wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:37 AM GMT

PDB ID	:	2HLD
Title	:	Crystal structure of yeast mitochondrial F1-ATPase
Authors	:	Kabaleeswaran, V.; Puri, N.; Walker, J.E.; Leslie, A.G.; Mueller, D.M.
Deposited on	:	2006-07-06
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

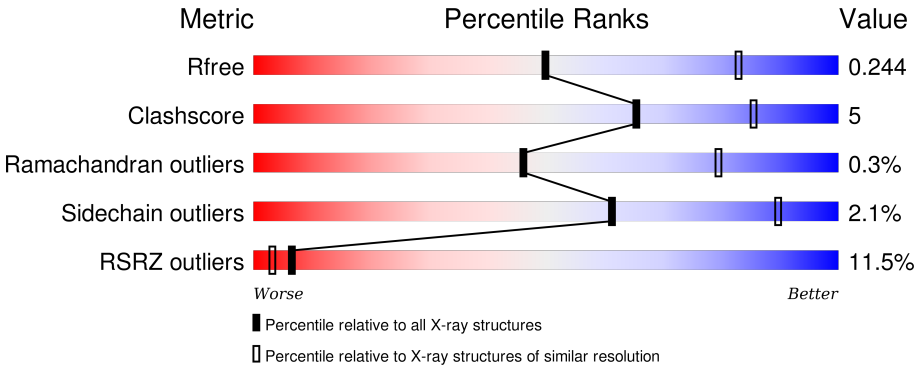
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	3% 83% 11% 5%
1	B	510	6% 81% 12% • 5%
1	C	510	6% 82% 12% • 5%
1	J	510	7% 85% 9% • 6%
1	K	510	9% 80% 14% • 5%

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Mol	Chain	Length	Quality of chain
1	L	510	5% 79% 14% • 5%
1	S	510	8% 83% 11% • 6%
1	T	510	18% 82% 12% • 6%
1	U	510	20% 83% 10% • 6%
2	D	478	6% 87% 11% • •
2	E	478	9% 84% 14% •
2	F	478	5% 84% 13% • •
2	M	478	5% 83% 15% • •
2	N	478	13% 87% 10% • •
2	O	478	7% 87% 10% • •
2	V	478	17% 85% 12% • •
2	W	478	17% 85% 13% •
2	X	478	14% 80% 17% •
3	G	278	10% 73% 21% • 5%
3	P	278	22% 65% 19% • 13%
3	Y	278	20% 55% 17% 28%
4	H	138	32% 78% 8% • 13%
4	Q	138	20% 56% 5% 39%
4	Z	138	7% 12% 88%
5	1	61	18% 38% 7% 56%
5	I	61	13% 69% 8% • 21%
5	R	61	16% 52% • 44%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 72841 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 alpha chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3674	2319	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3684	2326	652	703	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	480	Total	C	N	O	S	0	0	0
			3651	2307	645	696	3			
1	T	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			
1	U	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			

- Molecule 2 is a protein called ATP synthase beta chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			
2	M	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total	C	N	O	S	0	0	0
			3538	2244	602	686	6			
2	V	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3531	2240	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total	C	N	O	S	0	0	0
			2031	1277	355	389	10			
3	P	243	Total	C	N	O	S	0	0	0
			1851	1165	322	355	9			
3	Y	200	Total	C	N	O	S	0	0	0
			1517	944	273	291	9			

- Molecule 4 is a protein called ATP synthase delta chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	120	Total	C	N	O	S	0	0	0
			758	475	134	147	2			
4	Q	84	Total	C	N	O		0	0	0
			436	262	87	87				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

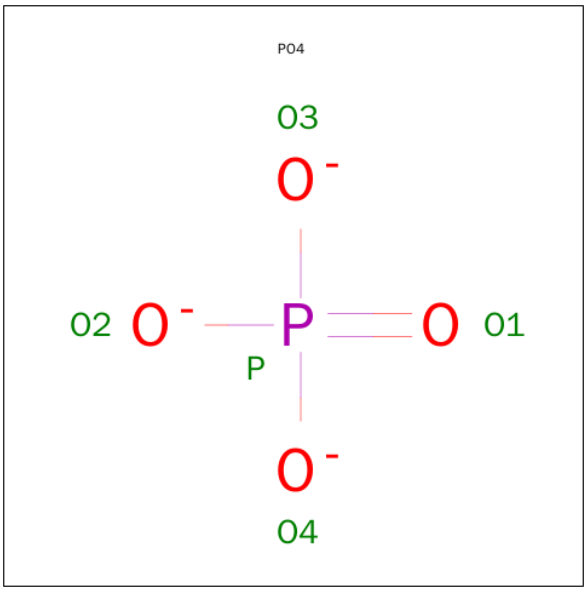
- Molecule 5 is a protein called ATP synthase epsilon chain, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	48	Total	C	N	O	0	0	0
			324	201	56	67			
5	R	34	Total	C	N	O	0	0	0
			170	102	34	34			
5	1	27	Total	C	N	O	0	0	0
			135	81	27	27			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

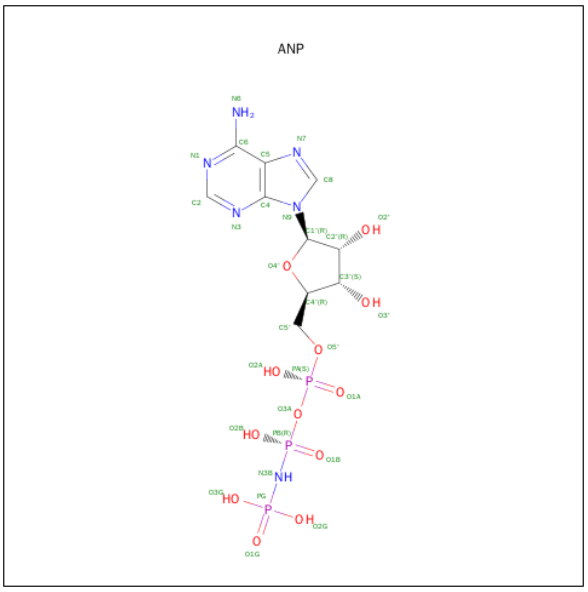
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0
6	K	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	V	1	Total Mg 1 1	0	0
6	A	1	Total Mg 1 1	0	0
6	T	1	Total Mg 1 1	0	0
6	U	1	Total Mg 1 1	0	0
6	X	1	Total Mg 1 1	0	0
6	O	1	Total Mg 1 1	0	0
6	L	1	Total Mg 1 1	0	0
6	S	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0
6	M	1	Total Mg 1 1	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	N	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	L	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	O	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	S	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	T	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	U	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	V	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
8	X	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	26	Total	O	0	0
			26	26		
9	B	18	Total	O	0	0
			18	18		
9	C	13	Total	O	0	0
			13	13		
9	D	20	Total	O	0	0
			20	20		
9	E	13	Total	O	0	0
			13	13		
9	F	11	Total	O	0	0
			11	11		

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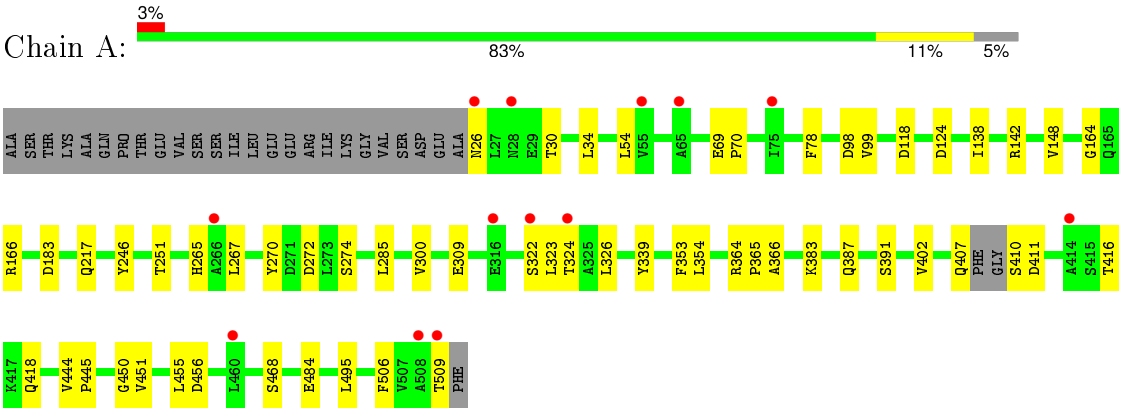
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	3	Total O 3 3	0	0
9	J	17	Total O 17 17	0	0
9	K	4	Total O 4 4	0	0
9	L	19	Total O 19 19	0	0
9	M	9	Total O 9 9	0	0
9	N	8	Total O 8 8	0	0
9	O	7	Total O 7 7	0	0
9	P	2	Total O 2 2	0	0
9	Q	1	Total O 1 1	0	0
9	S	6	Total O 6 6	0	0
9	T	1	Total O 1 1	0	0
9	U	3	Total O 3 3	0	0
9	X	2	Total O 2 2	0	0

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 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.

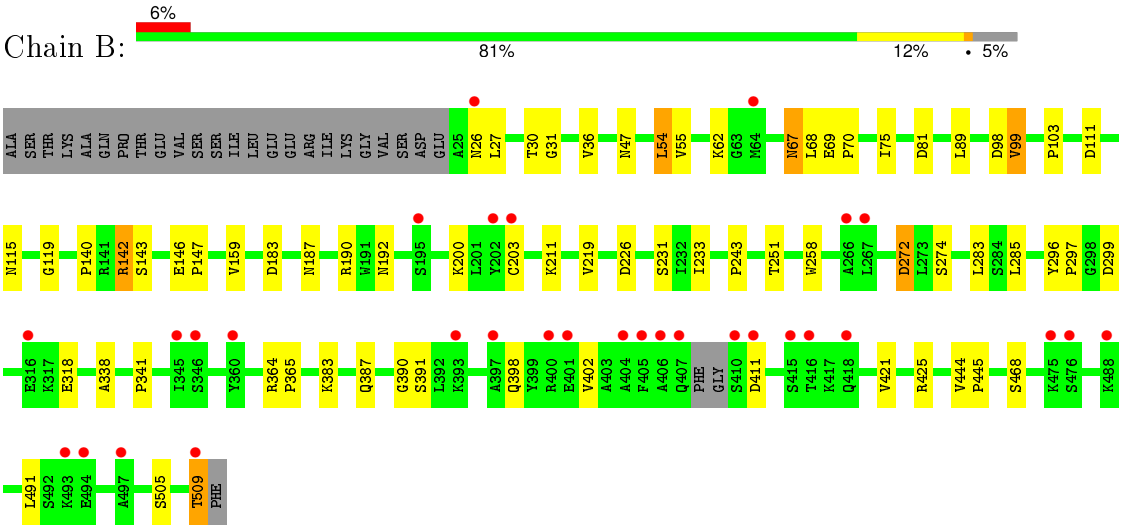
- Molecule 1: ATP synthase alpha chain, mitochondrial

Chain A:



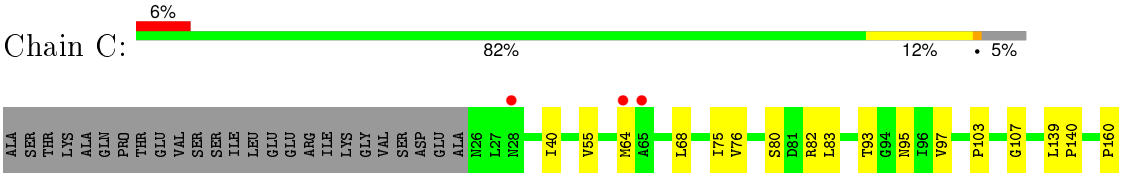
- Molecule 1: ATP synthase alpha chain, mitochondrial

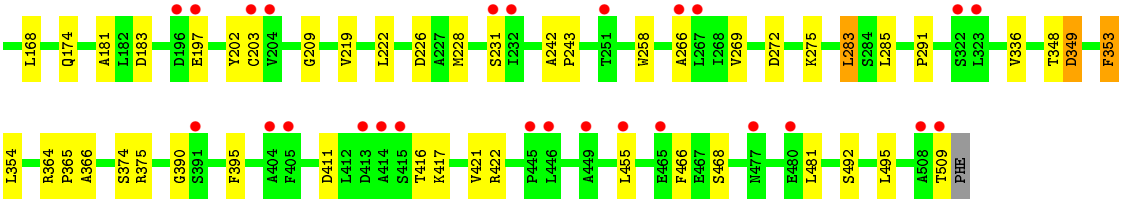
Chain B:



- Molecule 1: ATP synthase alpha chain, mitochondrial

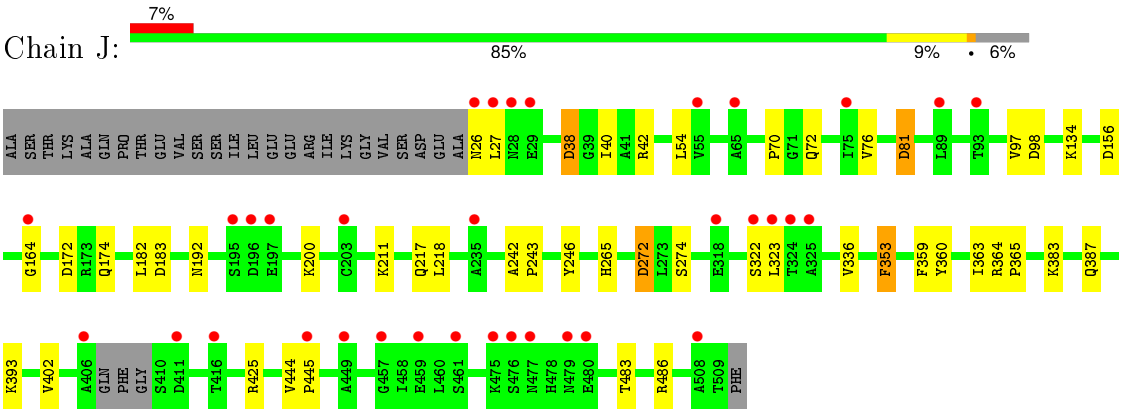
Chain C:





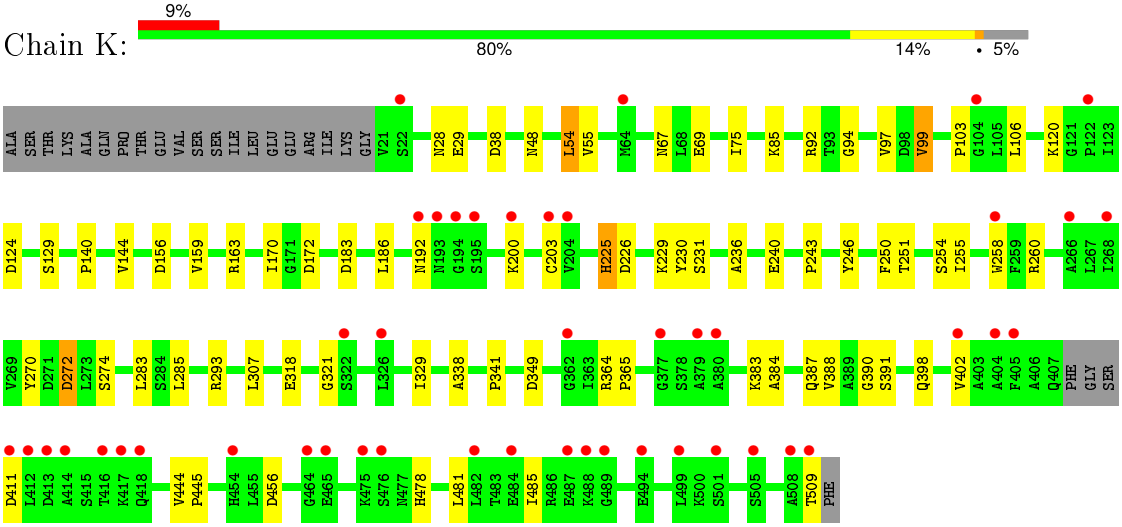
• Molecule 1: ATP synthase alpha chain, mitochondrial

Chain J:



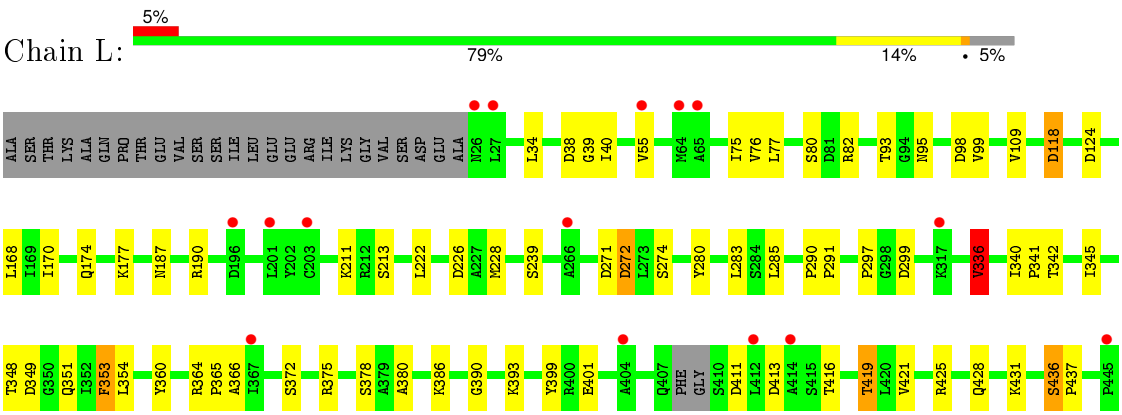
• Molecule 1: ATP synthase alpha chain, mitochondrial

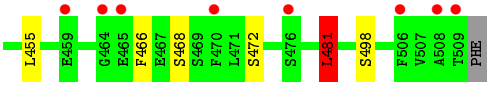
Chain K:



• Molecule 1: ATP synthase alpha chain, mitochondrial

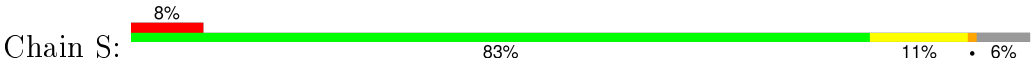
Chain L:

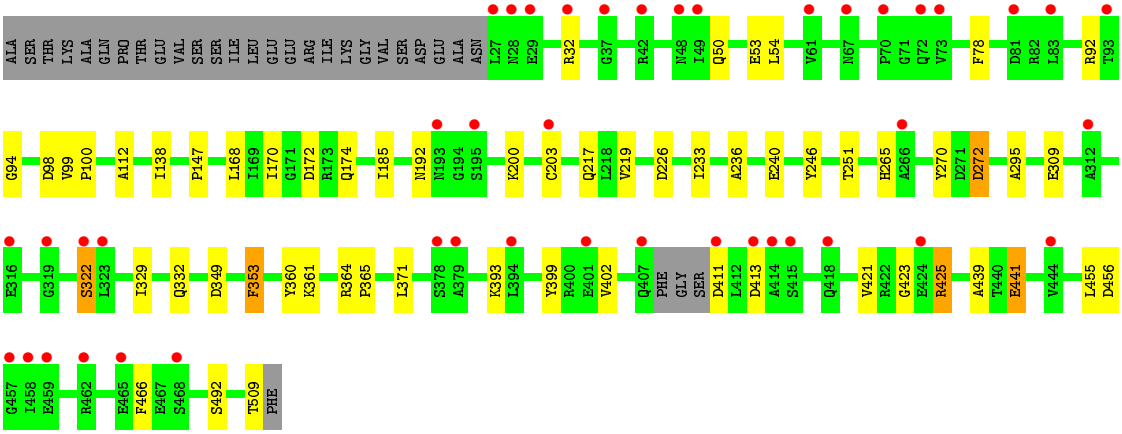




• Molecule 1: ATP synthase alpha chain, mitochondrial

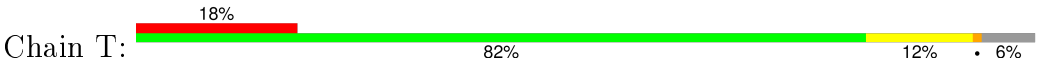
Chain S:

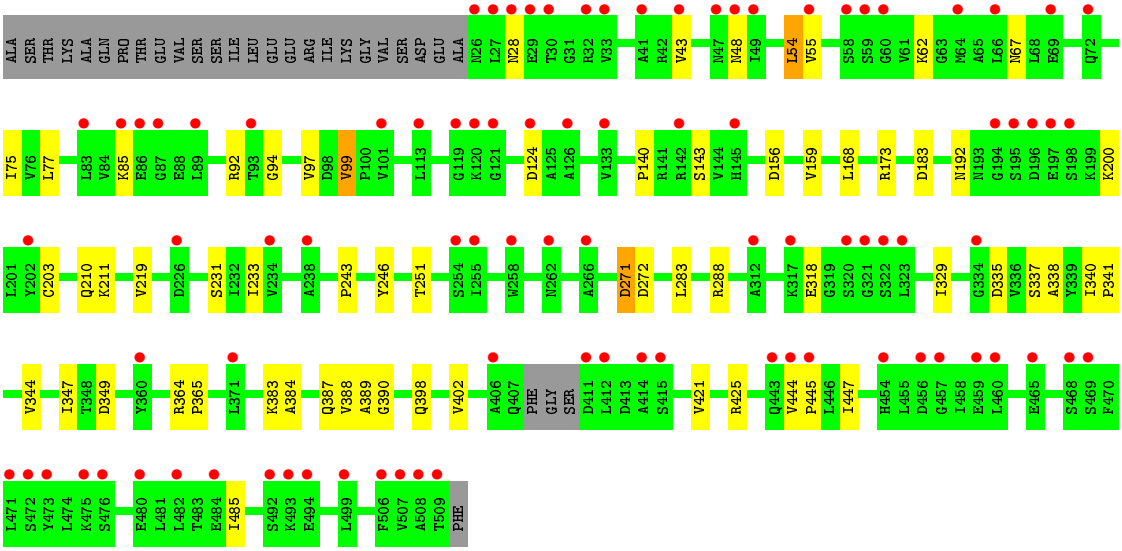




• Molecule 1: ATP synthase alpha chain, mitochondrial

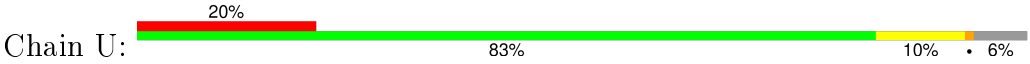
Chain T:

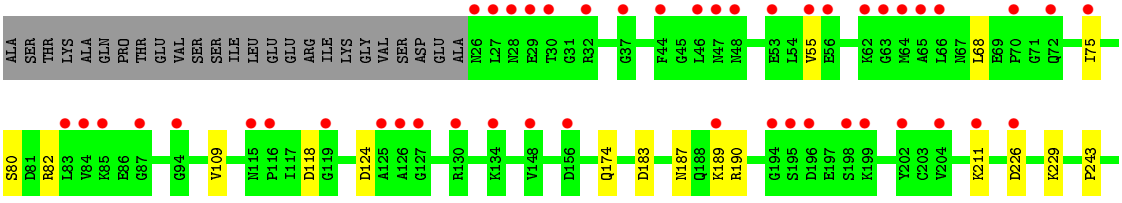


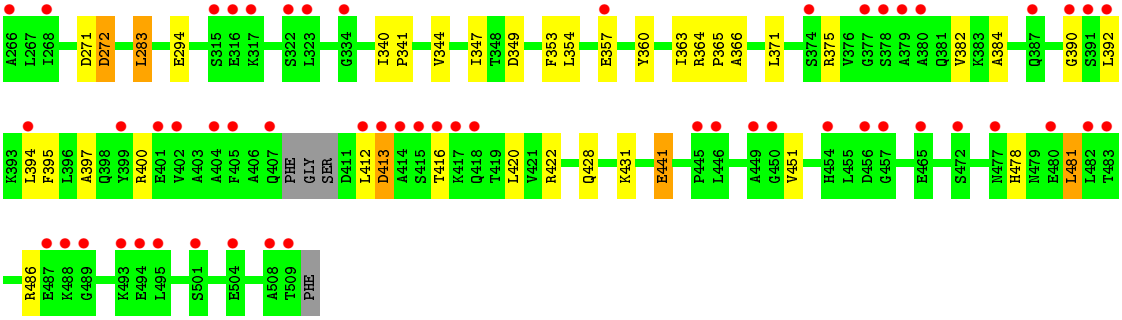


• Molecule 1: ATP synthase alpha chain, mitochondrial

Chain U:

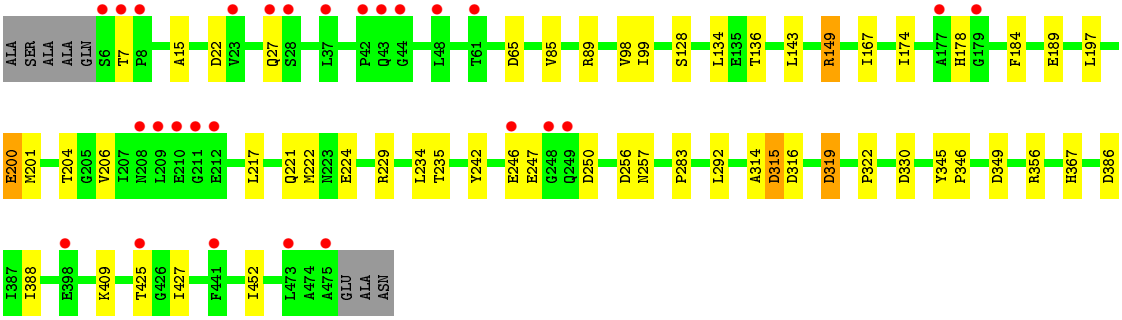






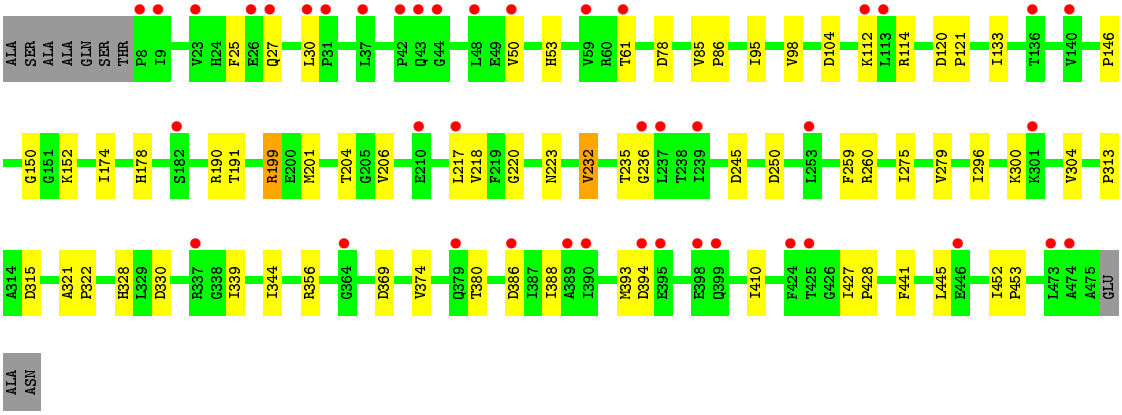
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain D:



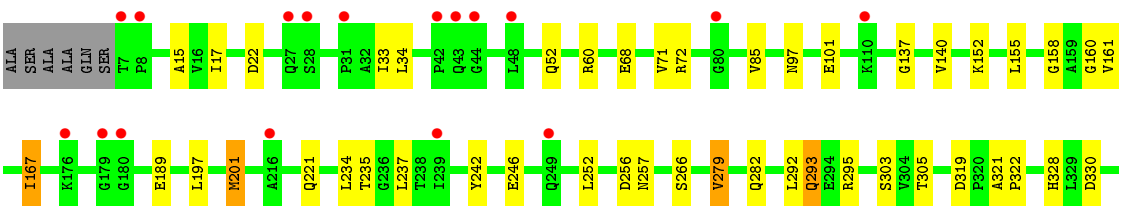
• Molecule 2: ATP synthase beta chain, mitochondrial

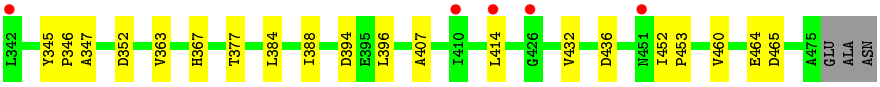
Chain E:



• Molecule 2: ATP synthase beta chain, mitochondrial

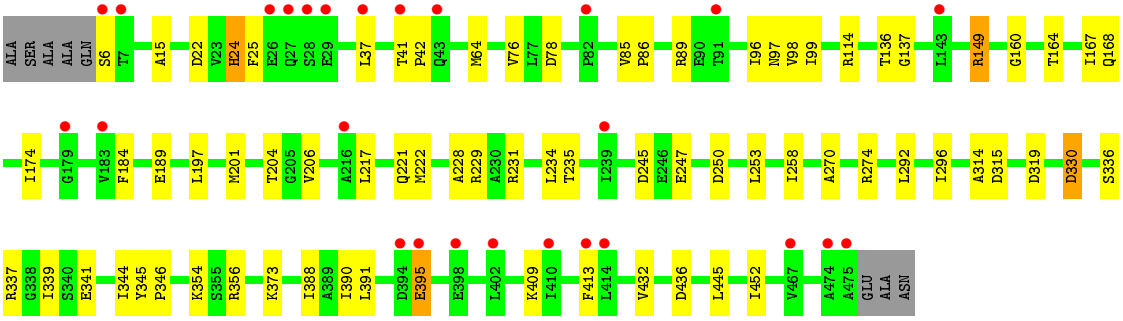
Chain F:





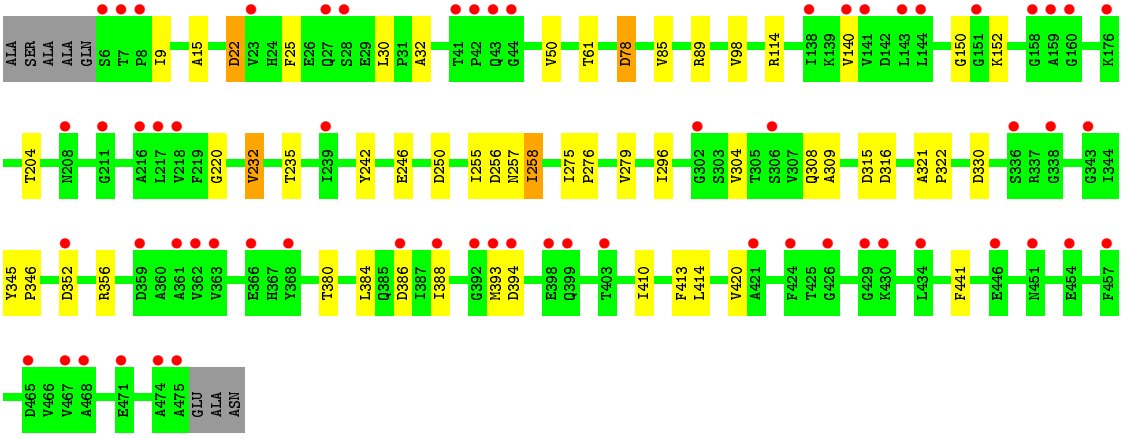
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain M:



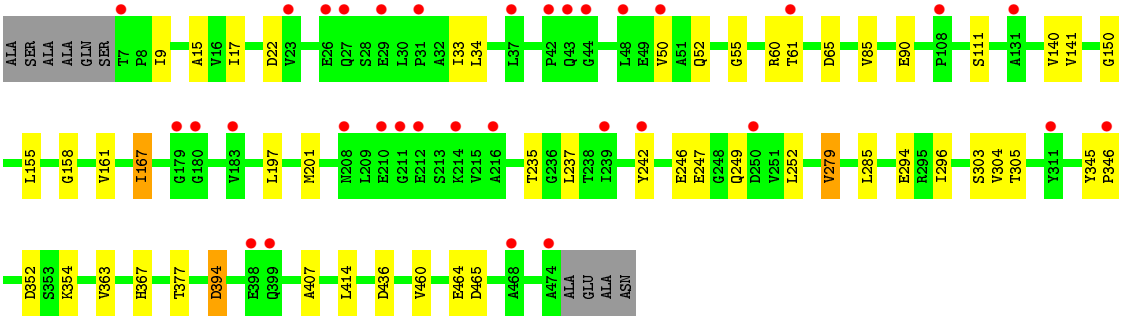
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain N:



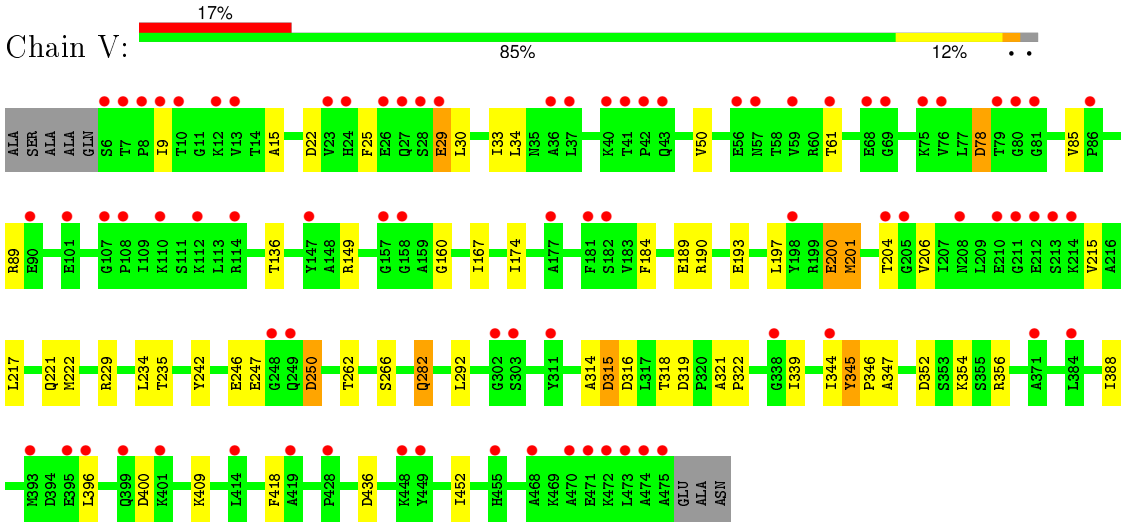
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain O:



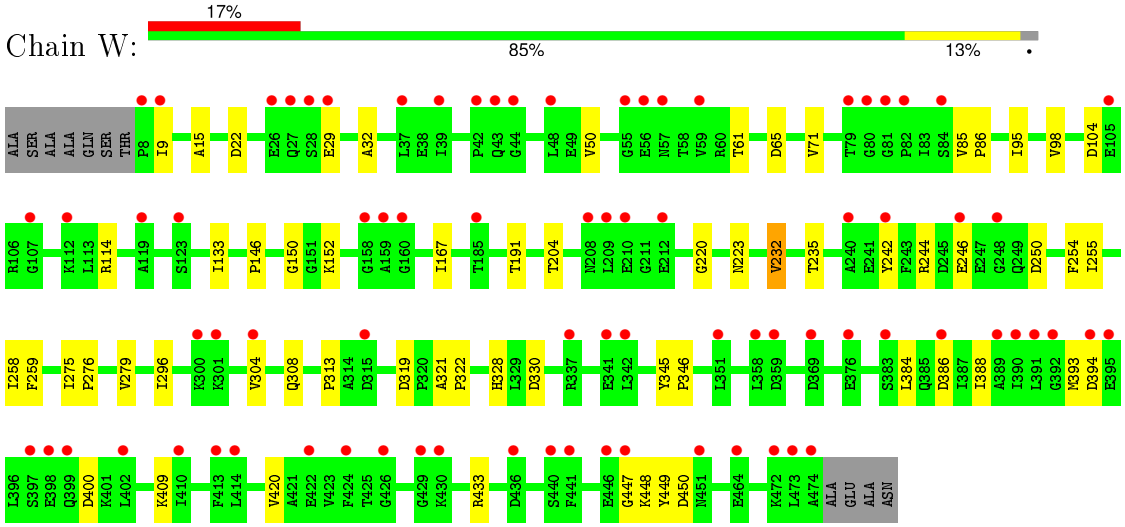
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain V:



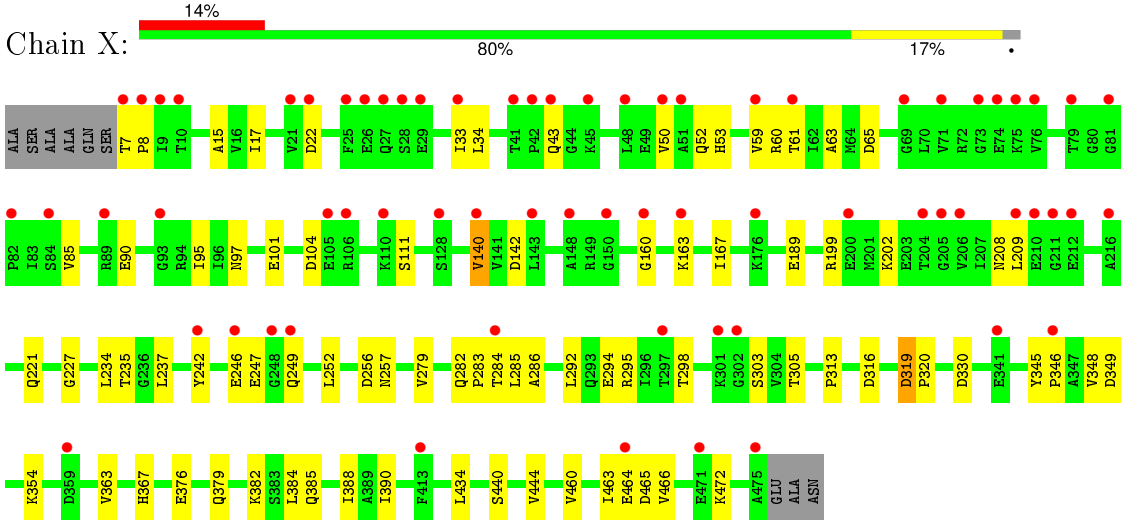
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain W:



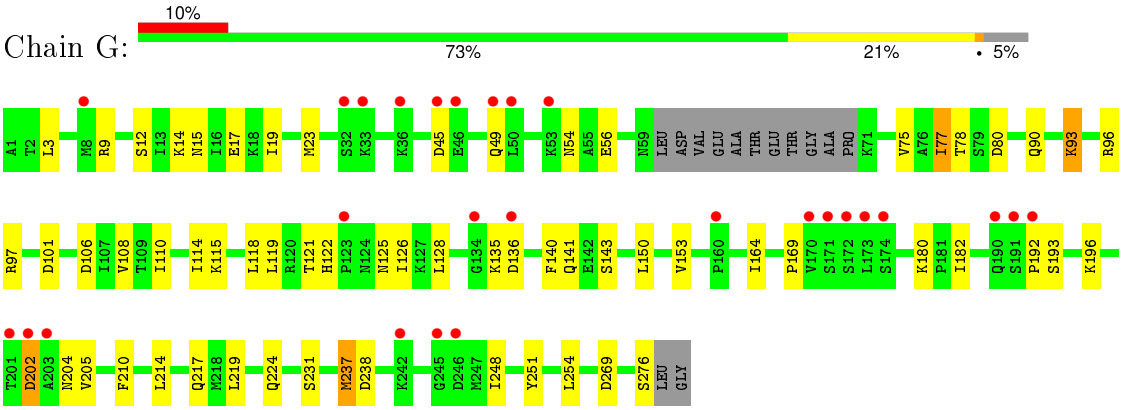
• Molecule 2: ATP synthase beta chain, mitochondrial

Chain X:



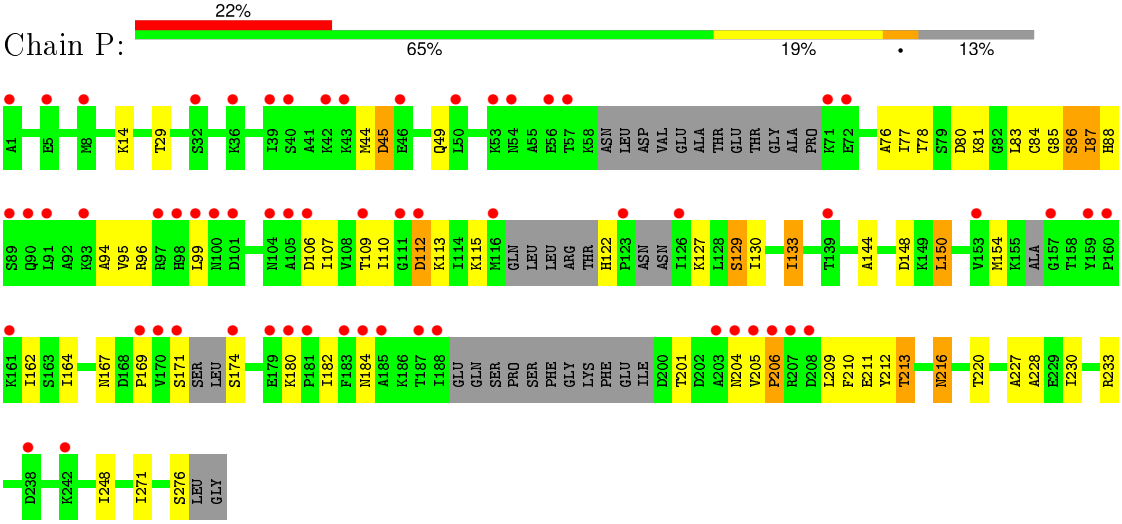
• Molecule 3: ATP synthase gamma chain, mitochondrial

Chain G:



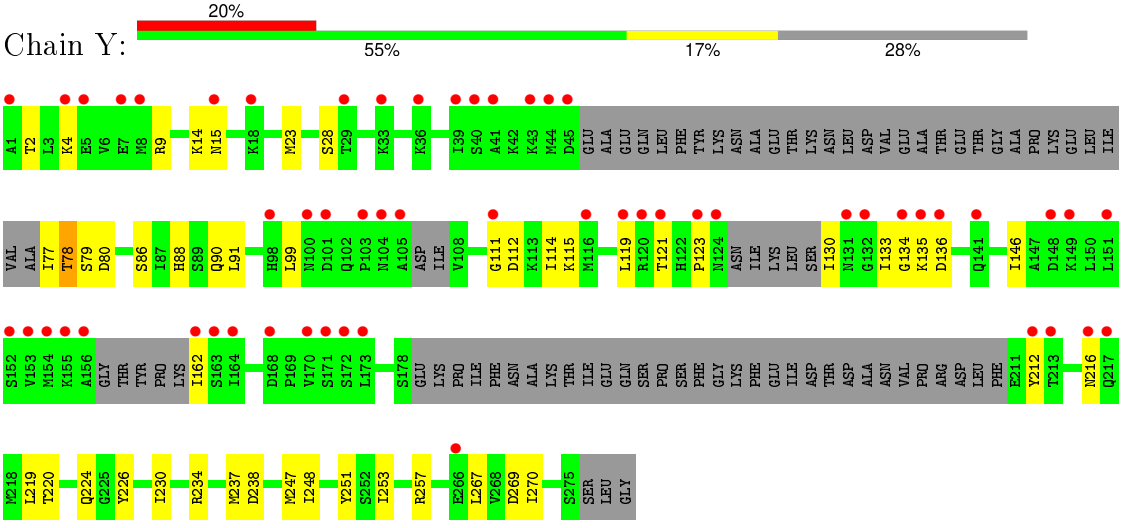
• Molecule 3: ATP synthase gamma chain, mitochondrial

Chain P:



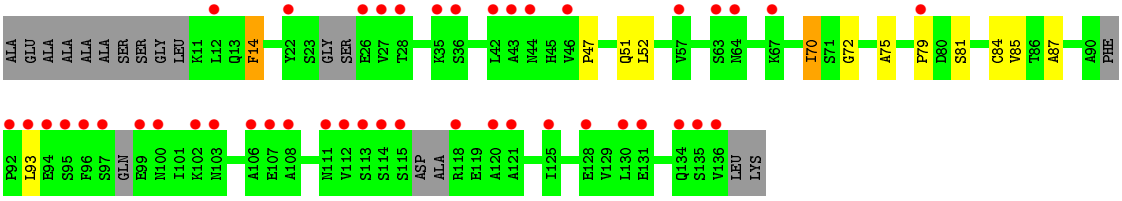
• Molecule 3: ATP synthase gamma chain, mitochondrial

Chain Y:



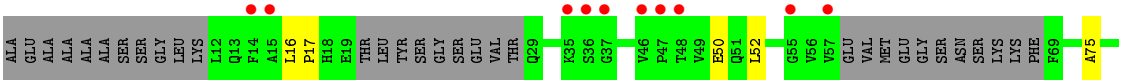
• Molecule 4: ATP synthase delta chain, mitochondrial

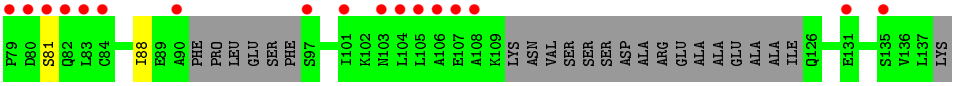
Chain H:



• Molecule 4: ATP synthase delta chain, mitochondrial

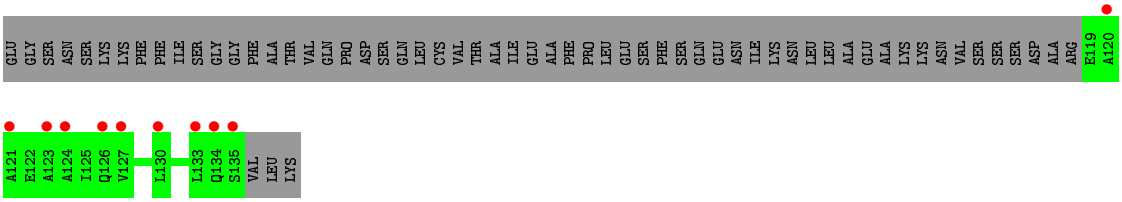
Chain Q:





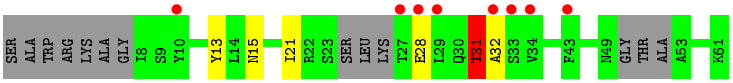
• Molecule 4: ATP synthase delta chain, mitochondrial

Chain Z:



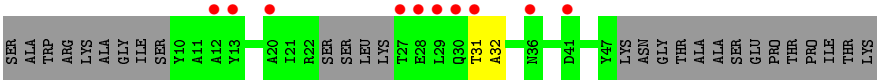
• Molecule 5: ATP synthase epsilon chain, mitochondrial

Chain I:



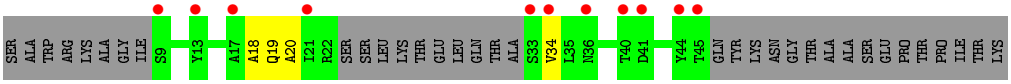
• Molecule 5: ATP synthase epsilon chain, mitochondrial

Chain R:



• Molecule 5: ATP synthase epsilon chain, mitochondrial

Chain 1:


SER
ALA
TRP
ARG
LYS
ALA
GLY
ILE
S9
Y13
A17
A18
Q19
A20
I21
R22
SER
SER
LEU
LYS
THR
GLU
LEU
GLN
THR
ALA
S33
V34
L35
N36
T40
D41
Y44
T45
GLN
TYR
LYS
ASN
GLY
THR
ALA
ALA
SER
GLU
PRO
THR
PRO
ILE
THR
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.52Å 294.13Å 190.43Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.80) 99.9 (19.99-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.244 0.211 , 0.244	Depositor DCC
R_{free} test set	5938 reflections (2.07%)	DCC
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 80.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 292845 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	72841	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, ANP, MG

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	0.64	0/3718	0.79	6/5032 (0.1%)
1	B	0.57	0/3723	0.76	6/5039 (0.1%)
1	C	0.57	0/3729	0.76	5/5048 (0.1%)
1	J	0.55	0/3709	0.74	7/5020 (0.1%)
1	K	0.46	0/3738	0.69	9/5060 (0.2%)
1	L	0.62	1/3718 (0.0%)	0.81	13/5032 (0.3%)
1	S	0.47	0/3705	0.72	8/5014 (0.2%)
1	T	0.38	0/3713	0.64	5/5025 (0.1%)
1	U	0.41	0/3713	0.68	6/5025 (0.1%)
2	D	0.57	0/3605	0.81	9/4889 (0.2%)
2	E	0.56	0/3592	0.76	10/4870 (0.2%)
2	F	0.54	0/3599	0.78	5/4881 (0.1%)
2	M	0.55	0/3605	0.80	5/4889 (0.1%)
2	N	0.48	0/3605	0.74	7/4889 (0.1%)
2	O	0.50	0/3594	0.75	4/4874 (0.1%)
2	V	0.43	0/3605	0.75	8/4889 (0.2%)
2	W	0.40	0/3587	0.69	6/4863 (0.1%)
2	X	0.42	0/3599	0.70	5/4881 (0.1%)
3	G	0.48	0/2056	0.74	6/2767 (0.2%)
3	P	0.47	0/1868	0.70	2/2508 (0.1%)
3	Y	0.37	0/1527	0.63	2/2048 (0.1%)
4	H	0.47	0/766	0.64	0/1051
4	Q	0.41	0/434	0.55	0/595
4	Z	0.42	0/84	0.51	0/116
5	1	0.38	0/133	0.44	0/183
5	I	0.55	0/326	0.69	0/445
5	R	0.45	0/168	0.51	0/232
All	All	0.51	1/73219 (0.0%)	0.74	134/99165 (0.1%)

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	S	0	1
2	D	0	1
2	V	0	1
2	W	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	353	PHE	CB-CG	-5.87	1.41	1.51

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	345	TYR	C-N-CD	-13.32	91.28	120.60
2	D	22	ASP	CB-CG-OD2	10.23	127.51	118.30
2	F	436	ASP	CB-CG-OD2	7.85	125.37	118.30
1	C	283	LEU	CA-CB-CG	7.74	133.09	115.30
2	M	319	ASP	CB-CG-OD2	7.57	125.11	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	7	THR	Peptide
1	S	147	PRO	Peptide
2	V	345	TYR	Peptide
2	W	447	GLY	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	3664	0	3748	27	0
1	B	3669	0	3752	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3674	0	3756	39	0
1	J	3655	0	3739	31	0
1	K	3684	0	3758	43	0
1	L	3664	0	3747	45	0
1	S	3651	0	3740	35	0
1	T	3659	0	3745	35	0
1	U	3659	0	3745	29	0
2	D	3549	0	3620	29	0
2	E	3536	0	3610	39	0
2	F	3543	0	3615	40	0
2	M	3549	0	3620	52	0
2	N	3549	0	3621	33	0
2	O	3538	0	3610	31	0
2	V	3549	0	3620	38	0
2	W	3531	0	3605	37	0
2	X	3543	0	3615	49	0
3	G	2031	0	2084	31	0
3	P	1851	0	1893	39	0
3	Y	1517	0	1561	28	0
4	H	758	0	602	9	0
4	Q	436	0	215	3	0
4	Z	85	0	45	0	0
5	1	135	0	70	1	0
5	I	324	0	249	2	0
5	R	170	0	87	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	1	0	0	0	0
6	X	1	0	0	0	0
7	N	5	0	0	0	0
8	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	31	0	13	0	0
8	C	31	0	13	1	0
8	D	31	0	13	0	0
8	F	31	0	13	2	0
8	J	31	0	13	0	0
8	K	31	0	13	1	0
8	L	31	0	13	1	0
8	M	31	0	13	6	0
8	O	31	0	13	0	0
8	S	31	0	13	1	0
8	T	31	0	13	0	0
8	U	31	0	13	0	0
8	V	31	0	13	3	0
8	X	31	0	13	4	0
9	A	26	0	0	2	0
9	B	18	0	0	0	0
9	C	13	0	0	0	0
9	D	20	0	0	0	0
9	E	13	0	0	1	0
9	F	11	0	0	0	0
9	G	3	0	0	0	0
9	J	17	0	0	0	0
9	K	4	0	0	0	0
9	L	19	0	0	0	0
9	M	9	0	0	0	0
9	N	8	0	0	0	0
9	O	7	0	0	0	0
9	P	2	0	0	0	0
9	Q	1	0	0	2	0
9	S	6	0	0	0	0
9	T	1	0	0	0	0
9	U	3	0	0	0	0
9	X	2	0	0	0	0
All	All	72841	0	73267	728	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 5.

The worst 5 of 728 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:V:85:VAL:HG11	2:V:235:THR:HG23	1.26	1.16
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.27	1.12
2:N:85:VAL:HG11	2:N:235:THR:HG23	1.28	1.11
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.25	1.11
3:G:96:ARG:HE	3:G:121:THR:HG21	1.10	1.09

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	478/510 (94%)	465 (97%)	13 (3%)	0	100	100
1	B	479/510 (94%)	462 (96%)	17 (4%)	0	100	100
1	C	482/510 (94%)	469 (97%)	12 (2%)	1 (0%)	52	84
1	J	477/510 (94%)	466 (98%)	11 (2%)	0	100	100
1	K	482/510 (94%)	469 (97%)	13 (3%)	0	100	100
1	L	478/510 (94%)	458 (96%)	19 (4%)	1 (0%)	52	84
1	S	476/510 (93%)	461 (97%)	15 (3%)	0	100	100
1	T	477/510 (94%)	466 (98%)	10 (2%)	1 (0%)	52	84
1	U	477/510 (94%)	462 (97%)	14 (3%)	1 (0%)	52	84
2	D	468/478 (98%)	452 (97%)	16 (3%)	0	100	100
2	E	466/478 (98%)	446 (96%)	19 (4%)	1 (0%)	52	84
2	F	467/478 (98%)	445 (95%)	19 (4%)	3 (1%)	30	65
2	M	468/478 (98%)	449 (96%)	19 (4%)	0	100	100
2	N	468/478 (98%)	454 (97%)	13 (3%)	1 (0%)	52	84
2	O	466/478 (98%)	446 (96%)	19 (4%)	1 (0%)	52	84
2	V	468/478 (98%)	448 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	W	465/478 (97%)	450 (97%)	14 (3%)	1 (0%)	52 84
2	X	467/478 (98%)	448 (96%)	18 (4%)	1 (0%)	52 84
3	G	261/278 (94%)	235 (90%)	23 (9%)	3 (1%)	17 50
3	P	229/278 (82%)	201 (88%)	21 (9%)	7 (3%)	5 17
3	Y	188/278 (68%)	172 (92%)	16 (8%)	0	100 100
4	H	110/138 (80%)	98 (89%)	10 (9%)	2 (2%)	11 34
4	Q	74/138 (54%)	59 (80%)	12 (16%)	3 (4%)	3 11
4	Z	15/138 (11%)	13 (87%)	2 (13%)	0	100 100
5	1	23/61 (38%)	20 (87%)	1 (4%)	2 (9%)	1 2
5	I	42/61 (69%)	35 (83%)	5 (12%)	2 (5%)	3 9
5	R	30/61 (49%)	23 (77%)	5 (17%)	2 (7%)	1 4
All	All	9481/10323 (92%)	9072 (96%)	376 (4%)	33 (0%)	46 79

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	135	LYS
5	I	31	THR
5	R	31	THR
5	R	32	ALA
3	G	204	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	388/412 (94%)	382 (98%)	6 (2%)	72 93
1	B	388/412 (94%)	380 (98%)	8 (2%)	61 90
1	C	389/412 (94%)	382 (98%)	7 (2%)	66 91
1	J	387/412 (94%)	382 (99%)	5 (1%)	76 94
1	K	388/412 (94%)	379 (98%)	9 (2%)	58 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	388/412 (94%)	378 (97%)	10 (3%)	54 86
1	S	387/412 (94%)	378 (98%)	9 (2%)	58 88
1	T	388/412 (94%)	382 (98%)	6 (2%)	72 93
1	U	388/412 (94%)	381 (98%)	7 (2%)	66 91
2	D	380/384 (99%)	374 (98%)	6 (2%)	70 93
2	E	378/384 (98%)	373 (99%)	5 (1%)	76 94
2	F	379/384 (99%)	374 (99%)	5 (1%)	76 94
2	M	380/384 (99%)	372 (98%)	8 (2%)	61 90
2	N	380/384 (99%)	373 (98%)	7 (2%)	66 91
2	O	379/384 (99%)	376 (99%)	3 (1%)	86 97
2	V	380/384 (99%)	372 (98%)	8 (2%)	61 90
2	W	378/384 (98%)	374 (99%)	4 (1%)	80 95
2	X	379/384 (99%)	374 (99%)	5 (1%)	76 94
3	G	219/236 (93%)	206 (94%)	13 (6%)	24 57
3	P	198/236 (84%)	183 (92%)	15 (8%)	16 42
3	Y	163/236 (69%)	157 (96%)	6 (4%)	41 76
4	H	54/112 (48%)	52 (96%)	2 (4%)	41 76
4	Q	5/112 (4%)	5 (100%)	0	100 100
5	I	23/48 (48%)	20 (87%)	3 (13%)	5 15
All	All	7566/8144 (93%)	7409 (98%)	157 (2%)	61 90

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	342	THR
2	N	114	ARG
2	W	433	ARG
1	L	401	GLU
2	M	6	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	398	GLN

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Mol	Chain	Res	Type
3	P	122	HIS
2	X	385	GLN
2	O	52	GLN
2	O	328	HIS

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 31 ligands modelled in this entry, 15 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
8	ANP	A	600	6	27,33,33	2.27	9 (33%)	30,52,52	2.23	8 (26%)
8	ANP	B	600	6	27,33,33	1.96	6 (22%)	30,52,52	2.30	7 (23%)
8	ANP	C	600	6	27,33,33	1.91	8 (29%)	30,52,52	2.47	8 (26%)
8	ANP	D	600	6	27,33,33	1.76	8 (29%)	30,52,52	2.27	9 (30%)
8	ANP	F	600	6	27,33,33	1.87	7 (25%)	30,52,52	2.56	7 (23%)
8	ANP	J	600	6	27,33,33	1.98	8 (29%)	30,52,52	2.59	6 (20%)
8	ANP	K	600	6	27,33,33	1.94	6 (22%)	30,52,52	2.42	7 (23%)
8	ANP	L	600	6	27,33,33	2.05	7 (25%)	30,52,52	2.53	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ANP	M	600	6	27,33,33	1.93	7 (25%)	30,52,52	2.65	8 (26%)
7	PO4	N	800	-	4,4,4	0.45	0	6,6,6	0.29	0
8	ANP	O	600	6	27,33,33	2.02	7 (25%)	30,52,52	2.30	10 (33%)
8	ANP	S	600	6	27,33,33	2.19	5 (18%)	30,52,52	2.67	12 (40%)
8	ANP	T	600	6	27,33,33	2.22	7 (25%)	30,52,52	2.21	6 (20%)
8	ANP	U	600	6	27,33,33	2.01	7 (25%)	30,52,52	2.06	7 (23%)
8	ANP	V	600	6	27,33,33	2.09	7 (25%)	30,52,52	2.30	7 (23%)
8	ANP	X	600	6	27,33,33	1.90	5 (18%)	30,52,52	2.75	9 (30%)

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
8	ANP	A	600	6	-	2/12/38/38	0/3/3/3
8	ANP	B	600	6	-	1/12/38/38	0/3/3/3
8	ANP	C	600	6	-	2/12/38/38	0/3/3/3
8	ANP	D	600	6	-	1/12/38/38	0/3/3/3
8	ANP	F	600	6	-	0/12/38/38	0/3/3/3
8	ANP	J	600	6	-	1/12/38/38	0/3/3/3
8	ANP	K	600	6	-	2/12/38/38	0/3/3/3
8	ANP	L	600	6	-	2/12/38/38	0/3/3/3
8	ANP	M	600	6	-	0/12/38/38	0/3/3/3
7	PO4	N	800	-	-	0/0/0/0	0/0/0/0
8	ANP	O	600	6	-	0/12/38/38	0/3/3/3
8	ANP	S	600	6	-	1/12/38/38	0/3/3/3
8	ANP	T	600	6	-	1/12/38/38	0/3/3/3
8	ANP	U	600	6	-	0/12/38/38	0/3/3/3
8	ANP	V	600	6	-	0/12/38/38	0/3/3/3
8	ANP	X	600	6	-	0/12/38/38	0/3/3/3

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ANP	PB-O2B	-2.93	1.48	1.56
8	C	600	ANP	PG-O2G	-2.83	1.48	1.56
8	A	600	ANP	PG-O2G	-2.67	1.49	1.56
8	J	600	ANP	PG-O2G	-2.59	1.49	1.56
8	L	600	ANP	PB-O2B	-2.50	1.49	1.56

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	600	ANP	N3-C2-N1	-9.66	121.50	128.89
8	X	600	ANP	N3-C2-N1	-8.94	122.05	128.89
8	S	600	ANP	N3-C2-N1	-8.77	122.18	128.89
8	J	600	ANP	O1G-PG-N3B	-8.65	98.62	111.90
8	M	600	ANP	N3-C2-N1	-8.27	122.56	128.89

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	600	ANP	O1G-PG-N3B-PB
8	J	600	ANP	O1B-PB-N3B-PG
8	A	600	ANP	O1G-PG-N3B-PB
8	B	600	ANP	O1B-PB-N3B-PG
8	A	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	600	ANP	1	0
8	F	600	ANP	2	0
8	K	600	ANP	1	0
8	L	600	ANP	1	0
8	M	600	ANP	6	0
8	S	600	ANP	1	0
8	V	600	ANP	3	0
8	X	600	ANP	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	482/510 (94%)	0.28	13 (2%) 58 45	41, 64, 77, 93	0
1	B	483/510 (94%)	0.56	31 (6%) 23 14	49, 69, 89, 110	0
1	C	484/510 (94%)	0.44	29 (5%) 25 15	48, 66, 86, 108	0
1	J	481/510 (94%)	0.50	34 (7%) 19 10	50, 65, 82, 103	0
1	K	486/510 (95%)	0.65	46 (9%) 10 5	55, 72, 84, 107	0
1	L	482/510 (94%)	0.37	23 (4%) 34 23	49, 66, 82, 100	0
1	S	480/510 (94%)	0.61	43 (8%) 12 6	59, 71, 84, 99	0
1	T	481/510 (94%)	1.07	91 (18%) 2 1	54, 68, 84, 123	0
1	U	481/510 (94%)	1.09	102 (21%) 1 1	51, 67, 86, 111	0
2	D	470/478 (98%)	0.43	27 (5%) 27 17	45, 67, 93, 107	0
2	E	468/478 (97%)	0.56	42 (8%) 12 6	44, 68, 87, 100	0
2	F	469/478 (98%)	0.41	22 (4%) 35 24	51, 67, 83, 104	0
2	M	470/478 (98%)	0.50	26 (5%) 29 18	46, 66, 90, 112	0
2	N	470/478 (98%)	0.72	62 (13%) 4 2	53, 69, 88, 115	0
2	O	468/478 (97%)	0.48	33 (7%) 19 10	50, 68, 85, 102	0
2	V	470/478 (98%)	1.03	80 (17%) 2 1	57, 74, 94, 135	0
2	W	467/478 (97%)	0.94	80 (17%) 2 1	54, 67, 85, 108	0
2	X	469/478 (98%)	0.97	68 (14%) 3 2	54, 72, 90, 124	0
3	G	265/278 (95%)	0.26	27 (10%) 9 4	21, 64, 90, 97	0
3	P	243/278 (87%)	1.10	61 (25%) 1 0	28, 93, 121, 127	0
3	Y	200/278 (71%)	1.25	56 (28%) 1 0	64, 107, 127, 132	0
4	H	120/138 (86%)	1.54	44 (36%) 0 0	60, 91, 129, 131	0
4	Q	84/138 (60%)	1.59	27 (32%) 1 0	88, 107, 134, 137	0
4	Z	17/138 (12%)	2.48	10 (58%) 0 0	132, 134, 140, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	1	27/61 (44%)	2.03	11 (40%) 0 0	107, 111, 115, 115	0
5	I	48/61 (78%)	0.88	8 (16%) 2 1	71, 84, 93, 94	0
5	R	34/61 (55%)	1.33	10 (29%) 1 0	95, 103, 112, 115	0
All	All	9599/10323 (92%)	0.69	1106 (11%) 6 3	21, 69, 99, 140	0

The worst 5 of 1106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	398	GLU	13.2
3	P	126	ILE	10.1
2	X	28	SER	7.8
1	U	509	THR	7.7
2	X	29	GLU	7.7

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
7	PO4	N	800	5/5	0.93	0.26	1.42	78,80,84,85	0
6	MG	F	700	1/1	0.98	0.26	0.31	44,44,44,44	0
8	ANP	T	600	31/31	0.95	0.27	0.29	66,89,91,97	0
8	ANP	K	600	31/31	0.97	0.23	-0.24	49,62,70,74	0
8	ANP	J	600	31/31	0.98	0.19	-0.55	23,46,52,53	0
8	ANP	U	600	31/31	0.94	0.20	-0.73	42,57,69,70	0
8	ANP	C	600	31/31	0.97	0.14	-1.30	25,41,50,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	ANP	L	600	31/31	0.97	0.15	-1.34	17,33,44,48	0
8	ANP	S	600	31/31	0.97	0.16	-1.45	37,52,58,63	0
8	ANP	F	600	31/31	0.96	0.14	-1.52	36,52,60,61	0
8	ANP	B	600	31/31	0.97	0.17	-1.57	29,37,41,44	0
6	MG	D	700	1/1	0.88	0.16	-2.03	46,46,46,46	0
8	ANP	X	600	31/31	0.95	0.15	-2.07	50,61,79,81	0
8	ANP	V	600	31/31	0.94	0.15	-2.09	61,74,81,90	0
8	ANP	A	600	31/31	0.98	0.13	-2.15	14,35,42,43	0
6	MG	V	700	1/1	0.81	0.14	-2.19	69,69,69,69	0
8	ANP	D	600	31/31	0.97	0.10	-2.31	37,51,57,64	0
8	ANP	O	600	31/31	0.97	0.10	-2.74	49,68,71,74	0
6	MG	O	700	1/1	0.80	0.12	-2.92	48,48,48,48	0
8	ANP	M	600	31/31	0.97	0.10	-3.04	31,52,59,65	0
6	MG	M	700	1/1	0.96	0.07	-3.10	52,52,52,52	0
6	MG	X	700	1/1	0.86	0.08	-5.79	67,67,67,67	0
6	MG	S	700	1/1	0.95	0.12	-	40,40,40,40	0
6	MG	B	700	1/1	0.95	0.08	-	43,43,43,43	0
6	MG	C	700	1/1	0.95	0.10	-	43,43,43,43	0
6	MG	U	700	1/1	0.95	0.12	-	78,78,78,78	0
6	MG	A	700	1/1	0.99	0.17	-	34,34,34,34	0
6	MG	L	700	1/1	0.97	0.14	-	49,49,49,49	0
6	MG	K	700	1/1	0.88	0.15	-	52,52,52,52	0
6	MG	T	700	1/1	0.86	0.22	-	70,70,70,70	0
6	MG	J	700	1/1	0.94	0.07	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.