Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Dec 28, 2016 – 06:29 AM EST

PDB ID	:	5T4Q
EMDB ID:	:	EMD-8359
Title	:	Autoinhibited E. coli ATP synthase state 3
Authors	:	Sobti, M.; Smits, C.; Wong, A.S.W.; Ishmukhametov, R.; Stock, D.; Sandin, S.; Stewart, A.G.
Deposited on	:	2016-08-29
Resolution	:	8.53 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 (i) symbol.

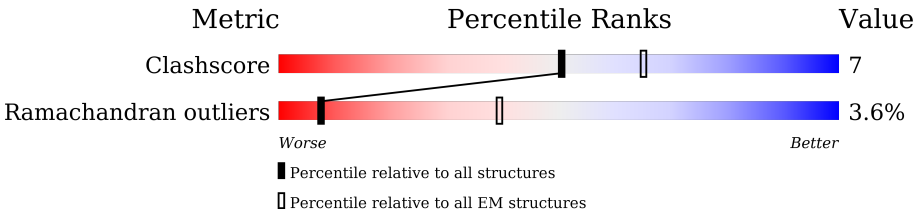
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 8.53 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	513	88% 12%
1	B	513	90% 10%
1	C	513	88% 11%
2	D	471	87% 12%
2	E	471	86% 13%
2	F	471	86% 13%
3	G	287	85% 13%
4	H	139	85% 13%
5	I	155	92% 8%
5	J	155	89% 11%
6	K	271	64% 13% 22%

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Mol	Chain	Length	Quality of chain
7	L	177	73% 18% 10%
8	M	79	80% 15% 5%
8	N	79	81% 14% 5%
8	O	79	85% 10% 5%
8	P	79	85% 10% 5%
8	Q	79	82% 13% 5%
8	R	79	78% 16% 5%
8	S	79	78% 16% 5%
8	T	79	78% 16% 5%
8	U	79	81% 14% 5%
8	V	79	78% 16% 5%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 23568 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 alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	511	Total 2507	C 1485	N 511	O 511	0	0
1	B	510	Total 2502	C 1482	N 510	O 510	0	0
1	C	508	Total 2492	C 1476	N 508	O 508	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	CYS	conflict	UNP B7MGF4
A	90	ALA	CYS	conflict	UNP B7MGF4
A	193	ALA	CYS	conflict	UNP B7MGF4
A	243	ALA	CYS	conflict	UNP B7MGF4
A	419	ASN	LYS	conflict	UNP B7MGF4
B	47	ALA	CYS	conflict	UNP B7MGF4
B	90	ALA	CYS	conflict	UNP B7MGF4
B	193	ALA	CYS	conflict	UNP B7MGF4
B	243	ALA	CYS	conflict	UNP B7MGF4
B	419	ASN	LYS	conflict	UNP B7MGF4
C	47	ALA	CYS	conflict	UNP B7MGF4
C	90	ALA	CYS	conflict	UNP B7MGF4
C	193	ALA	CYS	conflict	UNP B7MGF4
C	243	ALA	CYS	conflict	UNP B7MGF4
C	419	ASN	LYS	conflict	UNP B7MGF4

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	466	Total 2284	C 1352	N 466	O 466	0	0
2	E	466	Total 2284	C 1352	N 466	O 466	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	466	Total	C	N	O	0	0
			2284	1352	466	466		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP B7MGF2
D	-10	ARG	-	expression tag	UNP B7MGF2
D	-9	GLY	-	expression tag	UNP B7MGF2
D	-8	SER	-	expression tag	UNP B7MGF2
D	-7	HIS	-	expression tag	UNP B7MGF2
D	-6	HIS	-	expression tag	UNP B7MGF2
D	-5	HIS	-	expression tag	UNP B7MGF2
D	-4	HIS	-	expression tag	UNP B7MGF2
D	-3	HIS	-	expression tag	UNP B7MGF2
D	-2	HIS	-	expression tag	UNP B7MGF2
D	-1	GLY	-	expression tag	UNP B7MGF2
D	137	ALA	CYS	conflict	UNP B7MGF2
E	-11	MET	-	expression tag	UNP B7MGF2
E	-10	ARG	-	expression tag	UNP B7MGF2
E	-9	GLY	-	expression tag	UNP B7MGF2
E	-8	SER	-	expression tag	UNP B7MGF2
E	-7	HIS	-	expression tag	UNP B7MGF2
E	-6	HIS	-	expression tag	UNP B7MGF2
E	-5	HIS	-	expression tag	UNP B7MGF2
E	-4	HIS	-	expression tag	UNP B7MGF2
E	-3	HIS	-	expression tag	UNP B7MGF2
E	-2	HIS	-	expression tag	UNP B7MGF2
E	-1	GLY	-	expression tag	UNP B7MGF2
E	137	ALA	CYS	conflict	UNP B7MGF2
F	-11	MET	-	expression tag	UNP B7MGF2
F	-10	ARG	-	expression tag	UNP B7MGF2
F	-9	GLY	-	expression tag	UNP B7MGF2
F	-8	SER	-	expression tag	UNP B7MGF2
F	-7	HIS	-	expression tag	UNP B7MGF2
F	-6	HIS	-	expression tag	UNP B7MGF2
F	-5	HIS	-	expression tag	UNP B7MGF2
F	-4	HIS	-	expression tag	UNP B7MGF2
F	-3	HIS	-	expression tag	UNP B7MGF2
F	-2	HIS	-	expression tag	UNP B7MGF2
F	-1	GLY	-	expression tag	UNP B7MGF2
F	137	ALA	CYS	conflict	UNP B7MGF2

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	284	Total	C	N	O	0	0
			1400	832	284	284		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	ASP	GLU	conflict	UNP B7MGF3
G	87	ALA	CYS	conflict	UNP B7MGF3
G	112	ALA	CYS	conflict	UNP B7MGF3

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	136	Total	C	N	O	0	0
			668	396	136	136		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	155	Total	C	N	O	0	0
			772	462	155	155		
5	J	155	Total	C	N	O	0	0
			772	462	155	155		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	21	ALA	CYS	conflict	UNP P0ABA2
J	21	ALA	CYS	conflict	UNP P0ABA2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	211	Total	C	N	O	0	0
			1040	618	211	211		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	160	Total	C	N	O	0	0
			793	473	160	160		

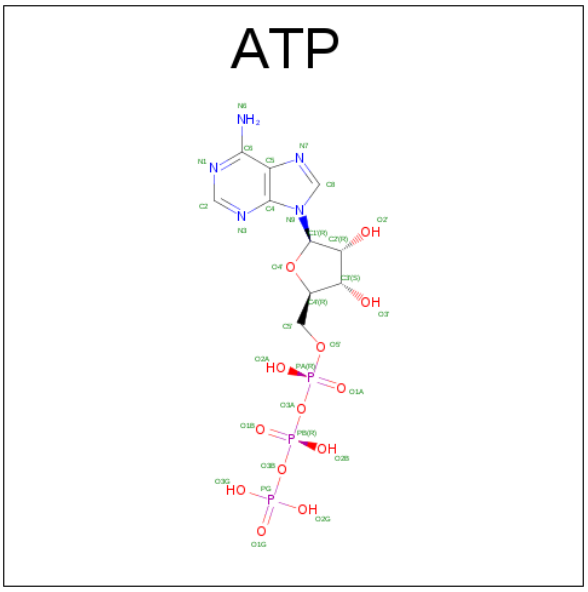
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	64	ALA	CYS	conflict	UNP B7MGF5
L	140	ALA	CYS	conflict	UNP B7MGF5

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

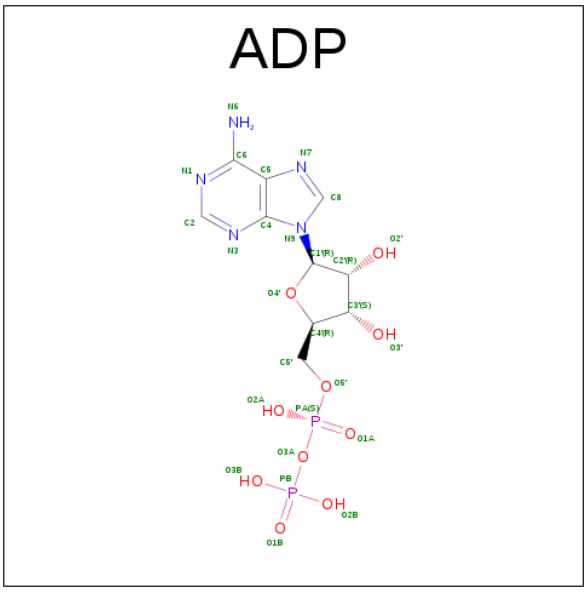
Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	75	Total	C	N	O	0	0
			365	215	75	75		
8	N	75	Total	C	N	O	0	0
			365	215	75	75		
8	O	75	Total	C	N	O	0	0
			365	215	75	75		
8	P	75	Total	C	N	O	0	0
			365	215	75	75		
8	Q	75	Total	C	N	O	0	0
			365	215	75	75		
8	R	75	Total	C	N	O	0	0
			365	215	75	75		
8	S	75	Total	C	N	O	0	0
			365	215	75	75		
8	T	75	Total	C	N	O	0	0
			365	215	75	75		
8	U	75	Total	C	N	O	0	0
			365	215	75	75		
8	V	75	Total	C	N	O	0	0
			365	215	75	75		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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



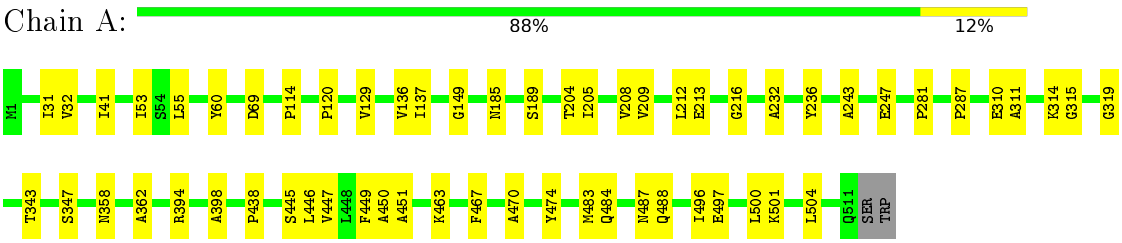
Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

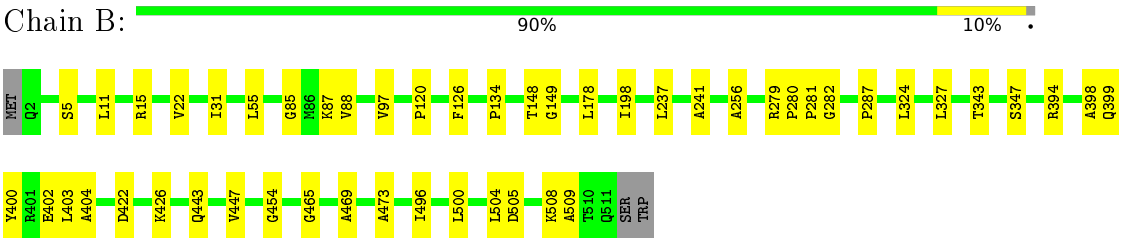
- Molecule 1: ATP synthase subunit alpha

Chain A:



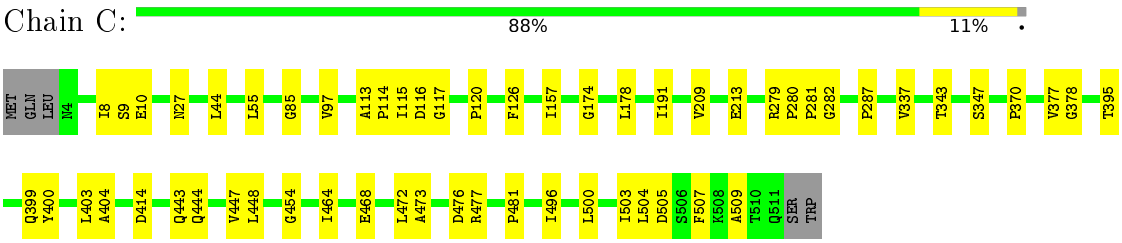
- Molecule 1: ATP synthase subunit alpha

Chain B:



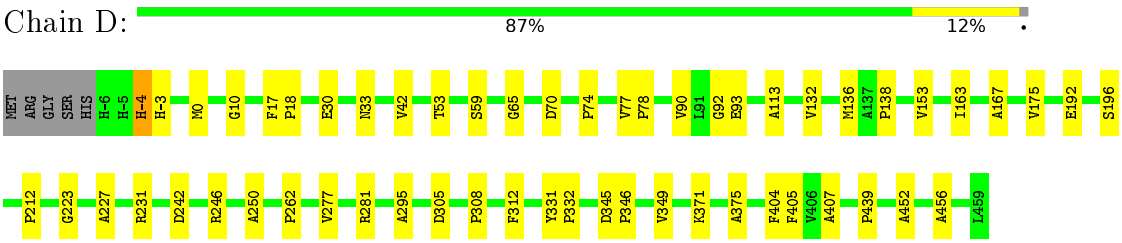
- Molecule 1: ATP synthase subunit alpha

Chain C:



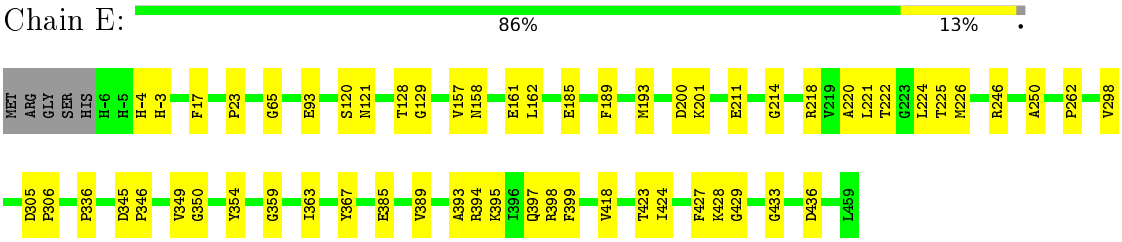
- Molecule 2: ATP synthase subunit beta

Chain D:



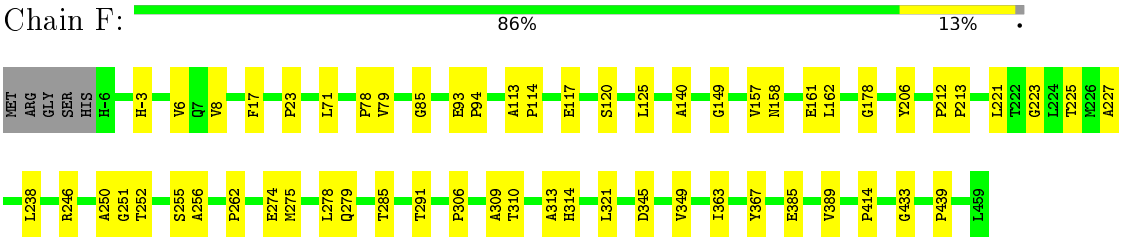
- Molecule 2: ATP synthase subunit beta

Chain E:



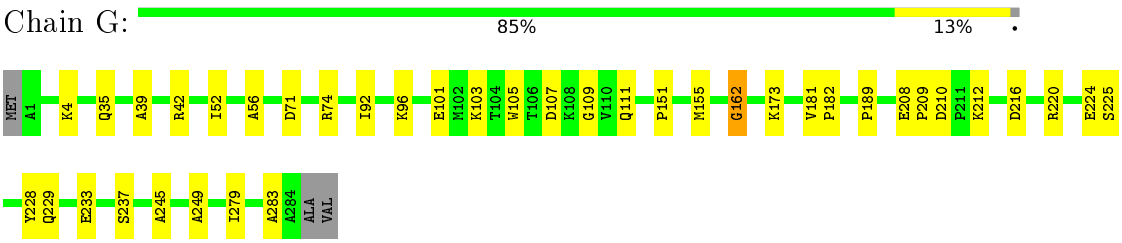
• Molecule 2: ATP synthase subunit beta

Chain F:



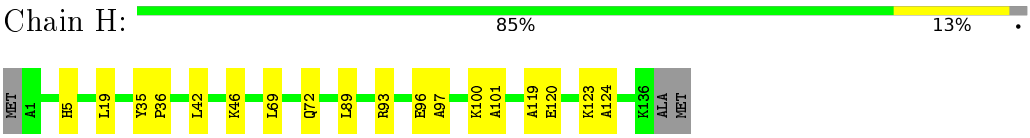
• Molecule 3: ATP synthase gamma chain

Chain G:



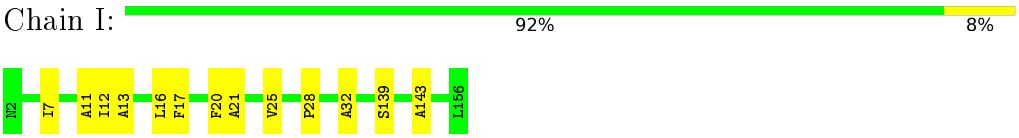
• Molecule 4: ATP synthase epsilon chain

Chain H:



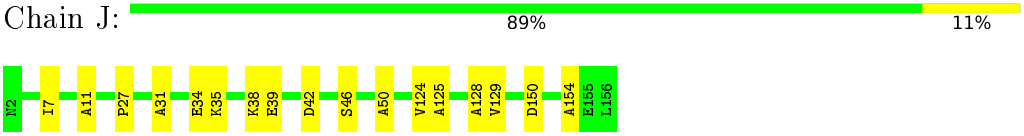
• Molecule 5: ATP synthase subunit b

Chain I:



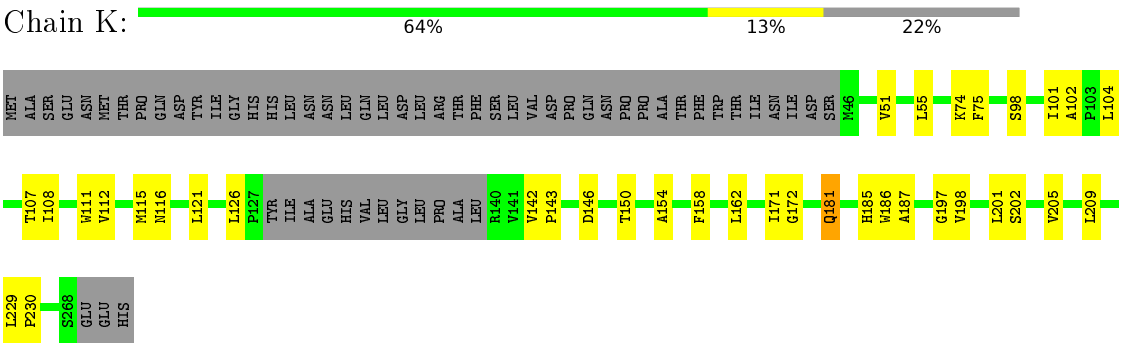
• Molecule 5: ATP synthase subunit b

Chain J:



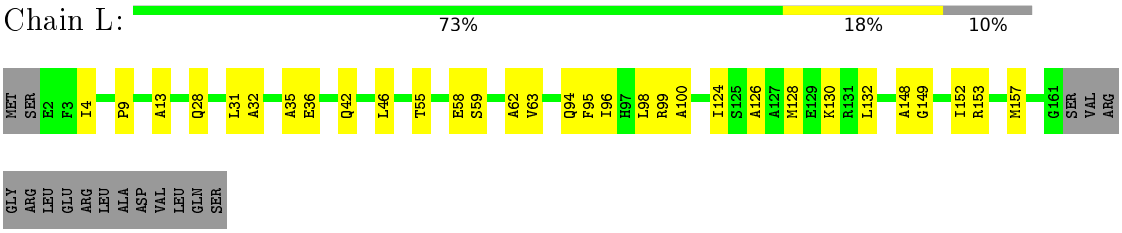
• Molecule 6: ATP synthase subunit a

Chain K:



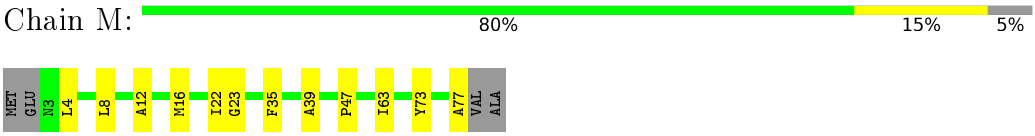
- Molecule 7: ATP synthase subunit delta

Chain L:



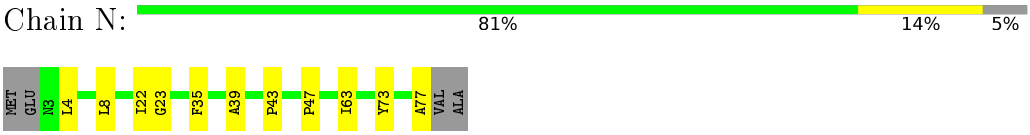
- Molecule 8: ATP synthase subunit c

Chain M:



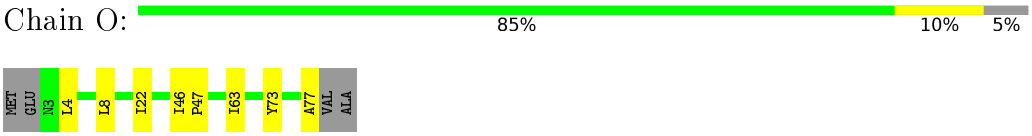
- Molecule 8: ATP synthase subunit c

Chain N:



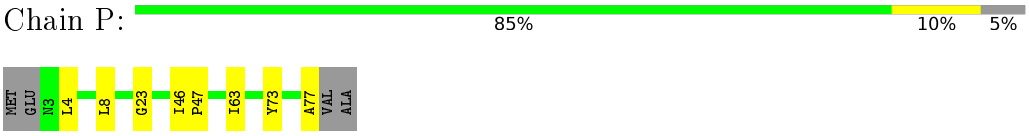
- Molecule 8: ATP synthase subunit c

Chain O:



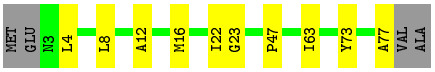
- Molecule 8: ATP synthase subunit c

Chain P:



- Molecule 8: ATP synthase subunit c

Chain Q:

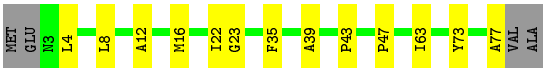


- Molecule 8: ATP synthase subunit c

Chain R:

- Molecule 8: ATP synthase subunit c

Chain S:

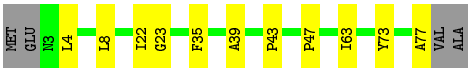


- Molecule 8: ATP synthase subunit c

Chain T:

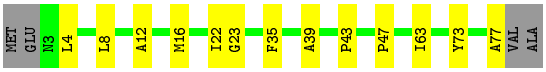
- Molecule 8: ATP synthase subunit c

Chain U:



- Molecule 8: ATP synthase subunit c

Chain V:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	95345	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 ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: 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	$\#\|Z\| > 2$
1	A	0.25	0/2506	0.43	0/3478
1	B	0.25	0/2501	0.43	0/3471
1	C	0.24	0/2491	0.43	0/3457
2	D	0.24	0/2283	0.42	0/3167
2	E	0.24	0/2283	0.43	0/3167
2	F	0.25	0/2283	0.45	0/3167
3	G	0.23	0/1399	0.39	0/1945
4	H	0.27	0/667	0.45	0/925
5	I	0.23	0/771	0.33	0/1076
5	J	0.23	0/771	0.34	0/1076
6	K	0.23	0/1038	0.41	0/1441
7	L	0.23	0/792	0.39	0/1103
8	M	0.23	0/364	0.34	0/502
8	N	0.24	0/364	0.34	0/502
8	O	0.23	0/364	0.33	0/502
8	P	0.23	0/364	0.34	0/502
8	Q	0.24	0/364	0.34	0/502
8	R	0.23	0/364	0.34	0/502
8	S	0.24	0/364	0.34	0/502
8	T	0.23	0/364	0.34	0/502
8	U	0.24	0/364	0.34	0/502
8	V	0.23	0/364	0.34	0/502
All	All	0.24	0/23425	0.41	0/32493

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2507	0	1240	23	0
1	B	2502	0	1235	20	0
1	C	2492	0	1231	20	0
2	D	2284	0	1065	16	0
2	E	2284	0	1065	24	0
2	F	2284	0	1065	23	0
3	G	1400	0	665	17	0
4	H	668	0	330	8	0
5	I	772	0	406	9	0
5	J	772	0	406	11	0
6	K	1040	0	464	18	0
7	L	793	0	407	17	0
8	M	365	0	192	7	0
8	N	365	0	192	5	0
8	O	365	0	192	3	0
8	P	365	0	192	3	0
8	Q	365	0	192	5	0
8	R	365	0	192	6	0
8	S	365	0	192	6	0
8	T	365	0	192	7	0
8	U	365	0	192	5	0
8	V	365	0	192	7	0
9	A	31	0	12	0	0
9	B	31	0	12	0	0
9	C	31	0	12	0	0
10	D	27	0	12	0	0
All	All	23568	0	11547	251	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 7.

All (251) 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)
2:E:128:THR:H	2:E:129:GLY:HA2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:58:GLU:O	7:L:62:ALA:HB3	1.91	0.71
1:C:97:VAL:O	1:C:126:PHE:HA	1.91	0.71
1:A:53:ILE:O	1:A:60:TYR:HA	1.91	0.71
5:J:124:VAL:O	5:J:128:ALA:HB3	1.94	0.68
5:J:27:PRO:O	5:J:31:ALA:HB3	1.92	0.68
2:F:238:LEU:HA	2:F:291:THR:O	1.94	0.67
1:B:237:LEU:O	1:B:241:ALA:HB3	1.96	0.65
6:K:186:TRP:H	6:K:187:ALA:C	2.00	0.65
1:A:446:LEU:O	1:A:450:ALA:HB3	2.00	0.62
2:F:309:ALA:O	2:F:313:ALA:HB3	2.00	0.62
2:D:371:LYS:O	2:D:375:ALA:HB3	1.99	0.61
2:F:178:GLY:O	2:F:206:TYR:HA	2.00	0.61
1:B:400:TYR:O	1:B:404:ALA:HB3	2.02	0.59
4:H:42:LEU:HA	4:H:69:LEU:O	2.03	0.58
1:A:394:ARG:O	1:A:398:ALA:HB3	2.03	0.58
5:I:139:SER:O	5:I:143:ALA:HB2	2.04	0.58
2:E:246:ARG:O	2:E:250:ALA:HB3	2.03	0.57
1:B:31:ILE:H	1:B:87:LYS:HA	1.71	0.56
7:L:9:PRO:O	7:L:13:ALA:HB3	2.07	0.55
2:E:128:THR:N	2:E:129:GLY:HA2	2.20	0.55
8:S:73:TYR:HA	8:S:77:ALA:HB3	1.90	0.54
5:J:150:ASP:O	5:J:154:ALA:HB3	2.07	0.54
8:Q:73:TYR:HA	8:Q:77:ALA:HB3	1.90	0.54
4:H:120:GLU:O	4:H:124:ALA:HB3	2.08	0.54
3:G:52:ILE:O	3:G:56:ALA:HB2	2.08	0.53
8:M:73:TYR:HA	8:M:77:ALA:HB3	1.90	0.53
8:U:73:TYR:HA	8:U:77:ALA:HB3	1.90	0.53
2:F:246:ARG:O	2:F:250:ALA:HB3	2.09	0.53
7:L:31:LEU:O	7:L:35:ALA:HB3	2.07	0.53
8:N:73:TYR:HA	8:N:77:ALA:HB3	1.90	0.53
8:V:73:TYR:HA	8:V:77:ALA:HB3	1.90	0.53
2:D:246:ARG:O	2:D:250:ALA:HB3	2.09	0.53
3:G:279:ILE:HA	3:G:283:ALA:HB3	1.90	0.52
1:B:256:ALA:O	1:B:324:LEU:HA	2.09	0.52
8:R:73:TYR:HA	8:R:77:ALA:HB3	1.90	0.52
8:O:73:TYR:HA	8:O:77:ALA:HB3	1.91	0.52
8:P:73:TYR:HA	8:P:77:ALA:HB3	1.91	0.52
1:B:97:VAL:O	1:B:126:PHE:HA	2.10	0.52
3:G:245:ALA:O	3:G:249:ALA:HB3	2.09	0.52
6:K:74:LYS:H	6:K:75:PHE:HA	1.75	0.51
1:A:447:VAL:O	1:A:451:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:23:GLY:HA3	8:Q:22:ILE:HA	1.93	0.51
4:H:97:ALA:O	4:H:101:ALA:HB3	2.11	0.51
8:T:73:TYR:HA	8:T:77:ALA:HB3	1.91	0.50
1:A:358:ASN:O	1:A:362:ALA:HB2	2.12	0.49
1:B:394:ARG:O	1:B:398:ALA:HB3	2.11	0.49
8:N:23:GLY:HA3	8:O:22:ILE:HA	1.94	0.49
4:H:5:HIS:HA	4:H:19:LEU:HA	1.95	0.49
1:B:465:GLY:O	1:B:469:ALA:HB3	2.13	0.48
8:S:23:GLY:HA3	8:T:22:ILE:HA	1.94	0.48
1:C:27:ASN:HA	1:C:44:LEU:HA	1.94	0.48
1:A:243:ALA:O	1:A:247:GLU:CB	2.62	0.48
1:C:116:ASP:HA	1:C:117:GLY:HA2	1.53	0.48
8:M:22:ILE:HA	8:V:23:GLY:HA3	1.96	0.48
1:C:400:TYR:O	1:C:404:ALA:HB3	2.13	0.47
2:E:200:ASP:HA	2:E:201:LYS:HA	1.53	0.47
8:Q:23:GLY:HA3	8:R:22:ILE:HA	1.95	0.47
2:D:-4:HIS:HA	2:D:-3:HIS:C	2.34	0.47
5:J:124:VAL:O	5:J:128:ALA:CB	2.62	0.47
7:L:42:GLN:O	7:L:46:LEU:CB	2.63	0.47
2:E:363:ILE:O	2:E:367:TYR:CB	2.63	0.47
5:J:7:ILE:O	5:J:11:ALA:HB3	2.14	0.47
8:U:23:GLY:HA3	8:V:22:ILE:HA	1.96	0.47
7:L:96:ILE:O	7:L:100:ALA:HB3	2.15	0.47
7:L:128:MET:O	7:L:132:LEU:CB	2.63	0.47
2:E:423:THR:O	2:E:427:PHE:CB	2.62	0.47
6:K:171:ILE:HA	6:K:172:GLY:HA3	1.69	0.46
2:D:163:ILE:O	2:D:167:ALA:HB3	2.16	0.46
2:F:310:THR:O	2:F:314:HIS:CB	2.64	0.46
6:K:74:LYS:N	6:K:75:PHE:HA	2.30	0.46
5:I:17:PHE:O	5:I:21:ALA:CB	2.64	0.46
5:I:28:PRO:O	5:I:32:ALA:HB3	2.16	0.46
1:A:314:LYS:HA	1:A:315:GLY:HA2	1.66	0.46
2:E:222:THR:O	2:E:226:MET:CB	2.64	0.46
5:J:38:LYS:O	5:J:42:ASP:CB	2.63	0.46
7:L:55:THR:O	7:L:59:SER:CB	2.63	0.46
6:K:111:TRP:O	6:K:115:MET:CB	2.64	0.46
2:E:424:ILE:O	2:E:428:LYS:CB	2.64	0.45
3:G:173:LYS:H	3:G:182:PRO:HA	1.81	0.45
2:D:227:ALA:O	2:D:231:ARG:CB	2.64	0.45
5:J:34:GLU:O	5:J:38:LYS:CB	2.65	0.45
5:I:16:LEU:O	5:I:20:PHE:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ILE:O	1:B:500:LEU:CB	2.65	0.45
2:E:395:LYS:O	2:E:399:PHE:CB	2.65	0.45
2:D:452:ALA:O	2:D:456:ALA:HB3	2.16	0.45
2:E:-4:HIS:HA	2:E:-3:HIS:HA	1.49	0.45
5:I:7:ILE:O	5:I:11:ALA:HB3	2.16	0.45
1:B:469:ALA:O	1:B:473:ALA:HB3	2.17	0.44
6:K:154:ALA:O	6:K:158:PHE:CB	2.65	0.44
6:K:198:VAL:O	6:K:202:SER:CB	2.65	0.44
1:A:497:GLU:O	1:A:501:LYS:CB	2.66	0.44
2:F:125:LEU:HA	2:F:140:ALA:HA	1.99	0.44
3:G:35:GLN:O	3:G:39:ALA:CB	2.66	0.44
1:C:157:ILE:HA	1:C:378:GLY:HA2	1.99	0.44
2:E:129:GLY:HA3	2:E:418:VAL:H	1.82	0.44
2:F:221:LEU:O	2:F:225:THR:CB	2.66	0.44
2:E:359:GLY:O	2:E:363:ILE:CB	2.66	0.44
1:C:468:GLU:O	1:C:472:LEU:CB	2.66	0.44
3:G:71:ASP:H	3:G:162:GLY:HA2	1.82	0.44
8:V:12:ALA:O	8:V:16:MET:CB	2.65	0.44
3:G:101:GLU:O	3:G:105:TRP:CB	2.65	0.44
3:G:220:ARG:O	3:G:224:GLU:CB	2.66	0.44
8:R:23:GLY:HA3	8:S:22:ILE:HA	2.00	0.44
1:A:232:ALA:O	1:A:236:TYR:CB	2.66	0.44
5:J:42:ASP:O	5:J:46:SER:CB	2.66	0.44
7:L:28:GLN:O	7:L:32:ALA:HB3	2.18	0.44
2:D:42:VAL:HA	2:D:53:THR:HA	1.99	0.44
3:G:225:SER:O	3:G:229:GLN:CB	2.66	0.44
6:K:158:PHE:O	6:K:162:LEU:CB	2.66	0.44
6:K:205:VAL:O	6:K:209:LEU:CB	2.66	0.44
7:L:149:GLY:O	7:L:153:ARG:CB	2.66	0.44
2:E:189:PHE:O	2:E:193:MET:CB	2.66	0.43
8:M:12:ALA:O	8:M:16:MET:CB	2.65	0.43
8:S:4:LEU:O	8:S:8:LEU:CB	2.66	0.43
1:C:399:GLN:O	1:C:403:LEU:CB	2.66	0.43
1:C:395:THR:O	1:C:399:GLN:CB	2.67	0.43
1:C:473:ALA:O	1:C:477:ARG:CB	2.66	0.43
8:U:4:LEU:O	8:U:8:LEU:CB	2.65	0.43
1:A:445:SER:O	1:A:449:PHE:CB	2.67	0.43
2:D:242:ASP:HA	2:D:295:ALA:HB3	2.00	0.43
2:F:252:THR:O	2:F:256:ALA:HB3	2.18	0.43
2:E:221:LEU:O	2:E:225:THR:CB	2.66	0.43
8:M:23:GLY:HA3	8:N:22:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:350:GLY:O	2:E:354:TYR:CB	2.67	0.43
2:E:394:ARG:O	2:E:398:ARG:CB	2.67	0.43
2:F:223:GLY:O	2:F:227:ALA:HB3	2.18	0.43
8:M:35:PHE:O	8:M:39:ALA:CB	2.66	0.43
1:B:465:GLY:O	1:B:469:ALA:CB	2.67	0.43
1:C:496:ILE:O	1:C:500:LEU:CB	2.67	0.43
8:N:4:LEU:O	8:N:8:LEU:CB	2.66	0.43
8:V:4:LEU:O	8:V:8:LEU:CB	2.67	0.43
1:C:472:LEU:O	1:C:476:ASP:CB	2.67	0.43
2:D:308:PRO:O	2:D:312:PHE:CB	2.67	0.43
3:G:173:LYS:CB	3:G:181:VAL:O	2.67	0.43
4:H:93:ARG:O	4:H:97:ALA:HB3	2.19	0.43
1:A:343:THR:O	1:A:347:SER:CB	2.67	0.42
2:D:30:GLU:H	2:D:70:ASP:HA	1.84	0.42
3:G:224:GLU:O	3:G:228:TYR:CB	2.67	0.42
4:H:96:GLU:O	4:H:100:LYS:CB	2.67	0.42
2:E:120:SER:HA	2:E:121:ASN:HA	1.49	0.42
5:J:35:LYS:O	5:J:39:GLU:CB	2.67	0.42
8:P:4:LEU:O	8:P:8:LEU:CB	2.67	0.42
8:S:12:ALA:O	8:S:16:MET:CB	2.67	0.42
8:V:35:PHE:O	8:V:39:ALA:CB	2.67	0.42
2:D:10:GLY:HA2	2:D:59:SER:H	1.85	0.42
6:K:104:LEU:O	6:K:108:ILE:CB	2.68	0.42
7:L:59:SER:O	7:L:63:VAL:CB	2.68	0.42
1:A:208:VAL:O	1:A:212:LEU:CB	2.68	0.42
1:B:469:ALA:O	1:B:473:ALA:CB	2.67	0.42
1:C:464:ILE:O	1:C:468:GLU:CB	2.67	0.42
6:K:146:ASP:O	6:K:150:THR:CB	2.67	0.42
2:F:246:ARG:O	2:F:250:ALA:CB	2.67	0.42
1:B:505:ASP:O	1:B:509:ALA:HB3	2.19	0.42
2:F:363:ILE:O	2:F:367:TYR:CB	2.67	0.42
5:I:17:PHE:O	5:I:21:ALA:HB3	2.20	0.42
6:K:107:THR:O	6:K:111:TRP:CB	2.68	0.42
8:O:4:LEU:O	8:O:8:LEU:CB	2.68	0.42
8:S:35:PHE:O	8:S:39:ALA:CB	2.68	0.42
3:G:151:PRO:O	3:G:155:MET:CB	2.67	0.42
8:Q:12:ALA:O	8:Q:16:MET:CB	2.68	0.42
8:T:35:PHE:O	8:T:39:ALA:CB	2.67	0.42
5:I:13:ALA:O	5:I:17:PHE:CB	2.68	0.42
6:K:197:GLY:O	6:K:201:LEU:CB	2.67	0.42
8:N:35:PHE:O	8:N:39:ALA:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:GLN:O	1:B:403:LEU:CB	2.68	0.42
1:B:422:ASP:O	1:B:426:LYS:CB	2.68	0.42
2:D:277:VAL:O	2:D:281:ARG:CB	2.68	0.42
3:G:233:GLU:O	3:G:237:SER:CB	2.68	0.42
7:L:31:LEU:O	7:L:35:ALA:CB	2.68	0.42
7:L:94:GLN:O	7:L:98:LEU:CB	2.68	0.42
8:M:4:LEU:O	8:M:8:LEU:CB	2.68	0.42
2:F:306:PRO:O	2:F:310:THR:CB	2.68	0.42
5:I:21:ALA:O	5:I:25:VAL:CB	2.68	0.42
5:J:125:ALA:O	5:J:129:VAL:CB	2.68	0.42
7:L:32:ALA:O	7:L:36:GLU:CB	2.67	0.42
8:T:35:PHE:O	8:T:39:ALA:HB3	2.20	0.42
1:A:500:LEU:O	1:A:504:LEU:CB	2.68	0.41
6:K:181:GLN:O	6:K:185:HIS:CB	2.67	0.41
7:L:126:ALA:O	7:L:130:LYS:CB	2.68	0.41
7:L:153:ARG:O	7:L:157:MET:CB	2.68	0.41
1:B:398:ALA:O	1:B:402:GLU:CB	2.68	0.41
1:C:500:LEU:O	1:C:504:LEU:CB	2.68	0.41
1:A:204:THR:O	1:A:208:VAL:CB	2.68	0.41
1:C:209:VAL:O	1:C:213:GLU:CB	2.69	0.41
2:F:385:GLU:O	2:F:389:VAL:CB	2.69	0.41
1:C:343:THR:O	1:C:347:SER:CB	2.68	0.41
2:E:157:VAL:O	2:E:161:GLU:CB	2.68	0.41
2:E:185:GLU:O	2:E:189:PHE:CB	2.68	0.41
2:F:275:MET:O	2:F:279:GLN:CB	2.68	0.41
2:F:149:GLY:HA3	2:F:321:LEU:H	1.84	0.41
8:R:35:PHE:O	8:R:39:ALA:CB	2.69	0.41
1:B:504:LEU:O	1:B:508:LYS:CB	2.69	0.41
1:A:209:VAL:O	1:A:213:GLU:CB	2.69	0.41
1:B:343:THR:O	1:B:347:SER:CB	2.69	0.41
2:D:404:PHE:H	2:D:407:ALA:HB3	1.86	0.41
3:G:103:LYS:O	3:G:107:ASP:CB	2.69	0.41
5:J:46:SER:O	5:J:50:ALA:CB	2.69	0.41
8:T:4:LEU:O	8:T:8:LEU:CB	2.68	0.41
1:A:496:ILE:O	1:A:500:LEU:CB	2.68	0.41
1:B:11:LEU:O	1:B:15:ARG:CB	2.68	0.41
1:C:444:GLN:O	1:C:448:LEU:CB	2.68	0.41
2:D:132:VAL:O	2:D:136:MET:CB	2.68	0.41
7:L:148:ALA:O	7:L:152:ILE:CB	2.68	0.41
8:Q:4:LEU:O	8:Q:8:LEU:CB	2.69	0.41
8:R:4:LEU:O	8:R:8:LEU:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:-3:HIS:HA	2:F:71:LEU:HA	2.02	0.41
6:K:51:VAL:O	6:K:55:LEU:CB	2.69	0.41
2:E:393:ALA:O	2:E:397:GLN:CB	2.68	0.41
2:F:157:VAL:O	2:F:161:GLU:CB	2.69	0.41
3:G:74:ARG:HA	3:G:111:GLN:H	1.85	0.41
8:M:35:PHE:O	8:M:39:ALA:HB3	2.20	0.41
8:V:35:PHE:O	8:V:39:ALA:HB3	2.20	0.41
1:A:185:ASN:O	1:A:189:SER:CB	2.68	0.41
1:C:8:ILE:O	1:C:10:GLU:N	2.54	0.41
2:D:192:GLU:O	2:D:196:SER:CB	2.69	0.41
2:F:274:GLU:O	2:F:278:LEU:CB	2.69	0.41
7:L:95:PHE:O	7:L:99:ARG:CB	2.69	0.41
1:A:31:ILE:HA	1:A:41:ILE:HA	2.03	0.40
1:C:503:ILE:O	1:C:507:PHE:CB	2.68	0.40
2:D:223:GLY:O	2:D:227:ALA:HB3	2.21	0.40
2:E:220:ALA:O	2:E:224:LEU:CB	2.69	0.40
2:F:251:GLY:O	2:F:255:SER:CB	2.69	0.40
4:H:97:ALA:O	4:H:101:ALA:CB	2.69	0.40
2:E:385:GLU:O	2:E:389:VAL:CB	2.69	0.40
2:F:223:GLY:O	2:F:227:ALA:CB	2.69	0.40
3:G:212:LYS:O	3:G:216:ASP:CB	2.69	0.40
6:K:150:THR:O	6:K:154:ALA:CB	2.70	0.40
8:T:23:GLY:HA3	8:U:22:ILE:HA	2.04	0.40
1:A:205:ILE:O	1:A:209:VAL:CB	2.69	0.40
1:A:463:LYS:O	1:A:467:PHE:CB	2.69	0.40
1:A:470:ALA:O	1:A:474:TYR:CB	2.69	0.40
1:A:484:GLN:O	1:A:488:GLN:CB	2.69	0.40
1:B:500:LEU:O	1:B:504:LEU:CB	2.69	0.40
2:E:158:ASN:O	2:E:162:LEU:CB	2.69	0.40
5:I:12:ILE:O	5:I:16:LEU:CB	2.69	0.40
6:K:112:VAL:O	6:K:116:ASN:CB	2.70	0.40
8:T:12:ALA:O	8:T:16:MET:CB	2.69	0.40
1:A:483:MET:O	1:A:487:ASN:CB	2.69	0.40
1:B:443:GLN:O	1:B:447:VAL:CB	2.70	0.40
1:C:505:ASP:O	1:C:509:ALA:HB2	2.21	0.40
2:F:158:ASN:O	2:F:162:LEU:CB	2.69	0.40
4:H:119:ALA:O	4:H:123:LYS:CB	2.70	0.40
6:K:108:ILE:O	6:K:112:VAL:CB	2.69	0.40
8:U:35:PHE:O	8:U:39:ALA:CB	2.70	0.40
1:C:443:GLN:O	1:C:447:VAL:CB	2.70	0.40
2:E:214:GLY:O	2:E:218:ARG:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:SER:H	2:F:285:THR:HA	1.86	0.40
2:F:309:ALA:O	2:F:313:ALA:CB	2.69	0.40
3:G:92:ILE:O	3:G:96:LYS:CB	2.69	0.40
8:R:12:ALA:O	8:R:16:MET:CB	2.69	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
1	A	509/513 (99%)	395 (78%)	98 (19%)	16 (3%)	5 42
1	B	508/513 (99%)	396 (78%)	94 (18%)	18 (4%)	4 39
1	C	506/513 (99%)	392 (78%)	93 (18%)	21 (4%)	3 34
2	D	464/471 (98%)	365 (79%)	73 (16%)	26 (6%)	2 28
2	E	464/471 (98%)	358 (77%)	90 (19%)	16 (3%)	5 40
2	F	464/471 (98%)	367 (79%)	77 (17%)	20 (4%)	3 34
3	G	282/287 (98%)	240 (85%)	34 (12%)	8 (3%)	6 44
4	H	134/139 (96%)	108 (81%)	21 (16%)	5 (4%)	4 38
5	I	153/155 (99%)	147 (96%)	6 (4%)	0	100 100
5	J	153/155 (99%)	146 (95%)	7 (5%)	0	100 100
6	K	207/271 (76%)	175 (84%)	22 (11%)	10 (5%)	3 32
7	L	158/177 (89%)	130 (82%)	26 (16%)	2 (1%)	15 60
8	M	73/79 (92%)	66 (90%)	5 (7%)	2 (3%)	6 45
8	N	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3 35
8	O	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3 35
8	P	73/79 (92%)	65 (89%)	5 (7%)	3 (4%)	3 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Q	73/79 (92%)	65 (89%)	6 (8%)	2 (3%)	6	45
8	R	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	35
8	S	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	35
8	T	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	35
8	U	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	35
8	V	73/79 (92%)	66 (90%)	4 (6%)	3 (4%)	3	35
All	All	4732/4926 (96%)	3877 (82%)	685 (14%)	170 (4%)	7	38

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	120	PRO
1	A	281	PRO
1	B	55	LEU
1	B	279	ARG
1	B	281	PRO
1	B	287	PRO
1	C	55	LEU
1	C	279	ARG
2	D	17	PHE
2	D	77	VAL
2	D	138	PRO
2	D	332	PRO
2	D	345	ASP
2	D	346	PRO
2	E	17	PHE
2	E	23	PRO
2	E	211	GLU
2	E	262	PRO
2	E	298	VAL
2	E	305	ASP
2	E	345	ASP
2	F	17	PHE
2	F	113	ALA
2	F	262	PRO
3	G	189	PRO
3	G	209	PRO
3	G	210	ASP
4	H	35	TYR

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Mol	Chain	Res	Type
4	H	72	GLN
6	K	102	ALA
6	K	126	LEU
6	K	143	PRO
6	K	181	GLN
6	K	230	PRO
8	M	47	PRO
8	M	63	ILE
8	N	47	PRO
8	N	63	ILE
8	O	47	PRO
8	O	63	ILE
8	P	47	PRO
8	P	63	ILE
8	Q	47	PRO
8	Q	63	ILE
8	R	47	PRO
8	R	63	ILE
8	S	47	PRO
8	S	63	ILE
8	T	47	PRO
8	T	63	ILE
8	U	47	PRO
8	U	63	ILE
8	V	47	PRO
8	V	63	ILE
1	A	137	ILE
1	A	438	PRO
1	C	9	SER
1	C	85	GLY
1	C	120	PRO
2	D	78	PRO
2	D	90	VAL
2	D	405	PHE
2	E	93	GLU
2	E	346	PRO
2	E	349	VAL
4	H	46	LYS
7	L	4	ILE
1	A	114	PRO
1	A	319	GLY
1	B	5	SER

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Mol	Chain	Res	Type
1	B	85	GLY
1	B	327	LEU
1	B	454	GLY
1	C	191	ILE
1	C	414	ASP
1	C	481	PRO
2	D	0	MET
2	D	74	PRO
2	E	65	GLY
2	F	79	VAL
2	F	93	GLU
2	F	117	GLU
2	F	212	PRO
2	F	414	PRO
2	F	439	PRO
3	G	4	LYS
3	G	42	ARG
3	G	162	GLY
4	H	89	LEU
6	K	142	VAL
8	O	46	ILE
1	A	69	ASP
1	A	149	GLY
1	A	310	GLU
1	A	311	ALA
1	B	88	VAL
1	B	178	LEU
1	C	114	PRO
1	C	174	GLY
1	C	178	LEU
1	C	287	PRO
2	D	18	PRO
2	D	65	GLY
2	D	93	GLU
2	D	439	PRO
2	E	336	PRO
2	E	429	GLY
2	E	436	ASP
2	F	6	VAL
2	F	94	PRO
2	F	349	VAL
3	G	208	GLU

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Mol	Chain	Res	Type
6	K	98	SER
6	K	229	LEU
1	A	216	GLY
1	A	287	PRO
1	B	22	VAL
1	B	120	PRO
1	B	134	PRO
1	B	280	PRO
1	C	280	PRO
1	C	281	PRO
2	D	305	ASP
2	D	349	VAL
2	F	23	PRO
2	F	78	PRO
2	F	85	GLY
2	F	213	PRO
2	F	345	ASP
3	G	109	GLY
8	P	46	ILE
1	A	129	VAL
1	B	148	THR
1	C	370	PRO
2	D	-4	HIS
2	D	33	ASN
2	E	306	PRO
2	E	433	GLY
1	B	149	GLY
1	C	113	ALA
2	D	331	TYR
6	K	121	LEU
1	A	136	VAL
1	C	282	GLY
2	D	262	PRO
2	F	433	GLY
4	H	36	PRO
1	B	198	ILE
1	C	377	VAL
1	C	454	GLY
2	D	113	ALA
2	D	175	VAL
2	D	212	PRO
6	K	101	ILE

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Mol	Chain	Res	Type
7	L	124	ILE
8	T	43	PRO
8	U	43	PRO
1	A	32	VAL
1	C	337	VAL
8	N	43	PRO
8	S	43	PRO
1	B	282	GLY
1	C	115	ILE
2	D	92	GLY
2	D	153	VAL
2	F	8	VAL
2	F	114	PRO
8	R	43	PRO
8	V	43	PRO

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)

4 ligands 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ATP	A	601	-	26,33,33	0.96	1 (3%)	26,52,52	1.64	1 (3%)
9	ATP	B	601	-	26,33,33	0.96	1 (3%)	26,52,52	1.63	1 (3%)
9	ATP	C	601	-	26,33,33	0.96	1 (3%)	26,52,52	1.63	1 (3%)
10	ADP	D	601	-	24,29,29	0.99	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
9	ATP	A	601	-	-	0/18/38/38	0/3/3/3
9	ATP	B	601	-	-	0/18/38/38	0/3/3/3
9	ATP	C	601	-	-	0/18/38/38	0/3/3/3
10	ADP	D	601	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	601	ADP	C5-C4	3.11	1.47	1.40
9	C	601	ATP	C5-C4	3.13	1.47	1.40
9	B	601	ATP	C5-C4	3.14	1.47	1.40
9	A	601	ATP	C5-C4	3.14	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	601	ATP	N3-C2-N1	-6.59	123.69	128.87
9	B	601	ATP	N3-C2-N1	-6.54	123.73	128.87
9	C	601	ATP	N3-C2-N1	-6.54	123.74	128.87
10	D	601	ADP	N3-C2-N1	-6.49	123.77	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)

There are no chain breaks in this entry.