wwPDB EM Validation Summary Report (i)

Apr 16, 2024 – 04:51 am BST

PDB ID	:	6RW4
EMDB ID	:	EMD-10021
Title	:	Structure of human mitochondrial 28S ribosome in complex with mitochondrial IF3
Authors	:	Itoh, Y.; Khawaja, A.; Rorbach, J.; Amunts, A.
Deposited on	:	2019-06-03
Resolution	:	2.97 Å(reported)
Based on initial model	:	3J9M

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

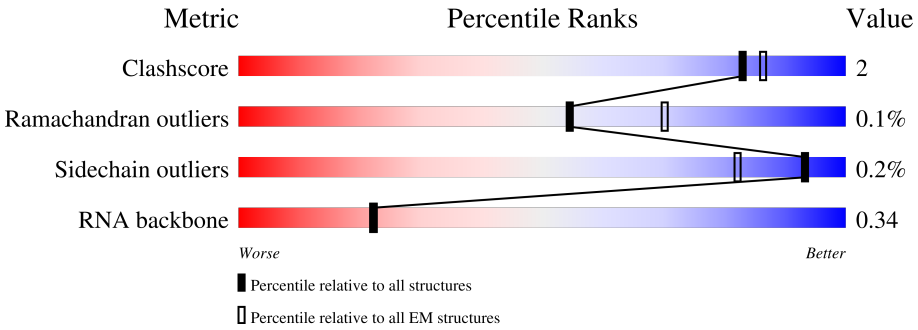
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	955	65% 30% ·
2	B	296	72% · 24%
3	C	167	65% 14% 21%
4	D	430	74% 5% 20%
5	E	125	93% 5% ·
6	F	242	81% 5% 14%
7	G	396	75% 8% 17%

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Mol	Chain	Length	Quality of chain
8	H	201	66% 30%
9	I	194	63% 8% 29%
10	J	138	74% 22%
11	K	128	70% 9% 21%
12	L	257	63% 5% 32%
13	M	137	84% 13%
14	N	130	79% 5% 15%
15	O	258	69% 6% 25%
16	P	142	63% 5% 32%
17	Q	86	91% 9%
18	R	360	76% 6% 18%
19	S	190	67% 29%
20	T	173	91% 6%
21	U	205	82% 14%
22	V	414	82% 6% 13%
23	W	187	50% 47%
24	X	398	83% 6% 12%
25	Y	395	36% 62%
26	Z	106	91% 6%
27	0	218	89% 10%
28	1	323	80% 5% 15%
29	2	117	93% 7%
30	3	199	33% 65%
31	4	689	78% 7% 15%
32	8	285	61% 6% 33%

2 Entry composition (i)

There are 42 unique types of molecules in this entry. The entry contains 128280 atoms, of which 59411 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	955	30595	9098	10313	3652	6577	955	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	225	3644	1164	1816	331	323	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	132	2172	699	1089	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	343	5536	1713	2805	518	487	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	122	1972	614	1000	177	177	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	208	3495	1104	1770	312	298	11	0	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	330	Total	C	H	N	O	S	0	0
			5434	1726	2718	485	491	14		

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	140	Total	C	H	N	O	S	0	0
			2336	745	1184	194	210	3		

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	137	Total	C	H	N	O	S	0	0
			2079	641	1060	193	181	4		

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	108	Total	C	H	N	O	S	0	0
			1727	521	888	169	143	6		

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	101	Total	C	H	N	O	S	0	0
			1748	537	886	179	141	5		

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	174	Total	C	H	N	O	S	0	0
			2994	925	1541	270	251	7		

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1908	594	966	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	110	Total	C	H	N	O	S	0	0
			1797	562	929	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	194	Total	C	H	N	O	S	0	0
			3165	1019	1566	295	278	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	97	Total	C	H	N	O	S	0	0
			1588	501	807	134	138	8		

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	86	Total	C	H	N	O	S	0	0
			1502	460	758	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	295	Total	C	H	N	O	S	0	0
			4838	1533	2429	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	135	Total	C	H	N	O	S	0	0
			2227	716	1116	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2764	877	1393	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	176	Total	C	H	N	O	S	0	0
			2988	916	1500	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	362	Total	C	H	N	O	S	0	0
			5933	1904	2964	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	100	Total	C	H	N	O	S	0	0
			1592	498	803	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	352	Total	C	H	N	O	S	0	0
			5694	1822	2845	499	517	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	149	Total	C	H	N	O	S	0	0
			2444	801	1198	207	234	4		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	100	Total	C	H	N	O	S	0	0
			1699	534	860	153	148	4		

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	215	Total	C	H	N	O	S	0	0
			3584	1130	1797	339	313	5		

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	276	Total	C	H	N	O	S	0	0
			4507	1419	2269	381	427	11		

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	117	Total	C	H	N	O	S	0	0
			1904	579	969	182	166	8		

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	70	Total	C	H	N	O	S	0	0
			1325	401	700	134	89	1		

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	588	Total	C	H	N	O	S	0	0
			9536	3053	4768	808	879	28		

- Molecule 32 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	8	191	Total	C	H	N	O	S	0	0
			3131	953	1588	289	293	8		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	68	ILE	THR	variant	UNP Q9H2K0
8	243	LEU	PHE	variant	UNP Q9H2K0
8	279	GLY	-	expression tag	UNP Q9H2K0
8	280	LEU	-	expression tag	UNP Q9H2K0
8	281	GLU	-	expression tag	UNP Q9H2K0

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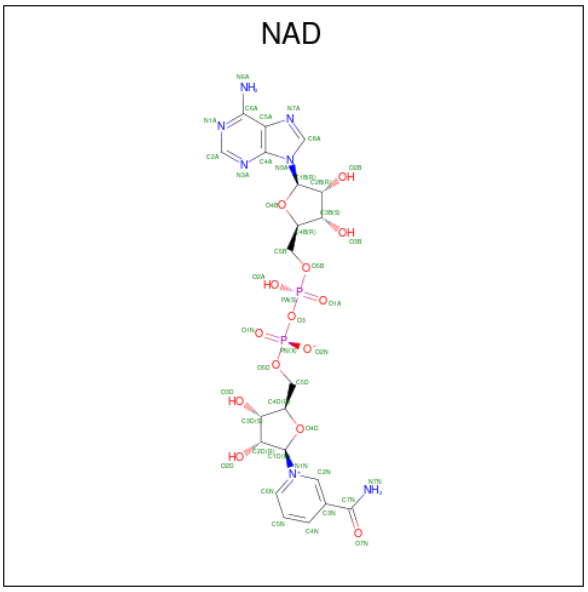
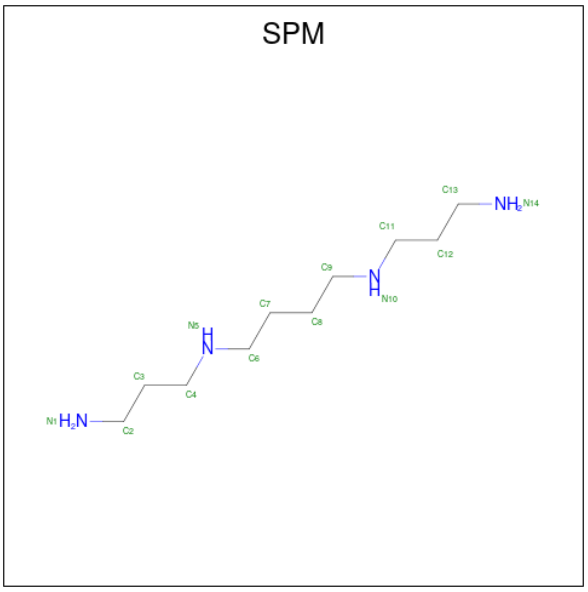
Chain	Residue	Modelled	Actual	Comment	Reference
8	282	VAL	-	expression tag	UNP Q9H2K0
8	283	LEU	-	expression tag	UNP Q9H2K0
8	284	PHE	-	expression tag	UNP Q9H2K0
8	285	GLN	-	expression tag	UNP Q9H2K0

- Molecule 33 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



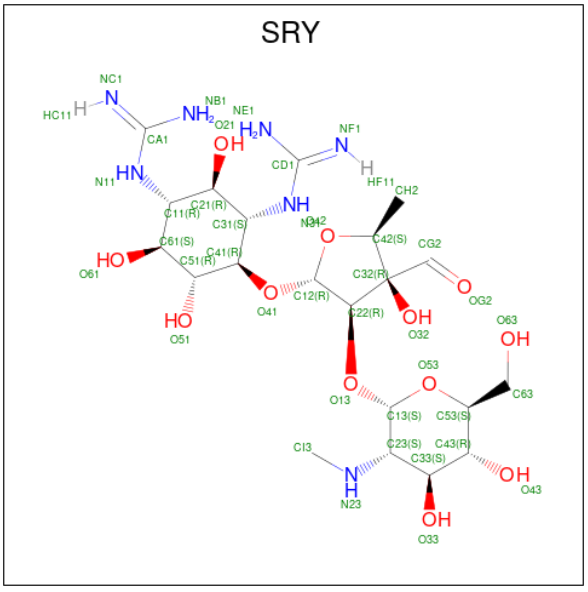
Mol	Chain	Residues	Atoms						AltConf
33	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 34 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
34	A	1	40	10	26	4	0

- Molecule 35 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
35	A	1	79	21	39	7	12	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
36	A	57	Total Mg 57 57	0
36	B	1	Total Mg 1 1	0
36	X	1	Total Mg 1 1	0
36	3	1	Total Mg 1 1	0

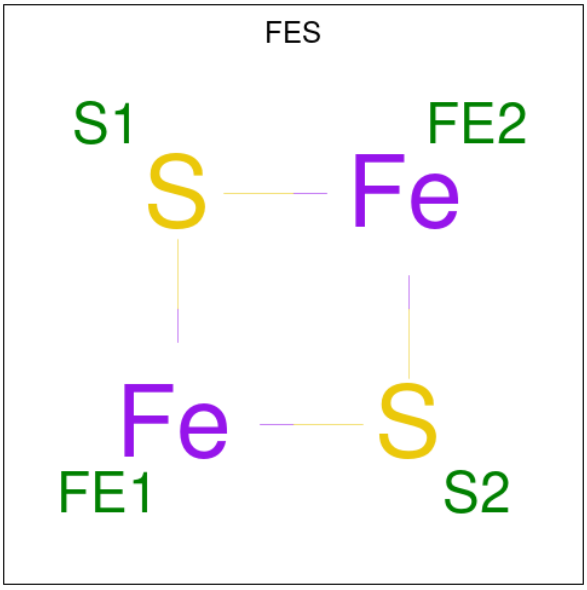
- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
37	A	17	Total K 17 17	0

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
38	O	1	Total Zn 1 1	0

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
39	P	1	Total Fe S 4 2 2	0

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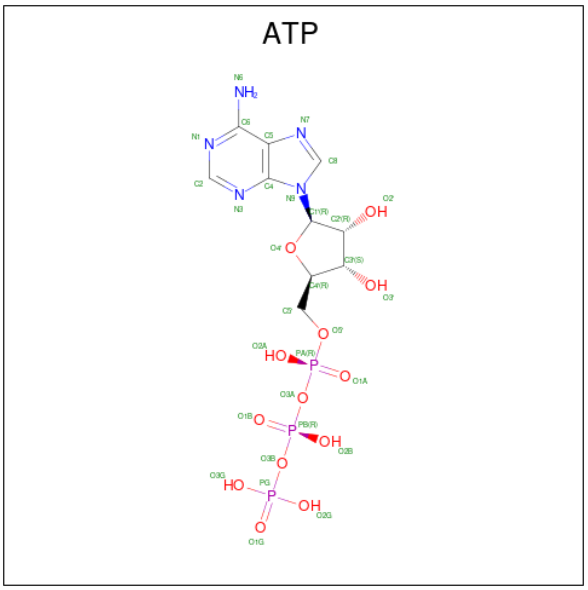
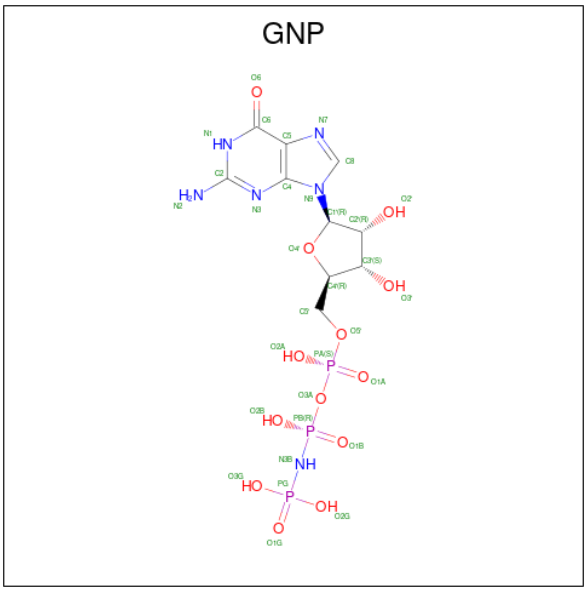
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
39	T	1	4	2	2	0

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
40	X	1	43	10	12	5	13	3	0

- Molecule 41 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
41	X	1	Total	C	H	N	O	P	0
			45	10	13	6	13	3	

- Molecule 42 is water.

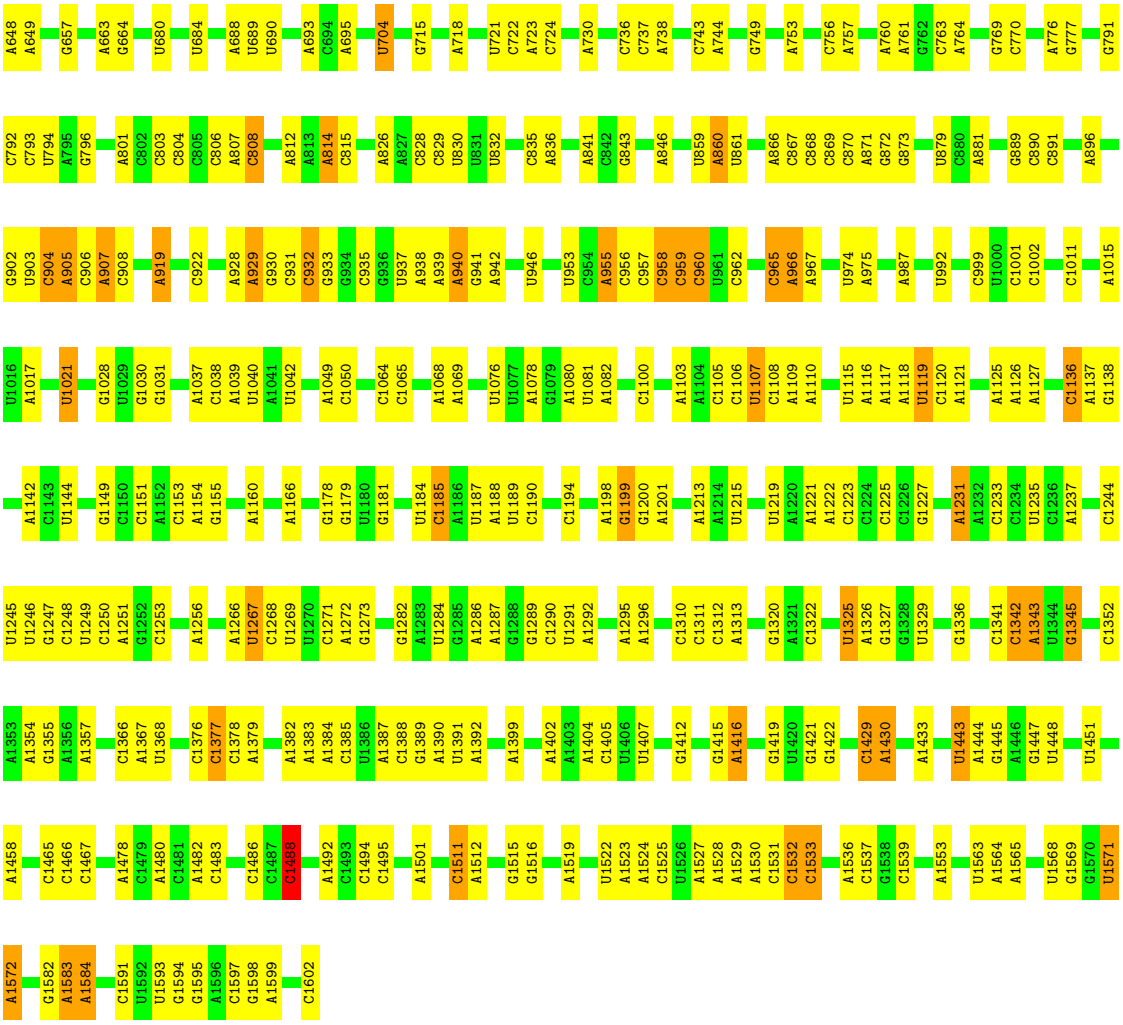
Mol	Chain	Residues	Atoms		AltConf
42	A	49	Total	O	0
			49	49	
42	C	2	Total	O	0
			2	2	
42	G	1	Total	O	0
			1	1	
42	I	1	Total	O	0
			1	1	
42	T	1	Total	O	0
			1	1	
42	X	3	Total	O	0
			3	3	
42	0	1	Total	O	0
			1	1	
42	2	1	Total	O	0
			1	1	

3 Residue-property plots (i)

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

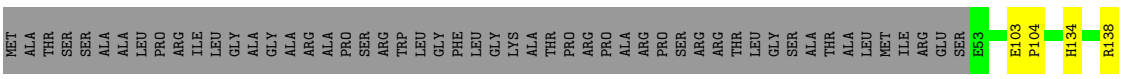
- Molecule 1: 12S mitochondrial rRNA

Chain A:



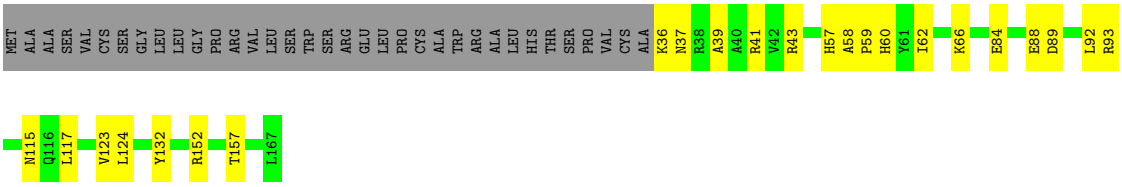
- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:



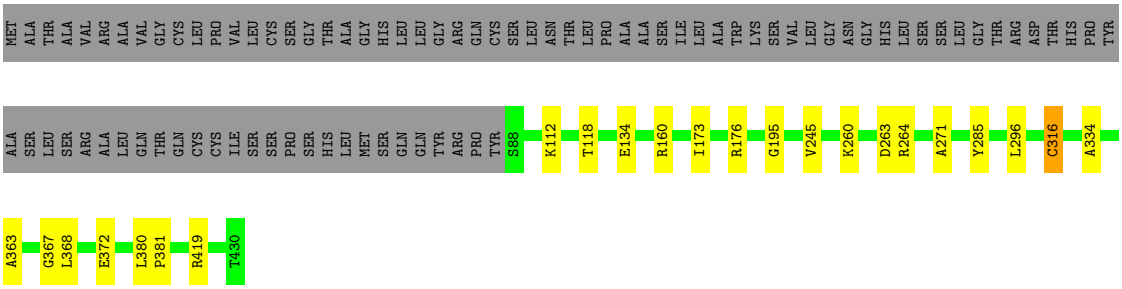
• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:



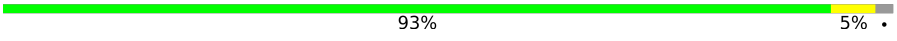
• Molecule 4: 28S ribosomal protein S5, mitochondrial

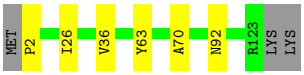
Chain D:



• Molecule 5: 28S ribosomal protein S6, mitochondrial

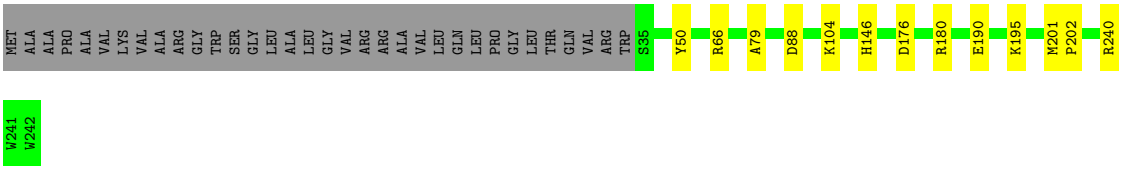
Chain E:





• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:

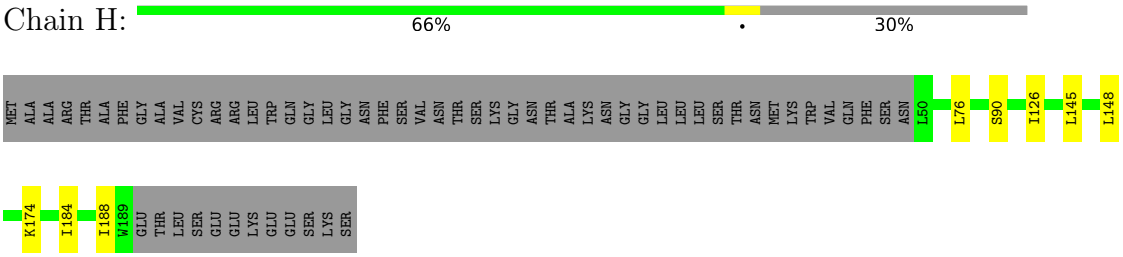


• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:

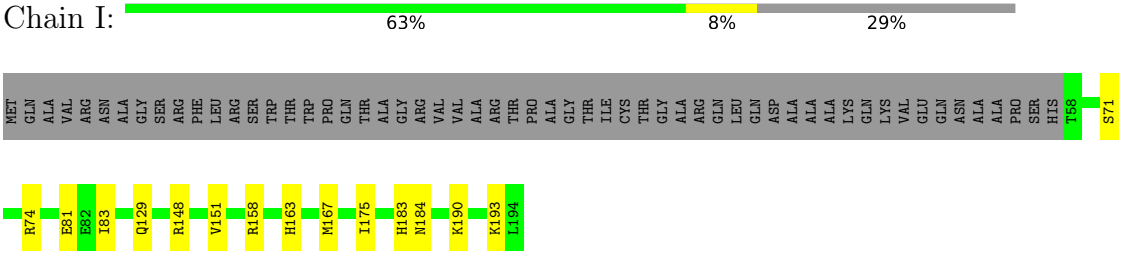
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



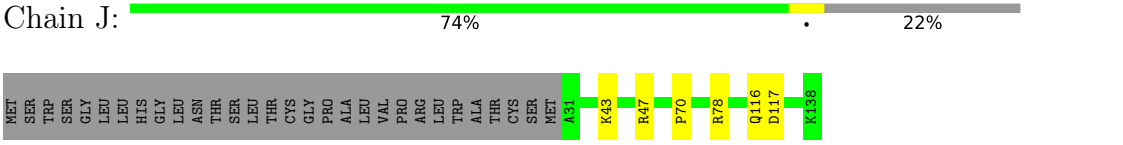
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



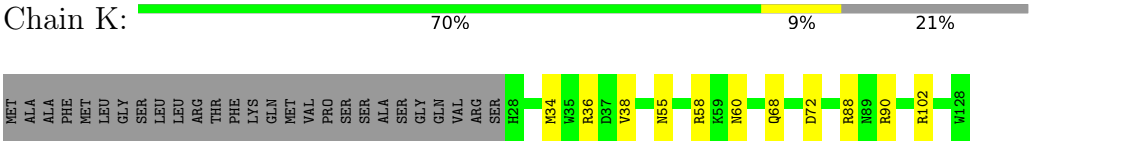
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



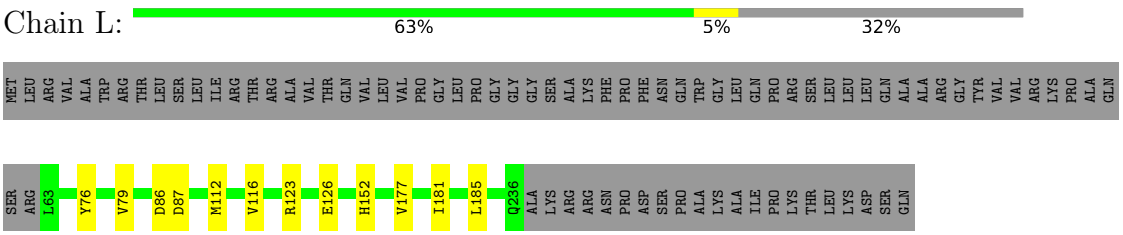
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



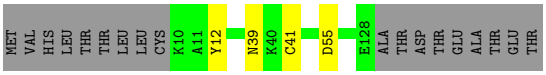
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



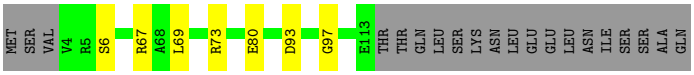
• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:



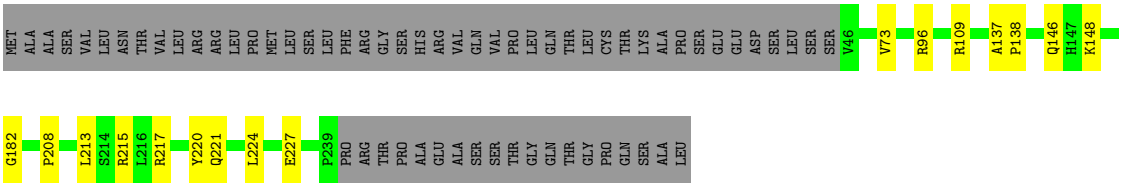
• Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain N:



• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:



• Molecule 16: 28S ribosomal protein S18c, mitochondrial

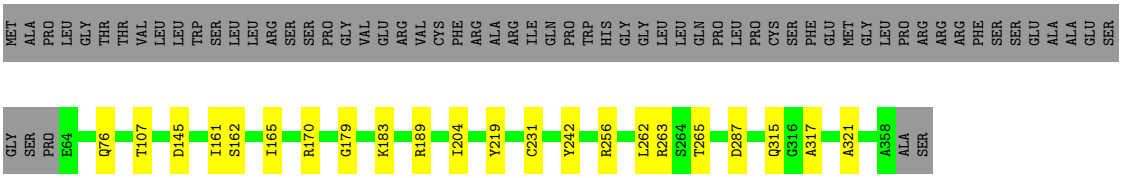
Chain P:

• Molecule 17: 28S ribosomal protein S21, mitochondrial

Chain Q:

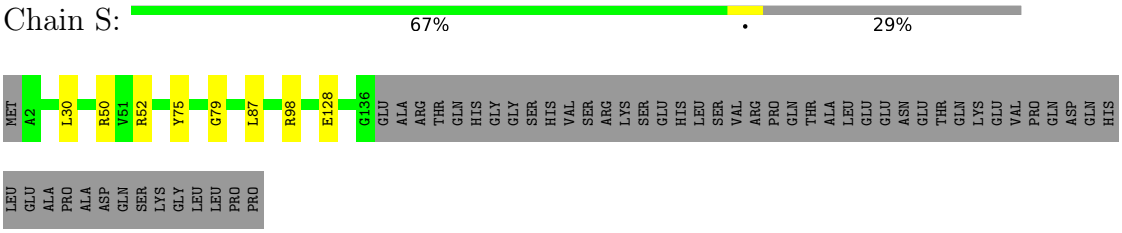
• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:



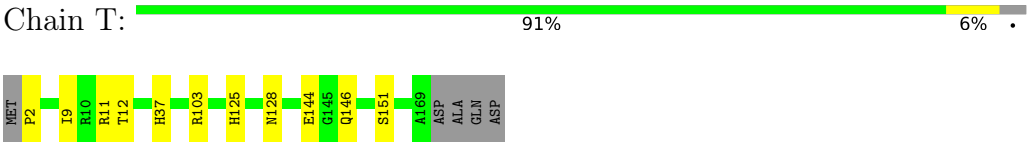
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



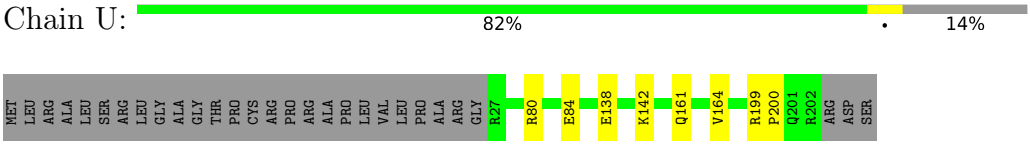
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



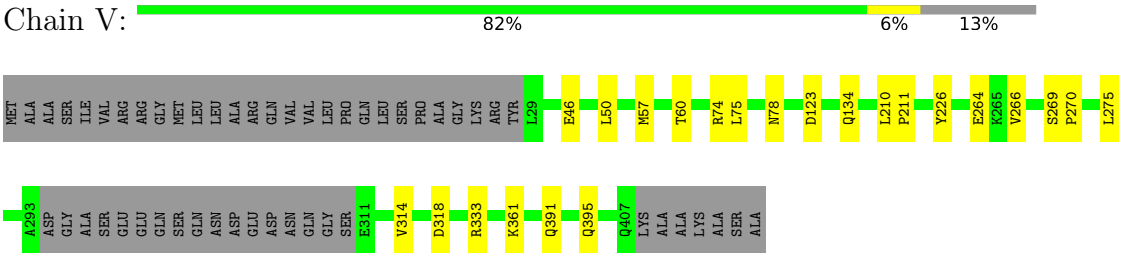
• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:



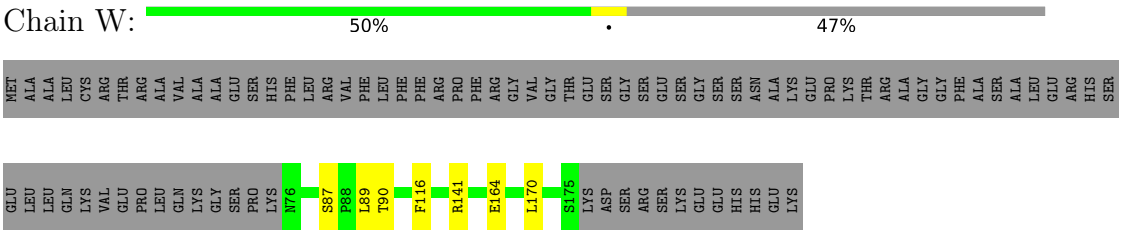
• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:



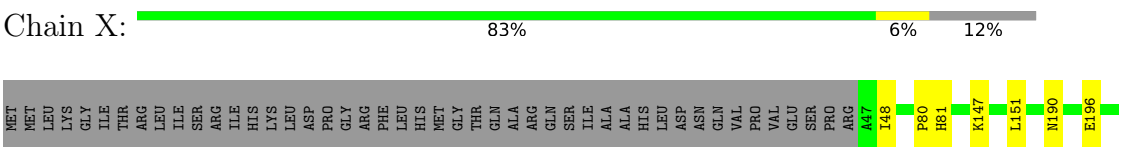
• Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain W:



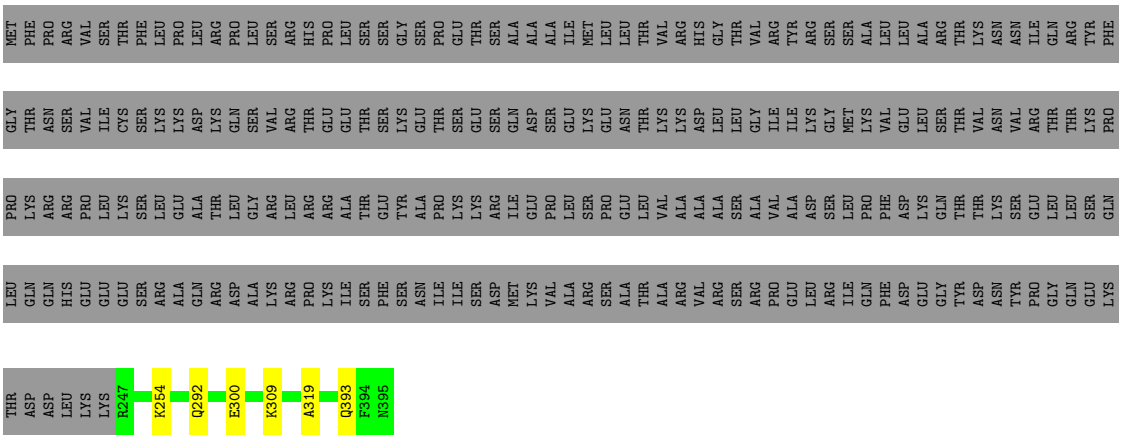
• Molecule 24: 28S ribosomal protein S29, mitochondrial

Chain X:



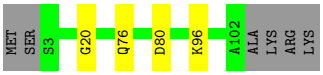
• Molecule 25: 28S ribosomal protein S31, mitochondrial

Chain Y:



• Molecule 26: 28S ribosomal protein S33, mitochondrial

Chain Z:

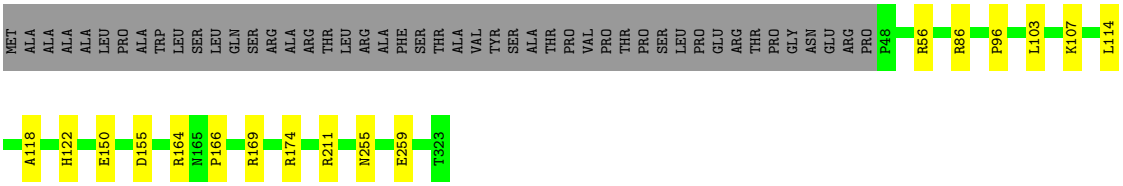


• Molecule 27: 28S ribosomal protein S34, mitochondrial

Chain 0:

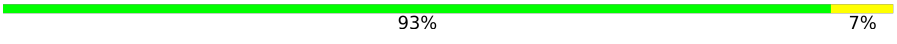
• Molecule 28: 28S ribosomal protein S35, mitochondrial

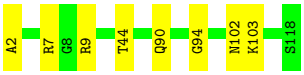
Chain 1:



• Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

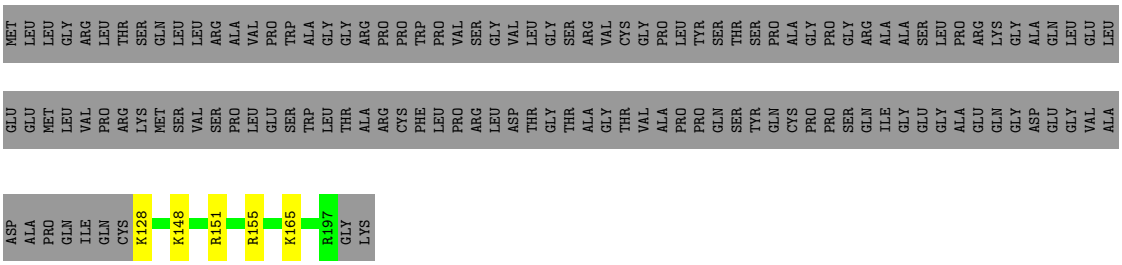
Chain 2:





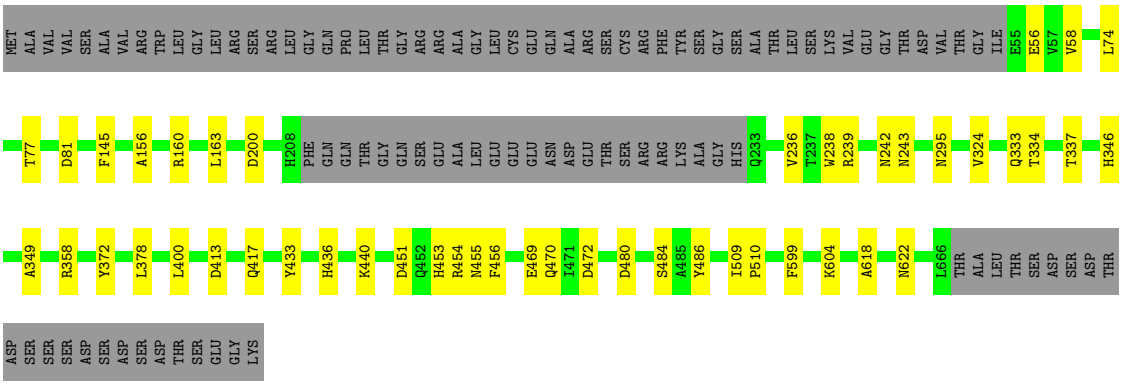
• Molecule 30: Aurora kinase A-interacting protein

Chain 3:



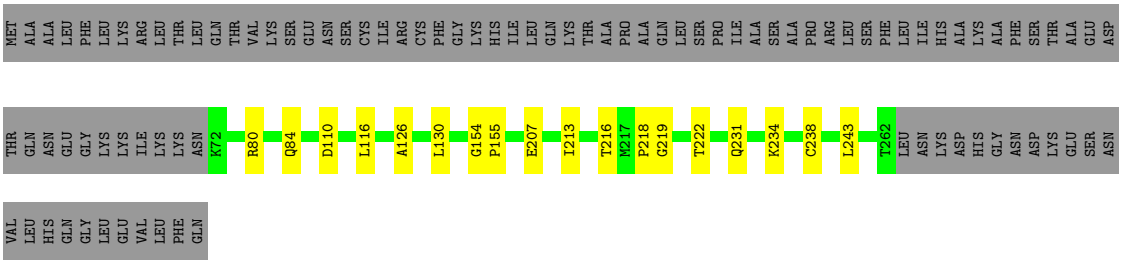
• Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:



• Molecule 32: Translation initiation factor IF-3, mitochondrial

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	250	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SRY, MA6, NAD, MG, SPM, 5MU, B8T, 5MC, ZN, FES, GNP, ATP, K, AYA

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	0.65	0/22562	0.78	0/35124
2	B	0.39	0/1871	0.45	0/2531
3	C	0.47	0/1113	0.48	0/1505
4	D	0.37	0/2783	0.47	0/3724
5	E	0.36	0/989	0.47	0/1335
6	F	0.33	0/1767	0.42	0/2373
7	G	0.36	0/2775	0.44	0/3720
8	H	0.43	0/1178	0.49	0/1598
9	I	0.41	0/1039	0.47	0/1400
10	J	0.39	0/855	0.49	0/1148
11	K	0.42	0/880	0.47	0/1182
12	L	0.37	0/1477	0.41	0/1974
13	M	0.41	0/963	0.49	0/1295
14	N	0.41	0/886	0.47	0/1199
15	O	0.41	0/1655	0.44	0/2254
16	P	0.41	0/798	0.42	0/1070
17	Q	0.43	0/748	0.47	0/994
18	R	0.36	0/2456	0.42	0/3317
19	S	0.36	0/1138	0.45	0/1533
20	T	0.41	0/1402	0.45	0/1883
21	U	0.34	0/1510	0.42	0/2025
22	V	0.33	0/3030	0.40	0/4093
23	W	0.35	0/801	0.48	0/1079
24	X	0.33	0/2921	0.42	0/3954
25	Y	0.35	0/1280	0.40	0/1725
26	Z	0.38	0/857	0.42	0/1141
27	0	0.38	0/1834	0.46	0/2484
28	1	0.37	0/2285	0.42	0/3090
29	2	0.30	0/941	0.44	0/1257
30	3	0.36	0/636	0.47	0/839
31	4	0.34	0/4877	0.41	0/6598
32	8	0.28	0/1560	0.47	0/2089

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.47	0/71867	0.58	0/101533

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
9	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	183	HIS	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	20282	10313	10297	75	0
2	B	1828	1816	1815	8	0
3	C	1083	1089	1088	14	0
4	D	2731	2805	2804	14	0
5	E	972	1000	1000	3	0
6	F	1725	1770	1769	8	0
7	G	2716	2718	2714	25	0
8	H	1152	1184	1183	6	0
9	I	1019	1060	1059	9	0
10	J	839	888	887	5	0
11	K	862	886	885	8	0
12	L	1453	1541	1540	7	0
13	M	942	966	965	3	0
14	N	868	929	928	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1599	1566	1565	12	0
16	P	781	807	806	4	0
17	Q	744	758	758	6	0
18	R	2409	2429	2428	14	0
19	S	1111	1116	1115	7	0
20	T	1371	1393	1393	10	0
21	U	1488	1500	1499	5	0
22	V	2969	2964	2961	14	0
23	W	789	803	802	5	0
24	X	2849	2845	2843	17	0
25	Y	1246	1198	1197	6	0
26	Z	839	860	858	3	0
27	0	1787	1797	1796	15	0
28	1	2238	2269	2269	11	0
29	2	935	969	969	5	0
30	3	625	700	699	4	0
31	4	4768	4768	4766	28	0
32	8	1543	1588	1587	10	0
33	A	44	26	26	0	0
34	A	14	26	26	1	0
35	A	40	39	39	0	0
36	3	1	0	0	0	0
36	A	57	0	0	0	0
36	B	1	0	0	0	0
36	X	1	0	0	0	0
37	A	17	0	0	0	0
38	O	1	0	0	0	0
39	P	4	0	0	0	0
39	T	4	0	0	0	0
40	X	31	12	12	0	0
41	X	32	13	13	0	0
42	0	1	0	0	0	0
42	2	1	0	0	0	0
42	A	49	0	0	3	0
42	C	2	0	0	0	0
42	G	1	0	0	2	0
42	I	1	0	0	0	0
42	T	1	0	0	1	0
42	X	3	0	0	0	0
All	All	68869	59411	59361	294	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 2.

The worst 5 of 294 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)
4:D:285:TYR:OH	4:D:372:GLU:OE2	1.92	0.86
1:A:1037:A:O2'	12:L:152:HIS:NE2	2.08	0.86
1:A:1021:U:OP2	29:2:9:ARG:NH2	2.09	0.86
3:C:37:ASN:O	3:C:43:ARG:NH2	2.14	0.81
31:4:470:GLN:NE2	31:4:472:ASP:OD2	2.16	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/296 (75%)	212 (95%)	11 (5%)	0	100	100
3	C	130/167 (78%)	126 (97%)	4 (3%)	0	100	100
4	D	341/430 (79%)	326 (96%)	15 (4%)	0	100	100
5	E	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
6	F	206/242 (85%)	202 (98%)	4 (2%)	0	100	100
7	G	326/396 (82%)	316 (97%)	10 (3%)	0	100	100
8	H	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	22	58
9	I	135/194 (70%)	128 (95%)	6 (4%)	1 (1%)	22	58
10	J	106/138 (77%)	100 (94%)	6 (6%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	172/257 (67%)	168 (98%)	4 (2%)	0	100	100
13	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
14	N	108/130 (83%)	102 (94%)	6 (6%)	0	100	100
15	O	192/258 (74%)	184 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	95/142 (67%)	93 (98%)	2 (2%)	0	100	100
17	Q	84/86 (98%)	84 (100%)	0	0	100	100
18	R	293/360 (81%)	287 (98%)	6 (2%)	0	100	100
19	S	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
22	V	358/414 (86%)	351 (98%)	7 (2%)	0	100	100
23	W	98/187 (52%)	93 (95%)	5 (5%)	0	100	100
24	X	350/398 (88%)	344 (98%)	6 (2%)	0	100	100
25	Y	147/395 (37%)	145 (99%)	2 (1%)	0	100	100
26	Z	98/106 (92%)	94 (96%)	4 (4%)	0	100	100
27	0	213/218 (98%)	206 (97%)	7 (3%)	0	100	100
28	1	274/323 (85%)	260 (95%)	14 (5%)	0	100	100
29	2	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
30	3	68/199 (34%)	65 (96%)	3 (4%)	0	100	100
31	4	584/689 (85%)	561 (96%)	23 (4%)	0	100	100
32	8	189/285 (66%)	183 (97%)	5 (3%)	1 (0%)	29	66
All	All	5852/7586 (77%)	5675 (97%)	174 (3%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	184	ASN
8	H	126	ILE
32	8	218	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	198/249 (80%)	197 (100%)	1 (0%)	88 95
3	C	115/143 (80%)	115 (100%)	0	100 100
4	D	286/357 (80%)	284 (99%)	2 (1%)	84 93
5	E	104/107 (97%)	103 (99%)	1 (1%)	76 91
6	F	185/209 (88%)	185 (100%)	0	100 100
7	G	288/342 (84%)	288 (100%)	0	100 100
8	H	130/180 (72%)	130 (100%)	0	100 100
9	I	105/147 (71%)	105 (100%)	0	100 100
10	J	93/118 (79%)	93 (100%)	0	100 100
11	K	91/113 (80%)	91 (100%)	0	100 100
12	L	158/226 (70%)	158 (100%)	0	100 100
13	M	97/113 (86%)	97 (100%)	0	100 100
14	N	96/115 (84%)	96 (100%)	0	100 100
15	O	175/230 (76%)	175 (100%)	0	100 100
16	P	88/123 (72%)	88 (100%)	0	100 100
17	Q	78/78 (100%)	78 (100%)	0	100 100
18	R	264/318 (83%)	264 (100%)	0	100 100
19	S	116/164 (71%)	116 (100%)	0	100 100
20	T	153/157 (98%)	153 (100%)	0	100 100
21	U	152/174 (87%)	152 (100%)	0	100 100
22	V	325/364 (89%)	324 (100%)	1 (0%)	92 97
23	W	87/158 (55%)	87 (100%)	0	100 100
24	X	311/351 (89%)	310 (100%)	1 (0%)	92 97
25	Y	137/357 (38%)	137 (100%)	0	100 100
26	Z	90/95 (95%)	90 (100%)	0	100 100
27	0	188/190 (99%)	188 (100%)	0	100 100
28	1	254/291 (87%)	254 (100%)	0	100 100
29	2	100/100 (100%)	100 (100%)	0	100 100
30	3	65/166 (39%)	65 (100%)	0	100 100
31	4	526/609 (86%)	525 (100%)	1 (0%)	93 98
32	8	172/253 (68%)	171 (99%)	1 (1%)	86 94
All	All	5227/6597 (79%)	5219 (100%)	8 (0%)	93 98

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	8	238	CYS
31	4	486	TYR
22	V	226	TYR
5	E	92	ASN
24	X	81	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
31	4	285	ASN
31	4	577	ASN
32	8	198	ASN
31	4	504	ASN
24	X	159	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	951/955 (99%)	281 (29%)	8 (0%)

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	649	A
1	A	657	G
1	A	680	U
1	A	688	A
1	A	689	U

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1532	C
1	A	1531	C
1	A	1488	5MC
1	A	1342	C
1	A	1512	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	B8T	A	1486	1	19,22,23	0.86	2 (10%)	26,31,34	1.01	1 (3%)
1	MA6	A	1584	1	18,26,27	1.15	2 (11%)	19,38,41	1.36	2 (10%)
1	5MU	A	1076	1	19,22,23	1.18	3 (15%)	28,32,35	2.12	9 (32%)
17	AYA	Q	2	17	6,7,8	1.42	1 (16%)	5,8,10	1.26	1 (20%)
29	AYA	2	2	29	6,7,8	1.28	1 (16%)	5,8,10	1.46	1 (20%)
1	MA6	A	1583	1	18,26,27	1.18	2 (11%)	19,38,41	1.45	3 (15%)
1	5MC	A	1488	1	18,22,23	1.24	2 (11%)	26,32,35	1.88	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B8T	A	1486	1	-	0/7/27/28	0/2/2/2
1	MA6	A	1584	1	-	1/7/29/30	0/3/3/3
1	5MU	A	1076	1	-	0/7/25/26	0/2/2/2
17	AYA	Q	2	17	-	1/4/6/8	-
29	AYA	2	2	29	-	0/4/6/8	-
1	MA6	A	1583	1	-	0/7/29/30	0/3/3/3
1	5MC	A	1488	1	-	0/7/25/26	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1584	MA6	C8-N7	-3.10	1.29	1.34
17	Q	2	AYA	CA-N	-3.09	1.43	1.46
1	A	1583	MA6	C4-N3	-2.90	1.31	1.35
1	A	1583	MA6	C8-N7	-2.84	1.29	1.34
1	A	1076	5MU	C2-N1	-2.72	1.34	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1076	5MU	C4-N3-C2	-5.32	120.46	127.35
1	A	1584	MA6	N3-C2-N1	-4.68	121.36	128.68
1	A	1583	MA6	N3-C2-N1	-4.64	121.42	128.68
1	A	1076	5MU	N3-C2-N1	4.53	120.91	114.89
1	A	1488	5MC	O3'-C3'-C4'	4.22	123.26	111.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	Q	2	AYA	C-CA-N-CT
1	A	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1584	MA6	4	0
1	A	1583	MA6	3	0
1	A	1488	5MC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 85 ligands modelled in this entry, 78 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
39	FES	T	201	20,13	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	ATP	X	501	36	26,33,33	0.91	1 (3%)	31,52,52	1.30	5 (16%)
34	SPM	A	1702	-	13,13,13	0.14	0	12,12,12	1.16	0
33	NAD	A	1701	36	42,48,48	1.09	5 (11%)	50,73,73	1.25	6 (12%)
41	GNP	X	503	-	29,34,34	1.59	7 (24%)	33,54,54	2.24	6 (18%)
35	SRY	A	1703	-	40,42,42	0.76	2 (5%)	49,63,63	1.33	5 (10%)
39	FES	P	201	5,16	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	ATP	X	501	36	-	0/18/38/38	0/3/3/3
39	FES	T	201	20,13	-	-	0/1/1/1
34	SPM	A	1702	-	-	0/11/11/11	-
33	NAD	A	1701	36	-	0/26/62/62	0/5/5/5
41	GNP	X	503	-	-	4/14/38/38	0/3/3/3
35	SRY	A	1703	-	-	1/20/87/87	0/3/3/3
39	FES	P	201	5,16	-	-	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	503	GNP	PB-O3A	4.33	1.64	1.59
41	X	503	GNP	PB-O1B	3.06	1.51	1.46
41	X	503	GNP	C6-N1	3.00	1.38	1.33
35	A	1703	SRY	CD1-N31	2.99	1.38	1.33
41	X	503	GNP	PG-N3B	2.91	1.71	1.63

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	X	503	GNP	C5-C6-N1	-8.45	111.87	123.43
41	X	503	GNP	C2-N1-C6	5.84	125.20	115.93
35	A	1703	SRY	C12-O42-C42	-4.57	101.19	108.38
33	A	1701	NAD	N3A-C2A-N1A	-4.13	122.23	128.68
35	A	1703	SRY	O42-C12-C22	-3.57	103.44	107.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	X	503	GNP	PG-N3B-PB-O3A
41	X	503	GNP	PA-O3A-PB-O1B
41	X	503	GNP	PA-O3A-PB-O2B
41	X	503	GNP	PG-N3B-PB-O1B
35	A	1703	SRY	C13-C23-N23-CI3

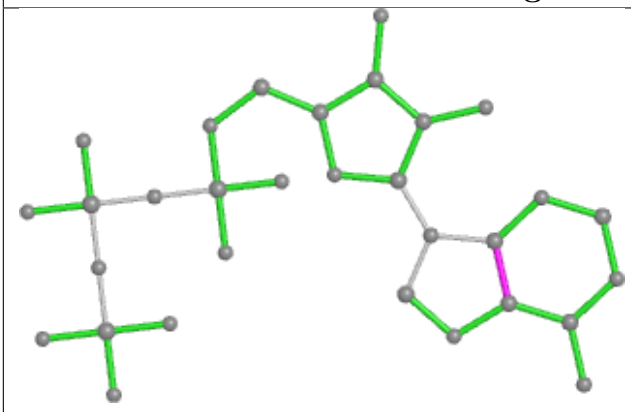
There are no ring outliers.

1 monomer is involved in 1 short contact:

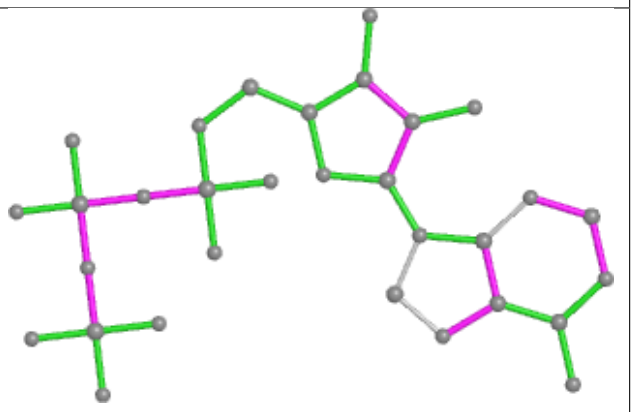
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	1702	SPM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

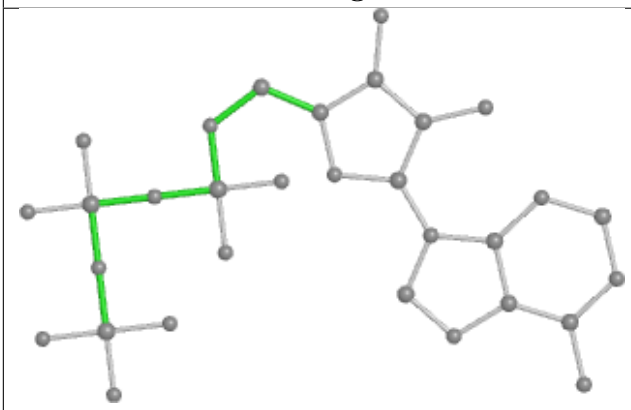
Ligand ATP X 501



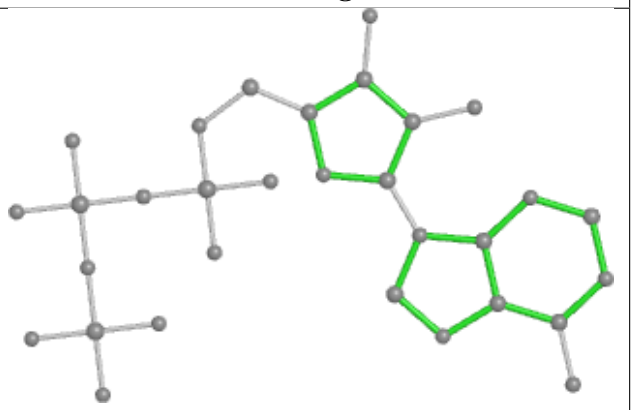
Bond lengths



Bond angles

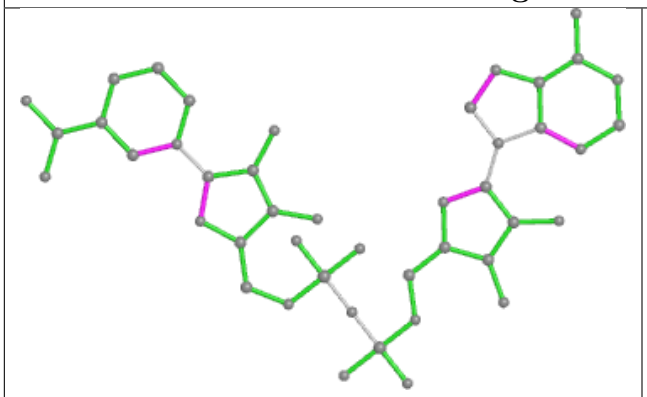


Torsions

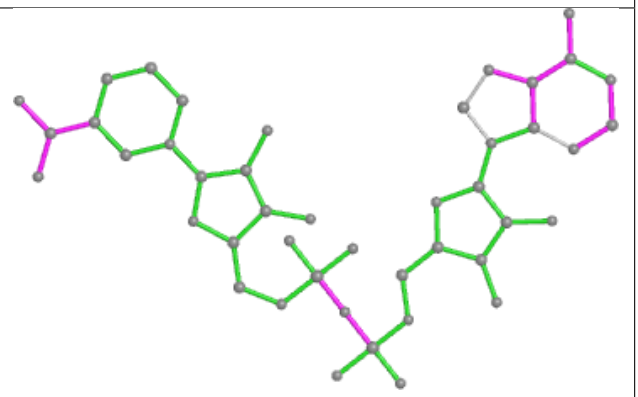


Rings

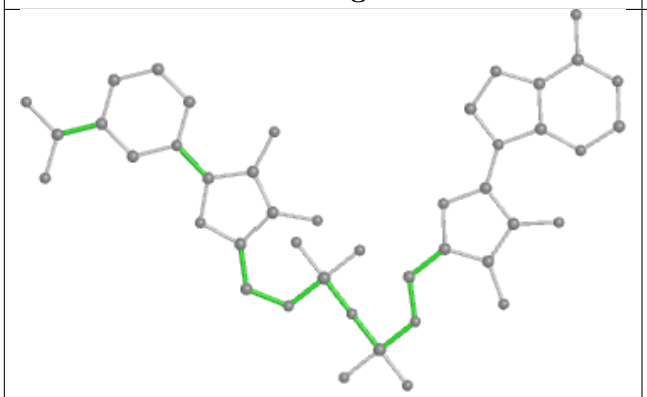
Ligand NAD A 1701



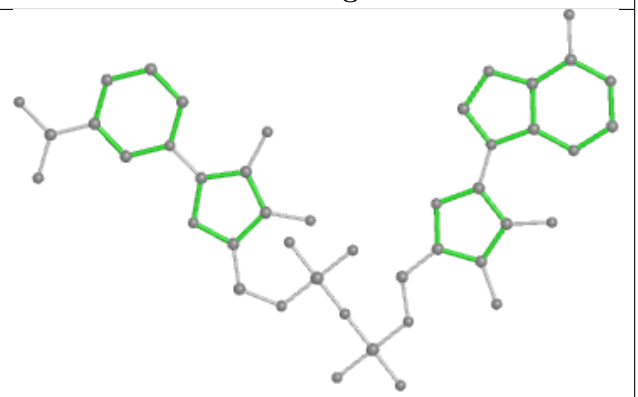
Bond lengths



Bond angles

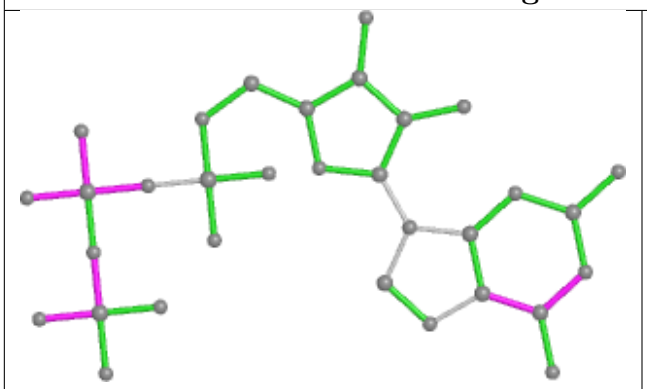


Torsions

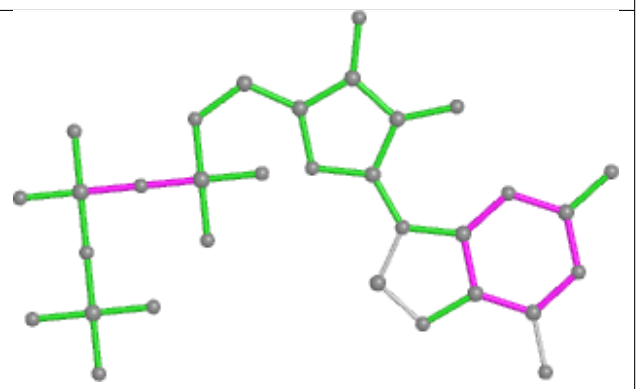


Rings

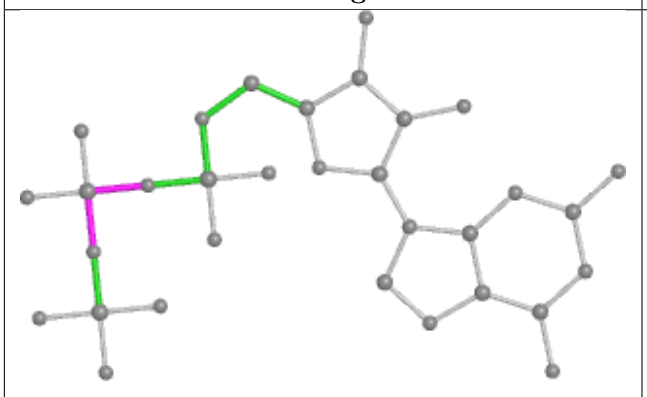
Ligand GNP X 503



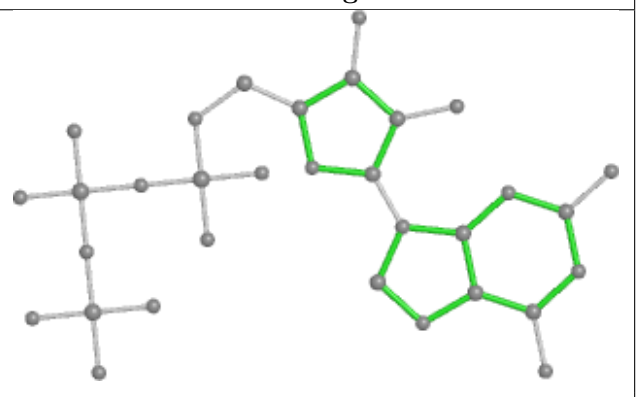
Bond lengths



Bond angles

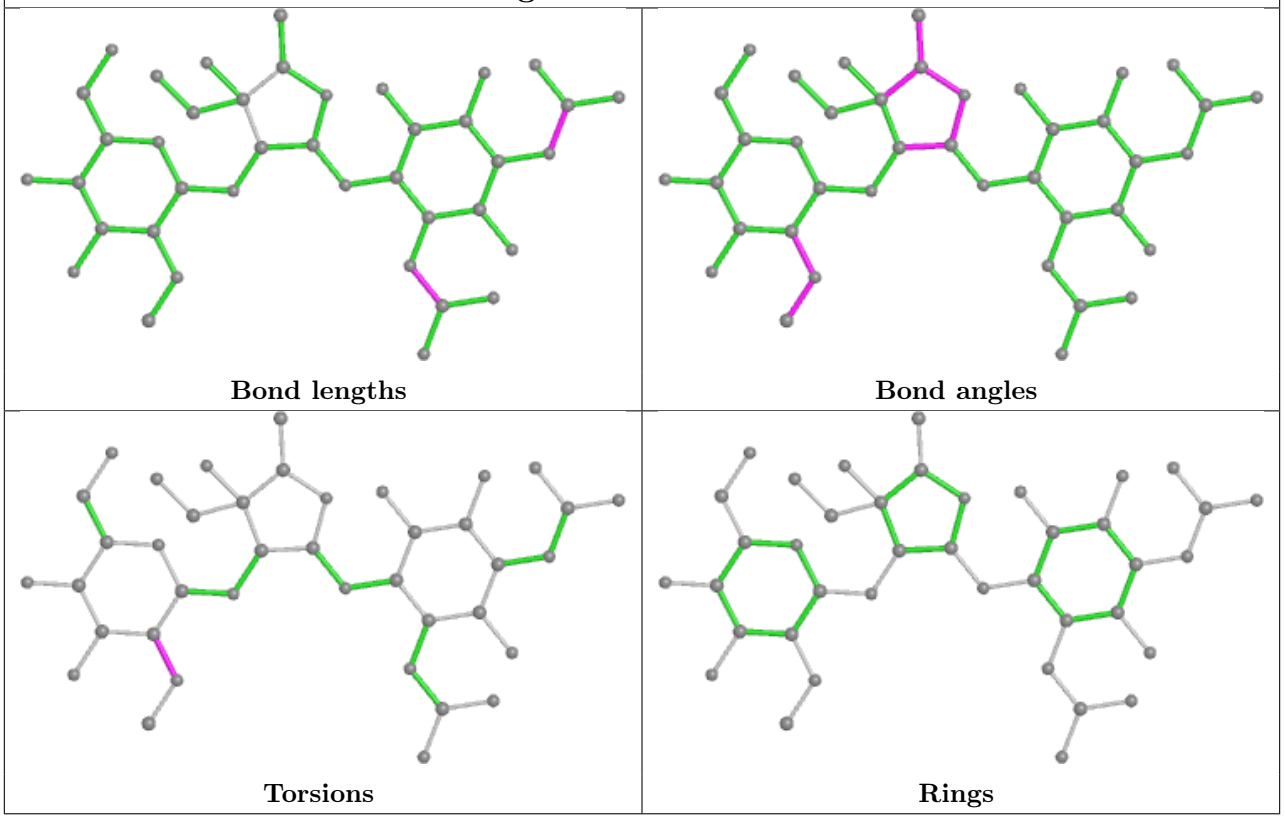


Torsions



Rings

Ligand SRY A 1703



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-10021. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.