wwPDB EM Validation Summary Report (i)

May 15, 2024 – 12:19 pm BST

PDB ID	:	6REU
EMDB ID	:	EMD-4857
Title	:	Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 3C, focussed refinement of F1 head and rotor
Authors	:	Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on	:	2019-04-12
Resolution	:	4.20 Å(reported)

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 (i)) were used in the production of this report:

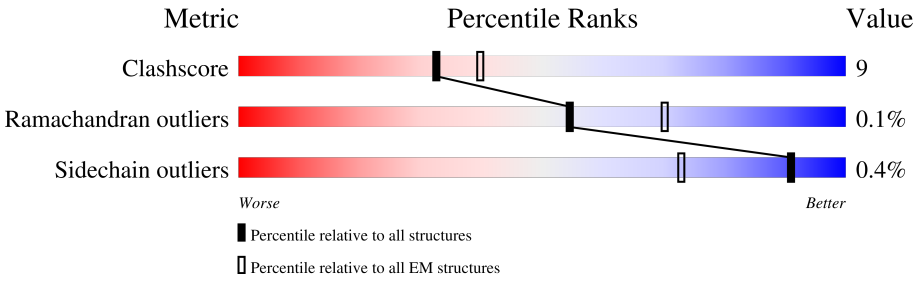
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.20 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	158937	4297
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%

Mol	Chain	Length	Quality of chain
1	A	127	43% 15% · 42%
1	B	127	39% 20% 42%
1	C	127	41% 17% 42%
1	D	127	44% 13% · 42%
1	E	127	45% 13% 42%
1	F	127	49% 9% 42%
1	G	127	42% 17% 42%
1	H	127	45% 13% 42%
1	I	127	47% 11% 42%

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Mol	Chain	Length	Quality of chain
1	J	127	50% 8% 42%
2	P	229	38% 11% 50%
3	Q	74	68% 30%
4	R	199	75% 14% 11%
5	S	317	68% 20% 13%
6	T	562	66% 19% 15%
6	U	562	71% 21% 7%
6	V	562	71% 21% 7%
7	X	574	68% 26% 6%
7	Y	574	72% 18% 9%
7	Z	574	71% 23% 6%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 33899 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 Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
1	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 2 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	114	Total	C	N	O	S	0	0
			895	576	147	171	1		

- Molecule 3 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 4 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 5 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	478	Total	C	N	O	S	0	0
			3609	2294	640	664	11		
6	U	523	Total	C	N	O	S	0	0
			3980	2537	703	729	11		
6	V	520	Total	C	N	O	S	0	0
			3962	2527	700	724	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	539	Total	C	N	O	S	0	0
			4095	2572	693	817	13		
7	Y	521	Total	C	N	O	S	0	0
			3957	2485	670	789	13		
7	Z	542	Total	C	N	O	S	0	0
			4115	2586	696	820	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41

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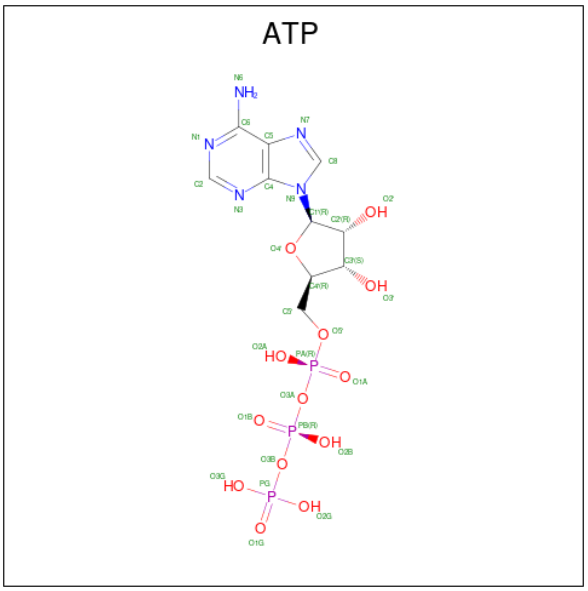
Chain	Residue	Modelled	Actual	Comment	Reference
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
8	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	T	1	Total	Mg	0
			1	1	
9	U	1	Total	Mg	0
			1	1	
9	V	1	Total	Mg	0
			1	1	
9	X	1	Total	Mg	0
			1	1	

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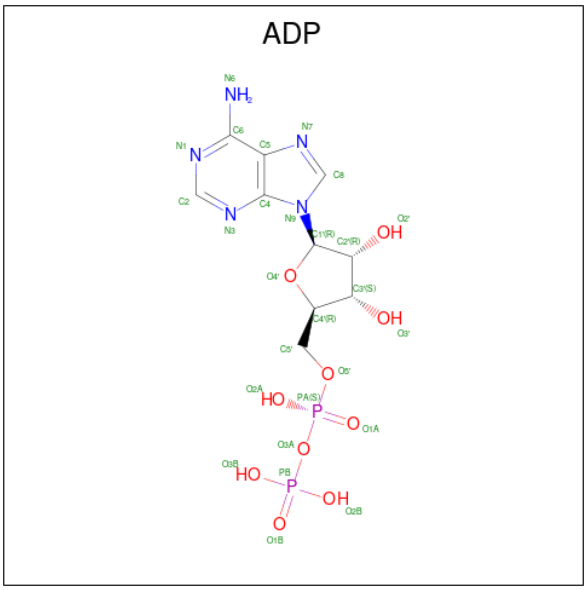
Mol	Chain	Residues	Atoms		AltConf
9	Z	1	Total	Mg	0
			1	1	

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



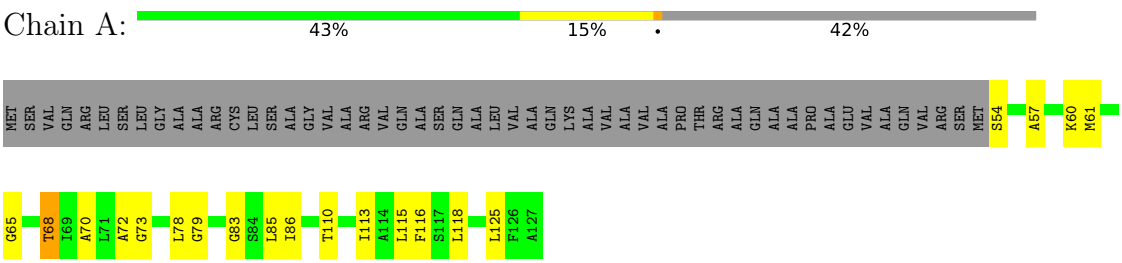
Mol	Chain	Residues	Atoms					AltConf
10	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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. 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.

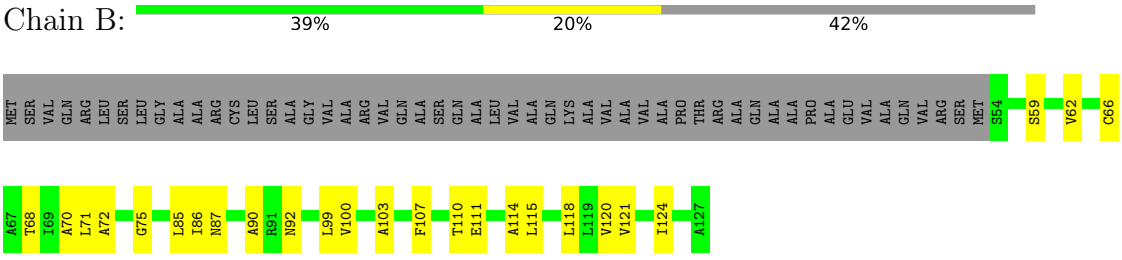
• Molecule 1: Mitochondrial ATP synthase subunit c

Chain A:



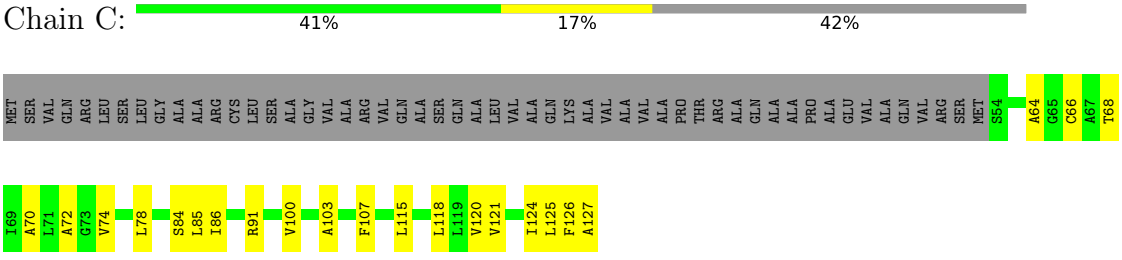
• Molecule 1: Mitochondrial ATP synthase subunit c

Chain B:



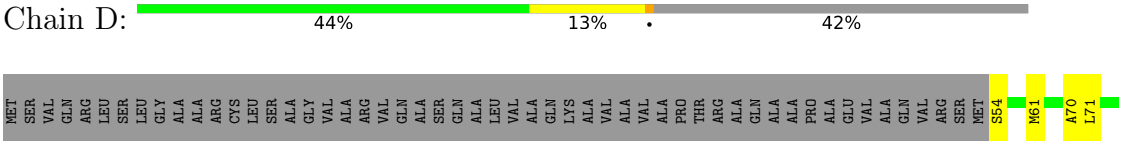
• Molecule 1: Mitochondrial ATP synthase subunit c

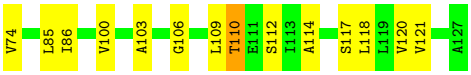
Chain C:



• Molecule 1: Mitochondrial ATP synthase subunit c

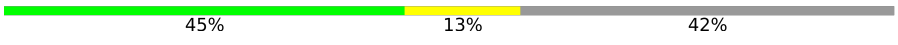
Chain D:

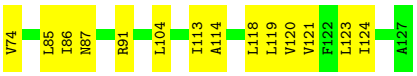




• Molecule 1: Mitochondrial ATP synthase subunit c

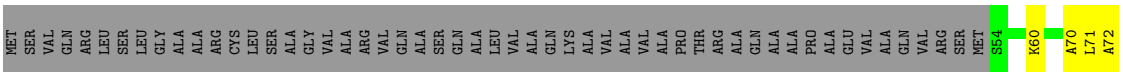
Chain E:





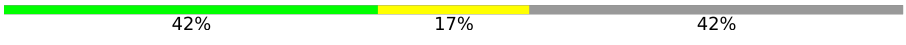
• Molecule 1: Mitochondrial ATP synthase subunit c

Chain F:



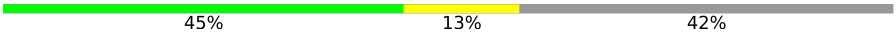
• Molecule 1: Mitochondrial ATP synthase subunit c

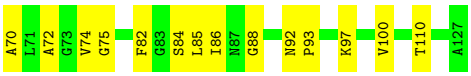
Chain G:



• Molecule 1: Mitochondrial ATP synthase subunit c

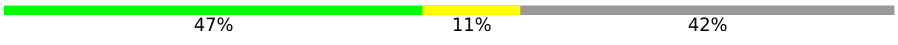
Chain H:

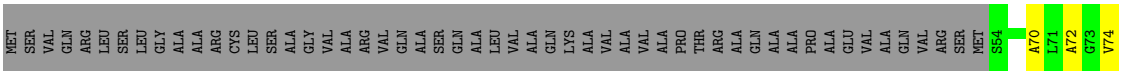




• Molecule 1: Mitochondrial ATP synthase subunit c

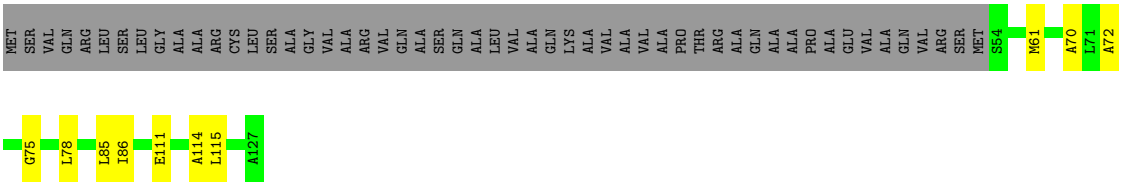
Chain I:





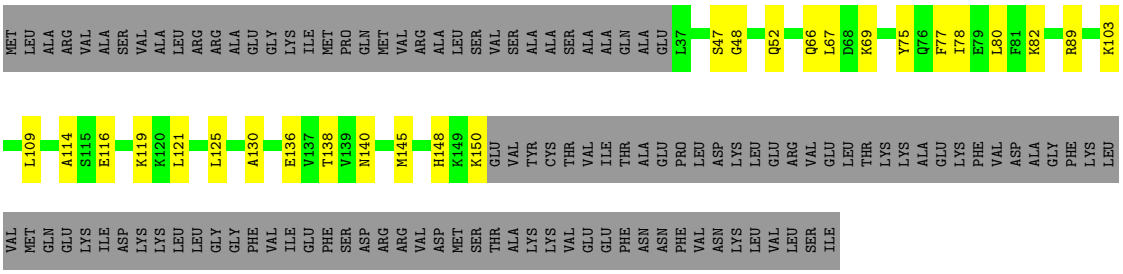
• Molecule 1: Mitochondrial ATP synthase subunit c

Chain J:



• Molecule 2: Mitochondrial ATP synthase subunit OSCP

Chain P:

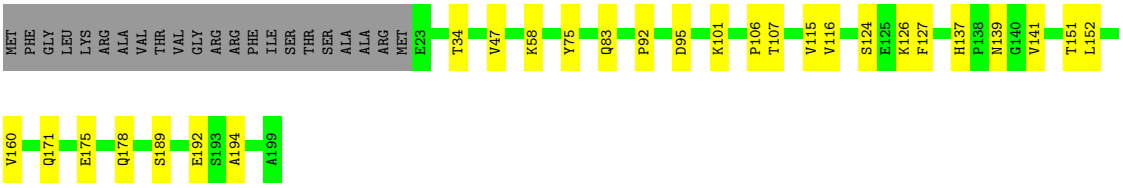


• Molecule 3: epsilon: Polytomella F-ATP synthase epsilon subunit

Chain Q:

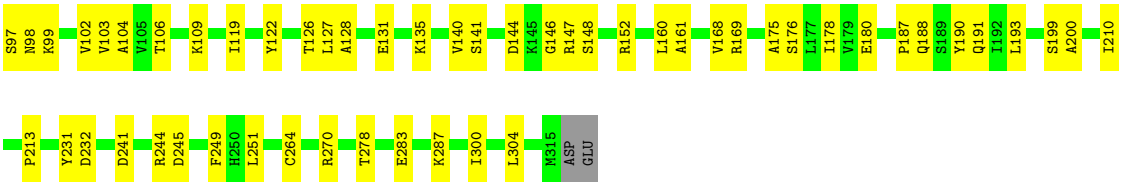
• Molecule 4: Mitochondrial ATP synthase subunit delta

Chain R:



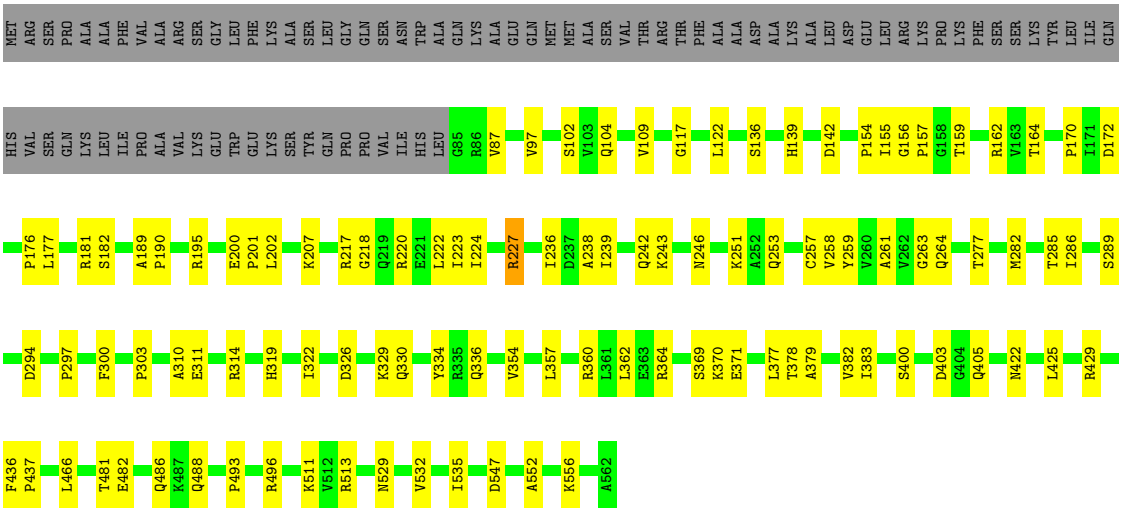
• Molecule 5: ATP synthase gamma chain, mitochondrial

Chain S:



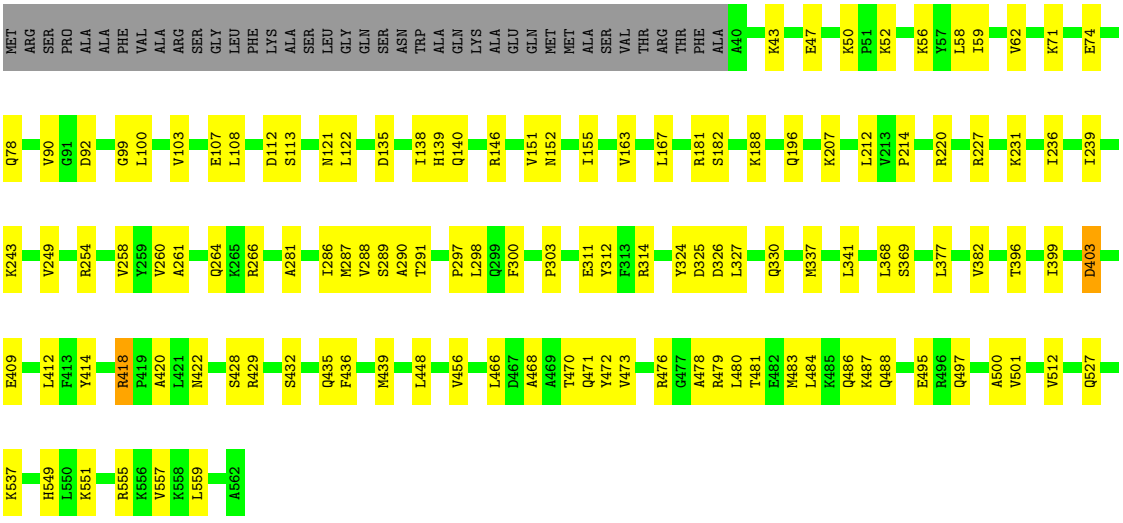
• Molecule 6: ATP synthase subunit alpha

Chain T:



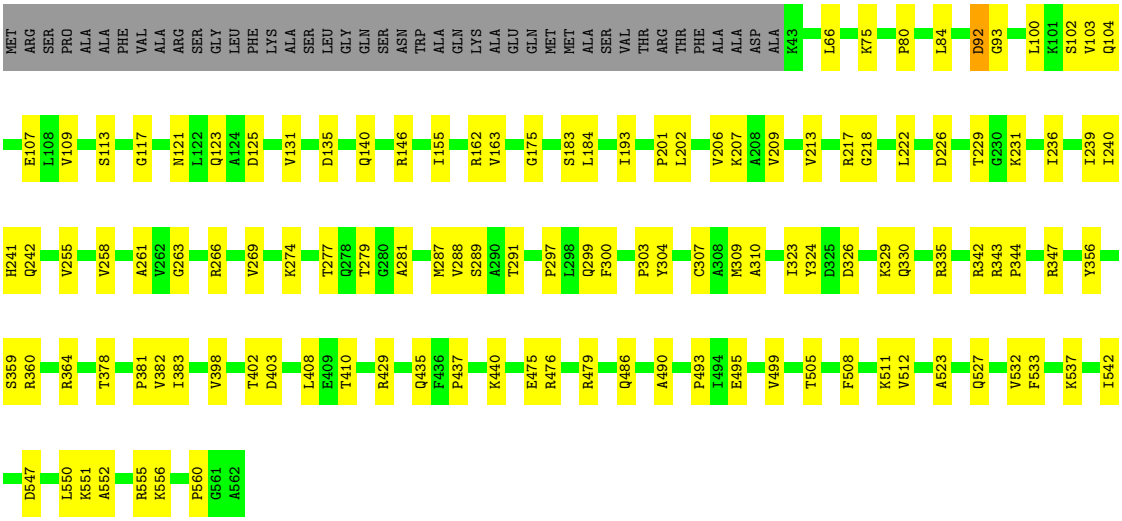
• Molecule 6: ATP synthase subunit alpha

Chain U:



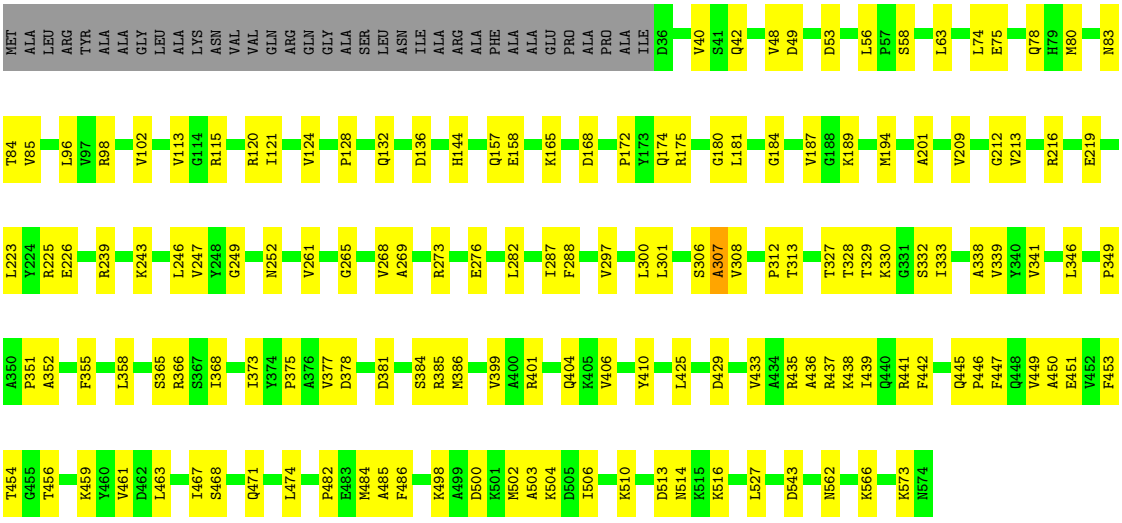
• Molecule 6: ATP synthase subunit alpha

Chain V:



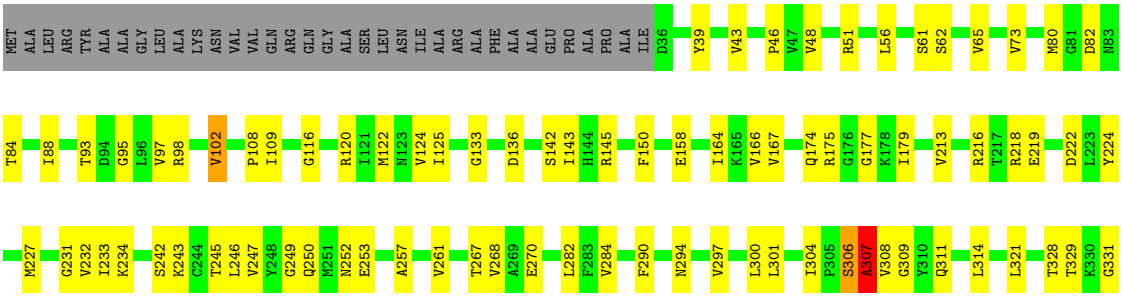
• Molecule 7: ATP synthase subunit beta

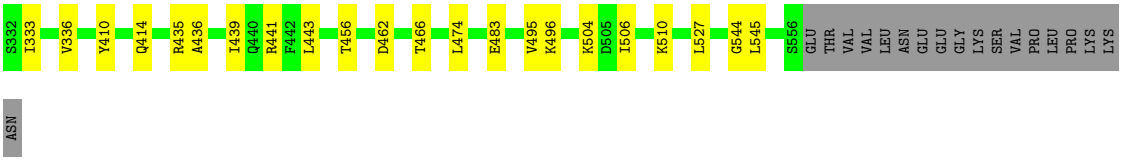
Chain X:



• Molecule 7: ATP synthase subunit beta

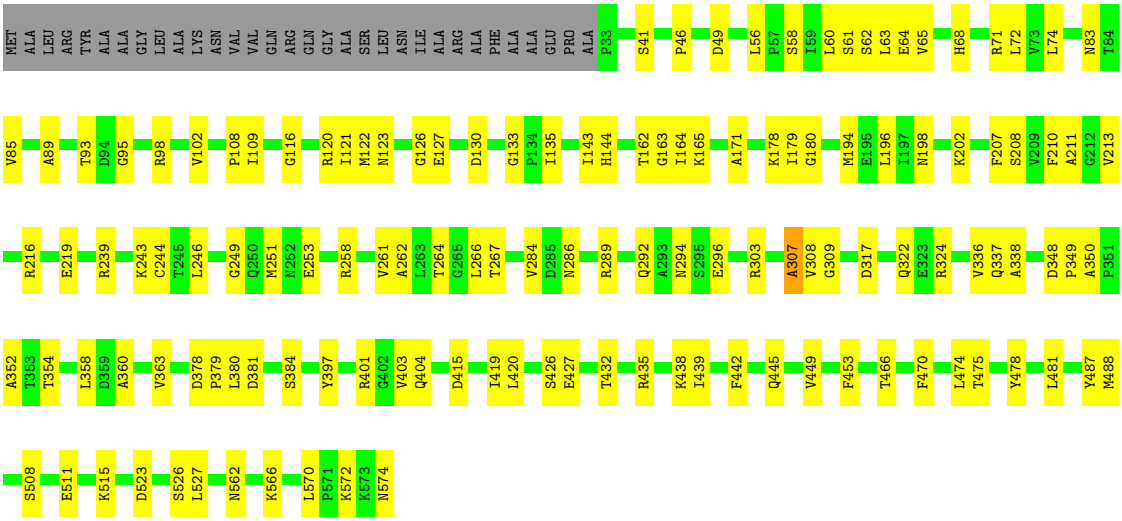
Chain Y:





• Molecule 7: ATP synthase subunit beta

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	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: ATP, MG, 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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/520	0.53	0/704
1	B	0.29	0/520	0.56	0/704
1	C	0.30	0/519	0.61	0/701
1	D	0.34	0/520	0.57	0/704
1	E	0.33	0/520	0.52	0/704
1	F	0.28	0/520	0.48	0/704
1	G	0.28	0/520	0.56	0/704
1	H	0.29	0/520	0.56	0/704
1	I	0.29	0/520	0.48	0/704
1	J	0.29	0/520	0.55	1/704 (0.1%)
2	P	0.36	0/908	0.55	0/1229
3	Q	0.33	0/574	0.54	0/774
4	R	0.34	0/1336	0.52	0/1827
5	S	0.33	0/2153	0.56	0/2901
6	T	0.36	0/3667	0.59	1/4965 (0.0%)
6	U	0.35	0/4049	0.57	0/5481
6	V	0.37	0/4031	0.56	1/5456 (0.0%)
7	X	0.34	0/4155	0.56	0/5630
7	Y	0.37	0/4015	0.56	0/5440
7	Z	0.37	0/4176	0.57	0/5659
All	All	0.35	0/34263	0.56	3/46399 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
7	X	0	1
7	Y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	Z	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	92	ASP	CB-CG-OD1	5.66	123.39	118.30
1	J	115	LEU	CA-CB-CG	5.34	127.58	115.30
6	T	466	LEU	CA-CB-CG	5.31	127.52	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	148	HIS	Mainchain
7	X	307	ALA	Peptide
7	Y	307	ALA	Peptide
7	Z	307	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	514	0	554	16	0
1	B	514	0	554	22	0
1	C	514	0	553	18	0
1	D	514	0	554	13	0
1	E	514	0	554	14	0
1	F	514	0	554	13	0
1	G	514	0	554	17	0
1	H	514	0	554	14	0
1	I	514	0	554	14	0
1	J	514	0	554	8	0
2	P	895	0	934	19	0
3	Q	561	0	565	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	1303	0	1266	18	0
5	S	2130	0	2180	42	0
6	T	3609	0	3732	71	0
6	U	3980	0	4119	85	0
6	V	3962	0	4105	87	0
7	X	4095	0	4113	95	0
7	Y	3957	0	3967	65	0
7	Z	4115	0	4138	86	0
8	T	31	0	12	1	0
8	U	31	0	12	1	0
8	V	31	0	12	1	0
9	T	1	0	0	0	0
9	U	1	0	0	0	0
9	V	1	0	0	0	0
9	X	1	0	0	0	0
9	Z	1	0	0	0	0
10	X	27	0	12	3	0
10	Z	27	0	12	0	0
All	All	33899	0	34718	639	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 9.

The worst 5 of 639 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)
7:X:498:LYS:O	7:X:502:MET:HG3	1.11	1.25
7:X:498:LYS:O	7:X:502:MET:CG	2.03	1.05
6:V:222:LEU:HD13	6:V:381:PRO:HG2	1.47	0.95
6:V:222:LEU:CD1	6:V:381:PRO:HG2	2.08	0.82
7:X:503:ALA:O	7:X:506:ILE:HG22	1.83	0.79

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	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	B	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	C	71/127 (56%)	69 (97%)	2 (3%)	0	100	100
1	D	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	E	72/127 (57%)	68 (94%)	4 (6%)	0	100	100
1	F	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	G	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
1	H	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	I	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
1	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
2	P	112/229 (49%)	103 (92%)	9 (8%)	0	100	100
3	Q	70/74 (95%)	62 (89%)	8 (11%)	0	100	100
4	R	175/199 (88%)	159 (91%)	16 (9%)	0	100	100
5	S	275/317 (87%)	261 (95%)	14 (5%)	0	100	100
6	T	476/562 (85%)	448 (94%)	28 (6%)	0	100	100
6	U	521/562 (93%)	493 (95%)	28 (5%)	0	100	100
6	V	518/562 (92%)	490 (95%)	27 (5%)	1 (0%)	47	80
7	X	537/574 (94%)	498 (93%)	38 (7%)	1 (0%)	47	80
7	Y	519/574 (90%)	490 (94%)	26 (5%)	3 (1%)	25	64
7	Z	540/574 (94%)	496 (92%)	43 (8%)	1 (0%)	47	80
All	All	4462/5497 (81%)	4200 (94%)	256 (6%)	6 (0%)	54	85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	X	308	VAL
7	Y	308	VAL
7	Z	308	VAL
7	Y	307	ALA
6	V	92	ASP

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
1	A	50/86 (58%)	49 (98%)	1 (2%)	55 73
1	B	50/86 (58%)	50 (100%)	0	100 100
1	C	50/86 (58%)	50 (100%)	0	100 100
1	D	50/86 (58%)	49 (98%)	1 (2%)	55 73
1	E	50/86 (58%)	50 (100%)	0	100 100
1	F	50/86 (58%)	50 (100%)	0	100 100
1	G	50/86 (58%)	50 (100%)	0	100 100
1	H	50/86 (58%)	50 (100%)	0	100 100
1	I	50/86 (58%)	50 (100%)	0	100 100
1	J	50/86 (58%)	50 (100%)	0	100 100
2	P	99/196 (50%)	98 (99%)	1 (1%)	76 86
3	Q	56/58 (97%)	55 (98%)	1 (2%)	59 76
4	R	134/151 (89%)	134 (100%)	0	100 100
5	S	235/265 (89%)	235 (100%)	0	100 100
6	T	378/448 (84%)	375 (99%)	3 (1%)	81 89
6	U	419/448 (94%)	415 (99%)	4 (1%)	76 86
6	V	418/448 (93%)	417 (100%)	1 (0%)	93 96
7	X	447/469 (95%)	446 (100%)	1 (0%)	93 96
7	Y	430/469 (92%)	428 (100%)	2 (0%)	88 93
7	Z	449/469 (96%)	449 (100%)	0	100 100
All	All	3565/4281 (83%)	3550 (100%)	15 (0%)	91 94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	U	220	ARG
7	Y	102	VAL
6	U	227	ARG

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Mol	Chain	Res	Type
7	Y	456	THR
6	V	213	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
6	V	244	ASN
7	X	294	ASN
7	Z	448	GLN
6	V	299	GLN
7	X	157	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
10	ADP	X	601	9	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ATP	U	1001	9	26,33,33	0.92	1 (3%)	31,52,52	1.56	5 (16%)
8	ATP	V	1001	9	26,33,33	0.92	1 (3%)	31,52,52	1.80	6 (19%)
8	ATP	T	1001	9	26,33,33	0.88	1 (3%)	31,52,52	1.56	5 (16%)
10	ADP	Z	601	9	24,29,29	0.95	1 (4%)	29,45,45	1.56	4 (13%)

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
10	ADP	X	601	9	-	3/12/32/32	0/3/3/3
8	ATP	U	1001	9	-	0/18/38/38	0/3/3/3
8	ATP	V	1001	9	-	1/18/38/38	0/3/3/3
8	ATP	T	1001	9	-	4/18/38/38	0/3/3/3
10	ADP	Z	601	9	-	1/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	1001	ATP	C5-C4	2.38	1.47	1.40
8	V	1001	ATP	C5-C4	2.32	1.47	1.40
10	X	601	ADP	C5-C4	2.22	1.46	1.40
8	T	1001	ATP	C5-C4	2.14	1.46	1.40
10	Z	601	ADP	C5-C4	2.11	1.46	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	1001	ATP	PA-O3A-PB	-4.65	116.87	132.83
8	V	1001	ATP	C3'-C2'-C1'	3.86	106.80	100.98
8	V	1001	ATP	PB-O3B-PG	-3.79	119.82	132.83
8	T	1001	ATP	PB-O3B-PG	-3.68	120.19	132.83
10	Z	601	ADP	PA-O3A-PB	-3.67	120.22	132.83

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	T	1001	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	X	601	ADP	C5'-O5'-PA-O1A
10	X	601	ADP	C5'-O5'-PA-O3A
8	T	1001	ATP	C3'-C4'-C5'-O5'
10	Z	601	ADP	O4'-C4'-C5'-O5'

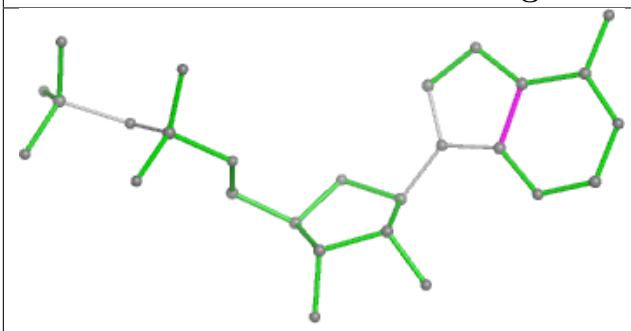
There are no ring outliers.

4 monomers are involved in 6 short contacts:

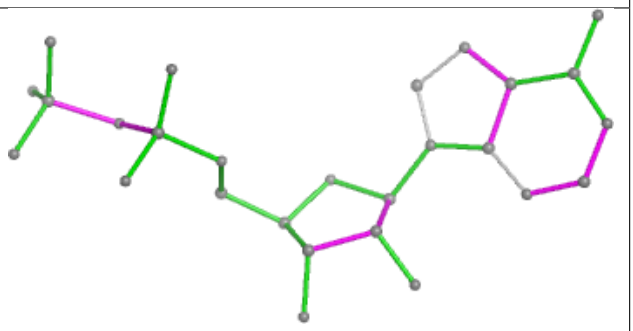
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	X	601	ADP	3	0
8	U	1001	ATP	1	0
8	V	1001	ATP	1	0
8	T	1001	ATP	1	0

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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

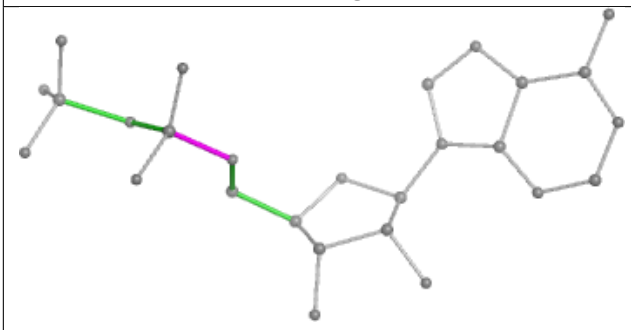
Ligand ADP X 601



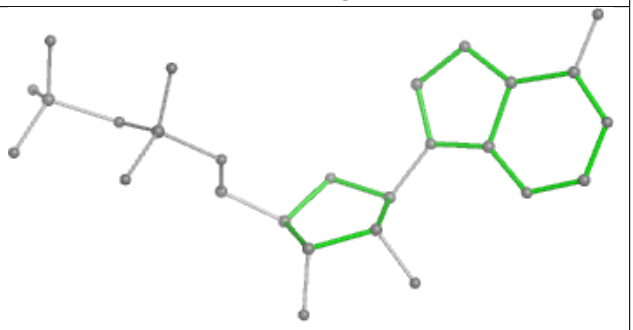
Bond lengths



Bond angles

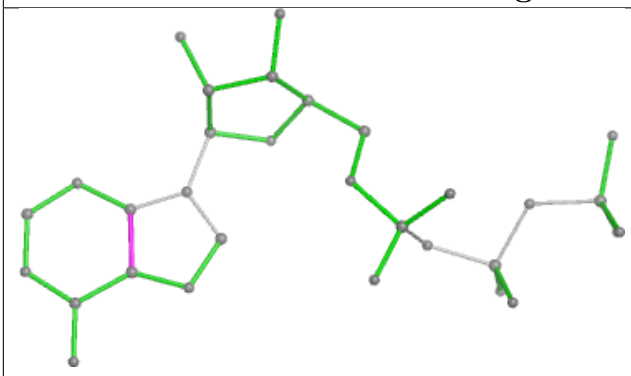


Torsions

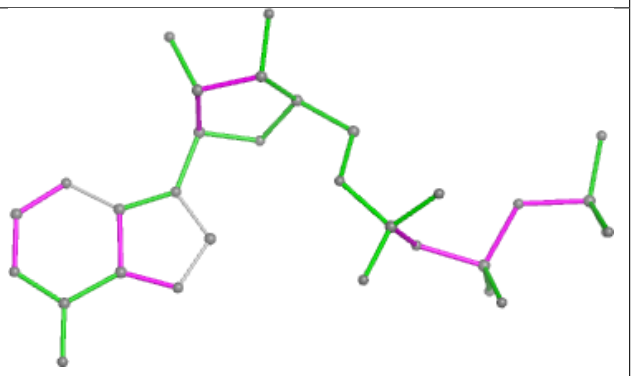


Rings

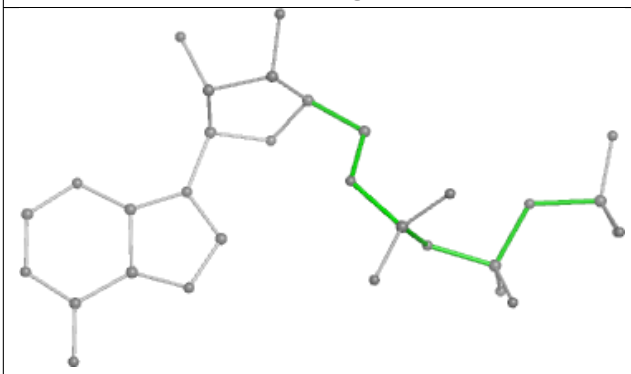
Ligand ATP U 1001



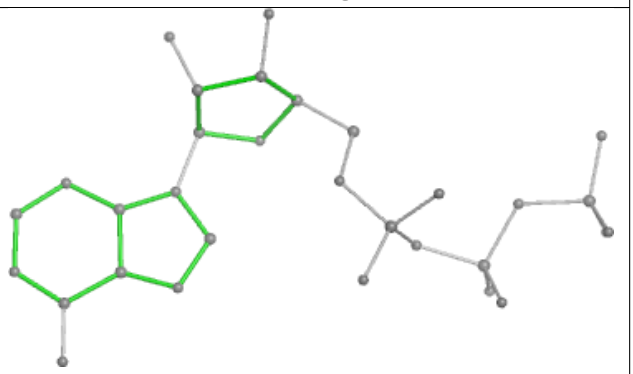
Bond lengths



Bond angles

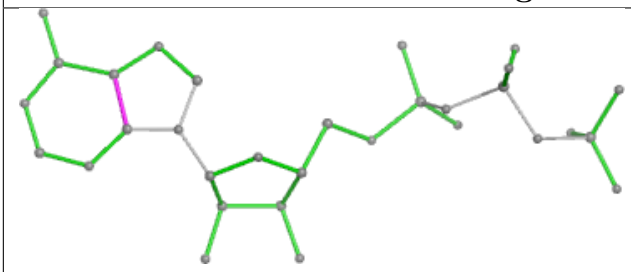


Torsions

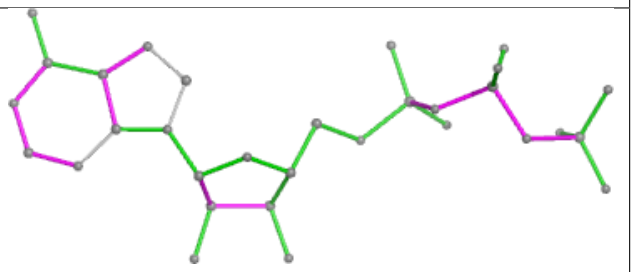


Rings

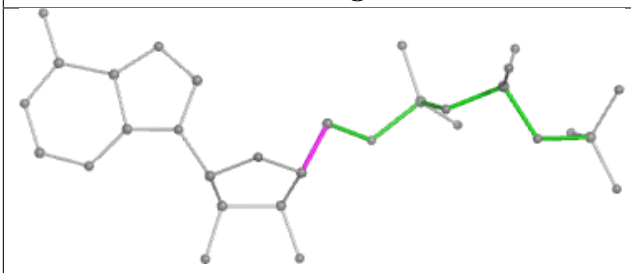
Ligand ATP V 1001



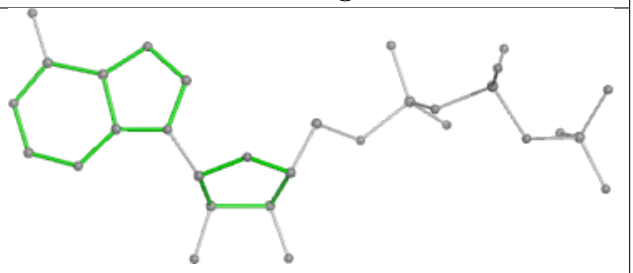
Bond lengths



Bond angles

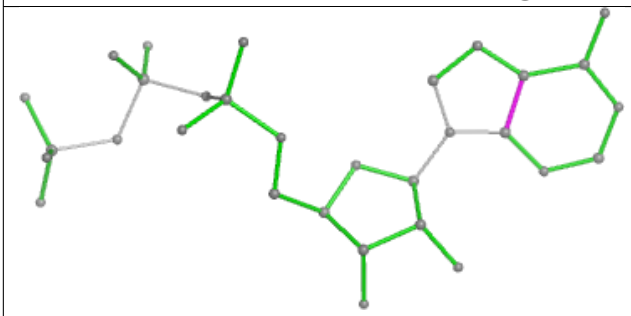


Torsions

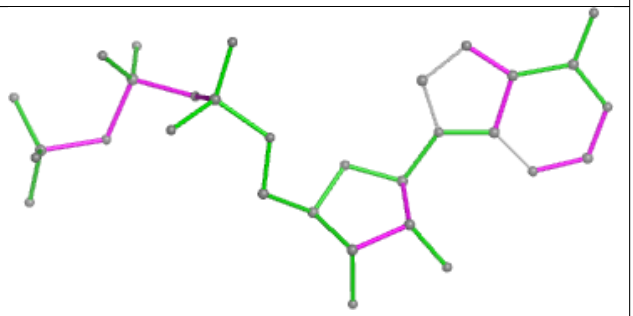


Rings

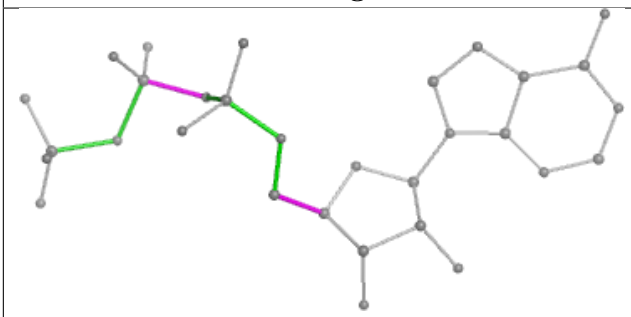
Ligand ATP T 1001



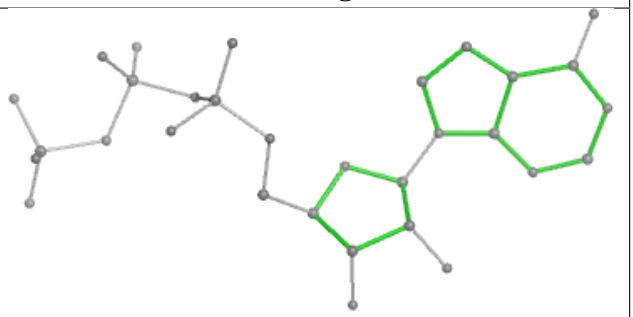
Bond lengths



Bond angles

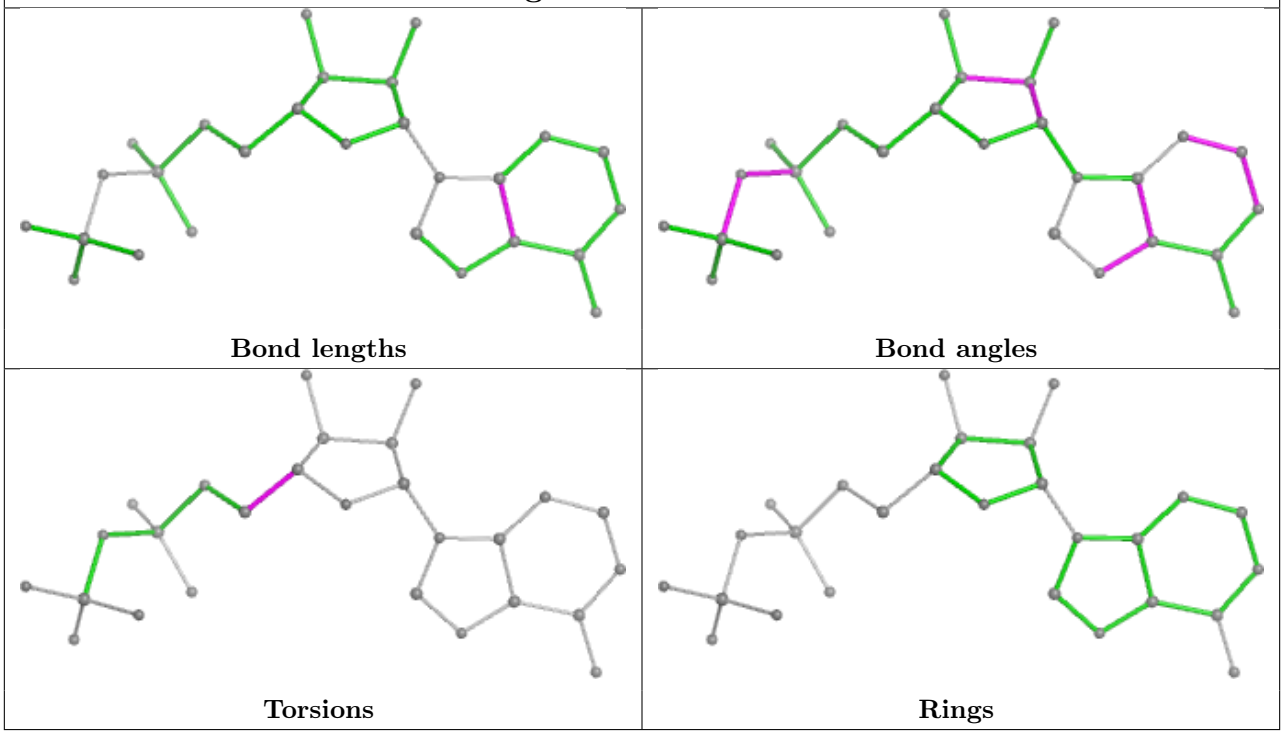


Torsions



Rings

Ligand ADP Z 601



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
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	3.47

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4857. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.