



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:43 PM GMT

PDB ID : 4PJ1
Title : Crystal structure of the human mitochondrial chaperonin symmetrical 'foot-ball' complex
Authors : Frolow, F.; Azem, A.; Nisemblat, S.
Deposited on : 2014-05-10
Resolution : 3.15 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

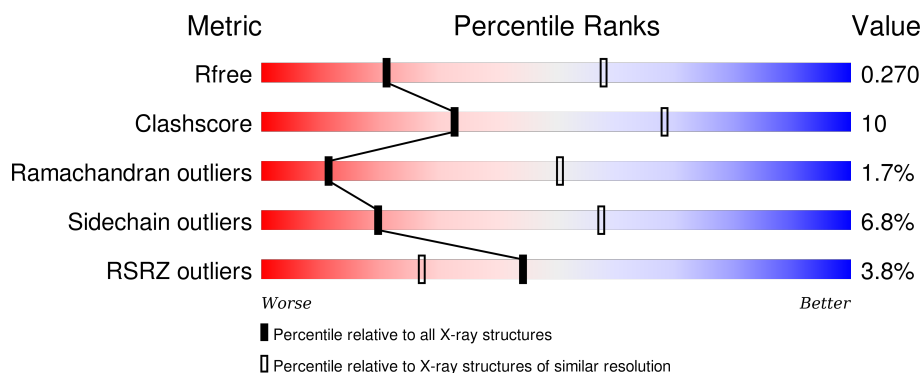
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	558	<div> <div>5%</div> <div>65% 27% 6%</div> </div>
1	B	558	<div> <div>9%</div> <div>62% 27% 5% 6%</div> </div>
1	C	558	<div> <div>2%</div> <div>69% 23% 6%</div> </div>
1	D	558	<div> <div>4%</div> <div>65% 25% 6%</div> </div>
1	E	558	<div> <div>3%</div> <div>69% 22% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	558	
1	G	558	
1	H	558	
1	I	558	
1	J	558	
1	K	558	
1	L	558	
1	M	558	
1	N	558	
2	1	114	
2	2	114	
2	O	114	
2	P	114	
2	Q	114	
2	R	114	
2	S	114	
2	T	114	
2	U	114	
2	V	114	
2	W	114	
2	X	114	
2	Y	114	
2	Z	114	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 65963 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 60 kDa heat shock protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	B	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	C	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	D	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	E	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	F	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	G	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	H	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	I	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	J	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	K	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	L	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	M	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			
1	N	526	Total	C	N	O	S	0	0	0
			3918	2457	670	777	14			

There are 406 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	GLY	-	expression tag	UNP P10809
A	-23	SER	-	expression tag	UNP P10809
A	-22	HIS	-	expression tag	UNP P10809
A	-21	HIS	-	expression tag	UNP P10809
A	-20	HIS	-	expression tag	UNP P10809
A	-19	HIS	-	expression tag	UNP P10809
A	-18	HIS	-	expression tag	UNP P10809
A	-17	HIS	-	expression tag	UNP P10809
A	-16	HIS	-	expression tag	UNP P10809
A	-15	HIS	-	expression tag	UNP P10809
A	-14	GLY	-	expression tag	UNP P10809
A	-13	SER	-	expression tag	UNP P10809
A	-12	ASP	-	expression tag	UNP P10809
A	-11	TYR	-	expression tag	UNP P10809
A	-10	ASP	-	expression tag	UNP P10809
A	-9	ILE	-	expression tag	UNP P10809
A	-8	PRO	-	expression tag	UNP P10809
A	-7	THR	-	expression tag	UNP P10809
A	-6	THR	-	expression tag	UNP P10809
A	-5	GLU	-	expression tag	UNP P10809
A	-4	ASN	-	expression tag	UNP P10809
A	-3	LEU	-	expression tag	UNP P10809
A	-2	TYR	-	expression tag	UNP P10809
A	-1	PHE	-	expression tag	UNP P10809
A	0	GLN	-	expression tag	UNP P10809
A	1	GLY	-	expression tag	UNP P10809
A	2	SER	-	expression tag	UNP P10809
A	323	LYS	GLU	engineered mutation	UNP P10809
B	-25	MET	-	expression tag	UNP P10809
B	-24	GLY	-	expression tag	UNP P10809
B	-23	SER	-	expression tag	UNP P10809
B	-22	HIS	-	expression tag	UNP P10809
B	-21	HIS	-	expression tag	UNP P10809
B	-20	HIS	-	expression tag	UNP P10809
B	-19	HIS	-	expression tag	UNP P10809
B	-18	HIS	-	expression tag	UNP P10809
B	-17	HIS	-	expression tag	UNP P10809
B	-16	HIS	-	expression tag	UNP P10809
B	-15	HIS	-	expression tag	UNP P10809
B	-14	GLY	-	expression tag	UNP P10809
B	-13	SER	-	expression tag	UNP P10809
B	-12	ASP	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	TYR	-	expression tag	UNP P10809
B	-10	ASP	-	expression tag	UNP P10809
B	-9	ILE	-	expression tag	UNP P10809
B	-8	PRO	-	expression tag	UNP P10809
B	-7	THR	-	expression tag	UNP P10809
B	-6	THR	-	expression tag	UNP P10809
B	-5	GLU	-	expression tag	UNP P10809
B	-4	ASN	-	expression tag	UNP P10809
B	-3	LEU	-	expression tag	UNP P10809
B	-2	TYR	-	expression tag	UNP P10809
B	-1	PHE	-	expression tag	UNP P10809
B	0	GLN	-	expression tag	UNP P10809
B	1	GLY	-	expression tag	UNP P10809
B	2	SER	-	expression tag	UNP P10809
B	323	LYS	GLU	engineered mutation	UNP P10809
C	-25	MET	-	expression tag	UNP P10809
C	-24	GLY	-	expression tag	UNP P10809
C	-23	SER	-	expression tag	UNP P10809
C	-22	HIS	-	expression tag	UNP P10809
C	-21	HIS	-	expression tag	UNP P10809
C	-20	HIS	-	expression tag	UNP P10809
C	-19	HIS	-	expression tag	UNP P10809
C	-18	HIS	-	expression tag	UNP P10809
C	-17	HIS	-	expression tag	UNP P10809
C	-16	HIS	-	expression tag	UNP P10809
C	-15	HIS	-	expression tag	UNP P10809
C	-14	GLY	-	expression tag	UNP P10809
C	-13	SER	-	expression tag	UNP P10809
C	-12	ASP	-	expression tag	UNP P10809
C	-11	TYR	-	expression tag	UNP P10809
C	-10	ASP	-	expression tag	UNP P10809
C	-9	ILE	-	expression tag	UNP P10809
C	-8	PRO	-	expression tag	UNP P10809
C	-7	THR	-	expression tag	UNP P10809
C	-6	THR	-	expression tag	UNP P10809
C	-5	GLU	-	expression tag	UNP P10809
C	-4	ASN	-	expression tag	UNP P10809
C	-3	LEU	-	expression tag	UNP P10809
C	-2	TYR	-	expression tag	UNP P10809
C	-1	PHE	-	expression tag	UNP P10809
C	0	GLN	-	expression tag	UNP P10809
C	1	GLY	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	SER	-	expression tag	UNP P10809
C	323	LYS	GLU	engineered mutation	UNP P10809
D	-25	MET	-	expression tag	UNP P10809
D	-24	GLY	-	expression tag	UNP P10809
D	-23	SER	-	expression tag	UNP P10809
D	-22	HIS	-	expression tag	UNP P10809
D	-21	HIS	-	expression tag	UNP P10809
D	-20	HIS	-	expression tag	UNP P10809
D	-19	HIS	-	expression tag	UNP P10809
D	-18	HIS	-	expression tag	UNP P10809
D	-17	HIS	-	expression tag	UNP P10809
D	-16	HIS	-	expression tag	UNP P10809
D	-15	HIS	-	expression tag	UNP P10809
D	-14	GLY	-	expression tag	UNP P10809
D	-13	SER	-	expression tag	UNP P10809
D	-12	ASP	-	expression tag	UNP P10809
D	-11	TYR	-	expression tag	UNP P10809
D	-10	ASP	-	expression tag	UNP P10809
D	-9	ILE	-	expression tag	UNP P10809
D	-8	PRO	-	expression tag	UNP P10809
D	-7	THR	-	expression tag	UNP P10809
D	-6	THR	-	expression tag	UNP P10809
D	-5	GLU	-	expression tag	UNP P10809
D	-4	ASN	-	expression tag	UNP P10809
D	-3	LEU	-	expression tag	UNP P10809
D	-2	TYR	-	expression tag	UNP P10809
D	-1	PHE	-	expression tag	UNP P10809
D	0	GLN	-	expression tag	UNP P10809
D	1	GLY	-	expression tag	UNP P10809
D	2	SER	-	expression tag	UNP P10809
D	323	LYS	GLU	engineered mutation	UNP P10809
E	-25	MET	-	expression tag	UNP P10809
E	-24	GLY	-	expression tag	UNP P10809
E	-23	SER	-	expression tag	UNP P10809
E	-22	HIS	-	expression tag	UNP P10809
E	-21	HIS	-	expression tag	UNP P10809
E	-20	HIS	-	expression tag	UNP P10809
E	-19	HIS	-	expression tag	UNP P10809
E	-18	HIS	-	expression tag	UNP P10809
E	-17	HIS	-	expression tag	UNP P10809
E	-16	HIS	-	expression tag	UNP P10809
E	-15	HIS	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	GLY	-	expression tag	UNP P10809
E	-13	SER	-	expression tag	UNP P10809
E	-12	ASP	-	expression tag	UNP P10809
E	-11	TYR	-	expression tag	UNP P10809
E	-10	ASP	-	expression tag	UNP P10809
E	-9	ILE	-	expression tag	UNP P10809
E	-8	PRO	-	expression tag	UNP P10809
E	-7	THR	-	expression tag	UNP P10809
E	-6	THR	-	expression tag	UNP P10809
E	-5	GLU	-	expression tag	UNP P10809
E	-4	ASN	-	expression tag	UNP P10809
E	-3	LEU	-	expression tag	UNP P10809
E	-2	TYR	-	expression tag	UNP P10809
E	-1	PHE	-	expression tag	UNP P10809
E	0	GLN	-	expression tag	UNP P10809
E	1	GLY	-	expression tag	UNP P10809
E	2	SER	-	expression tag	UNP P10809
E	323	LYS	GLU	engineered mutation	UNP P10809
F	-25	MET	-	expression tag	UNP P10809
F	-24	GLY	-	expression tag	UNP P10809
F	-23	SER	-	expression tag	UNP P10809
F	-22	HIS	-	expression tag	UNP P10809
F	-21	HIS	-	expression tag	UNP P10809
F	-20	HIS	-	expression tag	UNP P10809
F	-19	HIS	-	expression tag	UNP P10809
F	-18	HIS	-	expression tag	UNP P10809
F	-17	HIS	-	expression tag	UNP P10809
F	-16	HIS	-	expression tag	UNP P10809
F	-15	HIS	-	expression tag	UNP P10809
F	-14	GLY	-	expression tag	UNP P10809
F	-13	SER	-	expression tag	UNP P10809
F	-12	ASP	-	expression tag	UNP P10809
F	-11	TYR	-	expression tag	UNP P10809
F	-10	ASP	-	expression tag	UNP P10809
F	-9	ILE	-	expression tag	UNP P10809
F	-8	PRO	-	expression tag	UNP P10809
F	-7	THR	-	expression tag	UNP P10809
F	-6	THR	-	expression tag	UNP P10809
F	-5	GLU	-	expression tag	UNP P10809
F	-4	ASN	-	expression tag	UNP P10809
F	-3	LEU	-	expression tag	UNP P10809
F	-2	TYR	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	PHE	-	expression tag	UNP P10809
F	0	GLN	-	expression tag	UNP P10809
F	1	GLY	-	expression tag	UNP P10809
F	2	SER	-	expression tag	UNP P10809
F	323	LYS	GLU	engineered mutation	UNP P10809
G	-25	MET	-	expression tag	UNP P10809
G	-24	GLY	-	expression tag	UNP P10809
G	-23	SER	-	expression tag	UNP P10809
G	-22	HIS	-	expression tag	UNP P10809
G	-21	HIS	-	expression tag	UNP P10809
G	-20	HIS	-	expression tag	UNP P10809
G	-19	HIS	-	expression tag	UNP P10809
G	-18	HIS	-	expression tag	UNP P10809
G	-17	HIS	-	expression tag	UNP P10809
G	-16	HIS	-	expression tag	UNP P10809
G	-15	HIS	-	expression tag	UNP P10809
G	-14	GLY	-	expression tag	UNP P10809
G	-13	SER	-	expression tag	UNP P10809
G	-12	ASP	-	expression tag	UNP P10809
G	-11	TYR	-	expression tag	UNP P10809
G	-10	ASP	-	expression tag	UNP P10809
G	-9	ILE	-	expression tag	UNP P10809
G	-8	PRO	-	expression tag	UNP P10809
G	-7	THR	-	expression tag	UNP P10809
G	-6	THR	-	expression tag	UNP P10809
G	-5	GLU	-	expression tag	UNP P10809
G	-4	ASN	-	expression tag	UNP P10809
G	-3	LEU	-	expression tag	UNP P10809
G	-2	TYR	-	expression tag	UNP P10809
G	-1	PHE	-	expression tag	UNP P10809
G	0	GLN	-	expression tag	UNP P10809
G	1	GLY	-	expression tag	UNP P10809
G	2	SER	-	expression tag	UNP P10809
G	323	LYS	GLU	engineered mutation	UNP P10809
H	-25	MET	-	expression tag	UNP P10809
H	-24	GLY	-	expression tag	UNP P10809
H	-23	SER	-	expression tag	UNP P10809
H	-22	HIS	-	expression tag	UNP P10809
H	-21	HIS	-	expression tag	UNP P10809
H	-20	HIS	-	expression tag	UNP P10809
H	-19	HIS	-	expression tag	UNP P10809
H	-18	HIS	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	HIS	-	expression tag	UNP P10809
H	-16	HIS	-	expression tag	UNP P10809
H	-15	HIS	-	expression tag	UNP P10809
H	-14	GLY	-	expression tag	UNP P10809
H	-13	SER	-	expression tag	UNP P10809
H	-12	ASP	-	expression tag	UNP P10809
H	-11	TYR	-	expression tag	UNP P10809
H	-10	ASP	-	expression tag	UNP P10809
H	-9	ILE	-	expression tag	UNP P10809
H	-8	PRO	-	expression tag	UNP P10809
H	-7	THR	-	expression tag	UNP P10809
H	-6	THR	-	expression tag	UNP P10809
H	-5	GLU	-	expression tag	UNP P10809
H	-4	ASN	-	expression tag	UNP P10809
H	-3	LEU	-	expression tag	UNP P10809
H	-2	TYR	-	expression tag	UNP P10809
H	-1	PHE	-	expression tag	UNP P10809
H	0	GLN	-	expression tag	UNP P10809
H	1	GLY	-	expression tag	UNP P10809
H	2	SER	-	expression tag	UNP P10809
H	323	LYS	GLU	engineered mutation	UNP P10809
I	-25	MET	-	expression tag	UNP P10809
I	-24	GLY	-	expression tag	UNP P10809
I	-23	SER	-	expression tag	UNP P10809
I	-22	HIS	-	expression tag	UNP P10809
I	-21	HIS	-	expression tag	UNP P10809
I	-20	HIS	-	expression tag	UNP P10809
I	-19	HIS	-	expression tag	UNP P10809
I	-18	HIS	-	expression tag	UNP P10809
I	-17	HIS	-	expression tag	UNP P10809
I	-16	HIS	-	expression tag	UNP P10809
I	-15	HIS	-	expression tag	UNP P10809
I	-14	GLY	-	expression tag	UNP P10809
I	-13	SER	-	expression tag	UNP P10809
I	-12	ASP	-	expression tag	UNP P10809
I	-11	TYR	-	expression tag	UNP P10809
I	-10	ASP	-	expression tag	UNP P10809
I	-9	ILE	-	expression tag	UNP P10809
I	-8	PRO	-	expression tag	UNP P10809
I	-7	THR	-	expression tag	UNP P10809
I	-6	THR	-	expression tag	UNP P10809
I	-5	GLU	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	ASN	-	expression tag	UNP P10809
I	-3	LEU	-	expression tag	UNP P10809
I	-2	TYR	-	expression tag	UNP P10809
I	-1	PHE	-	expression tag	UNP P10809
I	0	GLN	-	expression tag	UNP P10809
I	1	GLY	-	expression tag	UNP P10809
I	2	SER	-	expression tag	UNP P10809
I	323	LYS	GLU	engineered mutation	UNP P10809
J	-25	MET	-	expression tag	UNP P10809
J	-24	GLY	-	expression tag	UNP P10809
J	-23	SER	-	expression tag	UNP P10809
J	-22	HIS	-	expression tag	UNP P10809
J	-21	HIS	-	expression tag	UNP P10809
J	-20	HIS	-	expression tag	UNP P10809
J	-19	HIS	-	expression tag	UNP P10809
J	-18	HIS	-	expression tag	UNP P10809
J	-17	HIS	-	expression tag	UNP P10809
J	-16	HIS	-	expression tag	UNP P10809
J	-15	HIS	-	expression tag	UNP P10809
J	-14	GLY	-	expression tag	UNP P10809
J	-13	SER	-	expression tag	UNP P10809
J	-12	ASP	-	expression tag	UNP P10809
J	-11	TYR	-	expression tag	UNP P10809
J	-10	ASP	-	expression tag	UNP P10809
J	-9	ILE	-	expression tag	UNP P10809
J	-8	PRO	-	expression tag	UNP P10809
J	-7	THR	-	expression tag	UNP P10809
J	-6	THR	-	expression tag	UNP P10809
J	-5	GLU	-	expression tag	UNP P10809
J	-4	ASN	-	expression tag	UNP P10809
J	-3	LEU	-	expression tag	UNP P10809
J	-2	TYR	-	expression tag	UNP P10809
J	-1	PHE	-	expression tag	UNP P10809
J	0	GLN	-	expression tag	UNP P10809
J	1	GLY	-	expression tag	UNP P10809
J	2	SER	-	expression tag	UNP P10809
J	323	LYS	GLU	engineered mutation	UNP P10809
K	-25	MET	-	expression tag	UNP P10809
K	-24	GLY	-	expression tag	UNP P10809
K	-23	SER	-	expression tag	UNP P10809
K	-22	HIS	-	expression tag	UNP P10809
K	-21	HIS	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-20	HIS	-	expression tag	UNP P10809
K	-19	HIS	-	expression tag	UNP P10809
K	-18	HIS	-	expression tag	UNP P10809
K	-17	HIS	-	expression tag	UNP P10809
K	-16	HIS	-	expression tag	UNP P10809
K	-15	HIS	-	expression tag	UNP P10809
K	-14	GLY	-	expression tag	UNP P10809
K	-13	SER	-	expression tag	UNP P10809
K	-12	ASP	-	expression tag	UNP P10809
K	-11	TYR	-	expression tag	UNP P10809
K	-10	ASP	-	expression tag	UNP P10809
K	-9	ILE	-	expression tag	UNP P10809
K	-8	PRO	-	expression tag	UNP P10809
K	-7	THR	-	expression tag	UNP P10809
K	-6	THR	-	expression tag	UNP P10809
K	-5	GLU	-	expression tag	UNP P10809
K	-4	ASN	-	expression tag	UNP P10809
K	-3	LEU	-	expression tag	UNP P10809
K	-2	TYR	-	expression tag	UNP P10809
K	-1	PHE	-	expression tag	UNP P10809
K	0	GLN	-	expression tag	UNP P10809
K	1	GLY	-	expression tag	UNP P10809
K	2	SER	-	expression tag	UNP P10809
K	323	LYS	GLU	engineered mutation	UNP P10809
L	-25	MET	-	expression tag	UNP P10809
L	-24	GLY	-	expression tag	UNP P10809
L	-23	SER	-	expression tag	UNP P10809
L	-22	HIS	-	expression tag	UNP P10809
L	-21	HIS	-	expression tag	UNP P10809
L	-20	HIS	-	expression tag	UNP P10809
L	-19	HIS	-	expression tag	UNP P10809
L	-18	HIS	-	expression tag	UNP P10809
L	-17	HIS	-	expression tag	UNP P10809
L	-16	HIS	-	expression tag	UNP P10809
L	-15	HIS	-	expression tag	UNP P10809
L	-14	GLY	-	expression tag	UNP P10809
L	-13	SER	-	expression tag	UNP P10809
L	-12	ASP	-	expression tag	UNP P10809
L	-11	TYR	-	expression tag	UNP P10809
L	-10	ASP	-	expression tag	UNP P10809
L	-9	ILE	-	expression tag	UNP P10809
L	-8	PRO	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	THR	-	expression tag	UNP P10809
L	-6	THR	-	expression tag	UNP P10809
L	-5	GLU	-	expression tag	UNP P10809
L	-4	ASN	-	expression tag	UNP P10809
L	-3	LEU	-	expression tag	UNP P10809
L	-2	TYR	-	expression tag	UNP P10809
L	-1	PHE	-	expression tag	UNP P10809
L	0	GLN	-	expression tag	UNP P10809
L	1	GLY	-	expression tag	UNP P10809
L	2	SER	-	expression tag	UNP P10809
L	323	LYS	GLU	engineered mutation	UNP P10809
M	-25	MET	-	expression tag	UNP P10809
M	-24	GLY	-	expression tag	UNP P10809
M	-23	SER	-	expression tag	UNP P10809
M	-22	HIS	-	expression tag	UNP P10809
M	-21	HIS	-	expression tag	UNP P10809
M	-20	HIS	-	expression tag	UNP P10809
M	-19	HIS	-	expression tag	UNP P10809
M	-18	HIS	-	expression tag	UNP P10809
M	-17	HIS	-	expression tag	UNP P10809
M	-16	HIS	-	expression tag	UNP P10809
M	-15	HIS	-	expression tag	UNP P10809
M	-14	GLY	-	expression tag	UNP P10809
M	-13	SER	-	expression tag	UNP P10809
M	-12	ASP	-	expression tag	UNP P10809
M	-11	TYR	-	expression tag	UNP P10809
M	-10	ASP	-	expression tag	UNP P10809
M	-9	ILE	-	expression tag	UNP P10809
M	-8	PRO	-	expression tag	UNP P10809
M	-7	THR	-	expression tag	UNP P10809
M	-6	THR	-	expression tag	UNP P10809
M	-5	GLU	-	expression tag	UNP P10809
M	-4	ASN	-	expression tag	UNP P10809
M	-3	LEU	-	expression tag	UNP P10809
M	-2	TYR	-	expression tag	UNP P10809
M	-1	PHE	-	expression tag	UNP P10809
M	0	GLN	-	expression tag	UNP P10809
M	1	GLY	-	expression tag	UNP P10809
M	2	SER	-	expression tag	UNP P10809
M	323	LYS	GLU	engineered mutation	UNP P10809
N	-25	MET	-	expression tag	UNP P10809
N	-24	GLY	-	expression tag	UNP P10809

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-23	SER	-	expression tag	UNP P10809
N	-22	HIS	-	expression tag	UNP P10809
N	-21	HIS	-	expression tag	UNP P10809
N	-20	HIS	-	expression tag	UNP P10809
N	-19	HIS	-	expression tag	UNP P10809
N	-18	HIS	-	expression tag	UNP P10809
N	-17	HIS	-	expression tag	UNP P10809
N	-16	HIS	-	expression tag	UNP P10809
N	-15	HIS	-	expression tag	UNP P10809
N	-14	GLY	-	expression tag	UNP P10809
N	-13	SER	-	expression tag	UNP P10809
N	-12	ASP	-	expression tag	UNP P10809
N	-11	TYR	-	expression tag	UNP P10809
N	-10	ASP	-	expression tag	UNP P10809
N	-9	ILE	-	expression tag	UNP P10809
N	-8	PRO	-	expression tag	UNP P10809
N	-7	THR	-	expression tag	UNP P10809
N	-6	THR	-	expression tag	UNP P10809
N	-5	GLU	-	expression tag	UNP P10809
N	-4	ASN	-	expression tag	UNP P10809
N	-3	LEU	-	expression tag	UNP P10809
N	-2	TYR	-	expression tag	UNP P10809
N	-1	PHE	-	expression tag	UNP P10809
N	0	GLN	-	expression tag	UNP P10809
N	1	GLY	-	expression tag	UNP P10809
N	2	SER	-	expression tag	UNP P10809
N	323	LYS	GLU	engineered mutation	UNP P10809

- Molecule 2 is a protein called 10 kDa heat shock protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	P	105	Total	C	N	O	S	0	0	0
			788	507	133	147	1			
2	Q	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	R	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	S	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	T	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	102	Total	C	N	O	S	0	0	0
			773	498	130	144	1			
2	V	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	W	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	X	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	Y	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	Z	108	Total	C	N	O	S	0	0	0
			815	524	138	152	1			
2	1	100	Total	C	N	O	S	0	0	0
			756	486	127	142	1			
2	2	104	Total	C	N	O	S	0	0	0
			783	504	132	146	1			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	103	LYS	-	expression tag	UNP P61604
O	104	LEU	-	expression tag	UNP P61604
O	105	ALA	-	expression tag	UNP P61604
O	106	ALA	-	expression tag	UNP P61604
O	107	ALA	-	expression tag	UNP P61604
O	108	LEU	-	expression tag	UNP P61604
O	109	GLU	-	expression tag	UNP P61604
O	110	HIS	-	expression tag	UNP P61604
O	111	HIS	-	expression tag	UNP P61604
O	112	HIS	-	expression tag	UNP P61604
O	113	HIS	-	expression tag	UNP P61604
O	114	HIS	-	expression tag	UNP P61604
P	103	LYS	-	expression tag	UNP P61604
P	104	LEU	-	expression tag	UNP P61604
P	105	ALA	-	expression tag	UNP P61604
P	106	ALA	-	expression tag	UNP P61604
P	107	ALA	-	expression tag	UNP P61604
P	108	LEU	-	expression tag	UNP P61604
P	109	GLU	-	expression tag	UNP P61604
P	110	HIS	-	expression tag	UNP P61604
P	111	HIS	-	expression tag	UNP P61604
P	112	HIS	-	expression tag	UNP P61604
P	113	HIS	-	expression tag	UNP P61604

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Chain	Residue	Modelled	Actual	Comment	Reference
P	114	HIS	-	expression tag	UNP P61604
Q	103	LYS	-	expression tag	UNP P61604
Q	104	LEU	-	expression tag	UNP P61604
Q	105	ALA	-	expression tag	UNP P61604
Q	106	ALA	-	expression tag	UNP P61604
Q	107	ALA	-	expression tag	UNP P61604
Q	108	LEU	-	expression tag	UNP P61604
Q	109	GLU	-	expression tag	UNP P61604
Q	110	HIS	-	expression tag	UNP P61604
Q	111	HIS	-	expression tag	UNP P61604
Q	112	HIS	-	expression tag	UNP P61604
Q	113	HIS	-	expression tag	UNP P61604
Q	114	HIS	-	expression tag	UNP P61604
R	103	LYS	-	expression tag	UNP P61604
R	104	LEU	-	expression tag	UNP P61604
R	105	ALA	-	expression tag	UNP P61604
R	106	ALA	-	expression tag	UNP P61604
R	107	ALA	-	expression tag	UNP P61604
R	108	LEU	-	expression tag	UNP P61604
R	109	GLU	-	expression tag	UNP P61604
R	110	HIS	-	expression tag	UNP P61604
R	111	HIS	-	expression tag	UNP P61604
R	112	HIS	-	expression tag	UNP P61604
R	113	HIS	-	expression tag	UNP P61604
R	114	HIS	-	expression tag	UNP P61604
S	103	LYS	-	expression tag	UNP P61604
S	104	LEU	-	expression tag	UNP P61604
S	105	ALA	-	expression tag	UNP P61604
S	106	ALA	-	expression tag	UNP P61604
S	107	ALA	-	expression tag	UNP P61604
S	108	LEU	-	expression tag	UNP P61604
S	109	GLU	-	expression tag	UNP P61604
S	110	HIS	-	expression tag	UNP P61604
S	111	HIS	-	expression tag	UNP P61604
S	112	HIS	-	expression tag	UNP P61604
S	113	HIS	-	expression tag	UNP P61604
S	114	HIS	-	expression tag	UNP P61604
T	103	LYS	-	expression tag	UNP P61604
T	104	LEU	-	expression tag	UNP P61604
T	105	ALA	-	expression tag	UNP P61604
T	106	ALA	-	expression tag	UNP P61604
T	107	ALA	-	expression tag	UNP P61604

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Chain	Residue	Modelled	Actual	Comment	Reference
T	108	LEU	-	expression tag	UNP P61604
T	109	GLU	-	expression tag	UNP P61604
T	110	HIS	-	expression tag	UNP P61604
T	111	HIS	-	expression tag	UNP P61604
T	112	HIS	-	expression tag	UNP P61604
T	113	HIS	-	expression tag	UNP P61604
T	114	HIS	-	expression tag	UNP P61604
U	103	LYS	-	expression tag	UNP P61604
U	104	LEU	-	expression tag	UNP P61604
U	105	ALA	-	expression tag	UNP P61604
U	106	ALA	-	expression tag	UNP P61604
U	107	ALA	-	expression tag	UNP P61604
U	108	LEU	-	expression tag	UNP P61604
U	109	GLU	-	expression tag	UNP P61604
U	110	HIS	-	expression tag	UNP P61604
U	111	HIS	-	expression tag	UNP P61604
U	112	HIS	-	expression tag	UNP P61604
U	113	HIS	-	expression tag	UNP P61604
U	114	HIS	-	expression tag	UNP P61604
V	103	LYS	-	expression tag	UNP P61604
V	104	LEU	-	expression tag	UNP P61604
V	105	ALA	-	expression tag	UNP P61604
V	106	ALA	-	expression tag	UNP P61604
V	107	ALA	-	expression tag	UNP P61604
V	108	LEU	-	expression tag	UNP P61604
V	109	GLU	-	expression tag	UNP P61604
V	110	HIS	-	expression tag	UNP P61604
V	111	HIS	-	expression tag	UNP P61604
V	112	HIS	-	expression tag	UNP P61604
V	113	HIS	-	expression tag	UNP P61604
V	114	HIS	-	expression tag	UNP P61604
W	103	LYS	-	expression tag	UNP P61604
W	104	LEU	-	expression tag	UNP P61604
W	105	ALA	-	expression tag	UNP P61604
W	106	ALA	-	expression tag	UNP P61604
W	107	ALA	-	expression tag	UNP P61604
W	108	LEU	-	expression tag	UNP P61604
W	109	GLU	-	expression tag	UNP P61604
W	110	HIS	-	expression tag	UNP P61604
W	111	HIS	-	expression tag	UNP P61604
W	112	HIS	-	expression tag	UNP P61604
W	113	HIS	-	expression tag	UNP P61604

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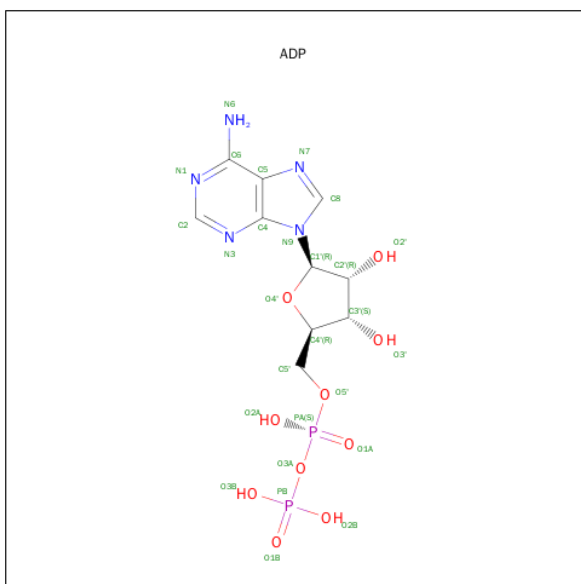
Chain	Residue	Modelled	Actual	Comment	Reference
W	114	HIS	-	expression tag	UNP P61604
X	103	LYS	-	expression tag	UNP P61604
X	104	LEU	-	expression tag	UNP P61604
X	105	ALA	-	expression tag	UNP P61604
X	106	ALA	-	expression tag	UNP P61604
X	107	ALA	-	expression tag	UNP P61604
X	108	LEU	-	expression tag	UNP P61604
X	109	GLU	-	expression tag	UNP P61604
X	110	HIS	-	expression tag	UNP P61604
X	111	HIS	-	expression tag	UNP P61604
X	112	HIS	-	expression tag	UNP P61604
X	113	HIS	-	expression tag	UNP P61604
X	114	HIS	-	expression tag	UNP P61604
Y	103	LYS	-	expression tag	UNP P61604
Y	104	LEU	-	expression tag	UNP P61604
Y	105	ALA	-	expression tag	UNP P61604
Y	106	ALA	-	expression tag	UNP P61604
Y	107	ALA	-	expression tag	UNP P61604
Y	108	LEU	-	expression tag	UNP P61604
Y	109	GLU	-	expression tag	UNP P61604
Y	110	HIS	-	expression tag	UNP P61604
Y	111	HIS	-	expression tag	UNP P61604
Y	112	HIS	-	expression tag	UNP P61604
Y	113	HIS	-	expression tag	UNP P61604
Y	114	HIS	-	expression tag	UNP P61604
Z	103	LYS	-	expression tag	UNP P61604
Z	104	LEU	-	expression tag	UNP P61604
Z	105	ALA	-	expression tag	UNP P61604
Z	106	ALA	-	expression tag	UNP P61604
Z	107	ALA	-	expression tag	UNP P61604
Z	108	LEU	-	expression tag	UNP P61604
Z	109	GLU	-	expression tag	UNP P61604
Z	110	HIS	-	expression tag	UNP P61604
Z	111	HIS	-	expression tag	UNP P61604
Z	112	HIS	-	expression tag	UNP P61604
Z	113	HIS	-	expression tag	UNP P61604
Z	114	HIS	-	expression tag	UNP P61604
1	103	LYS	-	expression tag	UNP P61604
1	104	LEU	-	expression tag	UNP P61604
1	105	ALA	-	expression tag	UNP P61604
1	106	ALA	-	expression tag	UNP P61604
1	107	ALA	-	expression tag	UNP P61604

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Chain	Residue	Modelled	Actual	Comment	Reference
1	108	LEU	-	expression tag	UNP P61604
1	109	GLU	-	expression tag	UNP P61604
1	110	HIS	-	expression tag	UNP P61604
1	111	HIS	-	expression tag	UNP P61604
1	112	HIS	-	expression tag	UNP P61604
1	113	HIS	-	expression tag	UNP P61604
1	114	HIS	-	expression tag	UNP P61604
2	103	LYS	-	expression tag	UNP P61604
2	104	LEU	-	expression tag	UNP P61604
2	105	ALA	-	expression tag	UNP P61604
2	106	ALA	-	expression tag	UNP P61604
2	107	ALA	-	expression tag	UNP P61604
2	108	LEU	-	expression tag	UNP P61604
2	109	GLU	-	expression tag	UNP P61604
2	110	HIS	-	expression tag	UNP P61604
2	111	HIS	-	expression tag	UNP P61604
2	112	HIS	-	expression tag	UNP P61604
2	113	HIS	-	expression tag	UNP P61604
2	114	HIS	-	expression tag	UNP P61604

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	N	1	Total 27	C 10	N 5	O 10	P 2	0	0

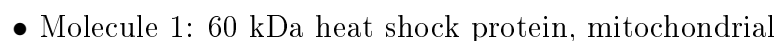
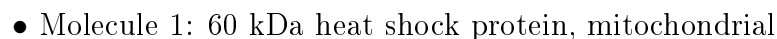
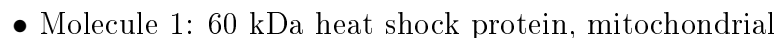
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

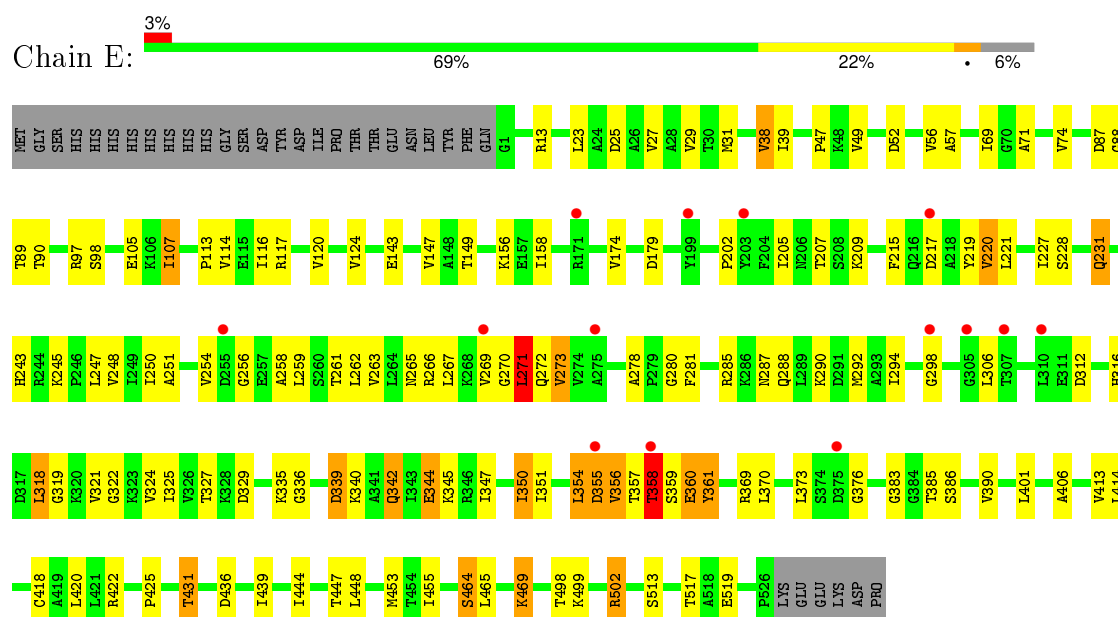
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

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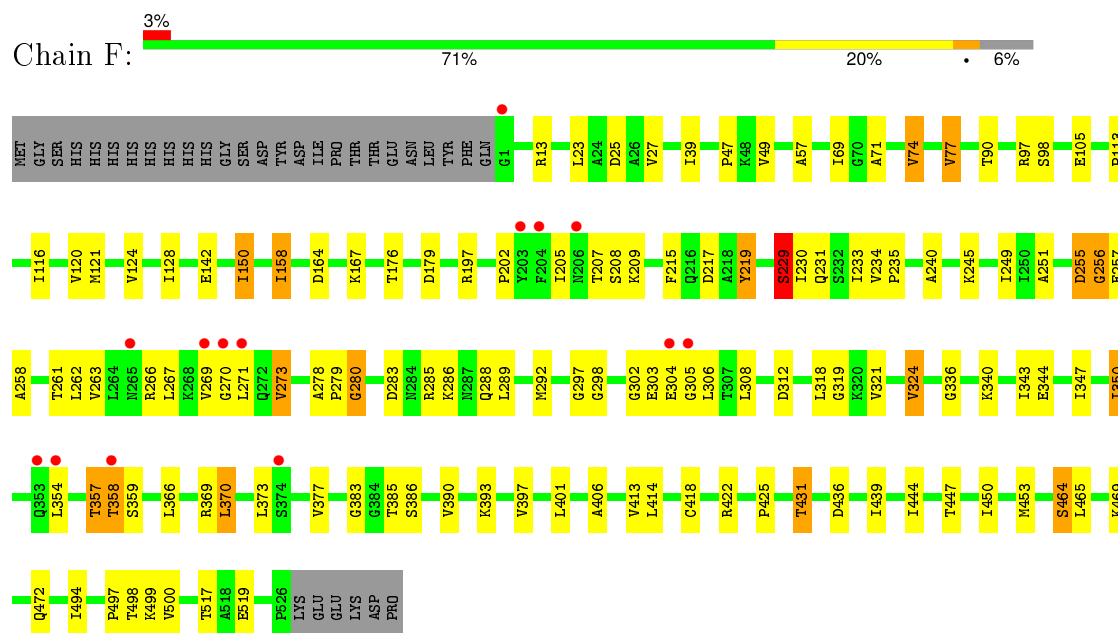
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

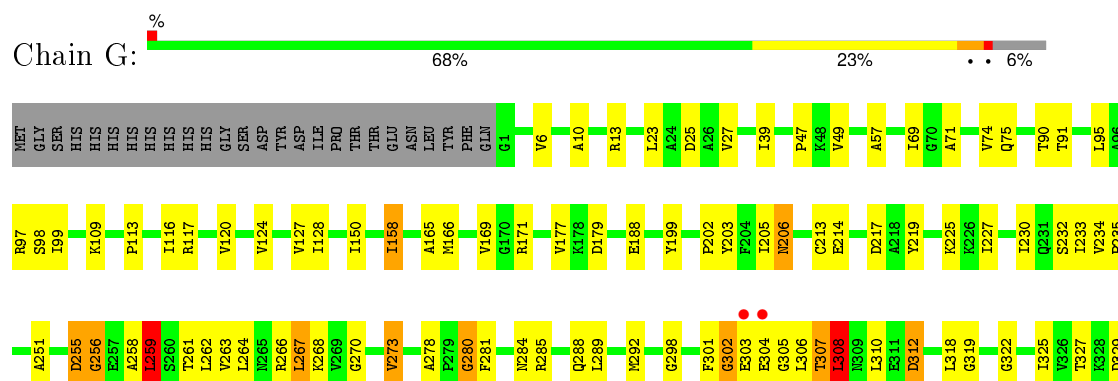


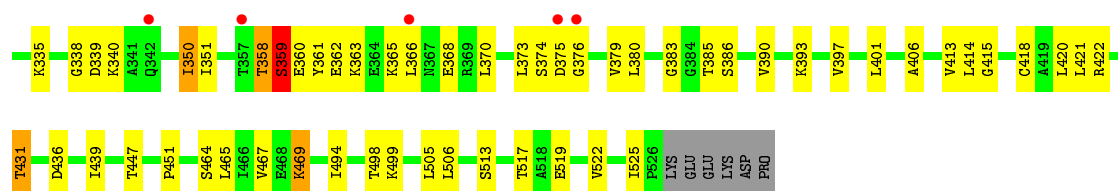


- Molecule 1: 60 kDa heat shock protein, mitochondrial

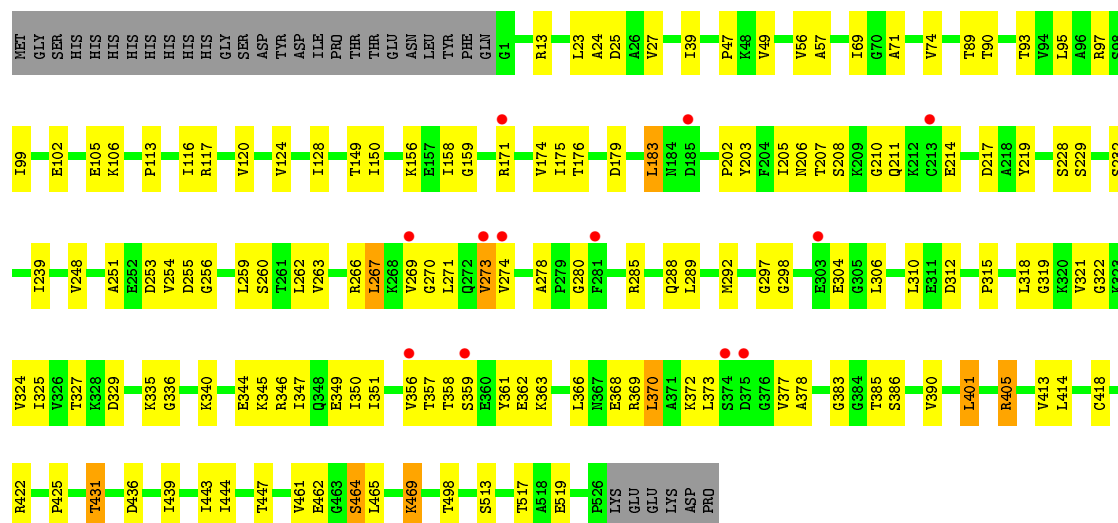


- Molecule 1: 60 kDa heat shock protein, mitochondrial

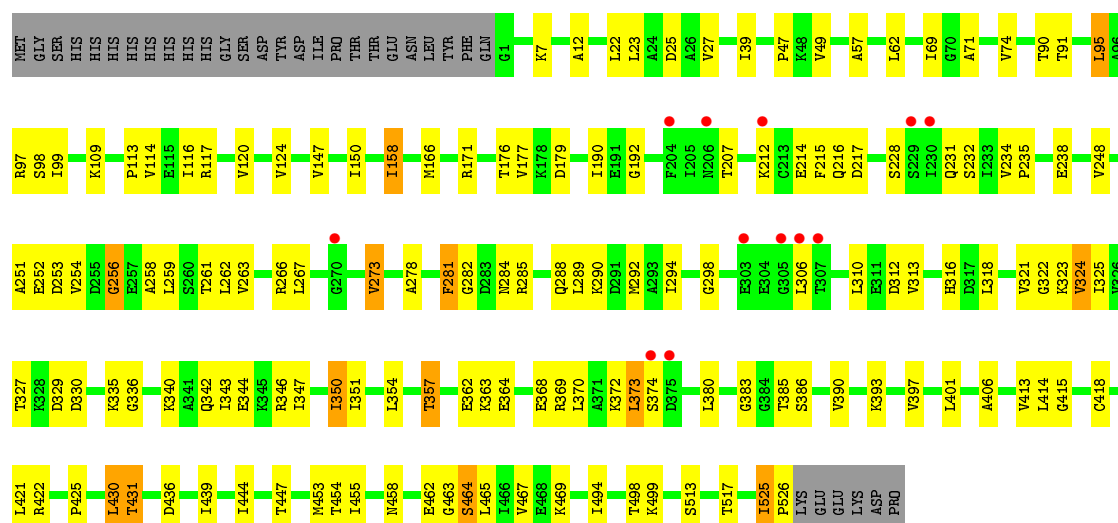




- Molecule 1: 60 kDa heat shock protein, mitochondrial

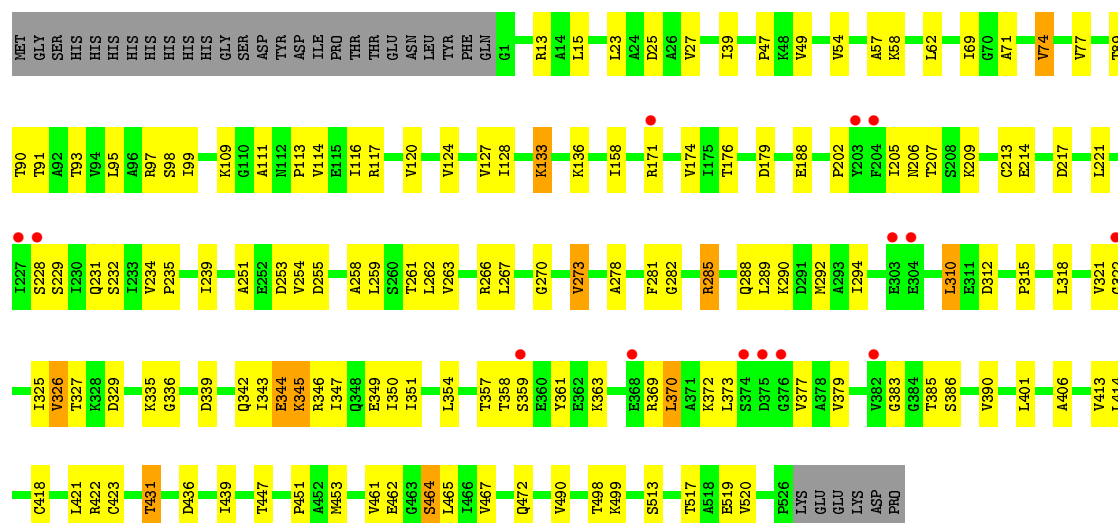


- Molecule 1: 60 kDa heat shock protein, mitochondrial

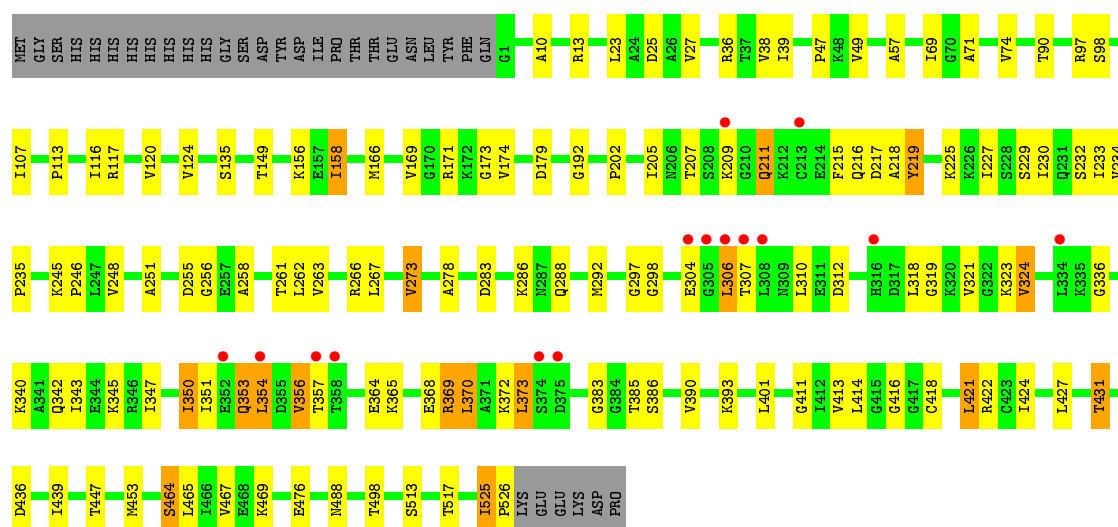


- Molecule 1: 60 kDa heat shock protein, mitochondrial

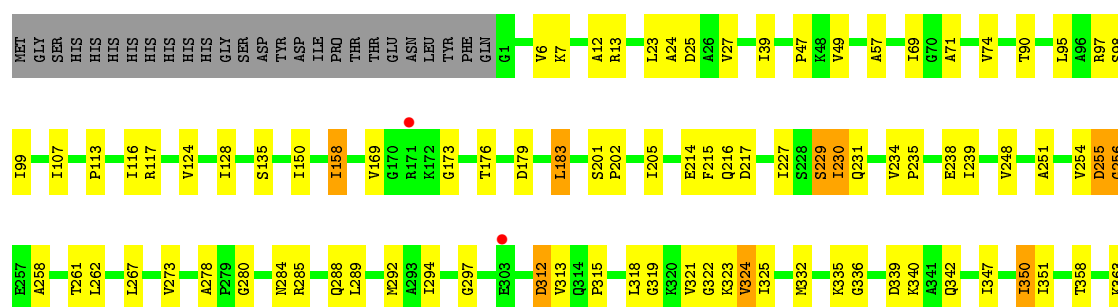


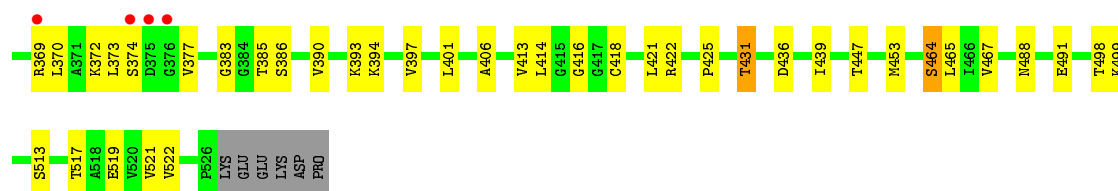


- Molecule 1: 60 kDa heat shock protein, mitochondrial

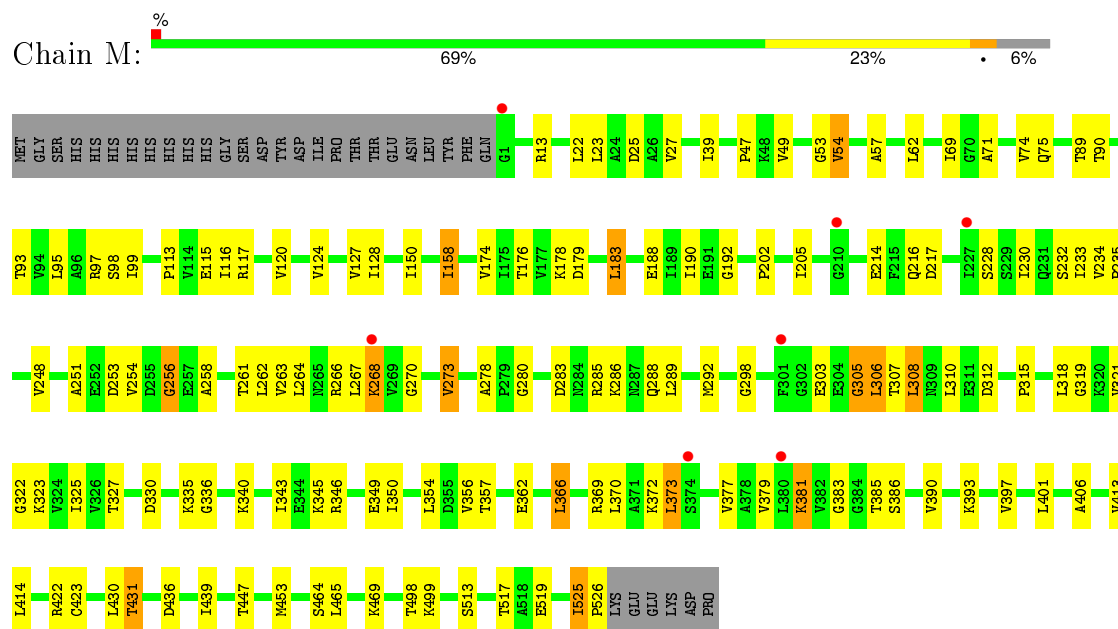


- Molecule 1: 60 kDa heat shock protein, mitochondrial

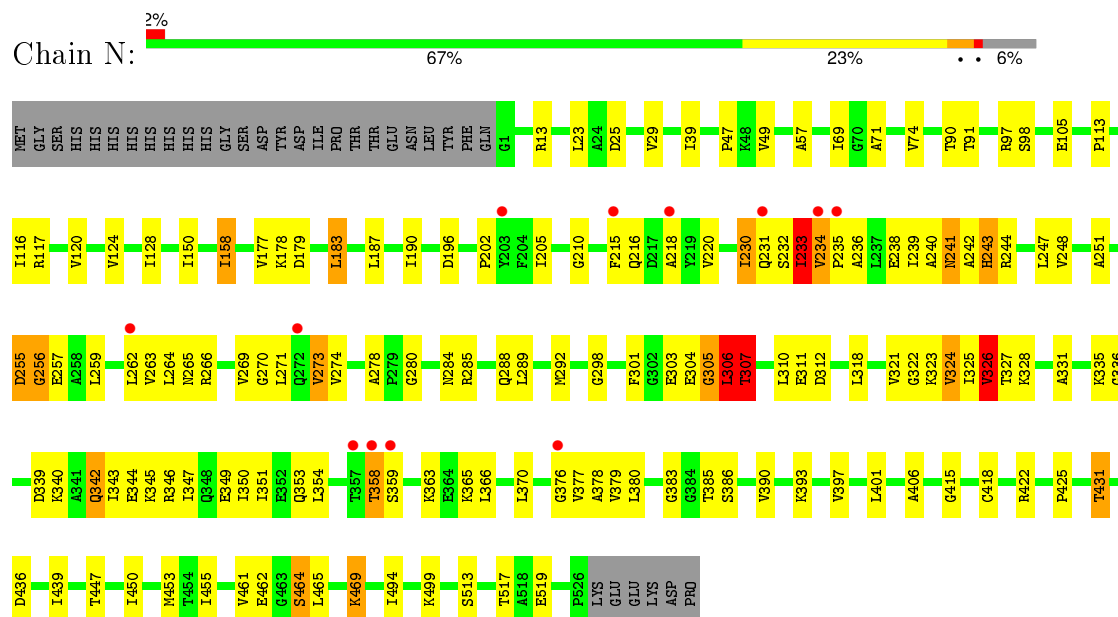




- Molecule 1: 60 kDa heat shock protein, mitochondrial



- Molecule 1: 60 kDa heat shock protein, mitochondrial



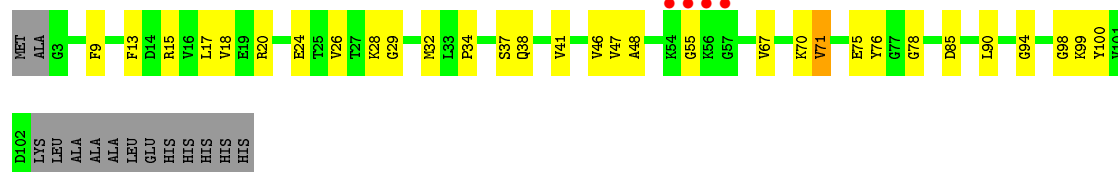
- Molecule 2: 10 kDa heat shock protein, mitochondrial



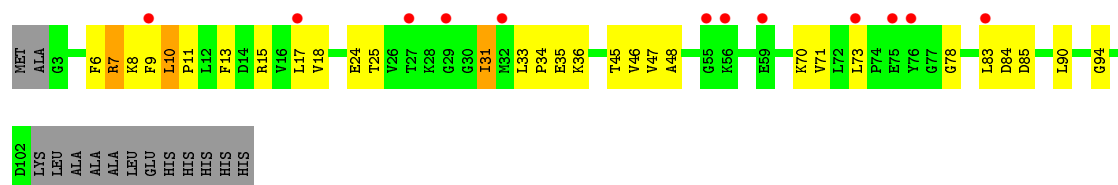
- Molecule 2: 10 kDa heat shock protein, mitochondrial



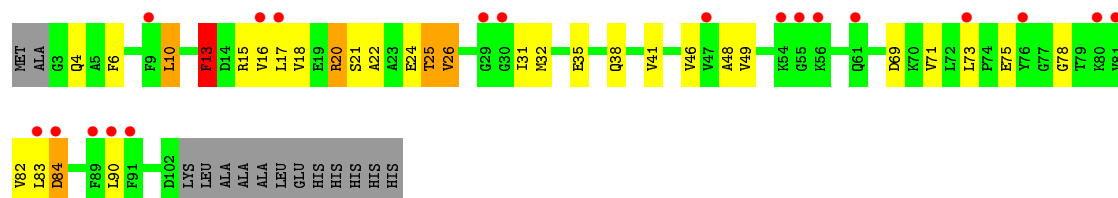
- Molecule 2: 10 kDa heat shock protein, mitochondrial



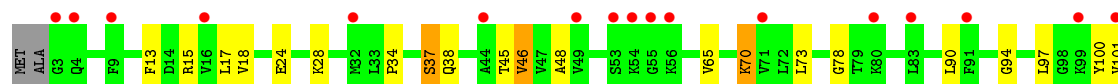
- Molecule 2: 10 kDa heat shock protein, mitochondrial

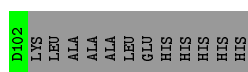


- Molecule 2: 10 kDa heat shock protein, mitochondrial

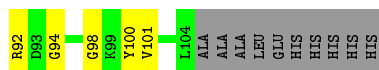
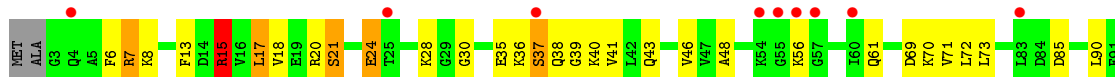


- Molecule 2: 10 kDa heat shock protein, mitochondrial

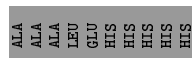
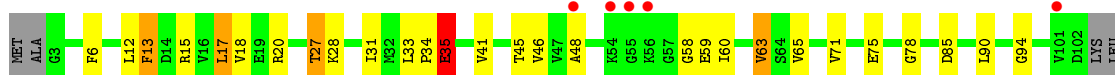




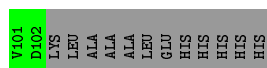
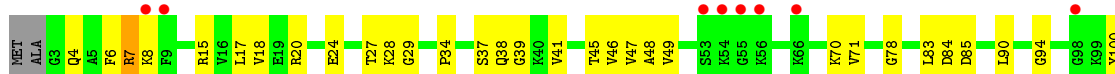
- Molecule 2: 10 kDa heat shock protein, mitochondrial



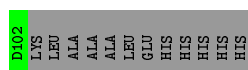
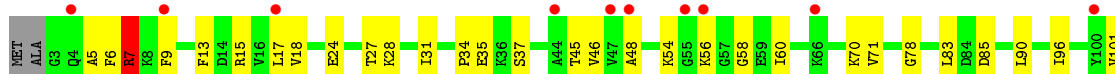
- Molecule 2: 10 kDa heat shock protein, mitochondrial



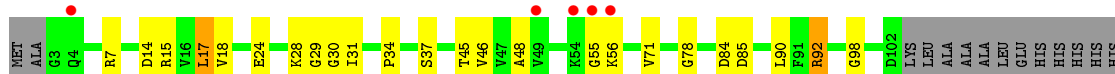
- Molecule 2: 10 kDa heat shock protein, mitochondrial



- Molecule 2: 10 kDa heat shock protein, mitochondrial

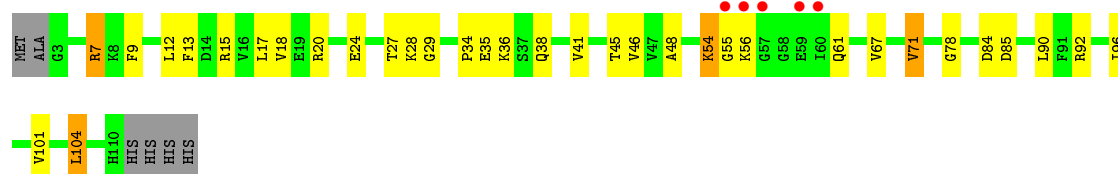


- Molecule 2: 10 kDa heat shock protein, mitochondrial



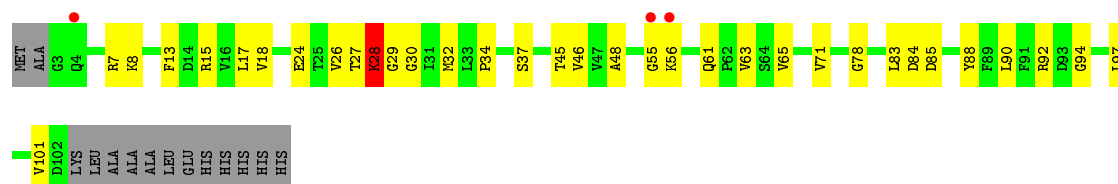
- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain Z: 



- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain 1: 



- Molecule 2: 10 kDa heat shock protein, mitochondrial

Chain 2: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	199.10Å 199.10Å 627.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.77 – 3.15 49.77 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.77-3.15) 99.4 (49.77-3.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.241 , 0.270 0.243 , 0.270	Depositor DCC
R_{free} test set	10852 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	102.6	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	7 of 215962 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	65963	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/3950	0.53	0/5328
1	B	0.27	0/3950	0.60	2/5328 (0.0%)
1	C	0.26	0/3950	0.51	1/5328 (0.0%)
1	D	0.25	0/3950	0.54	4/5328 (0.1%)
1	E	0.25	0/3950	0.52	1/5328 (0.0%)
1	F	0.25	0/3950	0.51	0/5328
1	G	0.26	0/3950	0.55	1/5328 (0.0%)
1	H	0.25	0/3950	0.51	0/5328
1	I	0.24	0/3950	0.49	0/5328
1	J	0.25	0/3950	0.51	0/5328
1	K	0.25	0/3950	0.51	0/5328
1	L	0.26	0/3950	0.52	0/5328
1	M	0.26	0/3950	0.51	0/5328
1	N	0.26	0/3950	0.55	2/5328 (0.0%)
2	1	0.25	0/767	0.61	1/1030 (0.1%)
2	2	0.27	0/794	0.63	0/1066
2	O	0.25	0/767	0.59	0/1030
2	P	0.26	0/799	0.61	0/1073
2	Q	0.25	0/767	0.59	0/1030
2	R	0.26	0/767	0.63	0/1030
2	S	0.29	0/767	0.71	1/1030 (0.1%)
2	T	0.24	0/767	0.62	0/1030
2	U	0.27	0/784	0.72	1/1052 (0.1%)
2	V	0.24	0/767	0.57	0/1030
2	W	0.26	0/767	0.59	0/1030
2	X	0.25	0/767	0.54	0/1030
2	Y	0.25	0/767	0.55	0/1030
2	Z	0.26	0/827	0.64	2/1111 (0.2%)
All	All	0.26	0/66174	0.54	16/89194 (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	B	0	3
1	D	0	1
1	G	0	3
1	K	0	1
1	N	0	5
2	S	0	1
2	U	0	2
2	V	0	1
2	Z	0	1
All	All	0	19

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	LEU	CA-CB-CG	8.52	134.88	115.30
1	B	247	LEU	CA-CB-CG	6.66	130.61	115.30
2	U	15	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	D	333	LEU	CA-CB-CG	6.37	129.94	115.30
1	N	210	GLY	N-CA-C	-5.92	98.31	113.10

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	SER	Peptide
1	B	303	GLU	Peptide
1	B	304	GLU	Peptide
1	B	339	ASP	Peptide
1	D	280	GLY	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	3918	0	4103	104	0
1	B	3918	0	4103	130	0
1	C	3918	0	4103	87	0
1	D	3918	0	4103	96	0
1	E	3918	0	4103	83	0
1	F	3918	0	4103	77	0
1	G	3918	0	4103	89	0
1	H	3918	0	4103	86	0
1	I	3918	0	4103	79	0
1	J	3918	0	4103	88	0
1	K	3918	0	4103	78	0
1	L	3918	0	4103	83	0
1	M	3918	0	4103	84	0
1	N	3918	0	4103	99	0
2	1	756	0	786	19	0
2	2	783	0	820	12	0
2	O	756	0	786	17	0
2	P	788	0	825	16	0
2	Q	756	0	786	16	0
2	R	756	0	786	14	0
2	S	756	0	786	20	0
2	T	756	0	786	10	0
2	U	773	0	810	26	0
2	V	756	0	786	12	0
2	W	756	0	786	16	0
2	X	756	0	786	14	0
2	Y	756	0	786	11	0
2	Z	815	0	849	16	0
3	A	27	0	12	2	0
3	B	27	0	12	2	0
3	C	27	0	12	2	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
3	I	27	0	12	1	0
3	J	27	0	12	0	0
3	K	27	0	12	1	0
3	L	27	0	12	1	0
3	M	27	0	12	0	0
3	N	27	0	12	2	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
All	All	65963	0	68774	1395	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 10.

The worst 5 of 1395 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:B:322:GLY:HA3	1:B:335:LYS:HB3	1.39	1.02
1:G:306:LEU:HA	1:G:307:THR:HB	1.52	0.91
1:G:206:ASN:ND2	1:G:213:CYS:SG	2.45	0.89
2:O:54:LYS:HA	2:O:60:ILE:HA	1.53	0.88
2:U:15:ARG:HG3	2:U:15:ARG:HH11	1.41	0.86

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	524/558 (94%)	494 (94%)	24 (5%)	6 (1%)	17	61
1	B	524/558 (94%)	487 (93%)	22 (4%)	15 (3%)	6	35
1	C	524/558 (94%)	492 (94%)	26 (5%)	6 (1%)	17	61
1	D	524/558 (94%)	494 (94%)	25 (5%)	5 (1%)	19	63
1	E	524/558 (94%)	489 (93%)	26 (5%)	9 (2%)	11	50
1	F	524/558 (94%)	490 (94%)	26 (5%)	8 (2%)	13	53
1	G	524/558 (94%)	489 (93%)	25 (5%)	10 (2%)	10	48
1	H	524/558 (94%)	493 (94%)	27 (5%)	4 (1%)	24	67
1	I	524/558 (94%)	493 (94%)	26 (5%)	5 (1%)	19	63
1	J	524/558 (94%)	497 (95%)	25 (5%)	2 (0%)	39	79
1	K	524/558 (94%)	496 (95%)	23 (4%)	5 (1%)	19	63
1	L	524/558 (94%)	494 (94%)	25 (5%)	5 (1%)	19	63
1	M	524/558 (94%)	489 (93%)	28 (5%)	7 (1%)	15	57
1	N	524/558 (94%)	486 (93%)	28 (5%)	10 (2%)	10	48
2	1	98/114 (86%)	88 (90%)	5 (5%)	5 (5%)	2	19
2	2	102/114 (90%)	94 (92%)	5 (5%)	3 (3%)	6	35
2	O	98/114 (86%)	85 (87%)	7 (7%)	6 (6%)	2	14
2	P	103/114 (90%)	97 (94%)	3 (3%)	3 (3%)	6	35
2	Q	98/114 (86%)	91 (93%)	4 (4%)	3 (3%)	5	32
2	R	98/114 (86%)	88 (90%)	6 (6%)	4 (4%)	3	25
2	S	98/114 (86%)	86 (88%)	6 (6%)	6 (6%)	2	14
2	T	98/114 (86%)	92 (94%)	4 (4%)	2 (2%)	9	46
2	U	100/114 (88%)	91 (91%)	5 (5%)	4 (4%)	4	25
2	V	98/114 (86%)	92 (94%)	3 (3%)	3 (3%)	5	32
2	W	98/114 (86%)	91 (93%)	5 (5%)	2 (2%)	9	46
2	X	98/114 (86%)	91 (93%)	4 (4%)	3 (3%)	5	32
2	Y	98/114 (86%)	92 (94%)	2 (2%)	4 (4%)	3	25
2	Z	106/114 (93%)	91 (86%)	10 (9%)	5 (5%)	3	21
All	All	8727/9408 (93%)	8152 (93%)	425 (5%)	150 (2%)	11	50

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	GLY
1	A	358	THR
1	B	217	ASP
1	B	231	GLN
1	B	269	VAL

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	425/455 (93%)	399 (94%)	26 (6%)	23	62
1	B	425/455 (93%)	389 (92%)	36 (8%)	13	46
1	C	425/455 (93%)	408 (96%)	17 (4%)	38	76
1	D	425/455 (93%)	391 (92%)	34 (8%)	15	50
1	E	425/455 (93%)	394 (93%)	31 (7%)	17	55
1	F	425/455 (93%)	401 (94%)	24 (6%)	26	66
1	G	425/455 (93%)	402 (95%)	23 (5%)	27	67
1	H	425/455 (93%)	400 (94%)	25 (6%)	24	63
1	I	425/455 (93%)	394 (93%)	31 (7%)	17	55
1	J	425/455 (93%)	399 (94%)	26 (6%)	23	62
1	K	425/455 (93%)	398 (94%)	27 (6%)	22	61
1	L	425/455 (93%)	402 (95%)	23 (5%)	27	67
1	M	425/455 (93%)	397 (93%)	28 (7%)	21	59
1	N	425/455 (93%)	400 (94%)	25 (6%)	24	63
2	1	81/91 (89%)	74 (91%)	7 (9%)	13	45
2	2	83/91 (91%)	75 (90%)	8 (10%)	10	38
2	O	81/91 (89%)	75 (93%)	6 (7%)	17	54
2	P	83/91 (91%)	76 (92%)	7 (8%)	14	47
2	Q	81/91 (89%)	74 (91%)	7 (9%)	13	45
2	R	81/91 (89%)	72 (89%)	9 (11%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	81/91 (89%)	73 (90%)	8 (10%)	10	36
2	T	81/91 (89%)	72 (89%)	9 (11%)	8	31
2	U	83/91 (91%)	75 (90%)	8 (10%)	10	38
2	V	81/91 (89%)	72 (89%)	9 (11%)	8	31
2	W	81/91 (89%)	75 (93%)	6 (7%)	17	54
2	X	81/91 (89%)	72 (89%)	9 (11%)	8	31
2	Y	81/91 (89%)	74 (91%)	7 (9%)	13	45
2	Z	86/91 (94%)	77 (90%)	9 (10%)	8	33
All	All	7095/7644 (93%)	6610 (93%)	485 (7%)	20	57

5 of 485 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	176	THR
1	J	465	LEU
2	X	35	GLU
1	I	281	PHE
1	I	525	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	206	ASN
1	I	284	ASN
1	K	216	GLN
1	C	342	GLN
1	J	216	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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
3	ADP	A	601	-	22,29,29	0.98	1 (4%)	27,45,45	1.90	3 (11%)
3	ADP	B	601	-	22,29,29	1.00	1 (4%)	27,45,45	1.85	3 (11%)
3	ADP	C	601	-	22,29,29	0.98	1 (4%)	27,45,45	1.90	3 (11%)
3	ADP	D	601	-	22,29,29	0.97	1 (4%)	27,45,45	1.93	4 (14%)
3	ADP	E	601	-	22,29,29	0.99	1 (4%)	27,45,45	1.85	4 (14%)
3	ADP	F	601	-	22,29,29	0.99	1 (4%)	27,45,45	1.87	4 (14%)
3	ADP	G	601	-	22,29,29	0.95	1 (4%)	27,45,45	1.88	4 (14%)
3	ADP	H	601	-	22,29,29	0.97	1 (4%)	27,45,45	1.91	3 (11%)
3	ADP	I	601	-	22,29,29	0.97	1 (4%)	27,45,45	2.06	6 (22%)
3	ADP	J	601	-	22,29,29	0.97	1 (4%)	27,45,45	1.88	3 (11%)
3	ADP	K	601	-	22,29,29	0.97	1 (4%)	27,45,45	1.93	4 (14%)
3	ADP	L	601	-	22,29,29	0.97	1 (4%)	27,45,45	1.91	3 (11%)
3	ADP	M	601	-	22,29,29	0.98	1 (4%)	27,45,45	1.85	4 (14%)
3	ADP	N	601	-	22,29,29	1.00	1 (4%)	27,45,45	1.99	6 (22%)

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
3	ADP	A	601	-	-	0/12/32/32	0/3/3/3
3	ADP	B	601	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	601	-	-	0/12/32/32	0/3/3/3
3	ADP	D	601	-	-	0/12/32/32	0/3/3/3
3	ADP	E	601	-	-	0/12/32/32	0/3/3/3
3	ADP	F	601	-	-	0/12/32/32	0/3/3/3
3	ADP	G	601	-	-	0/12/32/32	0/3/3/3
3	ADP	H	601	-	-	0/12/32/32	0/3/3/3
3	ADP	I	601	-	-	0/12/32/32	0/3/3/3
3	ADP	J	601	-	-	0/12/32/32	0/3/3/3
3	ADP	K	601	-	-	0/12/32/32	0/3/3/3
3	ADP	L	601	-	-	0/12/32/32	0/3/3/3
3	ADP	M	601	-	-	0/12/32/32	0/3/3/3
3	ADP	N	601	-	-	0/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	601	ADP	C5-C4	2.97	1.47	1.40
3	L	601	ADP	C5-C4	3.01	1.47	1.40
3	C	601	ADP	C5-C4	3.02	1.47	1.40
3	A	601	ADP	C5-C4	3.02	1.47	1.40
3	G	601	ADP	C5-C4	3.03	1.47	1.40

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	601	ADP	N3-C2-N1	-7.04	123.50	128.89
3	H	601	ADP	N3-C2-N1	-7.03	123.51	128.89
3	A	601	ADP	N3-C2-N1	-7.03	123.51	128.89
3	D	601	ADP	N3-C2-N1	-7.01	123.53	128.89
3	C	601	ADP	N3-C2-N1	-7.00	123.53	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	2	0
3	B	601	ADP	2	0
3	C	601	ADP	2	0
3	D	601	ADP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	601	ADP	1	0
3	K	601	ADP	1	0
3	L	601	ADP	1	0
3	N	601	ADP	2	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	526/558 (94%)	0.25	29 (5%) 29 15	65, 112, 194, 225	0
1	B	526/558 (94%)	0.56	49 (9%) 11 5	66, 116, 232, 279	0
1	C	526/558 (94%)	0.06	11 (2%) 67 50	66, 109, 169, 217	0
1	D	526/558 (94%)	0.20	21 (3%) 42 26	61, 107, 195, 228	0
1	E	526/558 (94%)	0.18	14 (2%) 58 42	66, 106, 202, 226	0
1	F	526/558 (94%)	0.14	14 (2%) 58 42	67, 110, 166, 192	0
1	G	526/558 (94%)	0.07	7 (1%) 79 67	67, 102, 153, 196	0
1	H	526/558 (94%)	0.08	12 (2%) 64 47	66, 103, 160, 191	0
1	I	526/558 (94%)	0.17	12 (2%) 64 47	64, 103, 179, 203	0
1	J	526/558 (94%)	0.15	14 (2%) 58 42	65, 107, 164, 191	0
1	K	526/558 (94%)	0.15	15 (2%) 55 39	61, 106, 167, 207	0
1	L	526/558 (94%)	0.09	6 (1%) 82 71	66, 101, 151, 182	0
1	M	526/558 (94%)	0.15	7 (1%) 79 67	66, 112, 169, 207	0
1	N	526/558 (94%)	0.16	12 (2%) 64 47	70, 110, 165, 202	0
2	1	100/114 (87%)	0.20	3 (3%) 54 37	94, 117, 179, 210	0
2	2	104/114 (91%)	0.41	6 (5%) 26 13	101, 135, 185, 200	0
2	O	100/114 (87%)	0.49	4 (4%) 42 26	107, 139, 185, 194	0
2	P	105/114 (92%)	0.14	1 (0%) 84 74	93, 121, 199, 209	0
2	Q	100/114 (87%)	0.31	4 (4%) 42 26	84, 114, 179, 199	0
2	R	100/114 (87%)	0.74	12 (12%) 6 3	97, 136, 187, 201	0
2	S	100/114 (87%)	0.88	19 (19%) 2 1	127, 158, 194, 202	0
2	T	100/114 (87%)	0.92	17 (17%) 2 1	123, 157, 195, 224	0
2	U	102/114 (89%)	0.60	9 (8%) 12 6	121, 145, 193, 223	0
2	V	100/114 (87%)	0.49	5 (5%) 32 17	107, 134, 181, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	100/114 (87%)	0.39	8 (8%) 15 7	118, 145, 182, 197	0
2	X	100/114 (87%)	0.76	10 (10%) 9 4	118, 141, 201, 210	0
2	Y	100/114 (87%)	0.23	5 (5%) 32 17	97, 124, 181, 216	0
2	Z	108/114 (94%)	0.19	5 (4%) 36 21	91, 118, 170, 216	0
All	All	8783/9408 (93%)	0.22	331 (3%) 44 27	61, 113, 185, 279	0

The worst 5 of 331 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	305	GLY	10.8
1	L	374	SER	10.7
2	Y	55	GLY	9.8
1	B	358	THR	9.4
1	B	269	VAL	8.6

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
3	ADP	H	601	27/27	0.92	0.27	1.37	75,87,95,98	0
3	ADP	C	601	27/27	0.92	0.26	1.14	69,90,104,110	0
3	ADP	I	601	27/27	0.92	0.27	1.05	61,86,93,96	0
3	ADP	L	601	27/27	0.94	0.26	0.87	63,85,94,95	0
3	ADP	F	601	27/27	0.92	0.26	0.70	62,87,92,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ADP	D	601	27/27	0.92	0.25	0.69	62,86,98,100	0
3	ADP	E	601	27/27	0.88	0.27	0.66	69,80,89,93	0
3	ADP	G	601	27/27	0.92	0.27	0.59	65,81,90,97	0
3	ADP	K	601	27/27	0.91	0.25	0.58	67,87,96,104	0
3	ADP	B	601	27/27	0.92	0.23	0.44	74,98,105,115	0
3	ADP	N	601	27/27	0.91	0.23	0.34	72,87,97,99	0
3	ADP	A	601	27/27	0.92	0.23	0.00	68,90,102,104	0
3	ADP	M	601	27/27	0.94	0.23	-0.09	69,87,93,95	0
3	ADP	J	601	27/27	0.91	0.23	-0.11	69,88,94,105	0
4	MG	I	602	1/1	0.96	0.29	-	60,60,60,60	0
4	MG	A	602	1/1	0.98	0.26	-	72,72,72,72	0
4	MG	B	602	1/1	0.94	0.28	-	74,74,74,74	0
4	MG	F	602	1/1	0.98	0.32	-	66,66,66,66	0
4	MG	L	602	1/1	0.98	0.32	-	72,72,72,72	0
4	MG	G	602	1/1	0.95	0.25	-	67,67,67,67	0
4	MG	D	602	1/1	0.94	0.28	-	77,77,77,77	0
4	MG	H	602	1/1	0.95	0.34	-	73,73,73,73	0
4	MG	K	602	1/1	0.98	0.27	-	61,61,61,61	0
4	MG	J	602	1/1	0.95	0.29	-	66,66,66,66	0
4	MG	E	602	1/1	0.98	0.30	-	62,62,62,62	0
4	MG	C	602	1/1	0.97	0.32	-	84,84,84,84	0
4	MG	M	602	1/1	0.99	0.29	-	60,60,60,60	0
4	MG	N	602	1/1	0.95	0.29	-	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.