



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:25 AM GMT

PDB ID : 2WSS
Title : THE STRUCTURE OF THE MEMBRANE EXTRINSIC REGION OF BOVINE ATP SYNTHASE
Authors : Rees, D.M.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2009-09-09
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

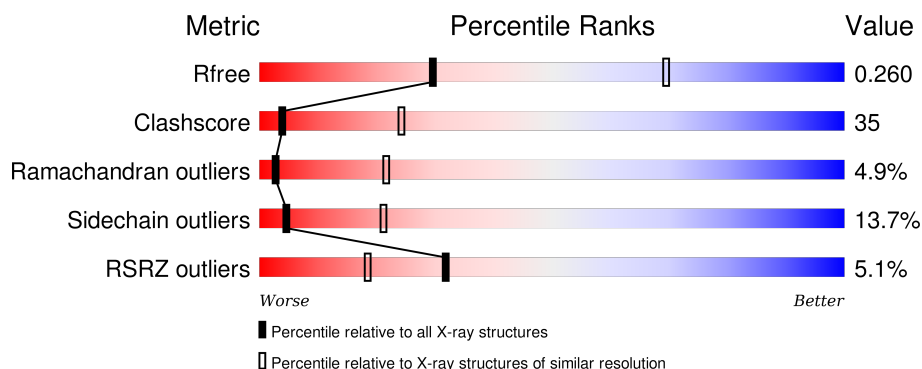
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	<div> <div>49%</div> <div>42%</div> <div>8%</div> <div>.</div> </div>
1	B	510	<div> <div>46%</div> <div>43%</div> <div>6%</div> <div>6%</div> </div>
1	C	510	<div> <div>3%</div> <div>36%</div> <div>48%</div> <div>10%</div> <div>5%</div> </div>
1	J	510	<div> <div>%</div> <div>43%</div> <div>44%</div> <div>8%</div> <div>5%</div> </div>
1	K	510	<div> <div>43%</div> <div>44%</div> <div>7%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	510	
2	D	482	
2	E	482	
2	F	482	
2	M	482	
2	N	482	
2	O	482	
3	G	272	
3	P	272	
4	H	146	
4	Q	146	
5	I	50	
5	R	50	
6	S	190	
6	W	190	
7	T	116	
7	X	116	
8	U	118	
9	V	76	
9	Z	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ANP	B	600	X	-	-	-
10	ANP	F	600	-	-	X	-
11	MG	D	601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MG	F	601	-	-	-	X
11	MG	M	601	-	-	-	X
11	MG	O	601	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 54949 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			3882	2442	684	744	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	484	Total	C	N	O	S	0	0	0
			3684	2323	653	696	12			
1	J	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	K	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	L	481	Total	C	N	O	S	0	0	0
			3670	2315	650	693	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
B	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
C	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
J	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
K	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
L	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	1	0
			3534	2242	600	681	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	N	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	O	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	260	Total	C	N	O	S	0	0	0
			2027	1273	351	395	8			
3	P	260	Total	C	N	O	S	0	0	0
			2027	1273	351	395	8			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			
4	Q	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			
5	R	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	S	167	Total	C	N	O	S	Se	0	0	0
			1292	820	223	242	1	6			
6	W	146	Total	C	N	O	S	Se	0	0	0
			1120	712	191	212	1	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	129	THR	ALA	CONFLICT	UNP P13621
W	129	THR	ALA	CONFLICT	UNP P13621

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	T	86	Total	C	N	O	S	Se	0	0	0
			733	459	139	130	1	4			
7	X	41	Total	C	N	O	S	Se	0	0	0
			336	211	62	59	1	3			

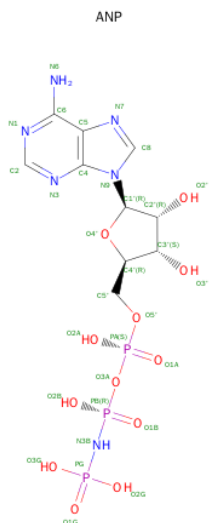
- Molecule 8 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	U	28	Total	C	N	O	0	0	0
			234	149	38	47			

- Molecule 9 is a protein called ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	66	Total	C	N	O	Se	0	0	0
			551	352	92	105	2			
9	Z	17	Total	C	N	O		0	0	0
			160	101	33	26				

- Molecule 10 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



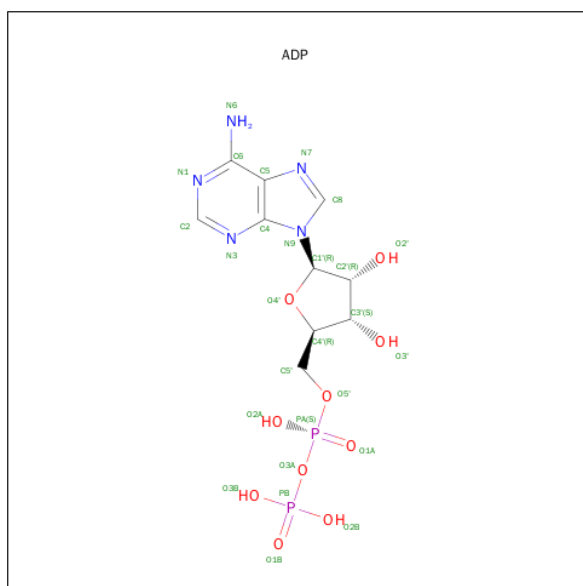
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	Mg	0	0
			1	1		
11	A	1	Total	Mg	0	0
			1	1		
11	O	1	Total	Mg	0	0
			1	1		
11	L	1	Total	Mg	0	0
			1	1		
11	F	1	Total	Mg	0	0
			1	1		
11	M	1	Total	Mg	0	0
			1	1		

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

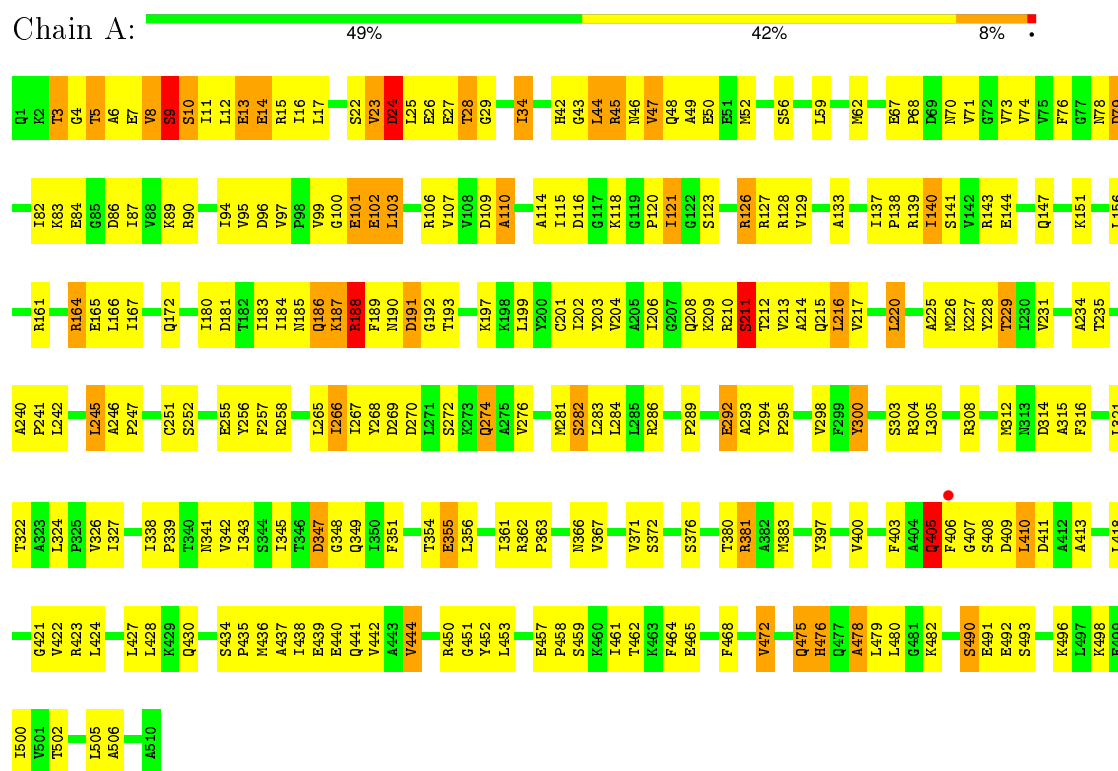


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
12	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

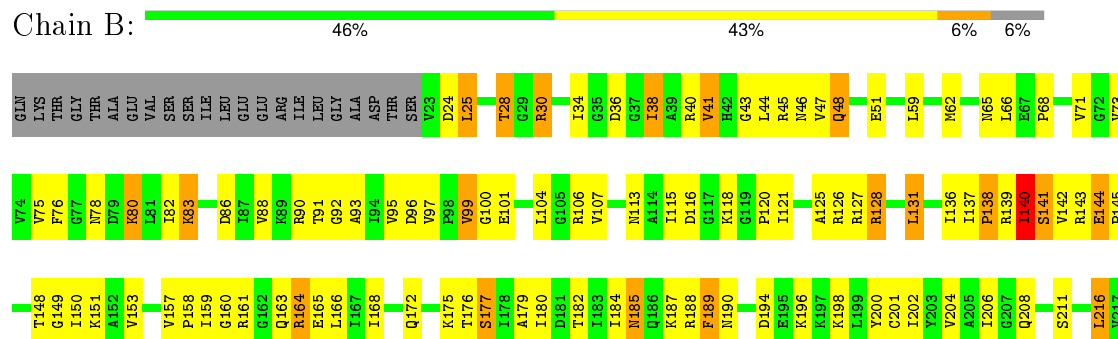
3 Residue-property plots

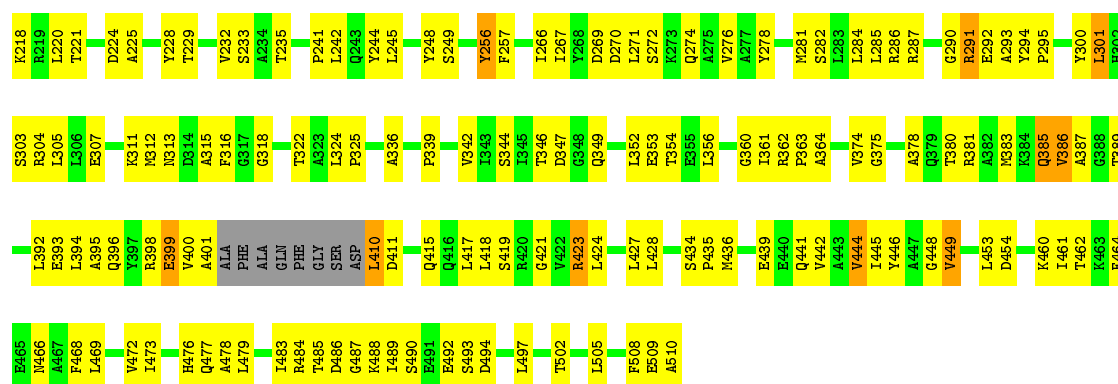
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

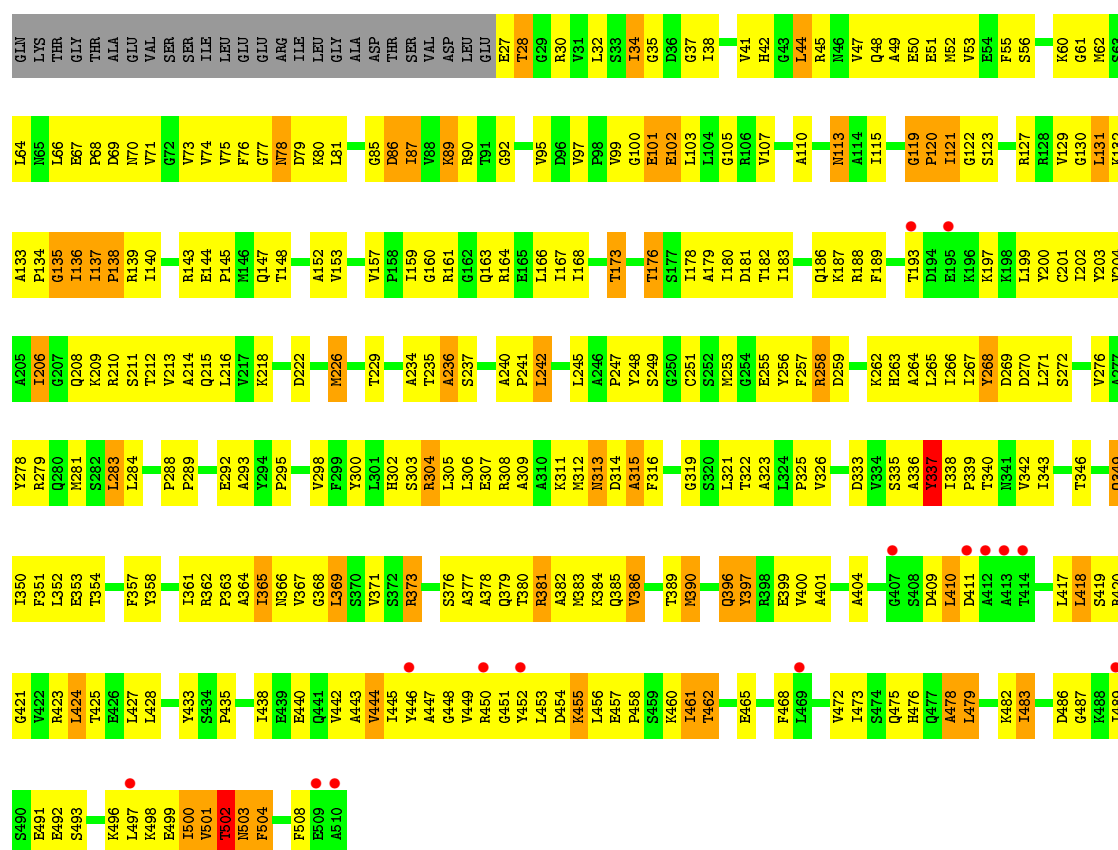


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

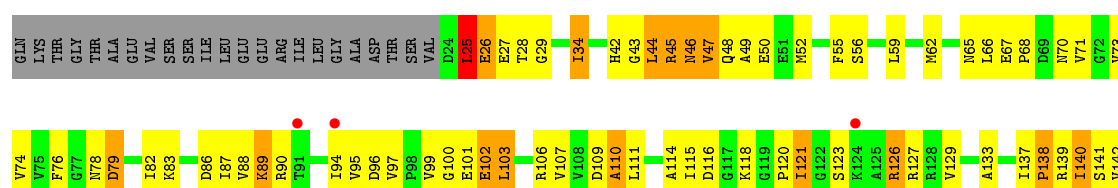
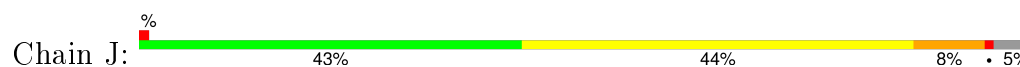


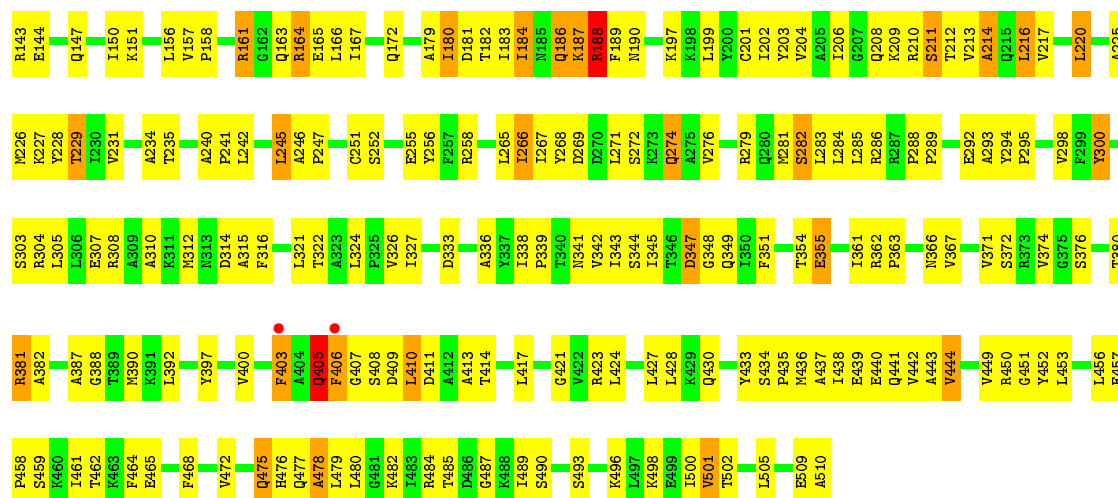


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



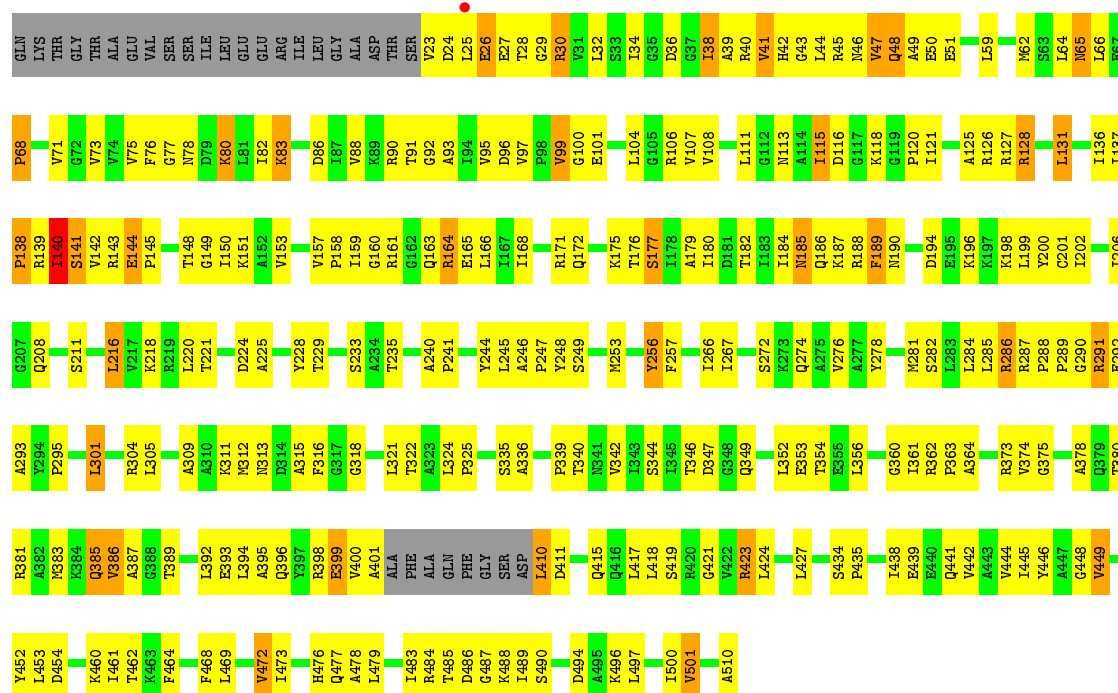
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL





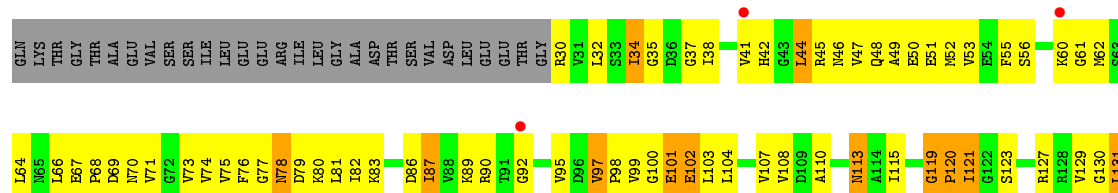
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

Chain K: 43% 44% 7% 6%

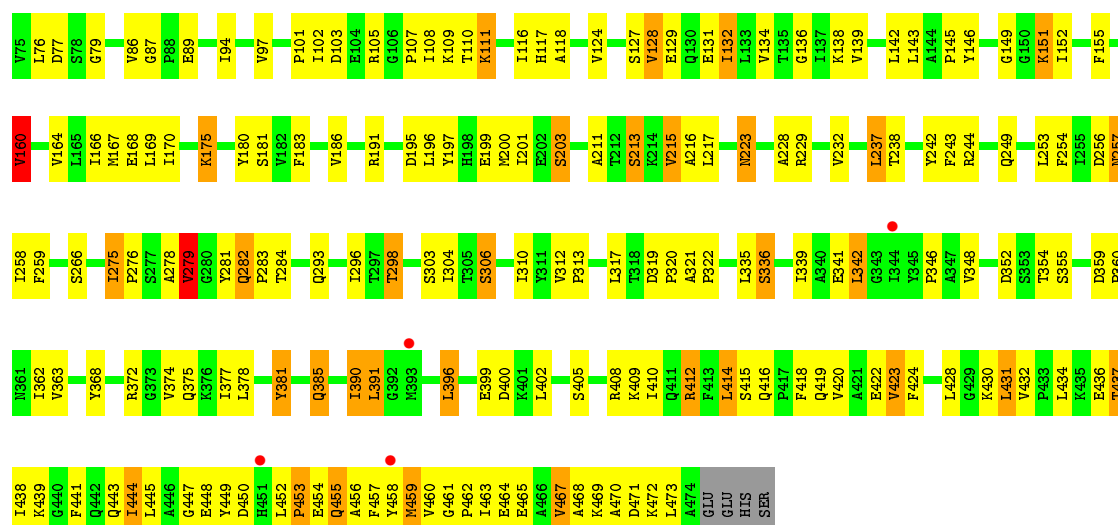


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

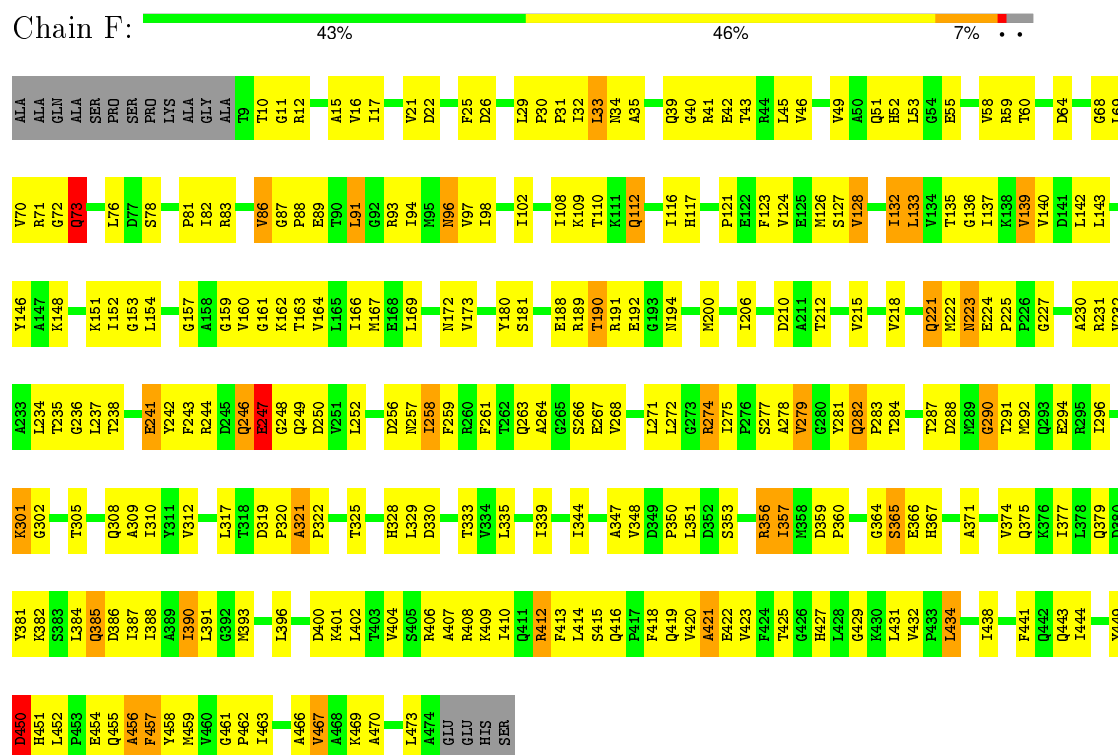
Chain L: 5% 34% 50% 10% 6%



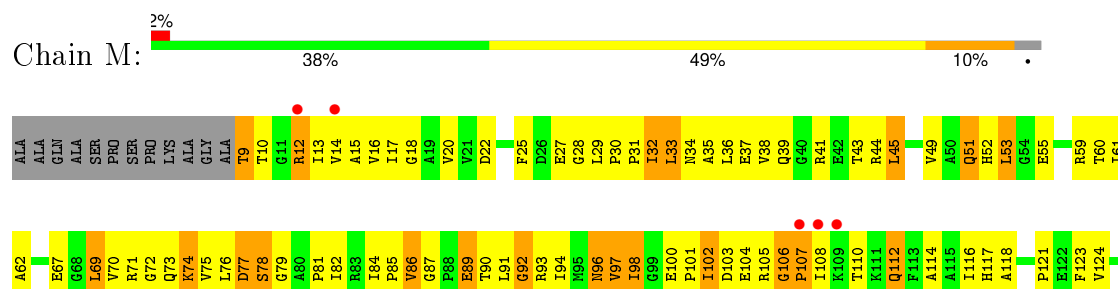


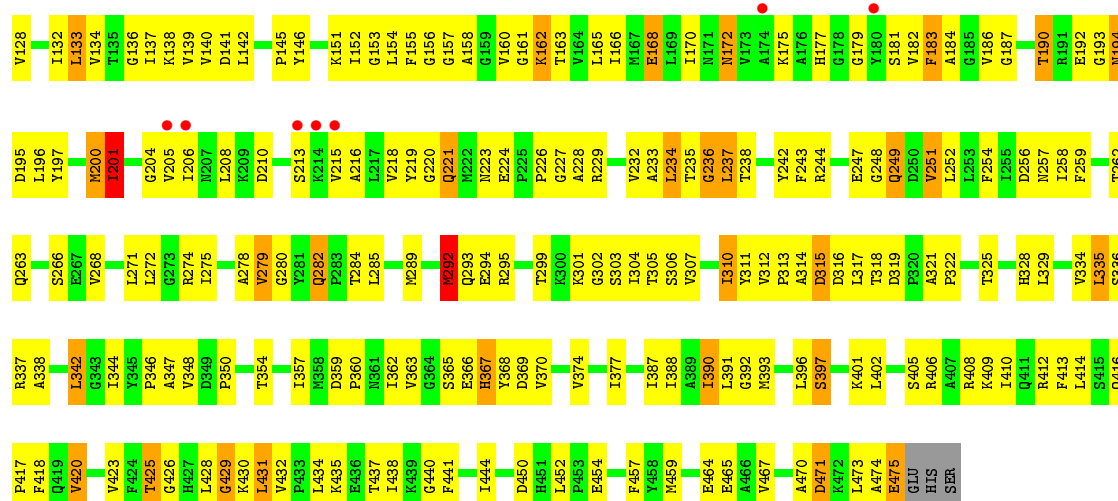


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



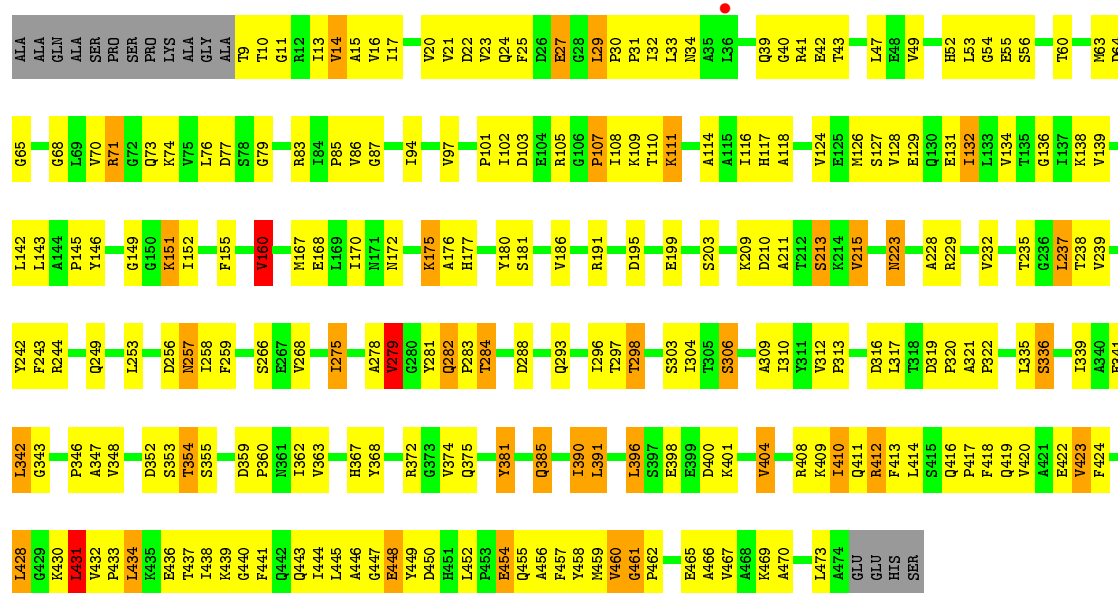
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





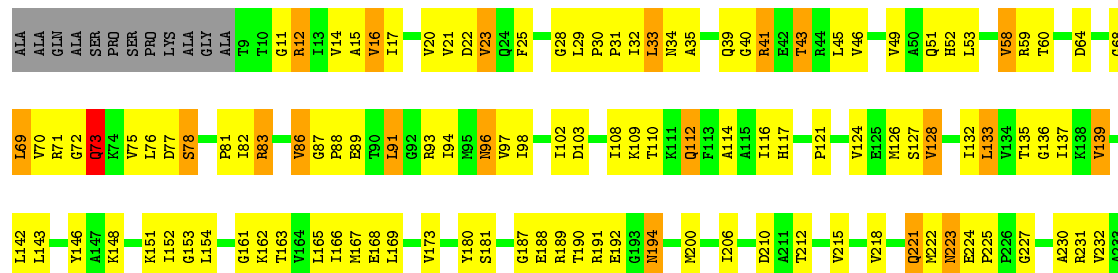
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

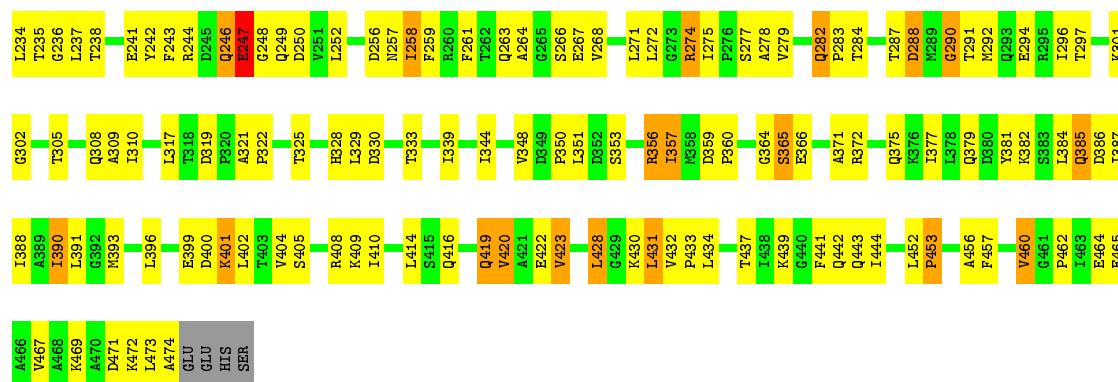
Chain N: 49% 39% 8%



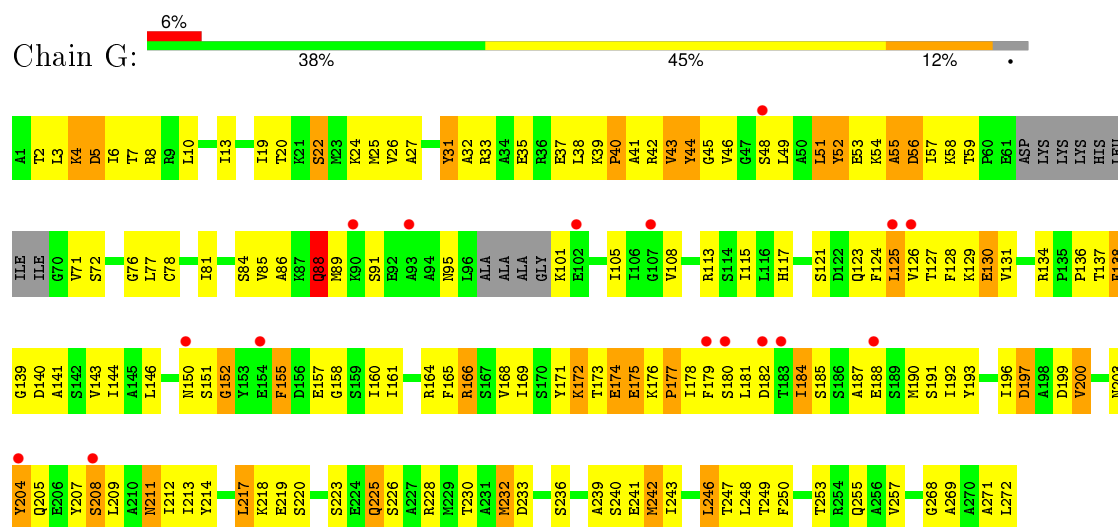
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain O: 46% 42% 8%

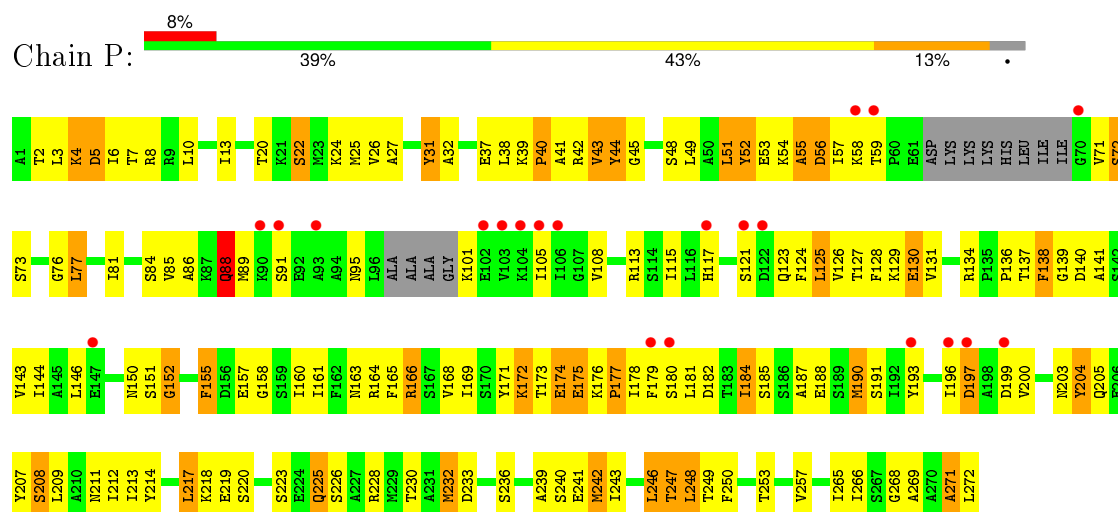




• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

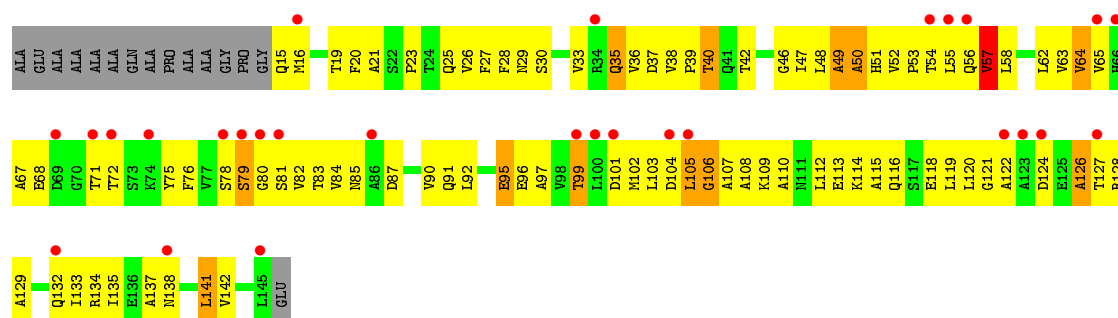


• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

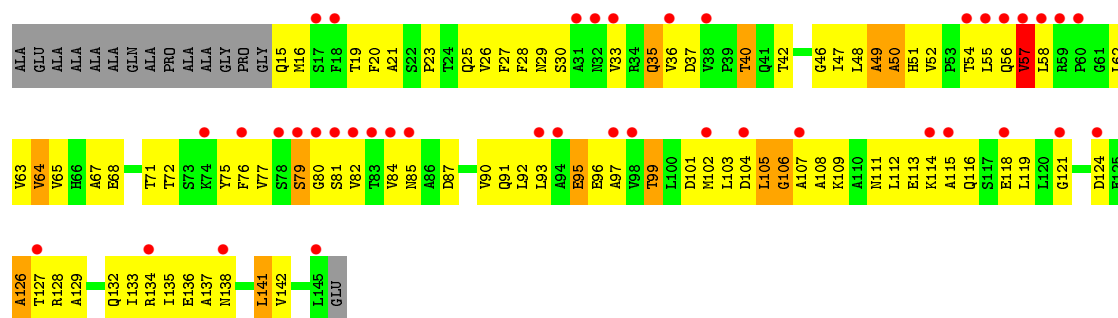


• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

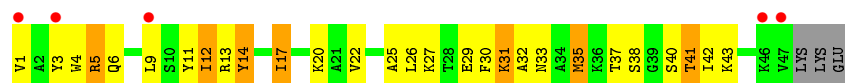
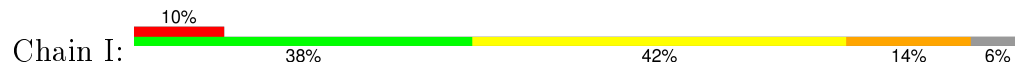




• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



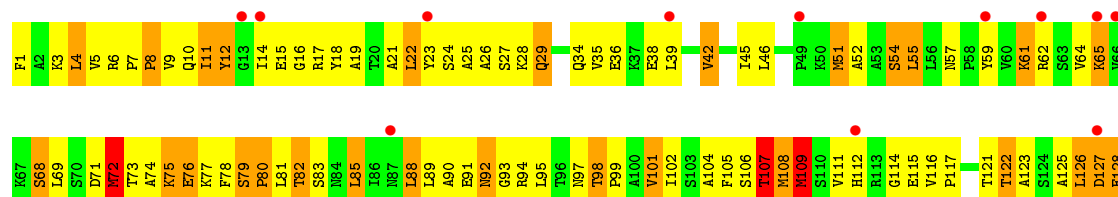
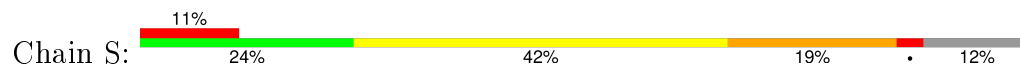
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



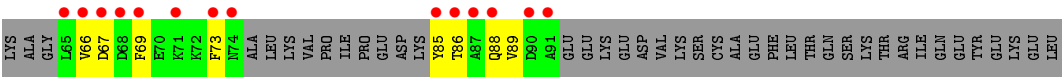
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL







● Molecule 9: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL



● Molecule 9: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	158.24Å 231.25Å 286.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.77 – 3.20 41.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.1 (41.77-3.20) 93.1 (41.77-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.217 , 0.271 0.203 , 0.260	Depositor DCC
R_{free} test set	8034 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 161021 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	54949	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, 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	0.80	1/3933 (0.0%)	0.75	2/5306 (0.0%)
1	B	0.55	0/3711	0.71	0/5005
1	C	0.46	0/3735	0.64	0/5038
1	J	0.58	0/3766	0.75	1/5080 (0.0%)
1	K	0.56	0/3711	0.73	0/5005
1	L	0.45	0/3721	0.65	0/5019
2	D	0.48	0/3596	0.65	0/4879
2	E	0.54	0/3587	0.70	1/4867 (0.0%)
2	F	0.51	0/3594	0.68	0/4877
2	M	0.47	0/3596	0.66	0/4879
2	N	0.52	0/3587	0.71	2/4867 (0.0%)
2	O	0.50	0/3587	0.70	0/4867
3	G	0.44	0/2050	0.61	0/2752
3	P	0.46	0/2050	0.61	0/2752
4	H	0.29	0/982	0.48	0/1337
4	Q	0.28	0/982	0.48	0/1337
5	I	0.29	0/374	0.46	0/501
5	R	0.28	0/374	0.45	0/501
6	S	0.39	0/1301	0.76	4/1740 (0.2%)
6	W	0.39	0/1131	0.74	3/1521 (0.2%)
7	T	0.31	0/739	0.61	3/982 (0.3%)
7	X	0.37	0/334	0.71	3/437 (0.7%)
8	U	0.27	0/236	0.47	0/315
9	V	0.34	0/562	0.61	2/751 (0.3%)
9	Z	0.28	0/160	0.46	0/207
All	All	0.51	1/55399 (0.0%)	0.68	21/74822 (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
1	A	0	1
1	J	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ASP	C-N	33.82	1.94	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ASP	C-N-CA	-10.48	100.28	122.30
6	S	72	MSE	CG-SE-CE	6.24	112.64	98.90
6	W	109	MSE	CG-SE-CE	6.17	112.47	98.90
7	T	165	MSE	CG-SE-CE	6.17	112.47	98.90
6	S	109	MSE	CG-SE-CE	5.97	112.04	98.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ASP	Peptide
1	J	269	ASP	Peptide

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	A	3882	0	3986	260	0
1	B	3663	0	3774	206	0
1	C	3684	0	3785	301	0
1	J	3715	0	3814	252	0
1	K	3663	0	3774	229	0
1	L	3670	0	3778	319	0
2	D	3539	0	3592	250	0
2	E	3530	0	3587	200	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3534	0	3595	251	0
2	M	3539	0	3592	280	0
2	N	3530	0	3587	208	0
2	O	3530	0	3586	258	0
3	G	2027	0	2082	167	0
3	P	2027	0	2082	167	0
4	H	970	0	972	98	0
4	Q	970	0	972	93	0
5	I	369	0	395	32	0
5	R	369	0	395	37	0
6	S	1292	0	1382	171	0
6	W	1120	0	1191	149	0
7	T	733	0	751	81	0
7	X	336	0	362	20	0
8	U	234	0	222	15	0
9	V	551	0	534	62	0
9	Z	160	0	171	11	0
10	A	31	0	13	2	0
10	B	31	0	12	1	0
10	C	31	0	13	0	0
10	F	31	0	13	9	0
10	J	31	0	13	2	0
10	K	31	0	13	4	0
10	L	31	0	13	2	0
10	O	31	0	13	6	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	F	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	O	1	0	0	0	0
12	D	27	0	12	3	0
12	M	27	0	12	4	0
All	All	54949	0	56088	3856	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 35.

The worst 5 of 3856 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)
1:A:191:ASP:C	1:A:192:GLY:N	1.93	1.20
1:L:179:ALA:HB1	1:L:267:ILE:HD13	1.23	1.15
1:C:212:THR:HG23	2:F:356:ARG:HH21	1.07	1.15
1:L:212:THR:HG23	2:O:356:ARG:HH21	1.10	1.14
1:A:16:ILE:HD13	6:S:22:LEU:HD21	1.29	1.14

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 X-ray entries followed by that with respect to entries of similar resolution.

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	508/510 (100%)	423 (83%)	61 (12%)	24 (5%)	3	22
1	B	476/510 (93%)	410 (86%)	60 (13%)	6 (1%)	15	59
1	C	482/510 (94%)	365 (76%)	88 (18%)	29 (6%)	2	16
1	J	485/510 (95%)	404 (83%)	61 (13%)	20 (4%)	3	27
1	K	476/510 (93%)	414 (87%)	54 (11%)	8 (2%)	11	52
1	L	479/510 (94%)	354 (74%)	100 (21%)	25 (5%)	2	19
2	D	465/482 (96%)	360 (77%)	84 (18%)	21 (4%)	3	24
2	E	464/482 (96%)	392 (84%)	61 (13%)	11 (2%)	7	43
2	F	465/482 (96%)	368 (79%)	78 (17%)	19 (4%)	3	27
2	M	465/482 (96%)	356 (77%)	79 (17%)	30 (6%)	1	13
2	N	464/482 (96%)	392 (84%)	60 (13%)	12 (3%)	7	40
2	O	464/482 (96%)	375 (81%)	70 (15%)	19 (4%)	3	27
3	G	254/272 (93%)	172 (68%)	65 (26%)	17 (7%)	1	12
3	P	254/272 (93%)	175 (69%)	62 (24%)	17 (7%)	1	12
4	H	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	1	5
4	Q	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	45/50 (90%)	28 (62%)	13 (29%)	4 (9%)	1	5
5	R	45/50 (90%)	28 (62%)	13 (29%)	4 (9%)	1	5
6	S	163/190 (86%)	97 (60%)	44 (27%)	22 (14%)	0	1
6	W	144/190 (76%)	81 (56%)	37 (26%)	26 (18%)	0	0
7	T	84/116 (72%)	68 (81%)	12 (14%)	4 (5%)	3	22
7	X	37/116 (32%)	25 (68%)	10 (27%)	2 (5%)	2	19
8	U	22/118 (19%)	20 (91%)	2 (9%)	0	100	100
9	V	64/76 (84%)	43 (67%)	19 (30%)	2 (3%)	5	34
9	Z	13/76 (17%)	5 (38%)	8 (62%)	0	100	100
All	All	7076/7770 (91%)	5545 (78%)	1185 (17%)	346 (5%)	3	22

5 of 346 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	22	SER
1	A	24	ASP
1	A	361	ILE
1	A	409	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	412/412 (100%)	358 (87%)	54 (13%)	5	24
1	B	389/412 (94%)	335 (86%)	54 (14%)	4	20
1	C	388/412 (94%)	333 (86%)	55 (14%)	4	19
1	J	393/412 (95%)	339 (86%)	54 (14%)	4	21
1	K	389/412 (94%)	333 (86%)	56 (14%)	4	19
1	L	388/412 (94%)	331 (85%)	57 (15%)	4	18
2	D	377/386 (98%)	321 (85%)	56 (15%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	376/386 (97%)	326 (87%)	50 (13%)	5	23
2	F	377/386 (98%)	332 (88%)	45 (12%)	6	28
2	M	377/386 (98%)	317 (84%)	60 (16%)	3	14
2	N	376/386 (97%)	330 (88%)	46 (12%)	6	27
2	O	376/386 (97%)	329 (88%)	47 (12%)	6	26
3	G	222/230 (96%)	184 (83%)	38 (17%)	2	12
3	P	222/230 (96%)	183 (82%)	39 (18%)	2	11
4	H	104/109 (95%)	95 (91%)	9 (9%)	13	45
4	Q	104/109 (95%)	95 (91%)	9 (9%)	13	45
5	I	38/41 (93%)	35 (92%)	3 (8%)	15	53
5	R	38/41 (93%)	34 (90%)	4 (10%)	8	35
6	S	146/158 (92%)	120 (82%)	26 (18%)	2	11
6	W	127/158 (80%)	107 (84%)	20 (16%)	3	15
7	T	81/100 (81%)	76 (94%)	5 (6%)	23	64
7	X	39/100 (39%)	37 (95%)	2 (5%)	29	70
8	U	26/100 (26%)	23 (88%)	3 (12%)	7	30
9	V	60/68 (88%)	55 (92%)	5 (8%)	14	49
9	Z	17/68 (25%)	14 (82%)	3 (18%)	2	11
All	All	5842/6300 (93%)	5042 (86%)	800 (14%)	4	21

5 of 800 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	14	TYR
1	K	256	TYR
6	S	42	VAL
1	J	101	GLU
1	J	408	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	35	GLN
1	K	172	GLN
4	Q	66	HIS

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Mol	Chain	Res	Type
4	H	138	ASN
1	J	430	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	ANP	A	600	11	27,33,33	4.07	12 (44%)	30,52,52	2.40	6 (20%)
10	ANP	B	600	11	27,33,33	4.11	12 (44%)	30,52,52	2.79	9 (30%)
10	ANP	C	600	11	27,33,33	3.98	12 (44%)	30,52,52	2.85	8 (26%)
12	ADP	D	600	11	22,29,29	1.95	6 (27%)	27,45,45	2.70	8 (29%)
10	ANP	F	600	11	27,33,33	3.72	12 (44%)	30,52,52	2.44	8 (26%)
10	ANP	J	600	11	27,33,33	3.98	12 (44%)	30,52,52	2.65	8 (26%)
10	ANP	K	600	11	27,33,33	3.95	12 (44%)	30,52,52	2.51	6 (20%)
10	ANP	L	600	11	27,33,33	4.14	12 (44%)	30,52,52	3.01	10 (33%)
12	ADP	M	600	11	22,29,29	2.18	7 (31%)	27,45,45	2.76	7 (25%)
10	ANP	O	600	11	27,33,33	3.68	12 (44%)	30,52,52	2.66	8 (26%)

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	ANP	A	600	11	-	1/12/38/38	0/3/3/3
10	ANP	B	600	11	2/2/7/8	1/12/38/38	0/3/3/3
10	ANP	C	600	11	-	0/12/38/38	0/3/3/3
12	ADP	D	600	11	-	0/12/32/32	0/3/3/3
10	ANP	F	600	11	-	0/12/38/38	0/3/3/3
10	ANP	J	600	11	-	1/12/38/38	0/3/3/3
10	ANP	K	600	11	-	0/12/38/38	0/3/3/3
10	ANP	L	600	11	-	0/12/38/38	0/3/3/3
12	ADP	M	600	11	-	0/12/32/32	0/3/3/3
10	ANP	O	600	11	-	0/12/38/38	0/3/3/3

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	600	ANP	PB-O2B	-3.73	1.46	1.56
10	A	600	ANP	PB-O2B	-3.60	1.46	1.56
10	K	600	ANP	PB-O2B	-3.47	1.47	1.56
10	L	600	ANP	PB-O2B	-3.46	1.47	1.56
10	C	600	ANP	PB-O2B	-3.43	1.47	1.56

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	600	ANP	N3-C2-N1	-12.23	119.53	128.89
10	C	600	ANP	N3-C2-N1	-12.22	119.54	128.89
10	B	600	ANP	N3-C2-N1	-11.63	119.99	128.89
12	D	600	ADP	N3-C2-N1	-11.26	120.28	128.89
12	M	600	ADP	N3-C2-N1	-10.97	120.50	128.89

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	600	ANP	C4'
10	B	600	ANP	C3'

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	600	ANP	O1B-PB-N3B-PG
10	B	600	ANP	O1B-PB-N3B-PG
10	A	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	600	ANP	2	0
10	B	600	ANP	1	0
12	D	600	ADP	3	0
10	F	600	ANP	9	0
10	J	600	ANP	2	0
10	K	600	ANP	4	0
10	L	600	ANP	2	0
12	M	600	ADP	4	0
10	O	600	ANP	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	510/510 (100%)	-0.40	1 (0%) 95 94	32, 60, 113, 179	0
1	B	480/510 (94%)	-0.54	0 100 100	34, 59, 91, 147	0
1	C	484/510 (94%)	-0.14	15 (3%) 52 38	50, 86, 171, 227	0
1	J	487/510 (95%)	-0.43	5 (1%) 84 75	32, 62, 98, 132	0
1	K	480/510 (94%)	-0.49	1 (0%) 95 94	33, 59, 95, 144	0
1	L	481/510 (94%)	-0.03	24 (4%) 32 19	51, 87, 170, 227	0
2	D	467/482 (96%)	-0.33	0 100 100	46, 79, 126, 169	0
2	E	466/482 (96%)	-0.45	4 (0%) 85 78	30, 64, 113, 174	0
2	F	466/482 (96%)	-0.27	0 100 100	39, 71, 105, 130	0
2	M	467/482 (96%)	-0.22	12 (2%) 59 45	46, 82, 127, 168	0
2	N	466/482 (96%)	-0.40	1 (0%) 95 94	31, 65, 119, 173	0
2	O	466/482 (96%)	-0.40	0 100 100	40, 71, 106, 139	0
3	G	260/272 (95%)	0.19	16 (6%) 24 13	33, 119, 237, 251	0
3	P	260/272 (95%)	0.32	21 (8%) 15 8	34, 118, 236, 252	0
4	H	131/146 (89%)	1.23	28 (21%) 1 1	117, 199, 238, 252	0
4	Q	131/146 (89%)	1.57	40 (30%) 1 0	123, 201, 239, 254	0
5	I	47/50 (94%)	0.62	5 (10%) 8 4	125, 193, 238, 252	0
5	R	47/50 (94%)	1.27	10 (21%) 1 1	124, 195, 239, 251	0
6	S	161/190 (84%)	0.66	20 (12%) 5 3	113, 159, 188, 206	0
6	W	142/190 (74%)	1.05	28 (19%) 1 1	115, 157, 191, 203	0
7	T	82/116 (70%)	2.44	49 (59%) 0 0	165, 233, 275, 288	0
7	X	38/116 (32%)	1.94	19 (50%) 0 0	164, 217, 238, 239	0
8	U	28/118 (23%)	2.58	21 (75%) 0 0	195, 232, 254, 261	0
9	V	64/76 (84%)	3.10	34 (53%) 0 0	157, 221, 291, 302	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
9	Z	17/76 (22%)	1.70	8 (47%) 0 0	175, 211, 230, 238	0
All	All	7128/7770 (91%)	-0.08	362 (5%) 32 18	30, 76, 216, 302	0

The worst 5 of 362 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	70	GLU	12.3
5	R	9	LEU	10.0
9	V	67	PRO	9.3
3	G	180	SER	9.2
9	V	8	VAL	9.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	MG	O	601	1/1	0.98	0.39	6.80	51,51,51,51	0
11	MG	D	601	1/1	0.98	0.50	5.21	66,66,66,66	0
11	MG	F	601	1/1	0.98	0.40	3.42	52,52,52,52	0
11	MG	M	601	1/1	0.97	0.42	3.03	64,64,64,64	0
12	ADP	M	600	27/27	0.92	0.28	1.55	46,66,79,86	0
12	ADP	D	600	27/27	0.95	0.27	1.05	53,70,80,84	0
10	ANP	A	600	31/31	0.96	0.22	0.91	51,64,82,93	0
10	ANP	J	600	31/31	0.96	0.21	0.72	50,70,85,95	0
10	ANP	K	600	31/31	0.95	0.19	0.68	40,95,115,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	ANP	B	600	31/31	0.94	0.19	0.68	44,92,104,109	0
10	ANP	O	600	31/31	0.97	0.19	0.21	44,55,67,81	0
10	ANP	L	600	31/31	0.94	0.20	-0.12	54,91,101,115	0
10	ANP	C	600	31/31	0.96	0.17	-0.16	78,98,114,115	0
10	ANP	F	600	31/31	0.96	0.20	-0.42	41,52,63,78	0
11	MG	J	601	1/1	0.98	0.37	-	81,81,81,81	0
11	MG	B	601	1/1	0.95	0.28	-	84,84,84,84	0
11	MG	A	601	1/1	0.96	0.31	-	49,49,49,49	0
11	MG	L	601	1/1	0.93	0.64	-	81,81,81,81	0
11	MG	C	601	1/1	0.96	0.36	-	76,76,76,76	0
11	MG	K	601	1/1	0.95	0.35	-	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.