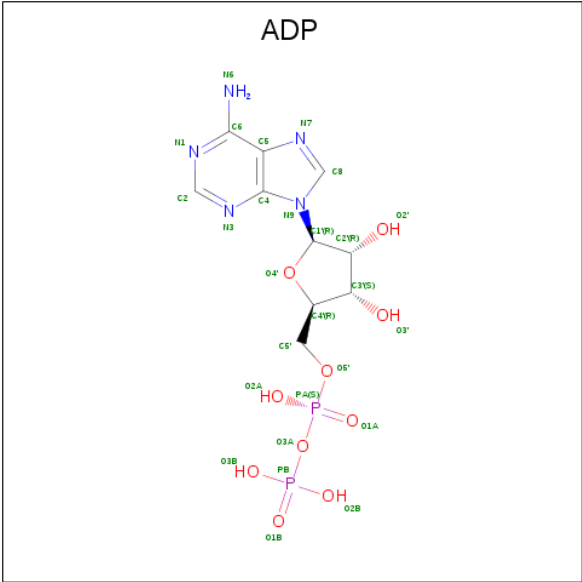
Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	122	Total	C	N	O	0	0
			601	357	122	122		

- 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
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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP synthase subunit f

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: ATP synthase subunit AAP1

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%



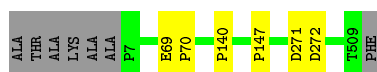
- Molecule 5: ATP synthase alpha subunit

Chain B:  95%



- Molecule 5: ATP synthase alpha subunit

Chain C:  97%



- Molecule 6: ATP synthase beta subunit

Chain D: 97% ..



- Molecule 6: ATP synthase beta subunit

Chain E: 96% ..



- Molecule 6: ATP synthase beta subunit

Chain F: 97% ..



- Molecule 7: ATP synthase gamma subunit

Chain G: 97% ..



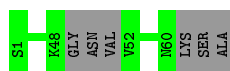
- Molecule 8: ATP synthase delta subunit

Chain H: 88% 5% 7%



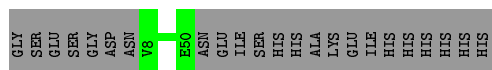
- Molecule 9: ATP synthase epsilon subunit

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:  88% 5% 7%



- Molecule 11: ATP synthase subunit c

Chain M:  86% 9% 5%



- Molecule 11: ATP synthase subunit c

Chain N:  89% 5% 5%



- Molecule 11: ATP synthase subunit c

Chain O:  92% . .



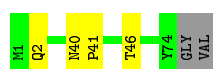
- Molecule 11: ATP synthase subunit c

Chain P:  93% . .



- Molecule 11: ATP synthase subunit c

Chain Q:  92% 5% .



- Molecule 11: ATP synthase subunit c

Chain R:  92%



- Molecule 11: ATP synthase subunit c

Chain S:  92%




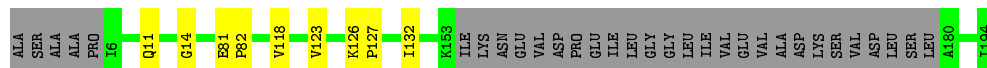
- Molecule 11: ATP synthase subunit c

Chain T:  91%



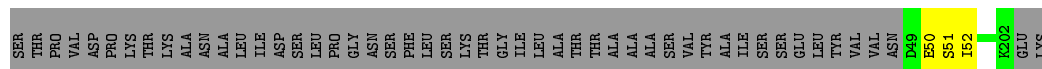
- Molecule 12: ATP synthase OSCP subunit

Chain U:  79%



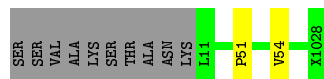
- Molecule 13: ATP synthase subunit b

Chain V:  74%



- Molecule 14: ATP synthase subunit d

Chain W:  92%



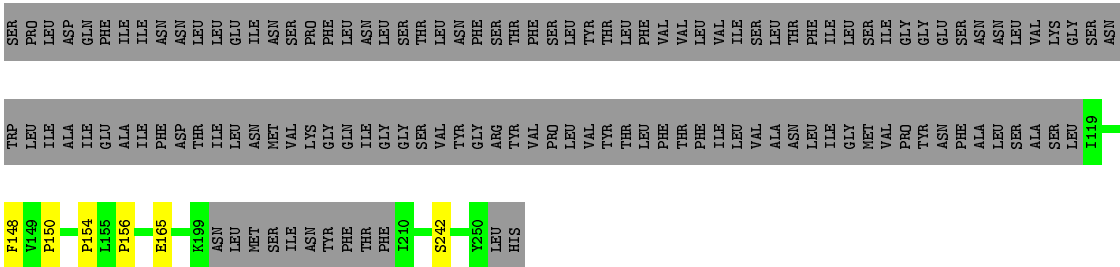
- Molecule 15: ATP synthase subunit h

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: ATP synthase subunit a

Chain Y:  46%



- Molecule 17: ATP synthase subunit a

Chain Z: 

84%

16%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF was estimated using the whole micrograph using all the frames. CTF was corrected per particle in RELION.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81395	Depositor
Image detector	FEI FALCON II (4k x 4k)	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	0.36	0/290
11	K	0.23	0/358	0.40	0/494
11	L	0.23	0/349	0.40	0/482
11	M	0.23	0/354	0.38	0/489
11	N	0.22	0/354	0.37	0/489
11	O	0.23	0/359	0.38	0/496
11	P	0.23	0/364	0.37	0/503
11	Q	0.23	0/364	0.38	0/503
11	R	0.23	0/359	0.39	0/496
11	S	0.23	0/359	0.39	0/496
11	T	0.23	0/354	0.38	0/489
12	U	0.23	0/808	0.41	0/1125
13	V	0.22	0/766	0.31	0/1069
14	W	0.23	0/582	0.38	0/812
16	Y	0.23	0/599	0.36	0/830
5	A	0.24	0/2483	0.42	0/3447
5	B	0.24	0/2413	0.43	0/3348
5	C	0.24	0/2468	0.42	0/3426
6	D	0.24	0/2305	0.42	0/3196
6	E	0.24	0/2296	0.43	0/3184
6	F	0.25	0/2300	0.43	0/3189
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	0/23040	0.41	0/31965

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	2484	0	1200	3	0
5	B	2415	0	1165	2	0
5	C	2469	0	1189	1	0
6	D	2306	0	1110	2	0
6	E	2297	0	1103	2	0
6	F	2301	0	1105	3	0
7	G	1323	0	630	1	0
8	H	633	0	316	2	0
9	I	284	0	140	0	0
10	J	211	0	116	0	0
11	K	359	0	197	0	0
11	L	350	0	192	1	0
11	M	355	0	197	3	0
11	N	355	0	197	1	0
11	O	360	0	199	1	0
11	P	365	0	201	0	0
11	Q	365	0	201	0	0
11	R	360	0	199	0	0
11	S	360	0	199	1	0
11	T	355	0	194	1	0
12	U	810	0	362	0	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	47	6	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	24199	0	11605	28	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 (28) 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)
17:Z:1017:UNK:O	17:Z:1021:UNK:CB	2.37	0.73
16:Y:242:SER:CB	17:Z:1020:UNK:CB	2.77	0.63
17:Z:1025:UNK:O	17:Z:1027:UNK:N	2.37	0.58
17:Z:1025:UNK:C	17:Z:1027:UNK:N	2.67	0.56
17:Z:1025:UNK:O	17:Z:1026:UNK:C	2.59	0.50
17:Z:1017:UNK:CB	17:Z:1028:UNK:CB	2.90	0.49
8:H:30:VAL:HA	8:H:59:VAL:HA	1.95	0.49
5:A:271:ASP:HA	5:A:272:ASP:HA	1.55	0.48
5:B:271:ASP:HA	5:B:272:ASP:HA	1.53	0.47
11:S:40:ASN:HA	11:S:41:PRO:HA	1.80	0.46
5:C:271:ASP:HA	5:C:272:ASP:HA	1.54	0.46
5:A:292:GLY:N	5:A:296:TYR:O	2.50	0.44
6:F:346:TYR:HA	6:F:347:PRO:HA	1.83	0.44
6:E:346:TYR:HA	6:E:347:PRO:HA	1.79	0.44
6:E:257:ASP:HA	6:E:258:ASN:HA	1.52	0.44
7:G:189:GLU:H	8:H:48:THR:HA	1.83	0.43
6:F:257:ASP:HA	6:F:258:ASN:HA	1.57	0.43
6:D:346:TYR:HA	6:D:347:PRO:HA	1.81	0.43
5:A:364:ARG:HA	5:A:365:PRO:HA	1.83	0.43
11:O:40:ASN:HA	11:O:41:PRO:HA	1.82	0.42
5:B:53:GLU:HA	5:B:96:ILE:HA	2.00	0.42
6:F:54:HIS:HA	6:F:60:VAL:HA	2.02	0.42
11:M:45:ASN:O	11:M:47:LEU:N	2.53	0.42
13:V:50:GLU:O	13:V:52:ILE:N	2.53	0.41
11:L:21:GLY:HA3	11:M:20:THR:HA	2.02	0.41
11:M:21:GLY:HA3	11:N:20:THR:HA	2.02	0.40
6:D:257:ASP:HA	6:D:258:ASN:HA	1.54	0.40
11:T:40:ASN:HA	11:T:41:PRO:HA	1.79	0.40

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	
5	A	504/510 (99%)	447 (89%)	51 (10%)	6 (1%)	15	57
5	B	488/510 (96%)	446 (91%)	41 (8%)	1 (0%)	51	84
5	C	501/510 (98%)	449 (90%)	48 (10%)	4 (1%)	22	67
6	D	469/476 (98%)	433 (92%)	31 (7%)	5 (1%)	17	60
6	E	467/476 (98%)	426 (91%)	34 (7%)	7 (2%)	12	53
6	F	468/476 (98%)	428 (92%)	36 (8%)	4 (1%)	20	63
7	G	265/269 (98%)	241 (91%)	19 (7%)	5 (2%)	9	47
8	H	126/138 (91%)	102 (81%)	20 (16%)	4 (3%)	5	35
9	I	53/63 (84%)	46 (87%)	7 (13%)	0	100	100
10	J	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
11	K	71/76 (93%)	66 (93%)	2 (3%)	3 (4%)	3	30
11	L	69/76 (91%)	63 (91%)	3 (4%)	3 (4%)	3	29
11	M	70/76 (92%)	67 (96%)	0	3 (4%)	3	29
11	N	70/76 (92%)	66 (94%)	1 (1%)	3 (4%)	3	29
11	O	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	3	30
11	P	72/76 (95%)	66 (92%)	3 (4%)	3 (4%)	3	30
11	Q	72/76 (95%)	66 (92%)	2 (3%)	4 (6%)	2	25
11	R	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	3	30
11	S	71/76 (93%)	66 (93%)	2 (3%)	3 (4%)	3	30
11	T	70/76 (92%)	63 (90%)	4 (6%)	3 (4%)	3	29
12	U	159/194 (82%)	122 (77%)	28 (18%)	9 (6%)	2	24
13	V	152/204 (74%)	147 (97%)	4 (3%)	1 (1%)	25	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	W	115/155 (74%)	111 (96%)	2 (2%)	2 (2%)	11	50
16	Y	118/252 (47%)	104 (88%)	9 (8%)	5 (4%)	3	30
All	All	4633/5059 (92%)	4195 (90%)	354 (8%)	84 (2%)	14	49

All (84) 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	82	PRO
12	U	126	LYS
12	U	127	PRO
16	Y	150	PRO
16	Y	154	PRO
16	Y	156	PRO
5	A	7	PRO
5	A	11	SER
5	C	147	PRO
6	E	340	ILE
6	F	323	PRO
11	M	46	THR
11	N	46	THR
12	U	118	VAL
12	U	132	ILE
13	V	51	SER
14	W	51	PRO
5	A	23	ASP
5	A	159	VAL
6	D	323	PRO
6	E	323	PRO
6	E	341	SER
8	H	23	THR
8	H	43	ALA
8	H	62	SER

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Mol	Chain	Res	Type
11	K	40	ASN
11	L	40	ASN
11	L	46	THR
11	O	46	THR
11	P	46	THR
11	Q	2	GLN
11	Q	40	ASN
11	Q	46	THR
11	R	40	ASN
11	R	46	THR
11	S	40	ASN
11	S	46	THR
12	U	11	GLN
12	U	14	GLY
12	U	123	VAL
16	Y	148	PHE
16	Y	165	GLU
5	A	26	ASN
6	F	163	GLY
6	F	221	GLY
11	K	46	THR
11	N	41	PRO
11	O	41	PRO
11	P	40	ASN
11	P	41	PRO
11	T	40	ASN
11	T	46	THR
5	C	69	GLU
6	D	82	ALA
6	D	225	GLU
6	E	82	ALA
6	E	145	LEU
6	E	225	GLU
6	F	42	GLY
7	G	183	PRO
11	N	40	ASN
6	D	221	GLY
7	G	196	ILE
8	H	63	SER
11	O	40	ASN
5	C	70	PRO
5	B	69	GLU

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Mol	Chain	Res	Type
5	C	140	PRO
6	E	16	VAL
7	G	127	VAL
7	G	164	VAL
14	W	54	VAL
5	A	204	VAL
6	D	83	PRO
11	M	40	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain 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	Percentiles	
11	K	1/55 (2%)	1 (100%)	0	100	100
11	L	1/55 (2%)	1 (100%)	0	100	100
11	M	1/55 (2%)	1 (100%)	0	100	100
11	N	1/55 (2%)	1 (100%)	0	100	100
11	O	1/55 (2%)	1 (100%)	0	100	100
11	P	1/55 (2%)	1 (100%)	0	100	100
11	Q	1/55 (2%)	1 (100%)	0	100	100
11	R	1/55 (2%)	1 (100%)	0	100	100
11	S	1/55 (2%)	1 (100%)	0	100	100
11	T	1/55 (2%)	1 (100%)	0	100	100
All	All	10/550 (2%)	10 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	27,33,33	0.96	1 (3%)	25,52,52	1.61	2 (8%)
20	ADP	B	600	19	25,29,29	0.99	1 (4%)	24,45,45	1.61	2 (8%)
20	ADP	C	600	19	25,29,29	0.99	1 (4%)	24,45,45	1.59	2 (8%)
20	ADP	D	600	19	25,29,29	0.99	1 (4%)	24,45,45	1.60	2 (8%)
20	ADP	E	600	-	25,29,29	0.99	1 (4%)	24,45,45	1.61	2 (8%)
20	ADP	F	600	19	25,29,29	0.98	1 (4%)	24,45,45	1.60	2 (8%)

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	C	600	ADP	C5-C4	3.10	1.47	1.40
20	F	600	ADP	C5-C4	3.11	1.47	1.40
20	E	600	ADP	C5-C4	3.12	1.47	1.40
18	A	600	ATP	C5-C4	3.13	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

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	600	ADP	N3-C2-N1	-5.95	123.68	128.86
20	E	600	ADP	N3-C2-N1	-5.93	123.69	128.86
20	D	600	ADP	N3-C2-N1	-5.92	123.71	128.86
18	A	600	ATP	N3-C2-N1	-5.91	123.71	128.86
20	F	600	ADP	N3-C2-N1	-5.86	123.75	128.86
20	C	600	ADP	N3-C2-N1	-5.81	123.80	128.86
20	E	600	ADP	C4-C5-N7	-2.94	106.57	109.41
20	B	600	ADP	C4-C5-N7	-2.94	106.57	109.41
20	F	600	ADP	C4-C5-N7	-2.93	106.58	109.41
20	C	600	ADP	C4-C5-N7	-2.91	106.59	109.41
20	D	600	ADP	C4-C5-N7	-2.91	106.60	109.41
18	A	600	ATP	C4-C5-N7	-2.88	106.62	109.41

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	1

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	5.36