Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 04:18 am BST

PDB ID	:	7QI4 / pdb_00007qi4
EMDB ID	:	EMD-13980
Title	:	Human mitochondrial ribosome at 2.2 A resolution (bound to partly built tRNAs and mRNA)
Authors	:	Singh, V.; Itoh, Y.; Amunts, A.
Deposited on	:	2021-12-14
Resolution	:	2.21 Å(reported)

This is a Full wwPDB EM Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

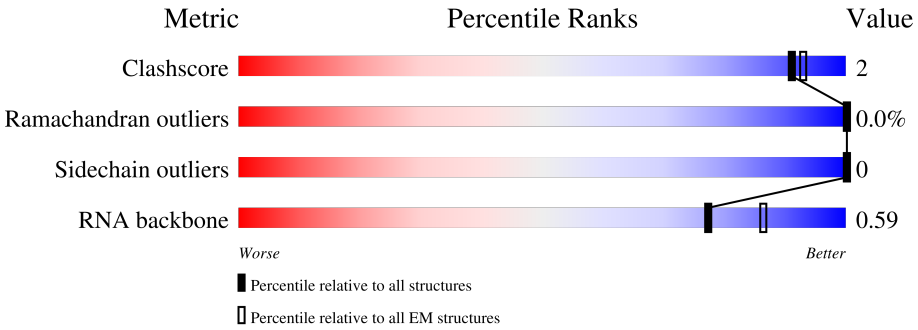
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

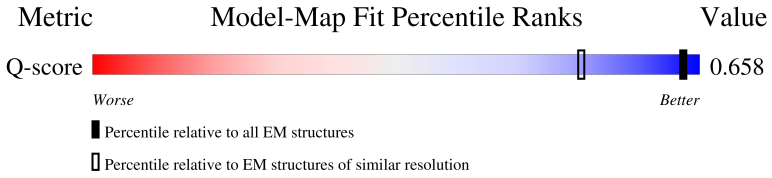
1 Overall quality at a glance

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

The reported resolution of this entry is 2.21 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3231 (1.71 - 2.71)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	954	80% 19%
2	AB	296	74% 24%
3	AC	167	74% 5% 21%

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Mol	Chain	Length	Quality of chain
4	AD	430	77% 20%
5	AE	125	94%
6	AF	242	81% 5% 14%
7	AG	396	5% 79% 17%
8	AH	201	65% 30%
9	AI	194	69% 29%
10	AJ	138	75% 22%
11	AK	128	76% 21%
12	AL	257	5% 66% 32%
13	AM	137	83% 13%
14	AN	130	80% 5% 15%
15	AO	258	72% 25%
16	AP	142	66% 32%
17	AQ	87	99%
18	AR	360	80% 18%
19	AS	190	7% 71% 29%
20	AT	173	95%
21	AU	205	85% 14%
22	AV	414	81% 7% 13%
23	AW	187	52% 47%
24	AX	398	84% 12%
25	AY	395	36% 62%
26	AZ	106	6% 92% 6%
27	A0	217	94% 5%
28	A1	323	83% 14%

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Mol	Chain	Length	Quality of chain
29	A2	118	10% 90% 9%
30	A3	199	32% 65%
31	A4	689	5% 83% 15%
32	Aw	22	59% 86% 9% 5%
33	Ax	70	70% 81% 19%
34	Az	34	56% 56% 41%
35	A	1558	5% 78% 20%
36	B	72	81% 18%
37	D	305	76% 22%
38	E	348	83% 12%
39	F	311	79% 19%
40	H	267	44% 69% 6% 24%
41	I	261	18% 79% 19%
42	J	192	5% 85% 6% 9%
43	K	178	96%
44	L	145	77% 21%
45	M	296	96%
46	N	251	84% 5% 12%
47	O	175	81% 7% 12%
48	P	180	79% 20%
49	Q	292	6% 79% 18%
50	R	149	93% 6%
51	S	205	76% 21%
52	T	206	76% 5% 19%
53	U	153	18% 95% 5%

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Mol	Chain	Length	Quality of chain
54	V	216	12% 86% 9% 5%
55	W	148	76% 22%
56	X	256	5% 94% 5%
57	Y	250	72% 28%
58	Z	161	72% 24%
59	0	188	57% 41%
60	1	65	6% 85% 14%
61	2	92	50% 50%
62	3	188	49% 49%
63	4	103	35% 63%
64	5	423	91% 7%
65	6	380	89% 7%
66	7	338	8% 83% 13%
67	8	206	13% 71% 27%
68	9	137	9% 88% 9%
69	a	142	9% 69% 30%
70	b	215	67% 30%
71	c	332	5% 83% 14%
72	d	306	16% 76% 21%
73	e	279	7% 82% 15%
74	f	212	8% 72% 26%
75	g	166	77% 19%
76	h	158	8% 67% 30%
77	i	128	75% 24%
78	j	123	8% 74% 24%

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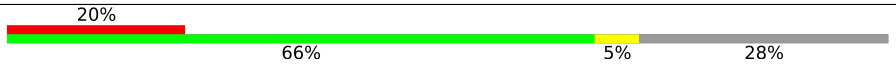
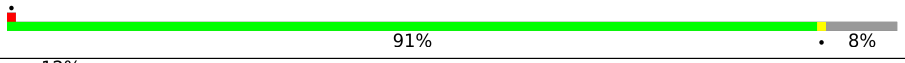
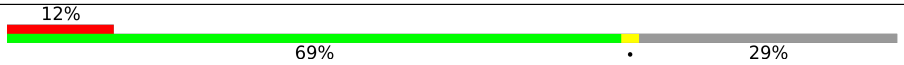
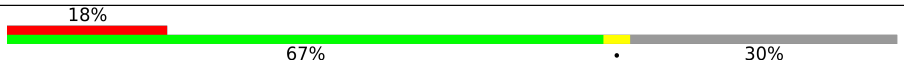
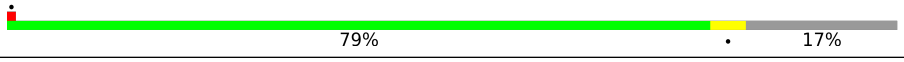
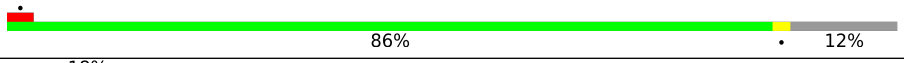
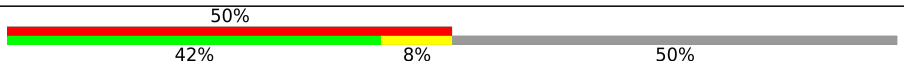
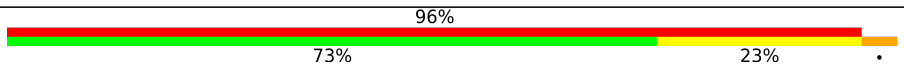
Mol	Chain	Length	Quality of chain
79	k	112	
80	l	138	
81	m	128	
82	o	102	
83	p	206	
84	q	222	
85	r	196	
86	s	439	
87	t	198	
87	u	198	
87	v	198	
87	w	198	
87	x	198	
87	y	198	
88	z	325	
89	Ay	52	

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 340116 atoms, of which 152427 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	AA	954	30564	9088	10304	3647	6571	954	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	AB	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	AC	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	AD	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	AE	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	AF	208	3496	1104	1771	312	298	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AG	327	Total	C	H	N	O	S	0	0
			5377	1710	2689	477	487	14		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AH	140	Total	C	H	N	O	S	0	0
			2339	745	1187	194	210	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AI	137	Total	C	H	N	O	S	0	0
			2081	642	1061	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	184	5F0	ASN	conflict	UNP P82912

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AJ	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	AK	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	AL	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	AM	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	AN	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	AO	193	Total	C	H	N	O	S	0	0
			3149	1014	1557	294	277	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AP	97	Total	C	H	N	O	S	0	0
			1587	501	806	134	138	8		

- Molecule 17 is a protein called MRPS21 isoform 1.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AR	295	Total	C	H	N	O	S	0	0
			4839	1533	2430	413	455	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AS	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	AT	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	AU	176	Total	C	H	N	O	S	0	0
			2989	916	1501	301	267	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AV	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	AW	100	Total	C	H	N	O	S	0	0
			1593	498	804	141	146	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	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	AY	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	AZ	100	Total	C	H	N	O	S	0	0
			1698	534	859	153	148	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A0	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	A1	279	Total	C	H	N	O	S	0	0
			4561	1435	2296	387	432	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
29	A2	117	Total	C	H	N	O	S	0	0
			1906	579	971	182	166	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	A3	70	Total	C	H	N	O	S	0	0
			1326	401	701	134	89	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
31	A4	588	Total	C	H	N	O	S	0	0
			9538	3053	4770	808	879	28		

- Molecule 32 is a RNA chain called A/A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Aw	22	Total	C	H	N	O	P	0	0
			701	209	237	82	151	22		

- Molecule 33 is a RNA chain called P/P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Ax	70	Total	C	H	N	O	P	0	0
			2233	665	751	260	487	70		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Az	34	Total	C	H	N	O	P	0	0
			1079	324	360	123	238	34		

- Molecule 35 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	A	1558	Total	C	H	N	O	P	0	0
			49871	14843	16801	5963	10706	1558		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 1563835895
A	?	-	C	deletion	GB 1563835895
A	?	-	U	deletion	GB 1563835895

- Molecule 36 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	B	72	Total	C	H	N	O	P	0	0
			2303	685	779	269	498	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	C	G	conflict	GB NC_012920.1
B	76	A	U	conflict	GB NC_012920.1

- Molecule 37 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	D	238	Total	C	H	N	O	S	0	0
			3780	1157	1921	376	317	9		

- Molecule 38 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	E	305	Total	C	H	N	O	S	0	0
			4822	1545	2416	418	432	11		

- Molecule 39 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	F	252	Total	C	H	N	O	S	0	0
			4097	1305	2066	370	350	6		

- Molecule 40 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	H	202	Total	C	H	N	O	S	0	0
			3397	1067	1736	304	286	4		

- Molecule 41 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	I	212	Total	C	H	N	O	S	0	0
			3481	1088	1786	304	292	11		

- Molecule 42 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	J	175	Total	C	H	N	O	S	0	0
			2738	847	1408	237	244	2		

- Molecule 43 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	K	177	Total	C	H	N	O	S	0	0
			2907	936	1452	259	253	7		

- Molecule 44 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	L	115	Total	C	H	N	O	S	0	0
			1832	559	942	171	155	5		

- Molecule 45 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	M	291	Total	C	H	N	O	S	0	0
			4723	1483	2396	430	408	6		

- Molecule 46 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	N	222	Total	C	H	N	O	S	0	0
			3604	1143	1818	326	307	10		

- Molecule 47 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	O	154	Total	C	H	N	O	S	0	0
			2554	792	1295	241	219	7		

- Molecule 48 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	P	144	Total	C	H	N	O	S	0	0
			2339	733	1166	224	211	5		

- Molecule 49 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	Q	239	Total	C	H	N	O	S	0	0
			4021	1277	2031	353	351	9		

- Molecule 50 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	R	140	Total	C	H	N	O	S	0	0
			2369	732	1215	231	187	4		

- Molecule 51 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	S	161	Total	C	H	N	O	S	0	0
			2659	835	1366	227	227	4		

- Molecule 52 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	T	166	Total	C	H	N	O	S	0	0
			2781	875	1412	254	233	7		

- Molecule 53 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	U	152	Total	C	H	N	O	S	0	0
			2483	788	1232	234	226	3		

- Molecule 54 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	V	205	Total	C	H	N	O	S	0	0
			3365	1068	1689	298	302	8		

- Molecule 55 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	W	116	Total	C	H	N	O	S	0	0
			1840	577	936	171	153	3		

- Molecule 56 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	X	244	Total	C	H	N	O	S	0	0
			4105	1322	2061	352	365	5		

- Molecule 57 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	Y	181	Total	C	H	N	O	S	0	0
			3154	995	1598	298	259	4		

- Molecule 58 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Z	122	Total	C	H	N	O	S	0	0
			2041	636	1045	186	171	3		

- Molecule 59 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	0	110	Total	C	H	N	O	S	0	0
			1815	554	917	176	162	6		

- Molecule 60 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	1	56	Total	C	H	N	O	S	0	0
			977	296	513	89	77	2		

- Molecule 61 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	2	46	Total	C	H	N	O	S	0	0
			784	233	407	83	60	1		

- Molecule 62 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	3	95	Total	C	H	N	O	S	0	0
			1716	539	884	162	128	3		

- Molecule 63 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	4	38	Total	C	H	N	O	S	0	0
			704	217	362	72	49	4		

- Molecule 64 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	5	394	Total	C	H	N	O	S	0	0
			6419	2073	3209	560	566	11		

- Molecule 65 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	6	354	Total	C	H	N	O	S	0	0
			5792	1881	2844	525	533	9		

- Molecule 66 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	7	294	Total	C	H	N	O	S	0	0
			4789	1529	2399	405	438	18		

- Molecule 67 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	8	151	Total	C	H	N	O	S	0	0
			2588	812	1310	226	238	2		

- Molecule 68 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	9	124	Total	C	H	N	O	S	0	0
			1985	644	988	170	181	2		

- Molecule 69 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	a	100	Total	C	H	N	O	S	0	0
			1652	529	812	152	154	5		

- Molecule 70 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	b	150	Total	C	H	N	O	S	0	0
			2392	744	1196	231	218	3		

- Molecule 71 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	c	286	Total	C	H	N	O	S	0	0
			4621	1470	2322	397	423	9		

- Molecule 72 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	d	241	Total	C	H	N	O	S	0	0
			3965	1273	1980	340	359	13		

- Molecule 73 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	e	238	Total	C	H	N	O	S	0	0
			3848	1222	1917	339	364	6		

- Molecule 74 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	f	157	Total	C	H	N	O	S	0	0
			2523	799	1271	207	242	4		

- Molecule 75 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	g	134	Total	C	H	N	O	S	0	0
			2210	719	1097	193	199	2		

- Molecule 76 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	h	110	Total	C	H	N	O	S	0	0
			1778	568	883	156	168	3		

- Molecule 77 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	i	97	Total	C	H	N	O	S	0	0
			1687	532	859	165	127	4		

- Molecule 78 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	j	94	Total	C	H	N	O	S	0	0
			1492	463	747	144	136	2		

- Molecule 79 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	k	101	Total	C	H	N	O	S	0	0
			1559	479	785	148	142	5		

- Molecule 80 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	l	82	Total	C	H	N	O	S	0	0
			1363	437	675	120	128	3		

- Molecule 81 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	m	92	Total	C	H	N	O	S	0	0
			1551	488	760	159	142	2		

- Molecule 82 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	o	94	Total	C	H	N	O	S	0	0
			1604	501	806	165	129	3		

- Molecule 83 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	p	147	Total	C	H	N	O	S	0	0
			2430	748	1225	228	225	4		

- Molecule 84 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	q	155	Total	C	H	N	O	S	0	0
			2571	809	1273	251	233	5		

- Molecule 85 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	r	162	Total	C	H	N	O	S	0	0
			2671	839	1349	252	223	8		

- Molecule 86 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	s	386	Total	C	H	N	O	S	0	0
			6300	2023	3145	559	559	14		

- Molecule 87 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	t	46	Total	C	H	N	O	0	0
			732	228	378	56	70		
87	u	32	Total	C	H	N	O	0	0
			541	168	284	40	49		

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Mol	Chain	Residues	Atoms					AltConf	Trace
87	v	32	Total	C	H	N	O	0	0
			541	168	284	40	49		
87	w	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
87	x	31	Total	C	H	N	O	0	0
			520	159	275	39	47		
87	y	31	Total	C	H	N	O	0	0
			520	159	275	39	47		

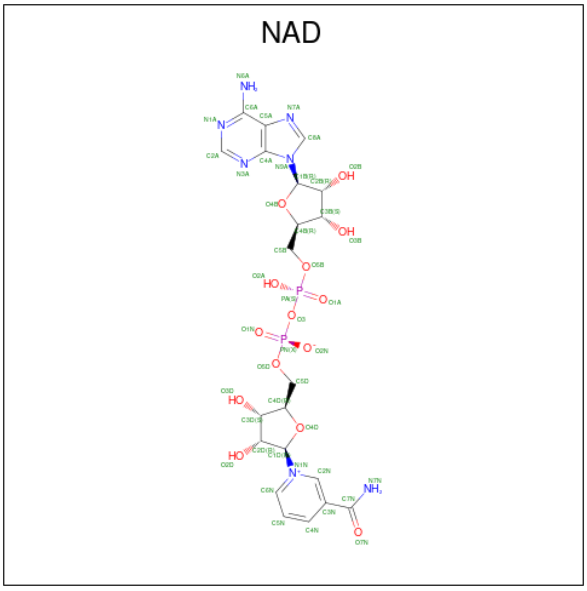
- Molecule 88 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	z	164	Total	C	H	N	O	S	0	0
			2682	856	1355	217	250	4		

- Molecule 89 is a RNA chain called E/E-tRNA.

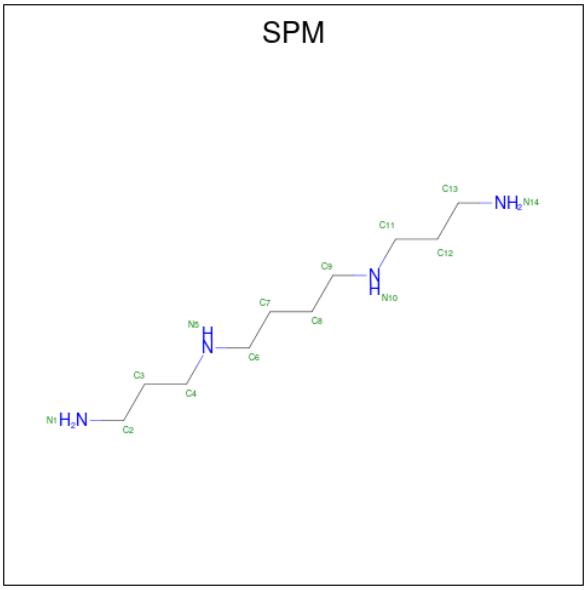
Mol	Chain	Residues	Atoms						AltConf	Trace
89	Ay	52	Total	C	H	N	O	P	0	0
			1667	496	560	199	360	52		

- Molecule 90 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



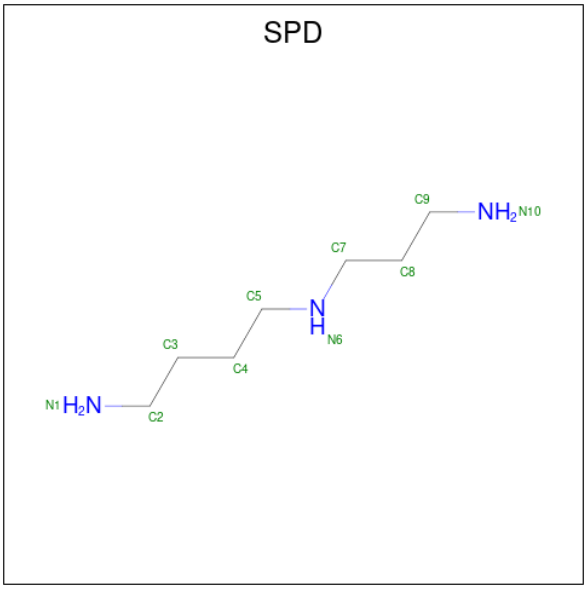
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
90	AA	1	70	21	26	7	14	2	0

- Molecule 91 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
91	AA	1	44	10	30	4	0

- Molecule 92 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
92	AA	1	Total 32	C 7	H 22	N 3	0
92	A	1	Total 32	C 7	H 22	N 3	0
92	A	1	Total 32	C 7	H 22	N 3	0
92	A	1	Total 32	C 7	H 22	N 3	0

- Molecule 93 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
93	AA	61	Total 61	Mg 61	0
93	AB	1	Total 1	Mg 1	0
93	AX	1	Total 1	Mg 1	0
93	A3	1	Total 1	Mg 1	0
93	Aw	1	Total 1	Mg 1	0
93	A	137	Total 137	Mg 137	0
93	D	2	Total 2	Mg 2	0
93	E	1	Total 1	Mg 1	0
93	g	1	Total 1	Mg 1	0

- Molecule 94 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
94	AA	18	Total 18	K 18	0
94	A	29	Total 29	K 29	0
94	D	1	Total 1	K 1	0
94	M	1	Total 1	K 1	0
94	W	1	Total 1	K 1	0

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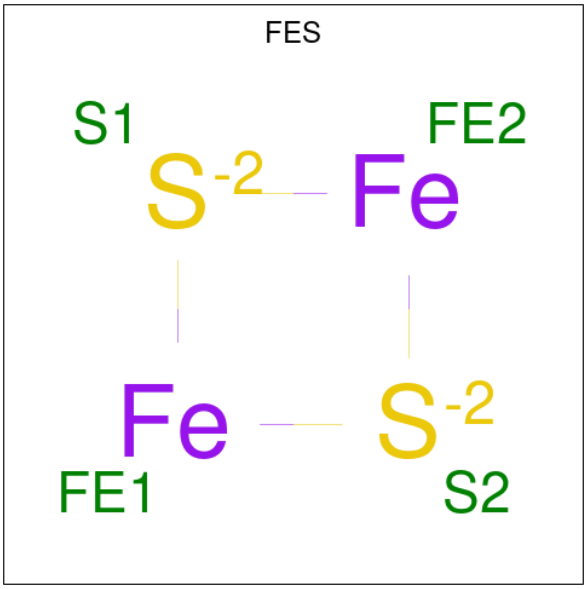
Mol	Chain	Residues	Atoms	AltConf
94	3	1	Total K 1 1	0
94	6	1	Total K 1 1	0
94	i	1	Total K 1 1	0
94	o	1	Total K 1 1	0

- Molecule 95 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
95	AO	1	Total Zn 1 1	0
95	0	1	Total Zn 1 1	0
95	4	1	Total Zn 1 1	0

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
96	AP	1	Total Fe S 4 2 2	0
96	AT	1	Total Fe S 4 2 2	0

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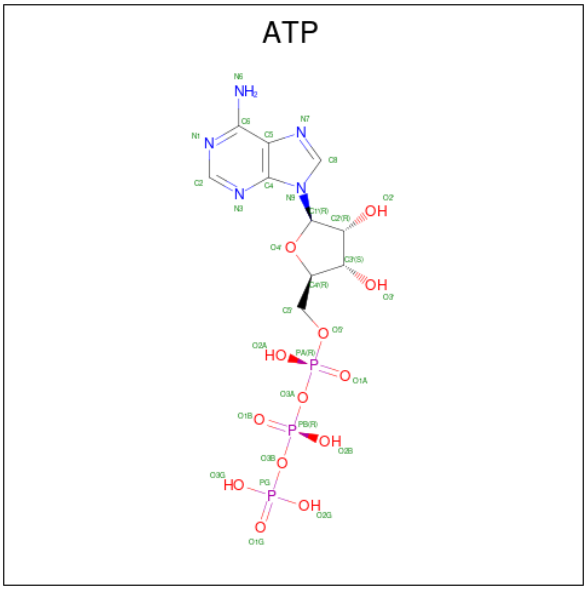
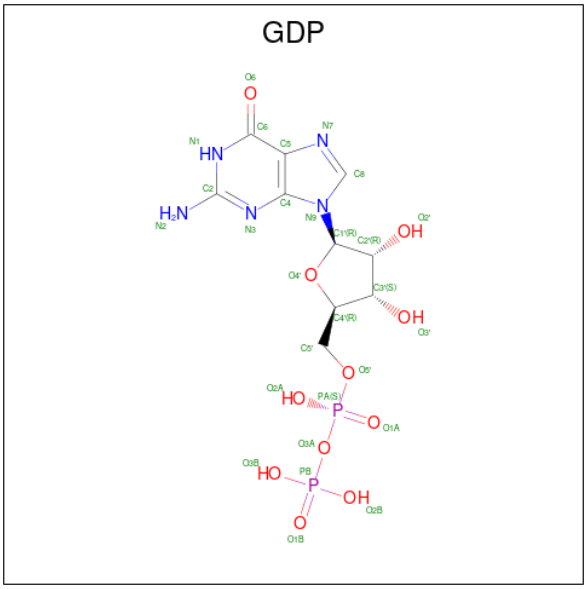
Mol	Chain	Residues	Atoms			AltConf
96	r	1	Total	Fe	S	0
			4	2	2	

- Molecule 97 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



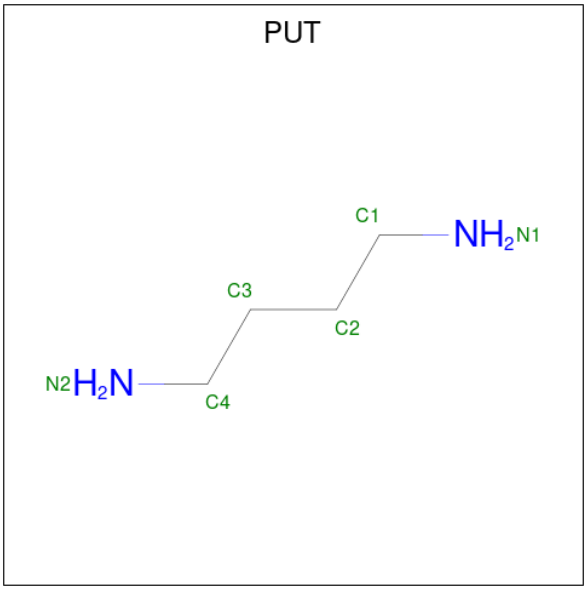
Mol	Chain	Residues	Atoms						AltConf
97	AX	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 98 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



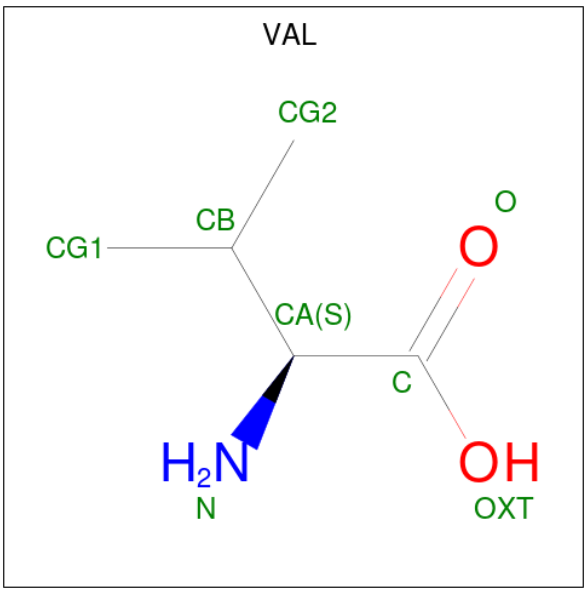
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
98	AX	1	40	10	12	5	11	2	0

- Molecule 99 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
99	A	1	20	4	14	2	0

- Molecule 100 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms					AltConf
100	B	1	Total	C	H	N	O	0
			18	5	11	1	1	

- Molecule 101 is water.

Mol	Chain	Residues	Atoms		AltConf
101	AA	2157	Total	O	0
			2157	2157	
101	AB	80	Total	O	0
			80	80	
101	AC	58	Total	O	0
			58	58	
101	AD	79	Total	O	0
			79	79	
101	AE	30	Total	O	0
			30	30	
101	AF	36	Total	O	0
			36	36	
101	AG	70	Total	O	0
			70	70	
101	AH	50	Total	O	0
			50	50	
101	AI	44	Total	O	0
			44	44	
101	AJ	29	Total	O	0
			29	29	
101	AK	51	Total	O	0
			51	51	
101	AL	43	Total	O	0
			43	43	
101	AM	21	Total	O	0
			21	21	
101	AN	34	Total	O	0
			34	34	
101	AO	37	Total	O	0
			37	37	
101	AP	31	Total	O	0
			31	31	
101	AQ	68	Total	O	0
			68	68	
101	AR	12	Total	O	0
			12	12	
101	AS	23	Total	O	0
			23	23	

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Mol	Chain	Residues	Atoms	AltConf
101	AT	43	Total O 43 43	0
101	AU	8	Total O 8 8	0
101	AW	15	Total O 15 15	0
101	AX	61	Total O 61 61	0
101	AY	20	Total O 20 20	0
101	AZ	27	Total O 27 27	0
101	A0	1	Total O 1 1	0
101	A1	36	Total O 36 36	0
101	A2	35	Total O 35 35	0
101	A3	52	Total O 52 52	0
101	A4	11	Total O 11 11	0
101	Aw	5	Total O 5 5	0
101	Ax	5	Total O 5 5	0
101	Az	15	Total O 15 15	0
101	A	3056	Total O 3056 3056	0
101	B	63	Total O 63 63	0
101	D	73	Total O 73 73	0
101	E	74	Total O 74 74	0
101	F	78	Total O 78 78	0
101	H	9	Total O 9 9	0
101	I	23	Total O 23 23	0

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Mol	Chain	Residues	Atoms	AltConf
101	J	1	Total O 1 1	0
101	K	65	Total O 65 65	0
101	L	25	Total O 25 25	0
101	M	66	Total O 66 66	0
101	N	60	Total O 60 60	0
101	O	38	Total O 38 38	0
101	P	89	Total O 89 89	0
101	Q	27	Total O 27 27	0
101	R	57	Total O 57 57	0
101	S	49	Total O 49 49	0
101	T	48	Total O 48 48	0
101	U	26	Total O 26 26	0
101	V	5	Total O 5 5	0
101	W	48	Total O 48 48	0
101	X	12	Total O 12 12	0
101	Y	29	Total O 29 29	0
101	Z	34	Total O 34 34	0
101	0	27	Total O 27 27	0
101	1	3	Total O 3 3	0
101	2	34	Total O 34 34	0
101	3	40	Total O 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
101	4	13	Total O 13 13	0
101	5	22	Total O 22 22	0
101	6	100	Total O 100 100	0
101	7	17	Total O 17 17	0
101	8	19	Total O 19 19	0
101	9	17	Total O 17 17	0
101	a	13	Total O 13 13	0
101	b	39	Total O 39 39	0
101	c	20	Total O 20 20	0
101	d	5	Total O 5 5	0
101	e	13	Total O 13 13	0
101	f	22	Total O 22 22	0
101	g	13	Total O 13 13	0
101	i	54	Total O 54 54	0
101	j	23	Total O 23 23	0
101	k	6	Total O 6 6	0
101	l	5	Total O 5 5	0
101	m	8	Total O 8 8	0
101	o	34	Total O 34 34	0
101	p	10	Total O 10 10	0
101	r	50	Total O 50 50	0

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Mol	Chain	Residues	Atoms	AltConf
101	s	51	Total O 51 51	0
101	Ay	1	Total O 1 1	0

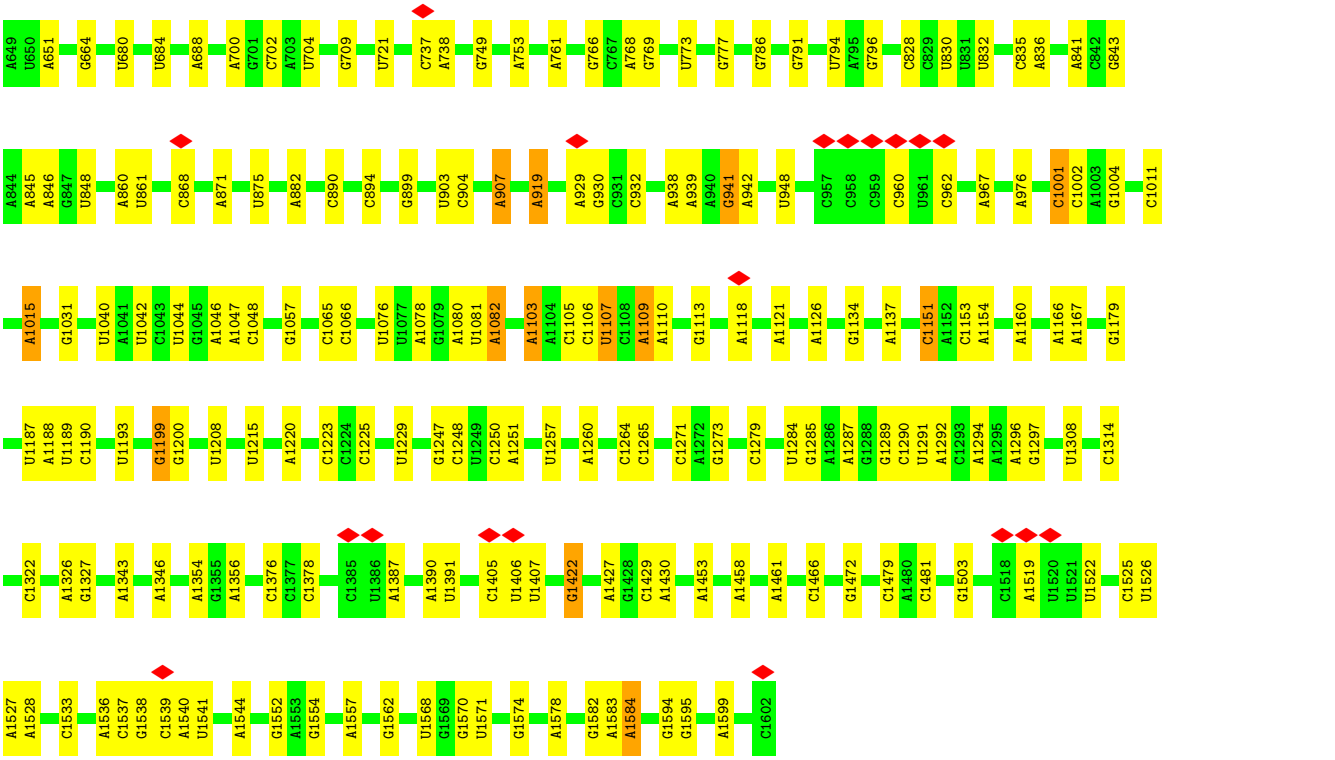
3 Residue-property plots (i)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 AA:

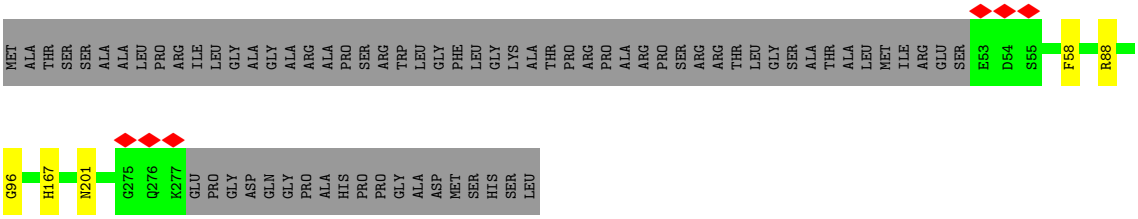




• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain AB:





• Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC:



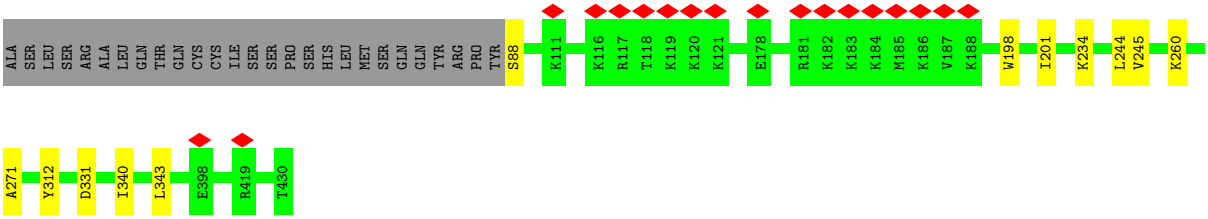


• Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain AD:

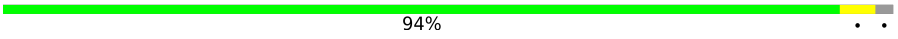


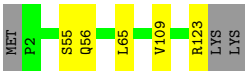




• Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain AE:

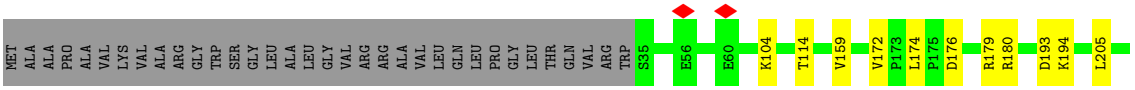




• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain AF:



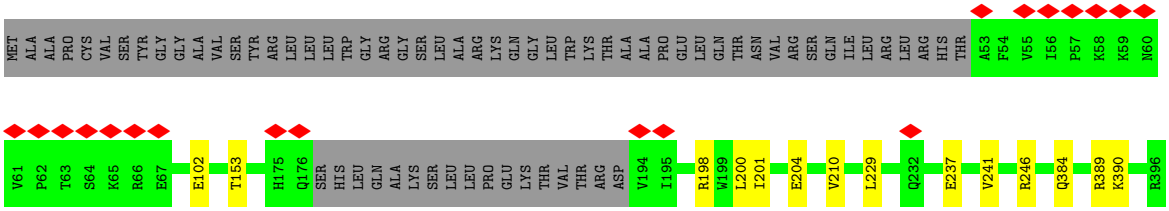




• Molecule 7: 28S ribosomal protein S9, mitochondrial

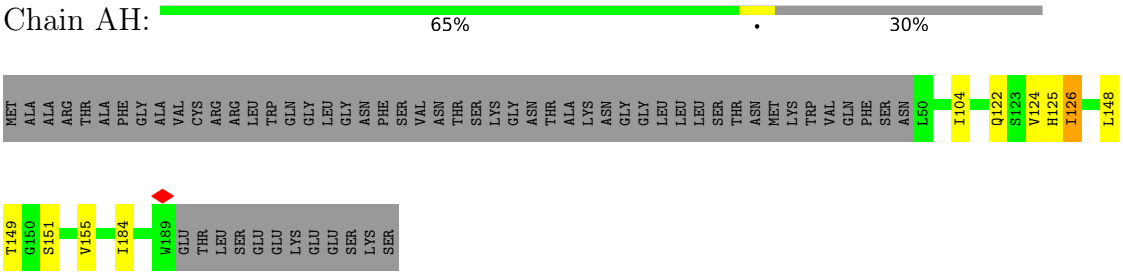
Chain AG:





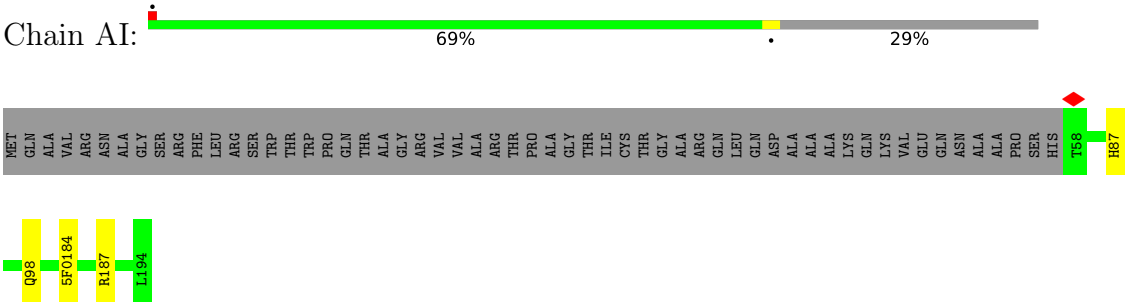
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain AH:



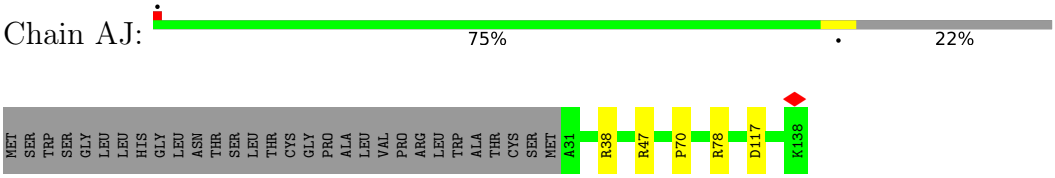
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain AI:



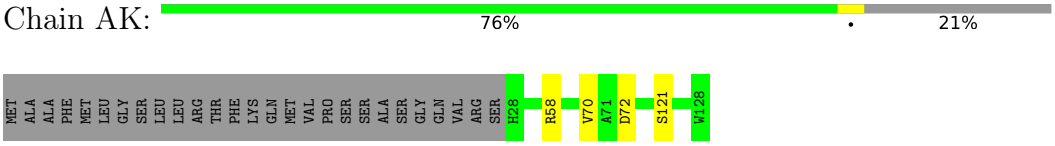
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain AJ:



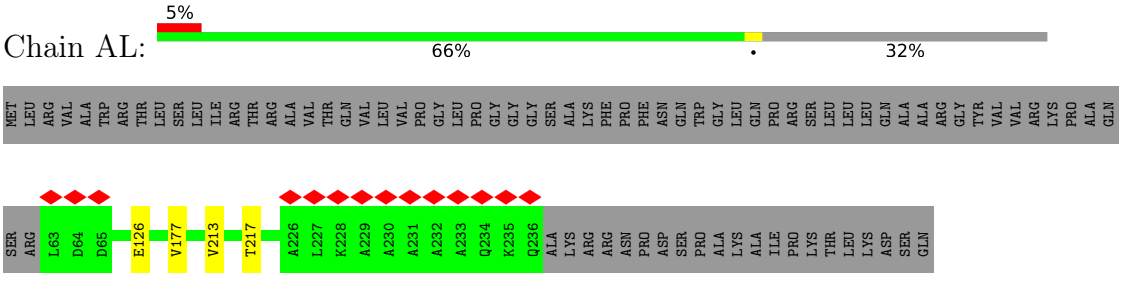
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain AK:



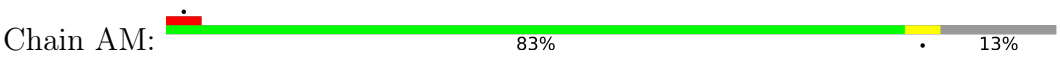
• Molecule 12: 28S ribosomal protein S15, mitochondrial

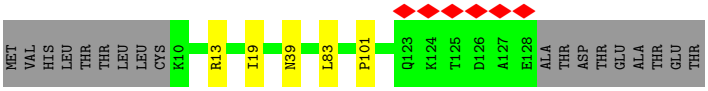
Chain AL:



• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain AM:

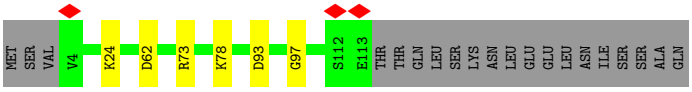




• Molecule 14: 28S ribosomal protein S17, mitochondrial

Chain AN:

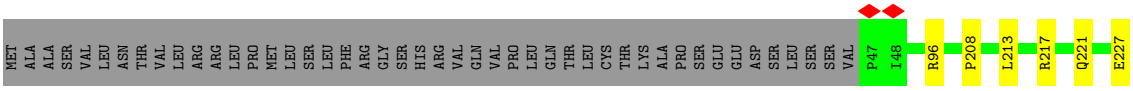


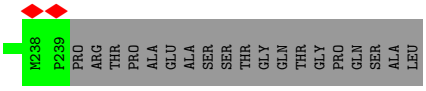


• Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain AO:



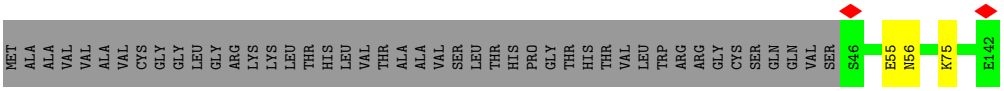




• Molecule 16: 28S ribosomal protein S18c, mitochondrial

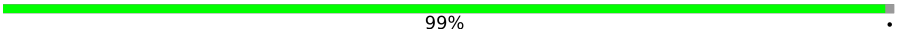
Chain AP:





• Molecule 17: MRPS21 isoform 1

Chain AQ:



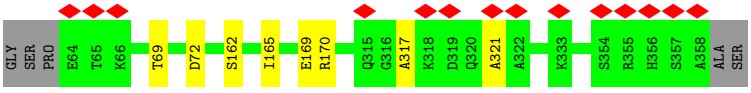


• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain AR:



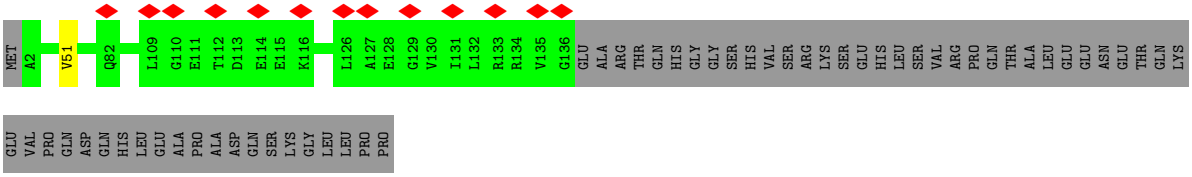




• Molecule 19: 28S ribosomal protein S23, mitochondrial

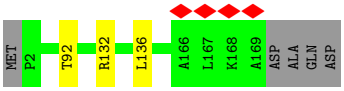
Chain AS:



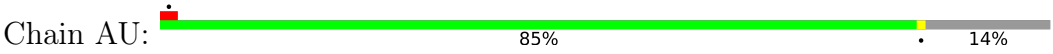


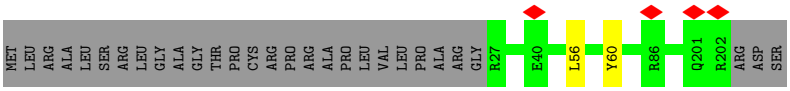
• Molecule 20: 28S ribosomal protein S25, mitochondrial



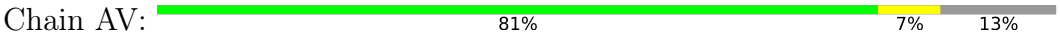


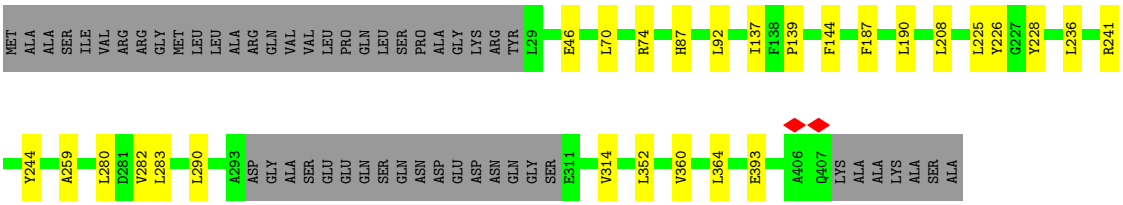
• Molecule 21: 28S ribosomal protein S26, mitochondrial





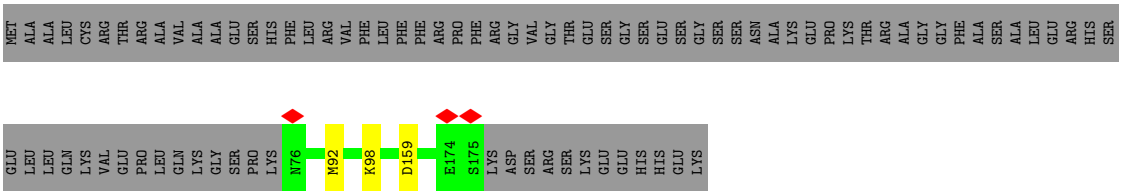
• Molecule 22: 28S ribosomal protein S27, mitochondrial



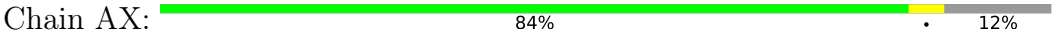


• Molecule 23: 28S ribosomal protein S28, mitochondrial

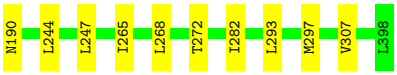




• Molecule 24: 28S ribosomal protein S29, mitochondrial



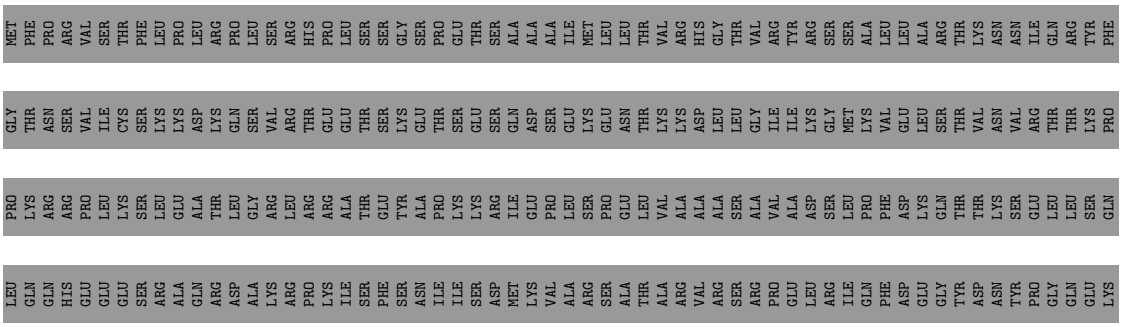


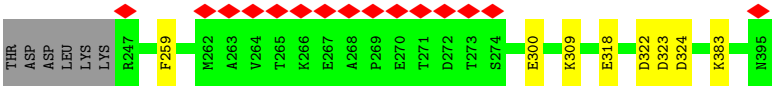


• Molecule 25: 28S ribosomal protein S31, mitochondrial

Chain AY:

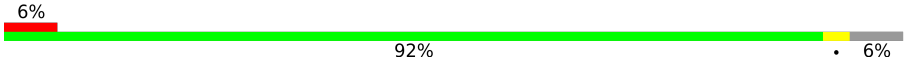


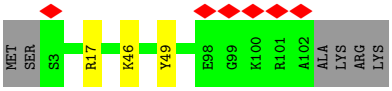




• Molecule 26: 28S ribosomal protein S33, mitochondrial

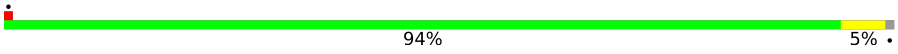
Chain AZ:





• Molecule 27: 28S ribosomal protein S34, mitochondrial

Chain A0:

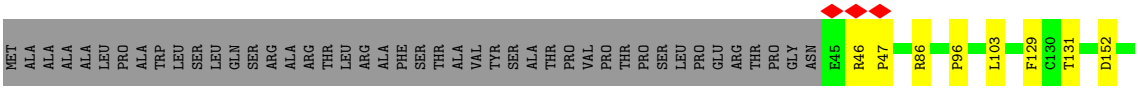


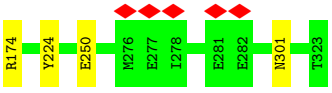


• Molecule 28: 28S ribosomal protein S35, mitochondrial

Chain A1:

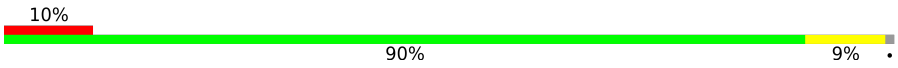


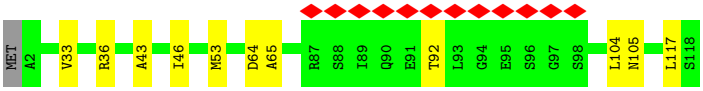




• Molecule 29: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2:

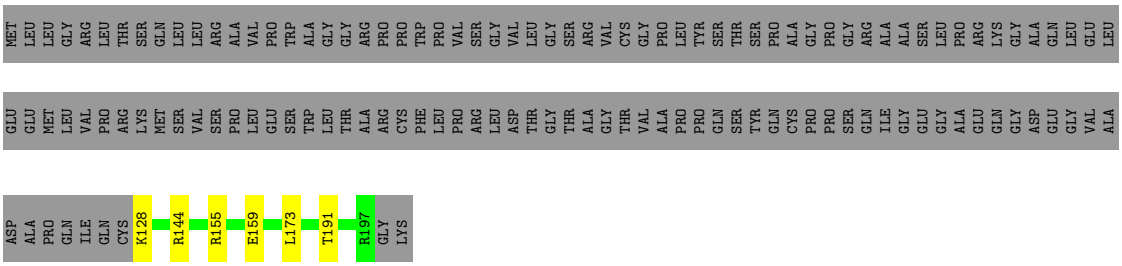




• Molecule 30: Aurora kinase A-interacting protein

Chain A3:

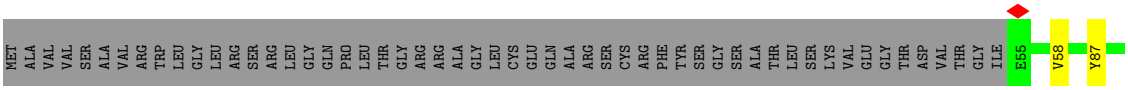


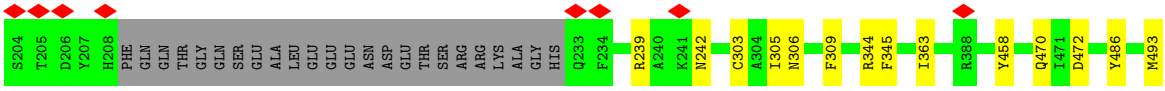


• Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4:





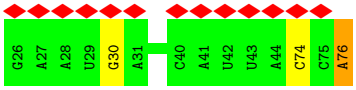




• Molecule 32: A/A-tRNA

Chain Aw:

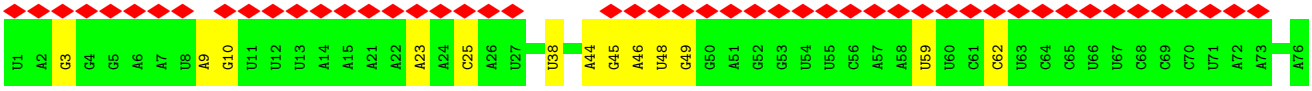




• Molecule 33: P/P-tRNA

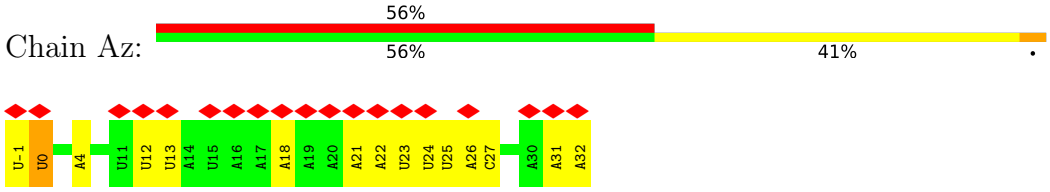
Chain Ax:





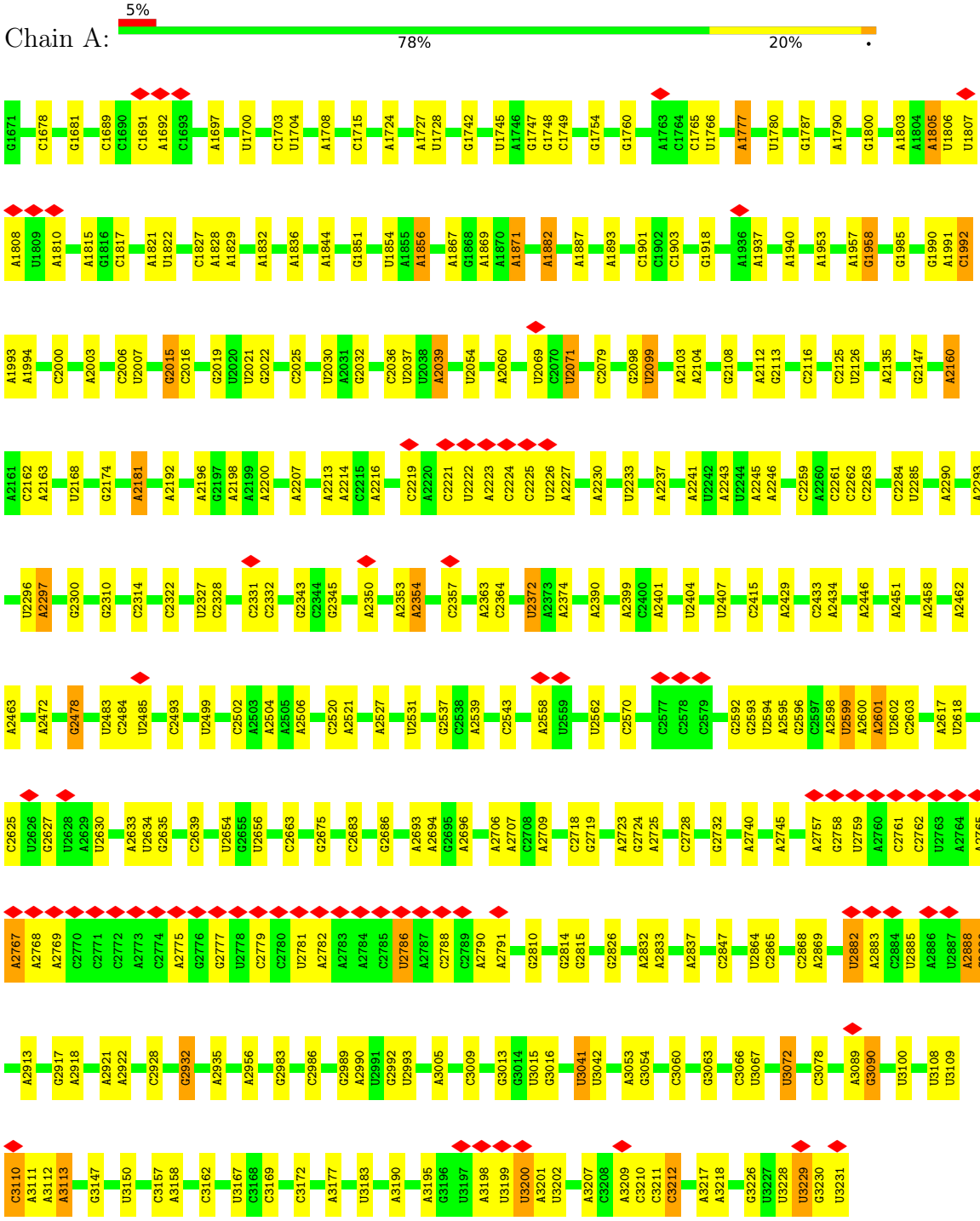
• Molecule 34: mRNA

Chain Az:



• Molecule 35: 16S mitochondrial rRNA

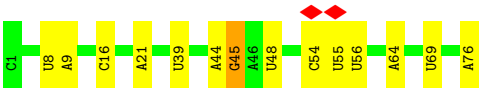
Chain A:



• Molecule 36: mitochondrial tRNAVal

Chain B:

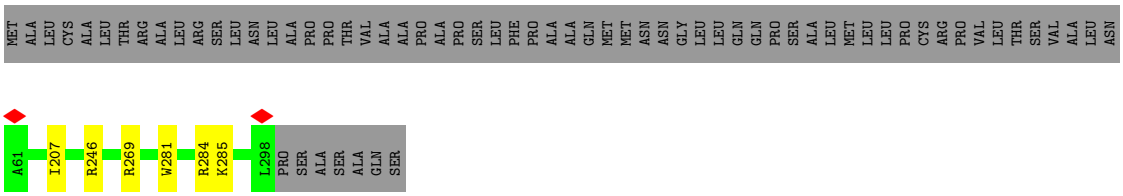




• Molecule 37: 39S ribosomal protein L2, mitochondrial

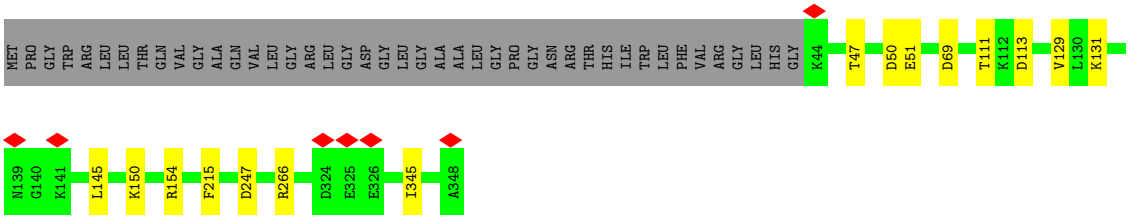
Chain D:





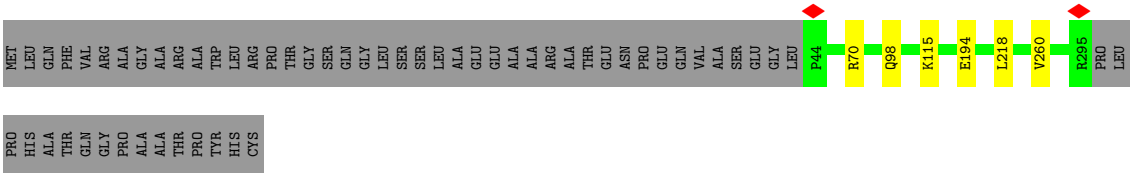
• Molecule 38: 39S ribosomal protein L3, mitochondrial

Chain E:



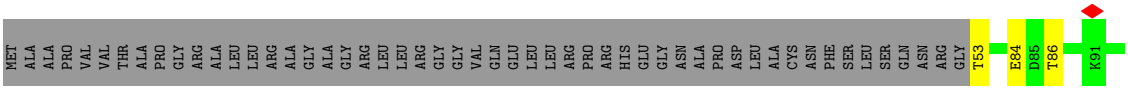
• Molecule 39: 39S ribosomal protein L4, mitochondrial

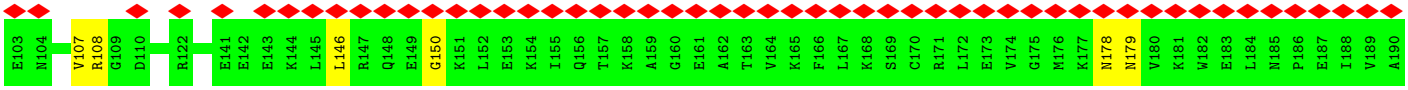
Chain F:



• Molecule 40: 39S ribosomal protein L9, mitochondrial

Chain H:



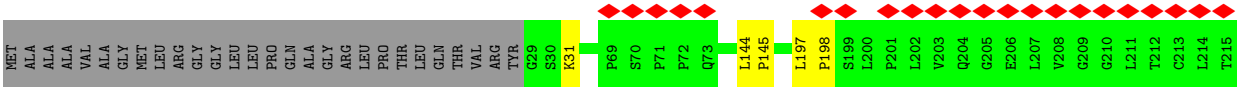


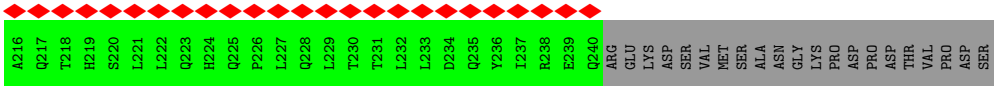


• Molecule 41: 39S ribosomal protein L10, mitochondrial

Chain I:



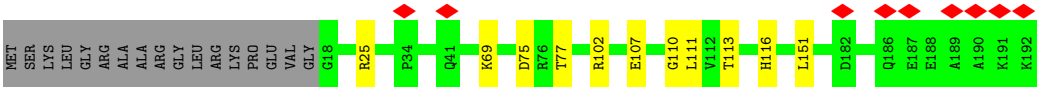




• Molecule 42: 39S ribosomal protein L11, mitochondrial

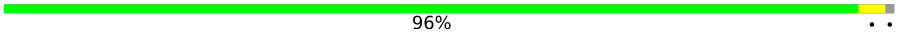
Chain J:

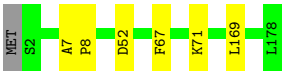




• Molecule 43: 39S ribosomal protein L13, mitochondrial

Chain K:





• Molecule 44: 39S ribosomal protein L14, mitochondrial

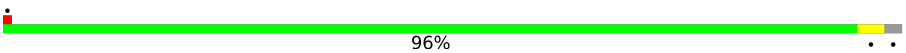
Chain L:

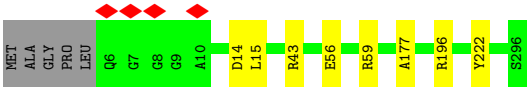




• Molecule 45: 39S ribosomal protein L15, mitochondrial

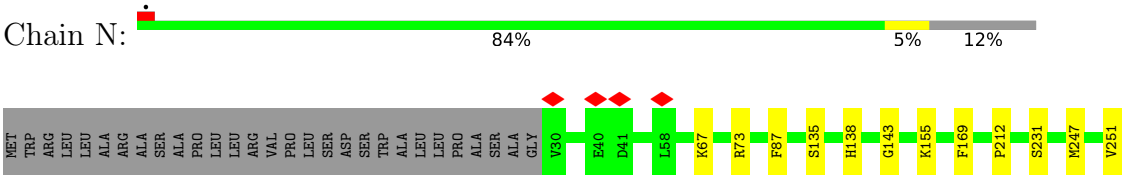
Chain M:





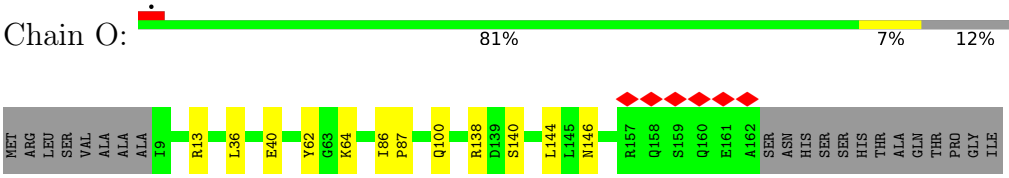
• Molecule 46: 39S ribosomal protein L16, mitochondrial

Chain N:



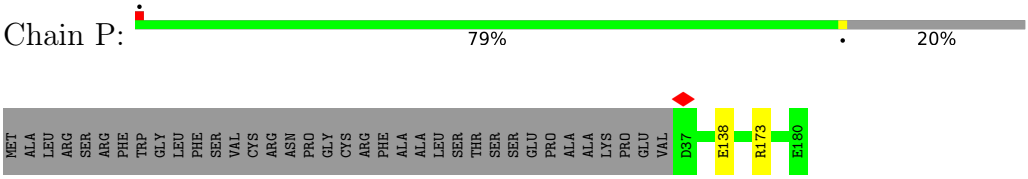
• Molecule 47: 39S ribosomal protein L17, mitochondrial

Chain O:



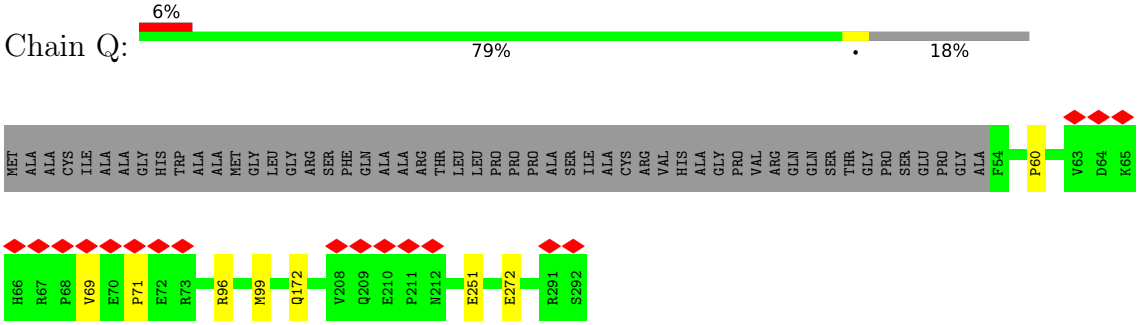
• Molecule 48: 39S ribosomal protein L18, mitochondrial

Chain P:



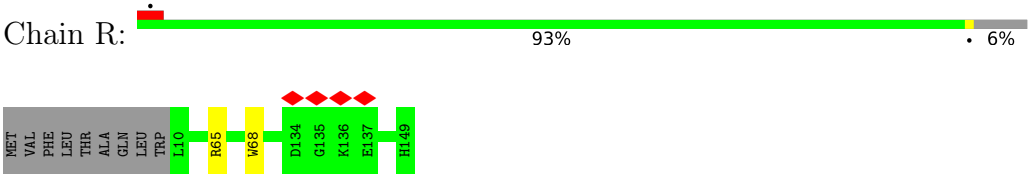
• Molecule 49: 39S ribosomal protein L19, mitochondrial

Chain Q:



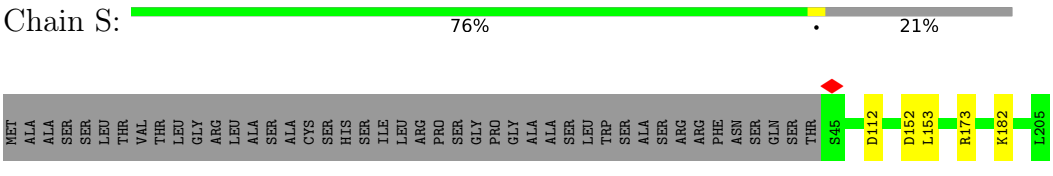
• Molecule 50: 39S ribosomal protein L20, mitochondrial

Chain R:



• Molecule 51: 39S ribosomal protein L21, mitochondrial

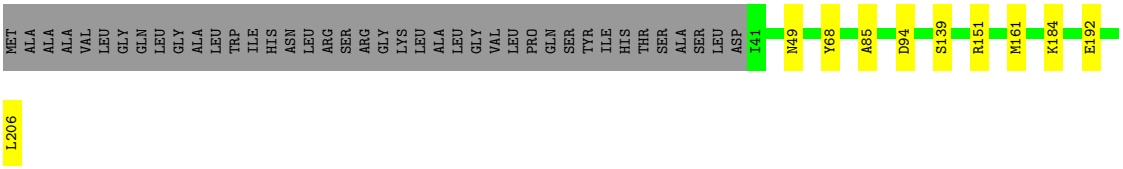
Chain S:



• Molecule 52: 39S ribosomal protein L22, mitochondrial

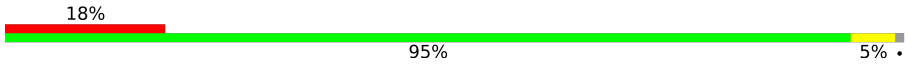
Chain T:

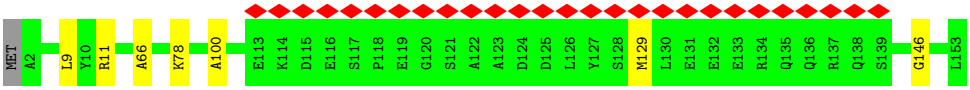




• Molecule 53: 39S ribosomal protein L23, mitochondrial

Chain U:

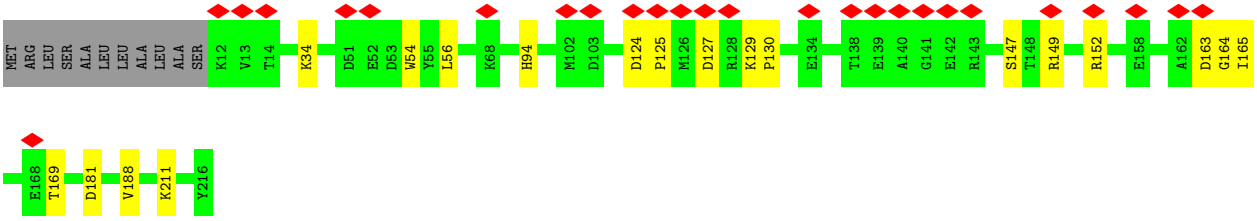




• Molecule 54: 39S ribosomal protein L24, mitochondrial

Chain V:

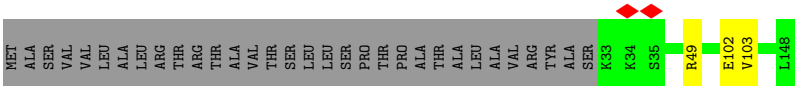




• Molecule 55: 39S ribosomal protein L27, mitochondrial

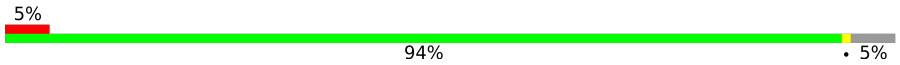
Chain W:

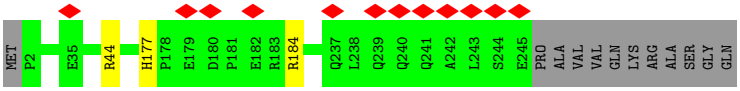




• Molecule 56: 39S ribosomal protein L28, mitochondrial

Chain X:



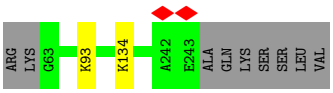


• Molecule 57: 39S ribosomal protein L47, mitochondrial

Chain Y:



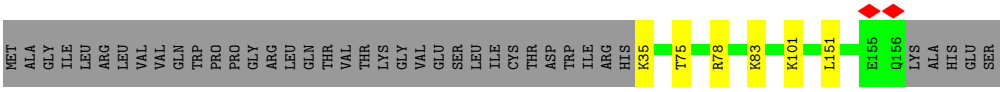




• Molecule 58: 39S ribosomal protein L30, mitochondrial

Chain Z:

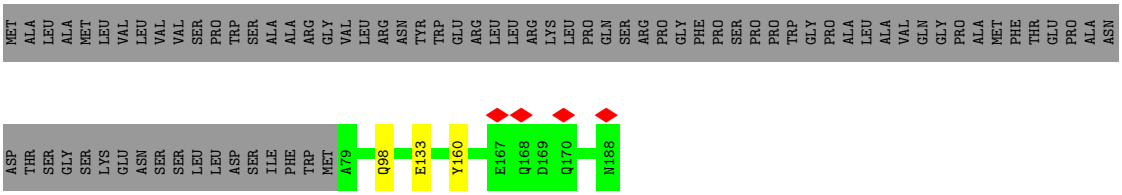




• Molecule 59: 39S ribosomal protein L32, mitochondrial

Chain 0:

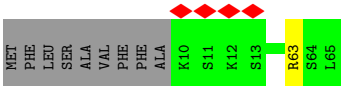




• Molecule 60: 39S ribosomal protein L33, mitochondrial

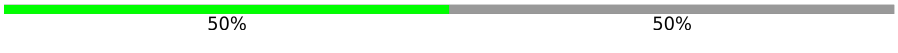
Chain 1:

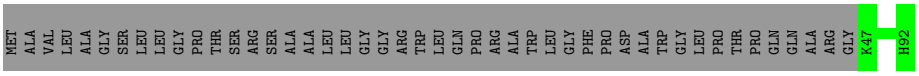




• Molecule 61: 39S ribosomal protein L34, mitochondrial

Chain 2:

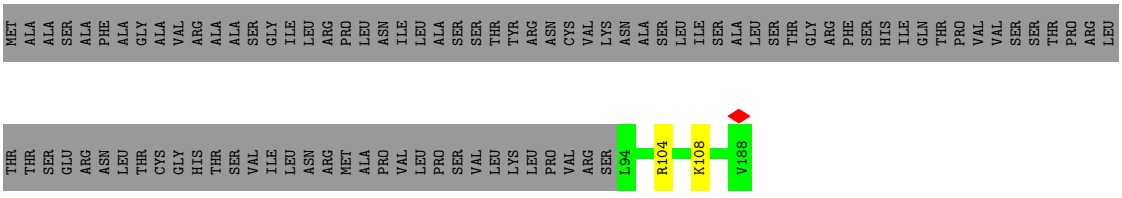




• Molecule 62: 39S ribosomal protein L35, mitochondrial

Chain 3:





• Molecule 63: 39S ribosomal protein L36, mitochondrial

Chain 4:



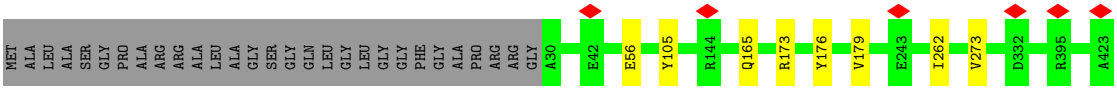




• Molecule 64: 39S ribosomal protein L37, mitochondrial

Chain 5:

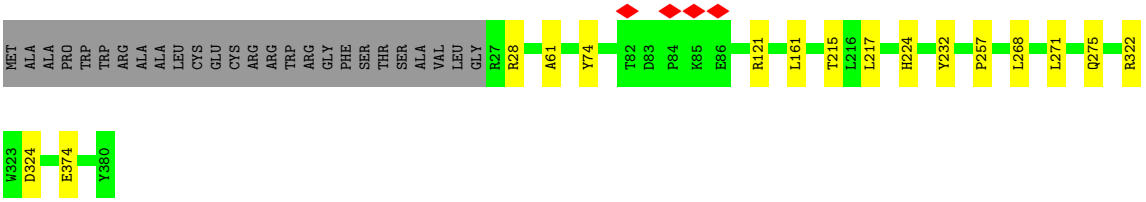




• Molecule 65: 39S ribosomal protein L38, mitochondrial

Chain 6:

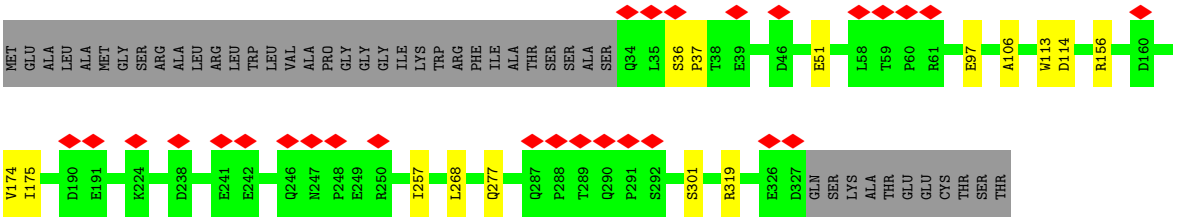




• Molecule 66: 39S ribosomal protein L39, mitochondrial

Chain 7:

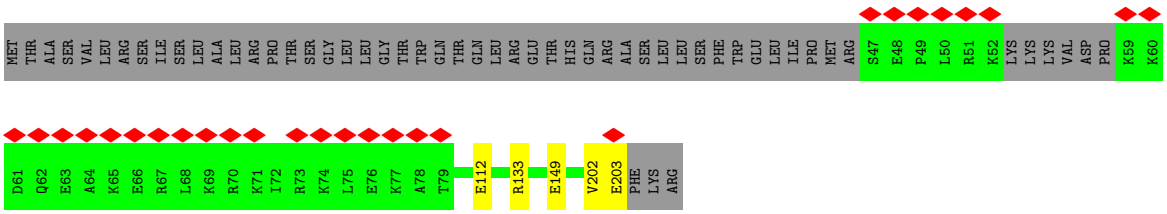




• Molecule 67: 39S ribosomal protein L40, mitochondrial

Chain 8:

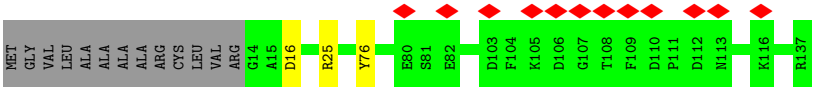




• Molecule 68: 39S ribosomal protein L41, mitochondrial

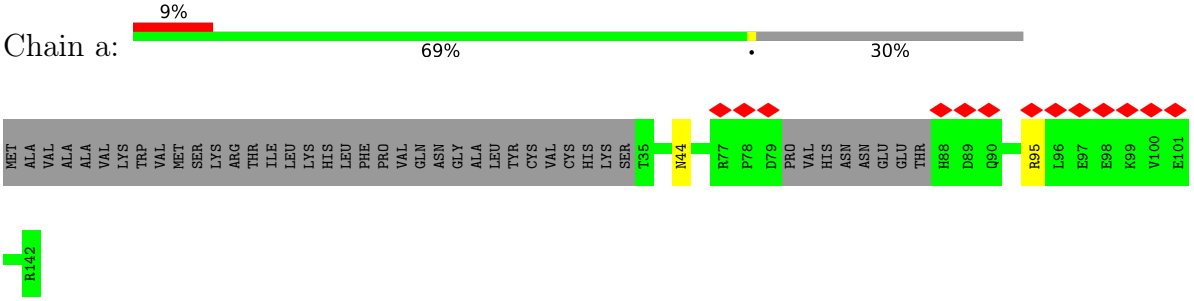
Chain 9:





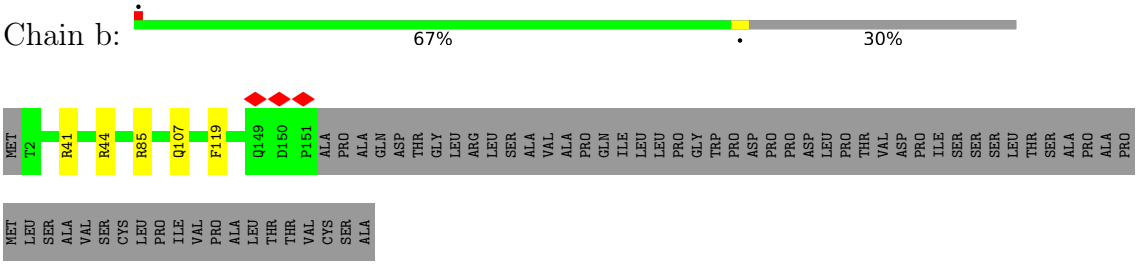
• Molecule 69: 39S ribosomal protein L42, mitochondrial

Chain a:



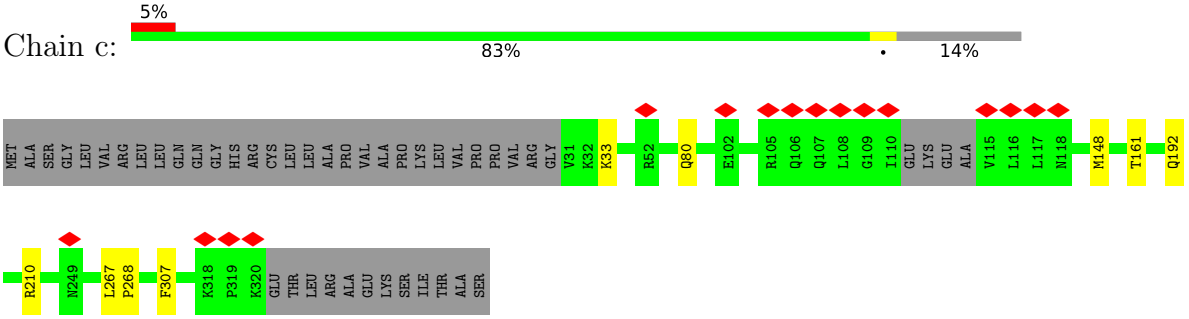
• Molecule 70: 39S ribosomal protein L43, mitochondrial

Chain b:



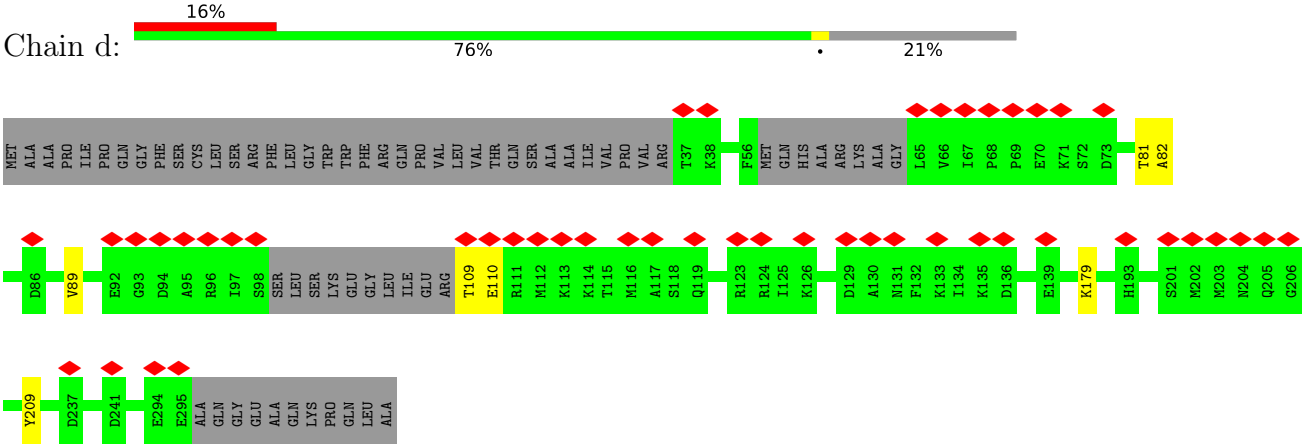
• Molecule 71: 39S ribosomal protein L44, mitochondrial

Chain c:



• Molecule 72: 39S ribosomal protein L45, mitochondrial

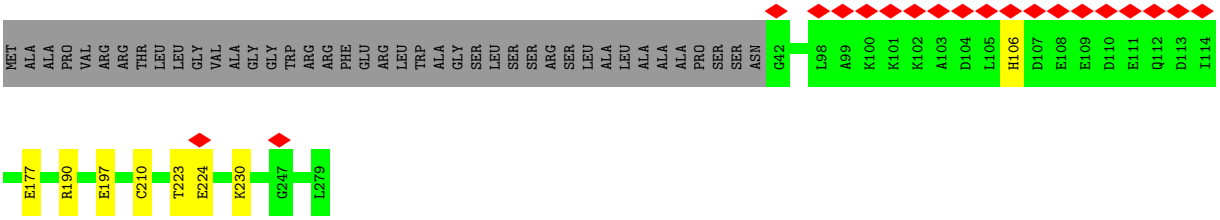
Chain d:



• Molecule 73: 39S ribosomal protein L46, mitochondrial

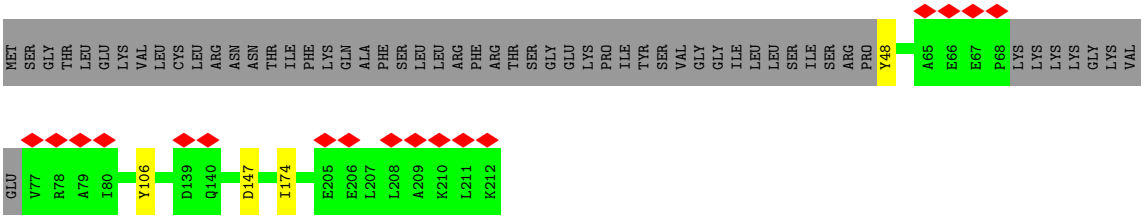
Chain e:



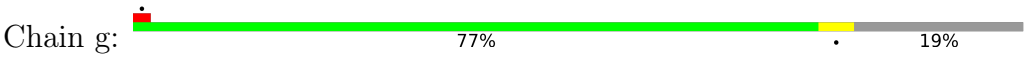


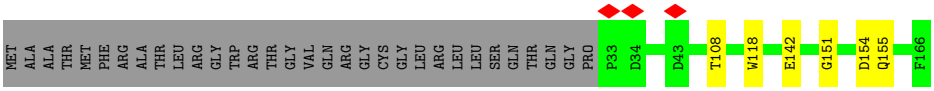
• Molecule 74: 39S ribosomal protein L48, mitochondrial





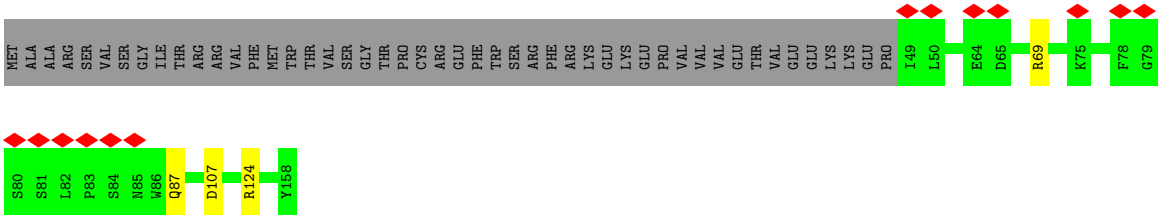
• Molecule 75: 39S ribosomal protein L49, mitochondrial





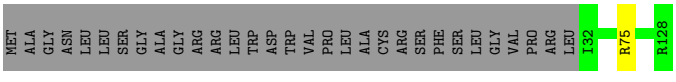
• Molecule 76: 39S ribosomal protein L50, mitochondrial





• Molecule 77: 39S ribosomal protein L51, mitochondrial



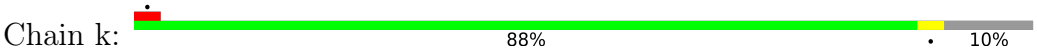


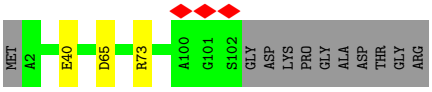
• Molecule 78: 39S ribosomal protein L52, mitochondrial





• Molecule 79: 39S ribosomal protein L53, mitochondrial





• Molecule 80: 39S ribosomal protein L54, mitochondrial

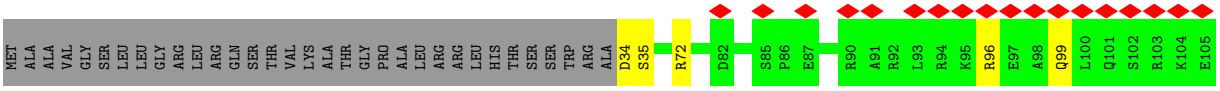


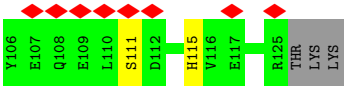




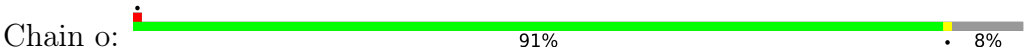
• Molecule 81: 39S ribosomal protein L55, mitochondrial

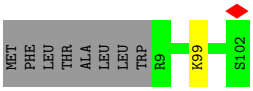






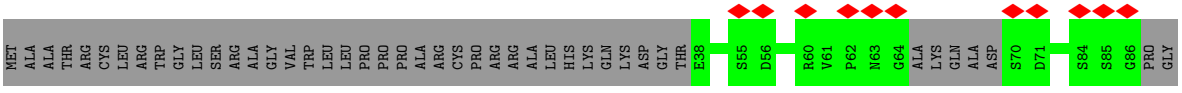
• Molecule 82: Ribosomal protein 63, mitochondrial

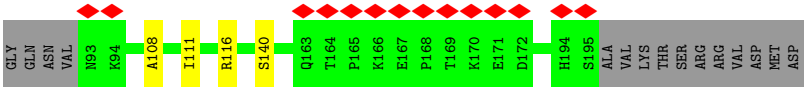




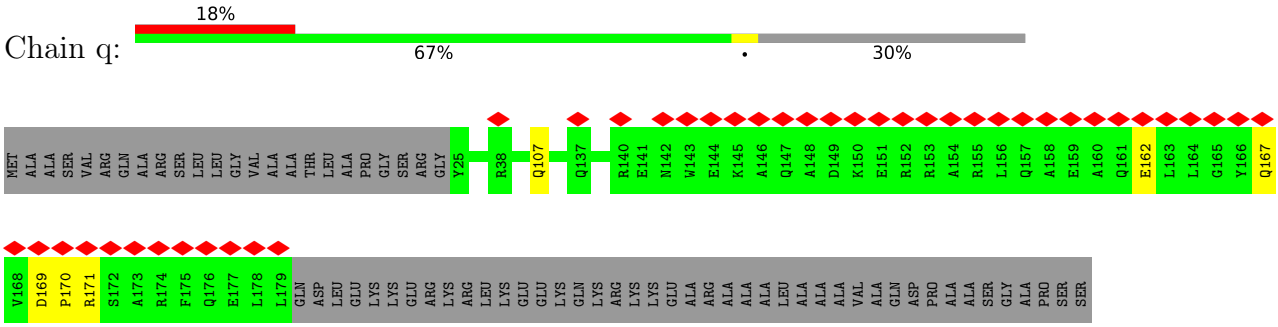
• Molecule 83: Peptidyl-tRNA hydrolase ICT1, mitochondrial



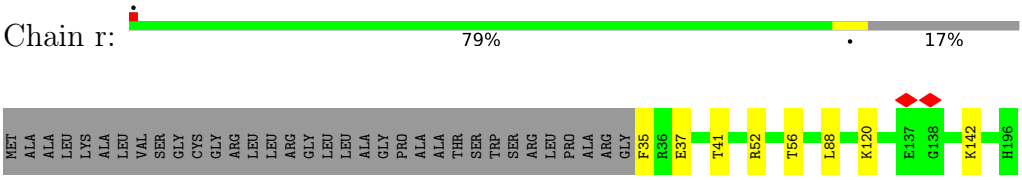




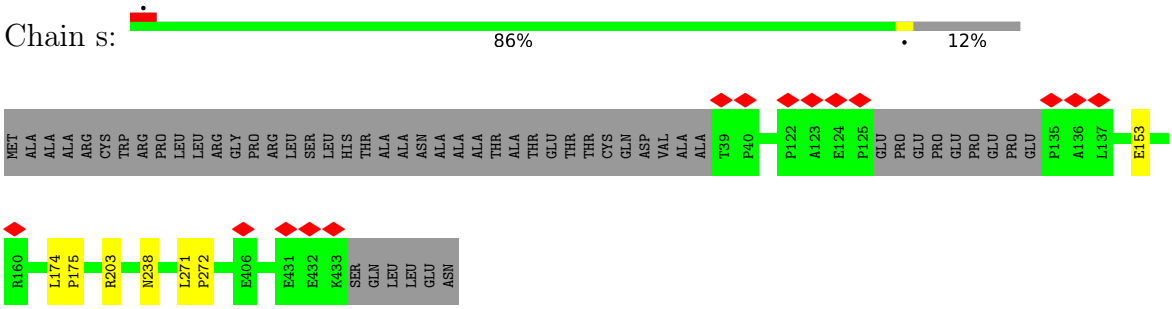
• Molecule 84: Growth arrest and DNA damage-inducible proteins-interacting protein 1



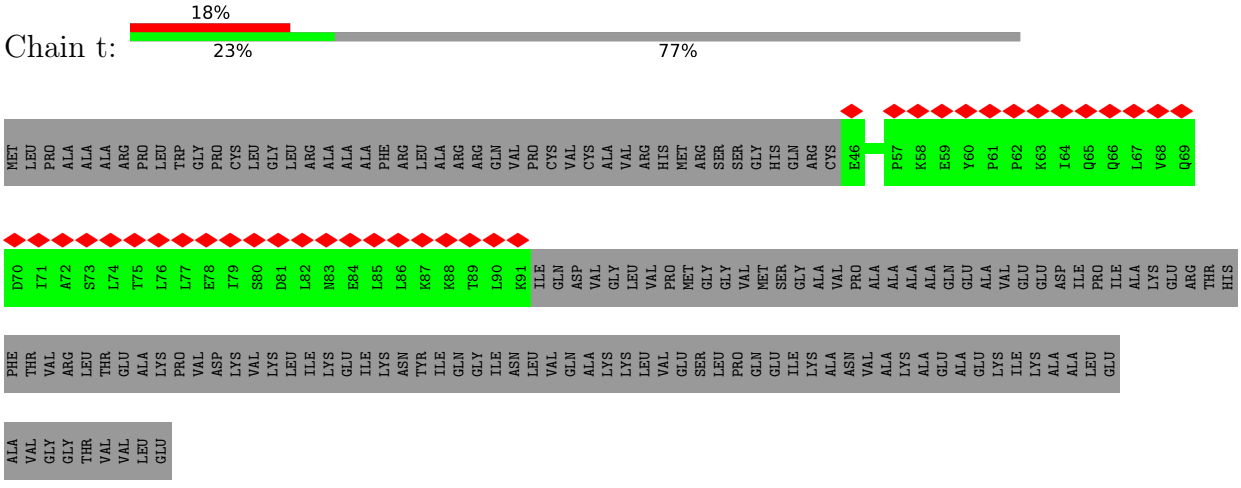
• Molecule 85: 39S ribosomal protein S18a, mitochondrial



• Molecule 86: 39S ribosomal protein S30, mitochondrial

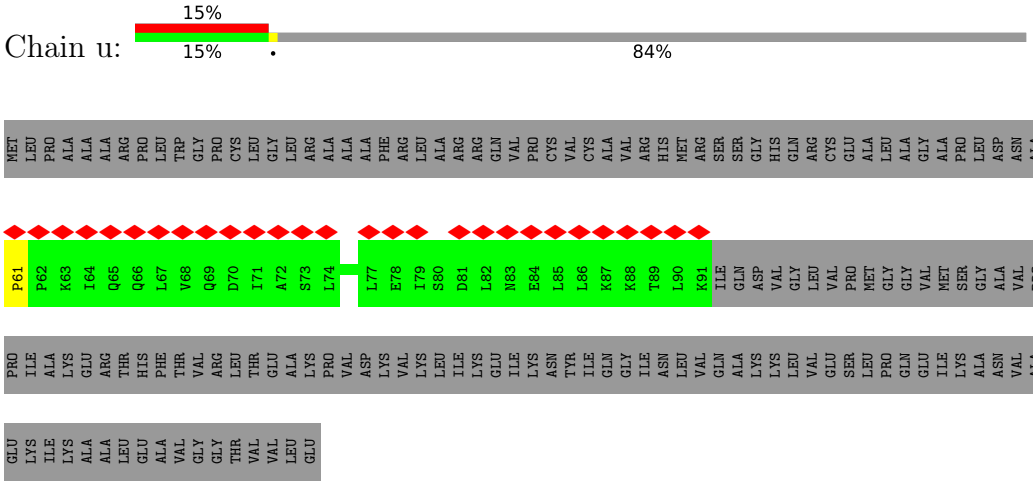


• Molecule 87: 39S ribosomal protein L12, mitochondrial



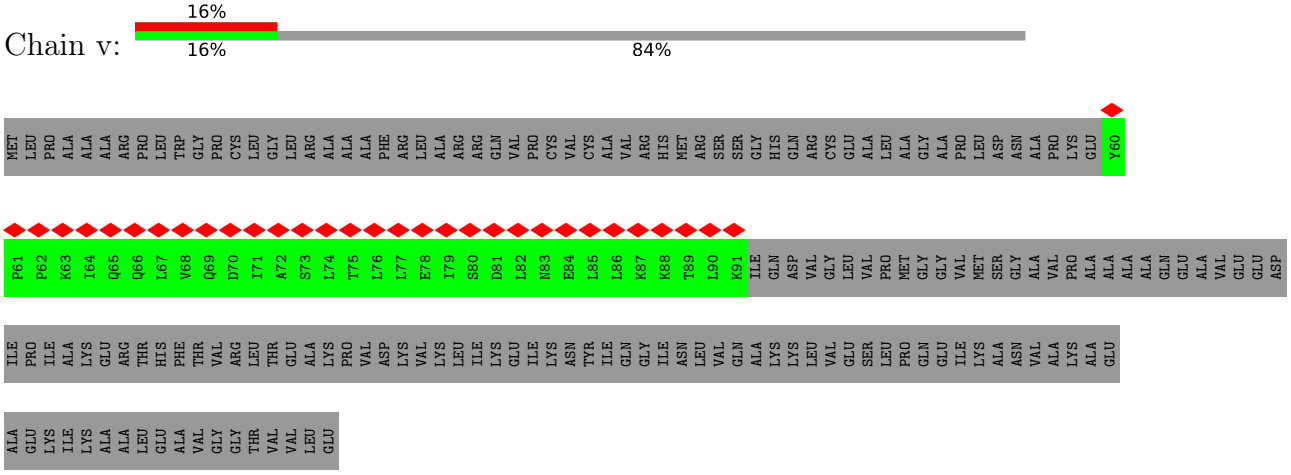
• Molecule 87: 39S ribosomal protein L12, mitochondrial

Chain u:



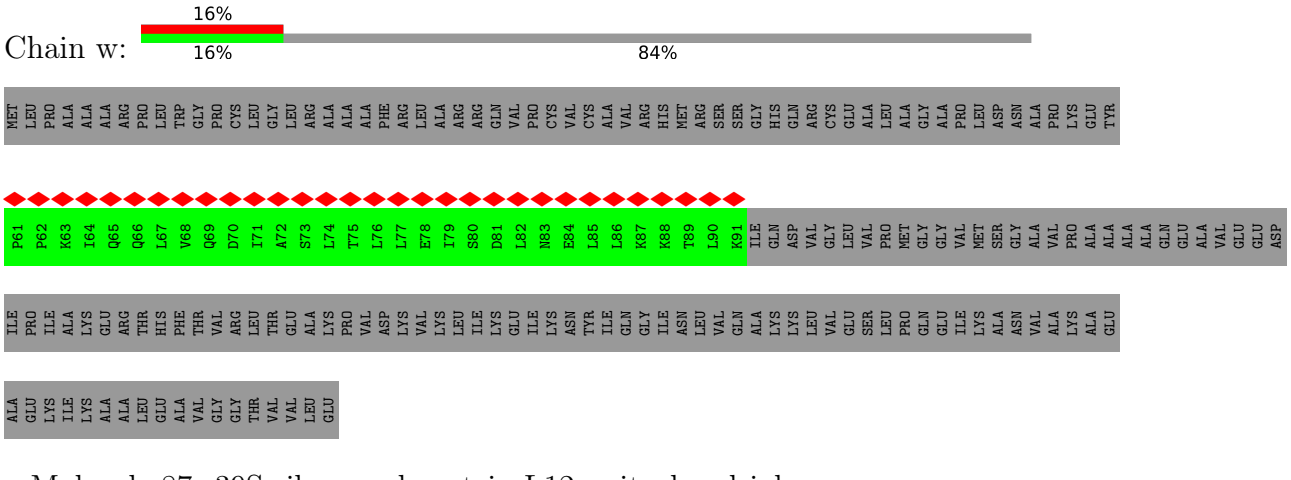
• Molecule 87: 39S ribosomal protein L12, mitochondrial

Chain v:



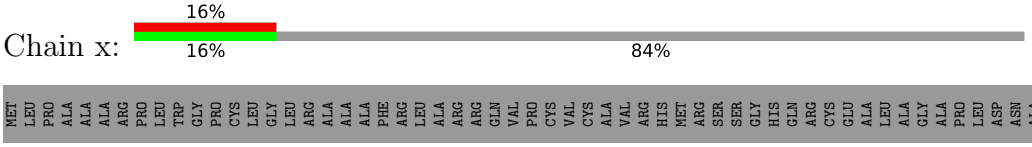
• Molecule 87: 39S ribosomal protein L12, mitochondrial

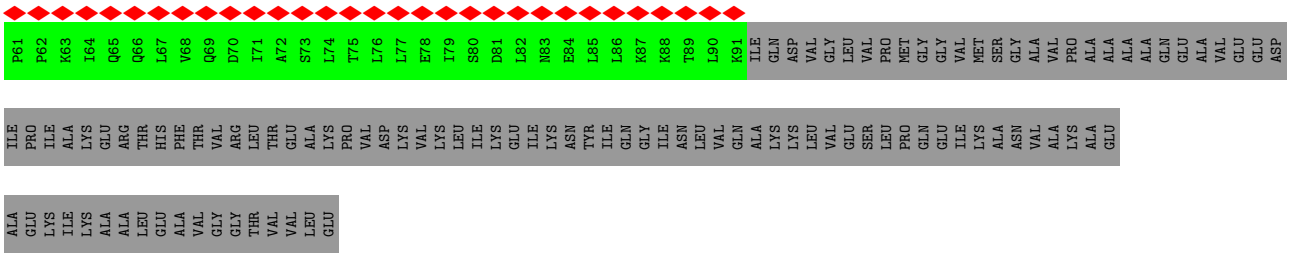
Chain w:



• Molecule 87: 39S ribosomal protein L12, mitochondrial

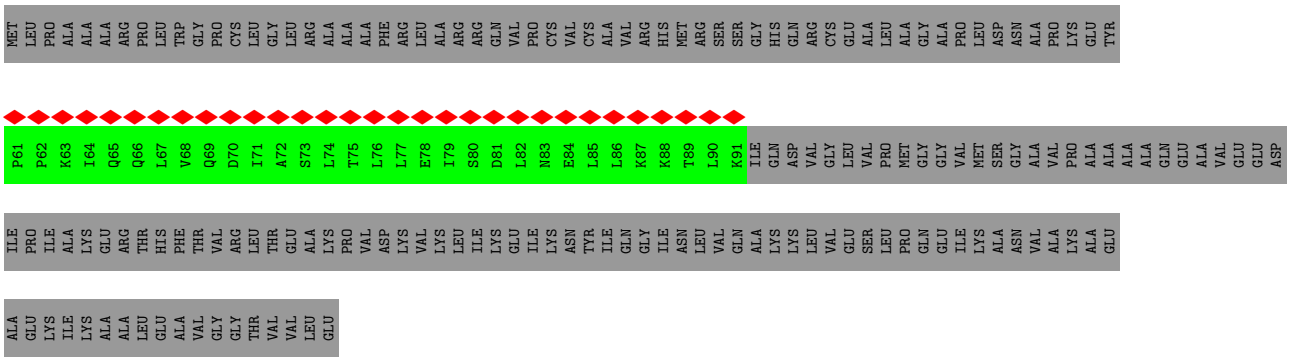
Chain x:



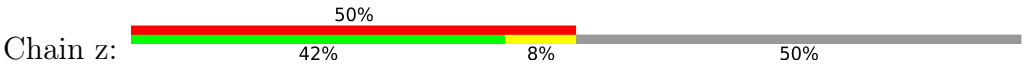


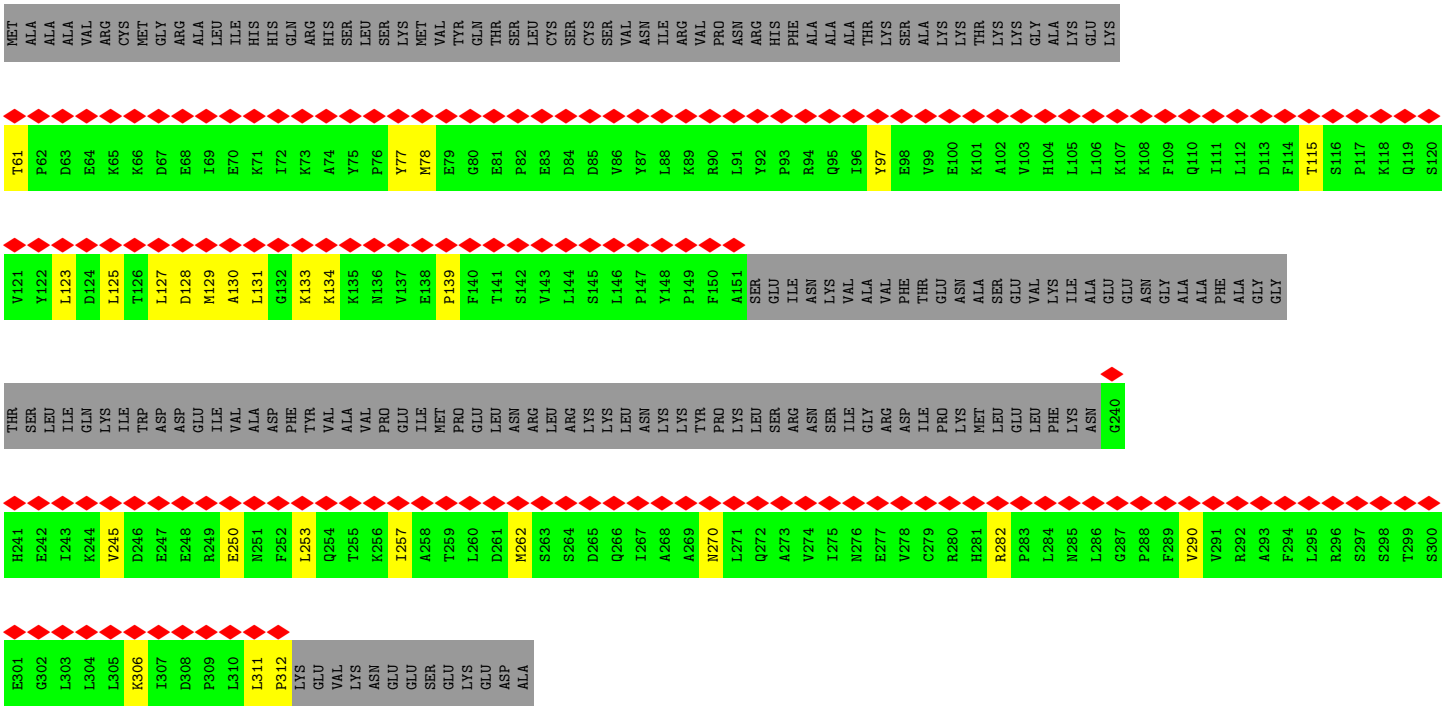
• Molecule 87: 39S ribosomal protein L12, mitochondrial





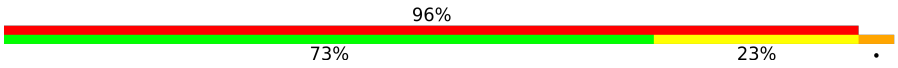
• Molecule 88: 39S ribosomal protein L1, mitochondrial





• Molecule 89: E/E-tRNA

Chain Ay:


96%
73%
23%


U1
A2
G3
G4
G5
A6
A7
U8
A9
G10
U11
U12
U13
A14
A15
A21
A22
A23
A24
C25
A26
G27
C43
A44
G45
A46
U48
G49
G50
A51
G52
G53
U54
A58
U59
U60
C61
G62
U63
C64
C65
U66
U67
C68
C69
C70
U71
A72
A73
C74
C75
A76

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	509691	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	71.473	Depositor
Minimum map value	-28.186	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.438	Depositor
Recommended contour level	4	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8T, 2MG, SPM, 1MA, OMG, K, NAD, SAC, ATP, 5MC, MG, 5MU, GDP, ZN, THC, AYA, MA6, PSU, SPD, 5F0, FES, OMU, PUT

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	AA	0.09	0/22537	0.19	0/35085
2	AB	0.09	0/1871	0.25	0/2531
3	AC	0.12	0/1113	0.29	0/1505
4	AD	0.09	0/2783	0.24	0/3724
5	AE	0.08	0/989	0.24	0/1335
6	AF	0.09	0/1767	0.22	0/2373
7	AG	0.08	0/2746	0.23	0/3681
8	AH	0.12	0/1178	0.27	0/1598
9	AI	0.09	0/1030	0.24	0/1386
10	AJ	0.10	0/855	0.26	0/1148
11	AK	0.09	0/880	0.21	0/1182
12	AL	0.08	0/1477	0.22	0/1974
13	AM	0.09	0/963	0.25	0/1295
14	AN	0.09	0/886	0.26	0/1199
15	AO	0.09	0/1648	0.24	0/2243
16	AP	0.09	0/798	0.24	0/1070
17	AQ	0.09	0/748	0.23	0/994
18	AR	0.08	0/2456	0.20	0/3317
19	AS	0.07	0/1138	0.20	0/1533
20	AT	0.08	0/1402	0.24	0/1883
21	AU	0.08	0/1510	0.20	0/2025
22	AV	0.12	0/3030	0.25	0/4093
23	AW	0.09	0/801	0.22	0/1079
24	AX	0.10	0/2921	0.26	0/3954
25	AY	0.09	0/1280	0.22	0/1725
26	AZ	0.09	0/857	0.24	0/1141
27	A0	0.11	0/1834	0.28	0/2484
28	A1	0.09	0/2313	0.24	0/3129
29	A2	0.08	0/941	0.25	0/1257
30	A3	0.09	0/636	0.26	0/839
31	A4	0.09	0/4877	0.22	0/6598

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	Aw	0.06	0/517	0.15	0/799
33	Ax	0.06	0/1655	0.15	0/2569
34	Az	0.08	0/803	0.19	0/1244
35	A	0.09	0/36876	0.23	0/57402
36	B	0.09	0/1627	0.18	0/2527
37	D	0.08	0/1896	0.26	0/2549
38	E	0.10	0/2475	0.27	0/3355
39	F	0.10	0/2090	0.28	0/2842
40	H	0.09	0/1698	0.25	0/2292
41	I	0.10	0/1731	0.29	0/2345
42	J	0.10	0/1348	0.24	0/1813
43	K	0.09	0/1490	0.26	0/2021
44	L	0.09	0/905	0.27	0/1218
45	M	0.10	0/2381	0.29	0/3212
46	N	0.09	0/1833	0.28	0/2468
47	O	0.08	0/1283	0.25	0/1727
48	P	0.10	0/1199	0.26	0/1623
49	Q	0.09	0/2039	0.25	0/2750
50	R	0.08	0/1175	0.24	0/1572
51	S	0.10	0/1320	0.28	0/1789
52	T	0.09	0/1403	0.27	0/1886
53	U	0.09	0/1274	0.26	0/1723
54	V	0.09	0/1721	0.25	0/2333
55	W	0.10	0/926	0.25	0/1244
56	X	0.09	0/2099	0.23	0/2837
57	Y	0.08	0/1593	0.22	0/2136
58	Z	0.09	0/1021	0.27	0/1378
59	0	0.09	0/913	0.24	0/1224
60	1	0.09	0/469	0.27	0/621
61	2	0.09	0/383	0.27	0/507
62	3	0.09	0/853	0.27	0/1136
63	4	0.08	0/350	0.23	0/461
64	5	0.09	0/3305	0.26	0/4502
65	6	0.11	0/3043	0.27	0/4140
66	7	0.10	0/2447	0.25	0/3310
67	8	0.09	0/1303	0.23	0/1750
68	9	0.10	0/1025	0.26	0/1379
69	a	0.10	0/866	0.28	0/1174
70	b	0.09	0/1211	0.27	0/1639
71	c	0.09	0/2347	0.23	0/3171
72	d	0.09	0/2039	0.25	0/2759
73	e	0.09	0/1970	0.23	0/2658
74	f	0.08	0/1273	0.22	0/1716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
75	g	0.10	0/1151	0.27	0/1569
76	h	0.08	0/918	0.21	0/1249
77	i	0.10	0/850	0.26	0/1135
78	j	0.11	0/760	0.26	0/1023
79	k	0.08	0/777	0.22	0/1048
80	l	0.09	0/707	0.27	0/960
81	m	0.08	0/805	0.22	0/1081
82	o	0.13	0/819	0.29	0/1097
83	p	0.08	0/1223	0.23	0/1641
84	q	0.07	0/1332	0.21	0/1801
85	r	0.11	0/1362	0.29	0/1846
86	s	0.09	0/3239	0.26	0/4400
87	t	0.06	0/358	0.19	0/486
87	u	0.08	0/259	0.19	0/350
87	v	0.07	0/259	0.16	0/350
87	w	0.08	0/246	0.19	0/331
87	x	0.07	0/246	0.17	0/331
87	y	0.07	0/246	0.17	0/331
88	z	0.12	0/1354	0.32	0/1831
89	Ay	0.07	0/1235	0.21	0/1912
All	All	0.09	0/188586	0.24	0/267953

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AA	20260	10304	10285	63	0
2	AB	1828	1816	1815	5	0
3	AC	1083	1089	1088	8	0
4	AD	2731	2805	2804	8	0
5	AE	972	1000	1000	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	1725	1771	1769	9	0
7	AG	2688	2689	2687	10	0
8	AH	1152	1187	1183	10	0
9	AI	1020	1061	1053	3	0
10	AJ	839	888	887	5	0
11	AK	862	886	885	3	0
12	AL	1453	1541	1540	3	0
13	AM	942	966	965	4	0
14	AN	868	929	928	5	0
15	AO	1592	1557	1557	4	0
16	AP	781	806	806	4	0
17	AQ	744	758	758	0	0
18	AR	2409	2430	2428	6	0
19	AS	1111	1116	1115	1	0
20	AT	1371	1393	1393	2	0
21	AU	1488	1501	1499	3	0
22	AV	2969	2964	2961	19	0
23	AW	789	804	802	2	0
24	AX	2849	2845	2843	12	0
25	AY	1246	1198	1197	6	0
26	AZ	839	859	858	2	0
27	A0	1787	1797	1796	7	0
28	A1	2265	2296	2294	12	0
29	A2	935	971	971	7	0
30	A3	625	701	699	5	0
31	A4	4768	4770	4766	13	0
32	Aw	464	237	238	2	0
33	Ax	1482	751	752	2	0
34	Az	719	360	360	2	0
35	A	33070	16801	16794	106	0
36	B	1524	779	779	1	0
37	D	1859	1921	1920	5	0
38	E	2406	2416	2415	11	0
39	F	2031	2066	2065	4	0
40	H	1661	1736	1734	10	0
41	I	1695	1786	1785	3	0
42	J	1330	1408	1407	7	0
43	K	1455	1452	1452	4	0
44	L	890	942	941	3	0
45	M	2327	2396	2395	6	0
46	N	1786	1818	1817	9	0
47	O	1259	1295	1294	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	P	1173	1166	1165	2	0
49	Q	1990	2031	2031	6	0
50	R	1154	1215	1214	1	0
51	S	1293	1366	1365	5	0
52	T	1369	1412	1410	6	0
53	U	1251	1232	1232	6	0
54	V	1676	1689	1687	13	0
55	W	904	936	935	3	0
56	X	2044	2061	2060	2	0
57	Y	1556	1598	1597	2	0
58	Z	996	1045	1044	5	0
59	0	898	917	916	2	0
60	1	464	513	511	1	0
61	2	377	407	406	0	0
62	3	832	884	883	2	0
63	4	342	362	361	2	0
64	5	3210	3209	3206	5	0
65	6	2948	2844	2841	12	0
66	7	2390	2399	2397	11	0
67	8	1278	1310	1308	4	0
68	9	997	988	987	3	0
69	a	840	812	810	2	0
70	b	1196	1196	1190	4	0
71	c	2299	2322	2320	5	0
72	d	1985	1980	1976	7	0
73	e	1931	1917	1916	5	0
74	f	1252	1271	1269	3	0
75	g	1113	1097	1097	3	0
76	h	895	883	881	2	0
77	i	828	859	857	1	0
78	j	745	747	746	3	0
79	k	774	785	784	2	0
80	l	688	675	674	1	0
81	m	791	760	796	6	0
82	o	798	806	804	1	0
83	p	1205	1225	1223	3	0
84	q	1298	1273	1272	4	0
85	r	1322	1349	1348	6	0
86	s	3155	3145	3139	4	0
87	t	354	378	377	0	0
87	u	257	284	283	1	0
87	v	257	284	283	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	w	245	275	275	0	0
87	x	245	275	275	0	0
87	y	245	275	275	0	0
88	z	1327	1355	1353	21	0
89	Ay	1107	560	563	3	0
90	AA	44	26	26	0	0
91	AA	14	30	26	0	0
92	A	30	66	57	0	0
92	AA	10	22	19	0	0
93	A	137	0	0	0	0
93	A3	1	0	0	0	0
93	AA	61	0	0	0	0
93	AB	1	0	0	0	0
93	AX	1	0	0	0	0
93	Aw	1	0	0	0	0
93	D	2	0	0	0	0
93	E	1	0	0	0	0
93	g	1	0	0	0	0
94	3	1	0	0	0	0
94	6	1	0	0	0	0
94	A	29	0	0	0	0
94	AA	18	0	0	0	0
94	D	1	0	0	0	0
94	M	1	0	0	0	0
94	W	1	0	0	0	0
94	i	1	0	0	0	0
94	o	1	0	0	0	0
95	0	1	0	0	0	0
95	4	1	0	0	0	0
95	AO	1	0	0	0	0
96	AP	4	0	0	0	0
96	AT	4	0	0	0	0
96	r	4	0	0	0	0
97	AX	31	12	12	1	0
98	AX	28	12	12	0	0
99	A	6	14	12	0	0
100	B	7	11	8	0	0
101	0	27	0	0	0	0
101	1	3	0	0	0	0
101	2	34	0	0	0	0
101	3	40	0	0	0	0
101	4	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	5	22	0	0	0	0
101	6	100	0	0	1	0
101	7	17	0	0	0	0
101	8	19	0	0	1	0
101	9	17	0	0	0	0
101	A	3056	0	0	21	0
101	A0	1	0	0	0	0
101	A1	36	0	0	0	0
101	A2	35	0	0	0	0
101	A3	52	0	0	1	0
101	A4	11	0	0	0	0
101	AA	2157	0	0	24	0
101	AB	80	0	0	1	0
101	AC	58	0	0	0	0
101	AD	79	0	0	1	0
101	AE	30	0	0	0	0
101	AF	36	0	0	0	0
101	AG	70	0	0	1	0
101	AH	50	0	0	0	0
101	AI	44	0	0	1	0
101	AJ	29	0	0	1	0
101	AK	51	0	0	0	0
101	AL	43	0	0	0	0
101	AM	21	0	0	0	0
101	AN	34	0	0	0	0
101	AO	37	0	0	0	0
101	AP	31	0	0	0	0
101	AQ	68	0	0	0	0
101	AR	12	0	0	0	0
101	AS	23	0	0	0	0
101	AT	43	0	0	0	0
101	AU	8	0	0	0	0
101	AW	15	0	0	0	0
101	AX	61	0	0	1	0
101	AY	20	0	0	1	0
101	AZ	27	0	0	0	0
101	Aw	5	0	0	0	0
101	Ax	5	0	0	0	0
101	Ay	1	0	0	0	0
101	Az	15	0	0	0	0
101	B	63	0	0	0	0
101	D	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
101	E	74	0	0	1	0
101	F	78	0	0	2	0
101	H	9	0	0	0	0
101	I	23	0	0	1	0
101	J	1	0	0	0	0
101	K	65	0	0	1	0
101	L	25	0	0	1	0
101	M	66	0	0	1	0
101	N	60	0	0	4	0
101	O	38	0	0	0	0
101	P	89	0	0	1	0
101	Q	27	0	0	0	0
101	R	57	0	0	0	0
101	S	49	0	0	2	0
101	T	48	0	0	0	0
101	U	26	0	0	0	0
101	V	5	0	0	0	0
101	W	48	0	0	0	0
101	X	12	0	0	0	0
101	Y	29	0	0	0	0
101	Z	34	0	0	0	0
101	a	13	0	0	0	0
101	b	39	0	0	1	0
101	c	20	0	0	1	0
101	d	5	0	0	0	0
101	e	13	0	0	1	0
101	f	22	0	0	1	0
101	g	13	0	0	0	0
101	i	54	0	0	0	0
101	j	23	0	0	0	0
101	k	6	0	0	1	0
101	l	5	0	0	0	0
101	m	8	0	0	0	0
101	o	34	0	0	0	0
101	p	10	0	0	0	0
101	r	50	0	0	0	0
101	s	51	0	0	0	0
All	All	187689	152427	152294	504	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.

All (504) 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)
66:7:156:ARG:O	69:a:95:ARG:NH2	2.04	0.90
32:Aw:74:C:N4	35:A:3041:U:O2	2.10	0.85
22:AV:226:TYR:HE1	22:AV:282:VAL:HG21	1.42	0.83
7:AG:389:ARG:NH1	7:AG:390:LYS:O	2.12	0.83
74:f:106:TYR:OH	74:f:174:ILE:O	1.96	0.82
6:AF:159:VAL:HG23	6:AF:172:VAL:HG21	1.63	0.80
35:A:3063:G:O2'	35:A:3066:C:OP2	2.00	0.79
88:z:127:LEU:HD22	88:z:290:VAL:HG22	1.64	0.79
35:A:3042:U:OP2	101:A:3501:HOH:O	2.00	0.79
35:A:3198:A:O2'	35:A:3200:U:O2'	2.01	0.78
53:U:9:LEU:O	53:U:11:ARG:NH1	2.16	0.78
1:AA:1472:G:O6	101:AA:1801:HOH:O	2.01	0.78
65:6:121:ARG:NH1	67:8:112:GLU:OE2	2.19	0.76
35:A:3147:G:OP1	101:A:3502:HOH:O	2.04	0.75
35:A:2098:G:O2'	35:A:2099:U:OP2	2.04	0.75
22:AV:92:LEU:HD21	22:AV:137:ILE:HD11	1.69	0.74
35:A:3226:G:O2'	35:A:3229:U:O4	2.04	0.74
31:A4:303:CYS:SG	31:A4:344:ARG:NH2	2.60	0.74
35:A:3041:U:OP1	101:A:3504:HOH:O	2.05	0.74
33:Ax:9:A:O2'	33:Ax:10:G:N7	2.21	0.74
35:A:3113:A:OP1	35:A:3167:U:O2'	2.04	0.73
24:AX:108:LEU:HD23	24:AX:141:VAL:HG21	1.71	0.73
86:s:203:ARG:NH1	86:s:238:ASN:OD1	2.21	0.73
39:F:115:LYS:NZ	101:F:401:HOH:O	2.21	0.72
1:AA:1287:A:OP2	4:AD:260:LYS:NZ	2.21	0.72
53:U:11:ARG:NH2	54:V:211:LYS:O	2.22	0.72
1:AA:941:G:OP1	101:AA:1802:HOH:O	2.07	0.72
83:p:111:ILE:O	83:p:116:ARG:NH1	2.22	0.72
35:A:2779:C:OP1	88:z:115:THR:OG1	2.08	0.71
22:AV:208:LEU:HD13	22:AV:226:TYR:HD2	1.56	0.71
22:AV:46:GLU:OE2	22:AV:74:ARG:NE	2.21	0.70
1:AA:1047:A:OP2	101:AA:1804:HOH:O	2.09	0.70
22:AV:226:TYR:CE1	22:AV:282:VAL:HG21	2.27	0.69
79:k:40:GLU:OE1	101:k:201:HOH:O	2.10	0.69
1:AA:1570:G:O6	101:AA:1803:HOH:O	2.09	0.69
65:6:217:LEU:HD11	65:6:271:LEU:HD12	1.74	0.69
35:A:1777:A:N6	35:A:1780:U:OP2	2.25	0.69
35:A:3015:U:OP1	101:A:3506:HOH:O	2.10	0.69
88:z:262:MET:SD	88:z:270:ASN:ND2	2.66	0.69
35:A:2290:A:N7	101:A:3533:HOH:O	2.26	0.69
25:AY:318:GLU:OE1	101:AY:401:HOH:O	2.11	0.68
89:Ay:75:C:O2'	89:Ay:76:A:OP1	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:272:THR:OG1	24:AX:282:ILE:O	2.10	0.68
31:A4:556:LYS:NZ	31:A4:560:GLU:OE2	2.27	0.68
85:r:35:PHE:N	85:r:56:THR:HG1	1.92	0.68
1:AA:976:A:N7	101:AA:1832:HOH:O	2.25	0.68
1:AA:1578:A:OP2	101:AA:1806:HOH:O	2.11	0.68
35:A:2181:A:OP1	101:A:3509:HOH:O	2.12	0.68
1:AA:1314:C:OP2	101:AA:1805:HOH:O	2.11	0.68
44:L:95:ARG:NH2	101:L:201:HOH:O	2.28	0.67
35:A:2562:U:O2'	37:D:284:ARG:O	2.09	0.67
51:S:112:ASP:OD2	101:S:301:HOH:O	2.13	0.67
46:N:73:ARG:O	46:N:155:LYS:NZ	2.27	0.67
35:A:2103:A:HO2'	58:Z:35:LYS:N	1.93	0.67
1:AA:1040:U:OP2	101:AA:1807:HOH:O	2.14	0.66
46:N:212:PRO:O	101:N:301:HOH:O	2.13	0.66
35:A:2543:C:OP1	101:A:3508:HOH:O	2.11	0.66
1:AA:1154:A:OP2	30:A3:155:ARG:NH2	2.29	0.66
1:AA:684:U:OP1	101:AA:1808:HOH:O	2.14	0.66
37:D:281:TRP:O	37:D:285:LYS:NZ	2.29	0.66
1:AA:1151:C:N3	101:AA:1843:HOH:O	2.29	0.66
40:H:178:ASN:OD1	40:H:179:ASN:N	2.28	0.66
46:N:143:GLY:O	101:N:302:HOH:O	2.14	0.66
64:5:165:GLN:NE2	64:5:179:VAL:HG21	2.11	0.66
35:A:2372:U:OP2	101:A:3511:HOH:O	2.14	0.66
28:A1:224:TYR:HH	81:m:115:HIS:HD1	0.69	0.66
97:AX:501:ATP:O1G	101:AX:601:HOH:O	2.15	0.65
35:A:1957:A:OP1	101:A:3510:HOH:O	2.13	0.65
35:A:2314:C:OP2	101:A:3512:HOH:O	2.14	0.65
1:AA:894:C:OP1	101:AA:1809:HOH:O	2.14	0.65
35:A:2160:A:OP2	63:4:88:TRP:NE1	2.29	0.65
65:6:322:ARG:NH1	101:6:502:HOH:O	2.29	0.65
1:AA:930:G:O6	10:AJ:47:ARG:NH2	2.29	0.65
67:8:133:ARG:NH1	101:8:301:HOH:O	2.24	0.65
31:A4:344:ARG:NH1	34:Az:31:A:OP1	2.30	0.64
35:A:1990:G:OP1	37:D:269:ARG:NH2	2.28	0.64
35:A:2826:G:OP1	55:W:49:ARG:NH1	2.31	0.64
35:A:1882:A:N7	101:A:3546:HOH:O	2.29	0.64
1:AA:828:C:OP2	101:AA:1810:HOH:O	2.15	0.64
35:A:2216:A:O2'	101:A:3505:HOH:O	2.09	0.64
35:A:2539:A:OP1	101:A:3515:HOH:O	2.15	0.64
35:A:1856:A:OP2	35:A:2986:C:O2'	2.16	0.64
35:A:2531:U:O4	37:D:246:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:1745:U:O4	62:3:108:LYS:NZ	2.30	0.63
4:AD:244:LEU:HD22	4:AD:343:LEU:HD23	1.81	0.63
7:AG:210:VAL:HG12	7:AG:210:VAL:O	1.98	0.63
25:AY:322:ASP:O	25:AY:324:ASP:N	2.32	0.62
35:A:2740:A:N3	35:A:2921:A:O2'	2.32	0.62
3:AC:109:VAL:HG23	28:A1:103:LEU:HD11	1.82	0.61
35:A:1871:A:N3	62:3:104:ARG:NH2	2.48	0.61
38:E:129:VAL:CG1	38:E:145:LEU:HD11	2.30	0.61
6:AF:174:LEU:O	6:AF:179:ARG:NH1	2.33	0.61
78:j:45:GLU:OE2	78:j:70:ARG:NH2	2.31	0.61
35:A:2767:A:O2'	35:A:2769:A:N7	2.33	0.61
47:O:62:TYR:OH	49:Q:272:GLU:OE2	2.18	0.61
1:AA:1458:A:OP1	6:AF:104:LYS:NZ	2.29	0.61
57:Y:134:LYS:NZ	68:9:76:TYR:OH	2.32	0.61
84:q:107:GLN:O	84:q:107:GLN:NE2	2.34	0.61
58:Z:78:ARG:O	58:Z:83:LYS:NZ	2.34	0.60
71:c:33:LYS:NZ	101:c:401:HOH:O	2.22	0.60
8:AH:104:ILE:HG23	8:AH:148:LEU:HD21	1.84	0.60
24:AX:265:ILE:HD11	24:AX:297:MET:HE2	1.82	0.60
1:AA:1554:G:OP2	101:AA:1814:HOH:O	2.17	0.60
1:AA:899:G:O2'	1:AA:907:A:N1	2.33	0.60
88:z:139:PRO:CB	88:z:245:VAL:HG21	2.32	0.59
35:A:1747:G:OP2	35:A:1749:C:N4	2.34	0.59
42:J:113:THR:OG1	42:J:116:HIS:ND1	2.26	0.59
66:7:175:ILE:O	66:7:319:ARG:NH2	2.35	0.59
35:A:3013:G:HO2'	63:4:66:PHE:N	2.01	0.59
29:A2:64:ASP:OD1	29:A2:65:ALA:N	2.36	0.59
41:I:31:LYS:NZ	101:I:301:HOH:O	2.35	0.59
68:9:16:ASP:OD1	68:9:25:ARG:NH2	2.35	0.59
84:q:167:GLN:O	84:q:171:ARG:NE	2.36	0.59
35:A:1958:G:OP1	101:A:3516:HOH:O	2.17	0.58
35:A:2104:A:OP1	46:N:231:SER:OG	2.21	0.58
35:A:2108:G:O6	46:N:67:LYS:NZ	2.36	0.58
1:AA:1308:U:O2'	3:AC:64:HIS:ND1	2.36	0.58
1:AA:1188:A:OP2	1:AA:1429:C:O2'	2.15	0.58
1:AA:1294:A:OP1	2:AB:201:ASN:ND2	2.36	0.58
35:A:2196:A:O2'	35:A:2213:A:N1	2.35	0.58
38:E:129:VAL:HG11	38:E:145:LEU:HD11	1.86	0.58
1:AA:769:G:OP2	14:AN:73:ARG:NH2	2.35	0.58
44:L:130:ARG:NH1	44:L:133:GLU:OE2	2.36	0.58
22:AV:208:LEU:HD13	22:AV:226:TYR:CD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:z:127:LEU:O	88:z:129:MET:N	2.37	0.58
1:AA:1208:U:OP1	101:AA:1813:HOH:O	2.16	0.57
101:AA:1827:HOH:O	5:AE:123:ARG:NH2	2.36	0.57
35:A:2021:U:OP1	101:A:3517:HOH:O	2.17	0.57
38:E:50:ASP:O	47:O:138:ARG:NH2	2.37	0.57
39:F:70:ARG:NH2	39:F:194:GLU:OE1	2.37	0.57
75:g:118:TRP:NE1	75:g:142:GLU:OE2	2.31	0.57
11:AK:58:ARG:NE	11:AK:72:ASP:OD1	2.36	0.57
35:A:3089:A:H3'	35:A:3090:G:C5'	2.34	0.57
88:z:139:PRO:HB3	88:z:245:VAL:HG21	1.86	0.57
28:A1:152:ASP:OD2	28:A1:174:ARG:NH1	2.31	0.57
35:A:3110:C:O2'	38:E:266:ARG:NH1	2.38	0.57
1:AA:1015:A:OP2	101:AA:1816:HOH:O	2.18	0.56
18:AR:69:THR:N	18:AR:72:ASP:OD2	2.38	0.56
1:AA:1109:A:OP2	101:AA:1815:HOH:O	2.17	0.56
2:AB:88:ARG:NH1	101:AB:403:HOH:O	2.38	0.56
4:AD:245:VAL:HG22	4:AD:271:ALA:HB1	1.86	0.56
6:AF:172:VAL:HG12	6:AF:240:ARG:HD3	1.86	0.56
58:Z:101:LYS:NZ	78:j:83:GLU:OE1	2.39	0.56
88:z:130:ALA:O	88:z:282:ARG:NH1	2.38	0.56
73:e:177:GLU:O	73:e:190:ARG:NH2	2.38	0.56
29:A2:43:ALA:HB1	29:A2:46:ILE:HD11	1.88	0.56
35:A:2364:C:OP2	53:U:78:LYS:NZ	2.38	0.56
42:J:25:ARG:NH1	80:l:58:ASP:OD1	2.37	0.55
88:z:61:THR:HG22	88:z:131:LEU:CD2	2.37	0.55
22:AV:236:LEU:CD1	22:AV:290:LEU:HD13	2.36	0.55
48:P:138:GLU:OE2	101:P:201:HOH:O	2.18	0.55
1:AA:1078:A:OP1	33:Ax:38:U:O2'	2.23	0.55
4:AD:340:ILE:HG22	4:AD:340:ILE:O	2.07	0.55
35:A:1760:G:OP1	45:M:196:ARG:NE	2.40	0.55
1:AA:1257:U:O2'	1:AA:1260:A:OP2	2.14	0.55
29:A2:33:VAL:HG21	29:A2:104:LEU:HD23	1.87	0.55
89:Ay:75:C:HO2'	89:Ay:76:A:P	2.29	0.55
35:A:1805:A:OP2	54:V:94:HIS:NE2	2.36	0.55
1:AA:1346:A:OP2	101:AA:1818:HOH:O	2.18	0.54
1:AA:845:A:H4'	21:AU:60:TYR:CE2	2.43	0.54
22:AV:228:TYR:HB3	22:AV:259:ALA:HB2	1.89	0.54
1:AA:843:G:N2	1:AA:846:A:OP2	2.35	0.54
1:AA:1044:U:OP1	1:AA:1110:A:O2'	2.22	0.54
22:AV:236:LEU:HD12	22:AV:290:LEU:HD13	1.89	0.54
24:AX:151:LEU:CD2	24:AX:247:LEU:HD22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:2016:C:OP2	45:M:59:ARG:NH1	2.41	0.54
1:AA:1264:C:H1'	8:AH:124:VAL:HG13	1.90	0.53
10:AJ:117:ASP:OD1	101:AJ:201:HOH:O	2.17	0.53
52:T:184:LYS:NZ	52:T:192:GLU:OE1	2.38	0.53
35:A:2761:C:O2	35:A:2786:U:N3	2.42	0.53
24:AX:108:LEU:HD21	24:AX:307:VAL:HG11	1.90	0.53
35:A:2462:A:N3	101:A:3569:HOH:O	2.34	0.53
8:AH:149:THR:HG1	28:A1:131:THR:HG1	1.55	0.53
8:AH:184:ILE:O	8:AH:184:ILE:HG22	2.08	0.53
35:A:2071:U:O2'	65:6:28:ARG:NH2	2.42	0.52
65:6:374:GLU:OE2	83:p:140:SER:OG	2.21	0.52
35:A:2354:A:O2'	101:A:3503:HOH:O	2.05	0.52
35:A:1953:A:O2'	35:A:2463:A:OP1	2.26	0.52
29:A2:36:ARG:NH2	29:A2:92:THR:HG23	2.25	0.52
7:AG:229:LEU:HD21	7:AG:241:VAL:HG11	1.91	0.52
1:AA:702:C:OP1	1:AA:848:U:O2'	2.26	0.52
7:AG:200:LEU:HD11	7:AG:204:GLU:HB3	1.91	0.52
65:6:161:LEU:HD13	65:6:271:LEU:HD11	1.91	0.52
75:g:154:ASP:OD1	75:g:155:GLN:N	2.43	0.52
64:5:173:ARG:HA	64:5:176:TYR:CE1	2.45	0.52
9:AI:87:HIS:NE2	101:AI:201:HOH:O	2.25	0.51
73:e:210:CYS:SG	101:e:309:HOH:O	2.43	0.51
35:A:3190:A:OP2	85:r:120:LYS:NZ	2.43	0.51
89:Ay:75:C:O2'	89:Ay:76:A:P	2.68	0.51
71:c:80:GLN:O	71:c:210:ARG:NH2	2.43	0.51
30:A3:144:ARG:NH2	101:A3:301:HOH:O	2.43	0.51
35:A:1749:C:OP2	35:A:2899:C:O2'	2.28	0.51
79:k:65:ASP:OD2	79:k:73:ARG:NH2	2.43	0.51
70:b:85:ARG:NH1	70:b:107:GLN:OE1	2.43	0.51
35:A:1742:G:O2'	35:A:1754:G:O6	2.23	0.51
54:V:163:ASP:OD1	54:V:164:GLY:N	2.44	0.51
72:d:81:THR:HG22	72:d:82:ALA:N	2.25	0.51
1:AA:1134:G:OP2	10:AJ:38:ARG:NH2	2.43	0.51
32:Aw:76:A:O3'	35:A:3072:U:O4	2.22	0.51
22:AV:187:PHE:CE1	22:AV:352:LEU:HD13	2.46	0.51
5:AE:65:LEU:HD11	16:AP:75:LYS:CD	2.41	0.51
6:AF:234:ARG:HB2	29:A2:53:MET:HE1	1.93	0.51
46:N:247:MET:SD	101:N:331:HOH:O	2.60	0.50
46:N:251:VAL:OXT	101:N:303:HOH:O	2.19	0.50
88:z:133:LYS:HG2	88:z:134:LYS:H	1.77	0.50
54:V:188:VAL:O	54:V:188:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:841:A:OP1	13:AM:39:ASN:ND2	2.42	0.50
22:AV:225:LEU:HD11	22:AV:283:LEU:HD22	1.94	0.50
24:AX:108:LEU:HD21	24:AX:307:VAL:CG1	2.42	0.50
24:AX:183:GLU:N	24:AX:183:GLU:OE1	2.42	0.50
28:A1:250:GLU:OE2	28:A1:301:ASN:ND2	2.45	0.50
56:X:177:HIS:O	56:X:184:ARG:NH1	2.44	0.50
73:e:106:HIS:CG	73:e:106:HIS:O	2.64	0.50
88:z:61:THR:HG23	88:z:134:LYS:HG3	1.94	0.50
35:A:2162:C:OP2	101:A:3519:HOH:O	2.19	0.49
66:7:277:GLN:O	66:7:301:SER:OG	2.26	0.49
35:A:2537:G:O2'	35:A:2634:U:OP2	2.26	0.49
72:d:89:VAL:HG23	72:d:89:VAL:O	2.12	0.49
28:A1:46:ARG:HB2	28:A1:47:PRO:HD3	1.93	0.49
1:AA:768:A:O2'	14:AN:24:LYS:NZ	2.45	0.49
1:AA:1004:G:O2'	9:AI:98:GLN:NE2	2.45	0.49
51:S:173:ARG:HB2	51:S:182:LYS:HG2	1.92	0.49
40:H:146:LEU:O	40:H:150:GLY:N	2.42	0.49
88:z:129:MET:HG2	88:z:129:MET:O	2.13	0.49
1:AA:1215:U:O4	101:AA:1819:HOH:O	2.18	0.49
43:K:52:ASP:OD1	101:K:201:HOH:O	2.19	0.49
29:A2:33:VAL:HG22	29:A2:105:ASN:OD1	2.13	0.49
35:A:2483:U:H2'	35:A:2484:C:O4'	2.13	0.49
1:AA:1103:A:N7	1:AA:1574:G:O2'	2.46	0.48
15:AO:208:PRO:HG2	15:AO:213:LEU:HD21	1.94	0.48
28:A1:46:ARG:HB2	28:A1:47:PRO:CD	2.43	0.48
24:AX:268:LEU:HD21	24:AX:293:LEU:HD23	1.96	0.48
54:V:169:THR:HG22	54:V:169:THR:O	2.12	0.48
3:AC:106:ASP:OD1	3:AC:107:GLN:N	2.43	0.48
6:AF:159:VAL:CG2	6:AF:172:VAL:HG21	2.40	0.48
26:AZ:17:ARG:NH2	81:m:111:SER:OG	2.42	0.48
7:AG:384:GLN:NE2	101:AG:404:HOH:O	2.47	0.48
31:A4:239:ARG:O	31:A4:242:ASN:ND2	2.44	0.48
35:A:2909:G:OP1	60:1:63:ARG:NH1	2.42	0.48
10:AJ:78:ARG:NH2	10:AJ:117:ASP:OD2	2.47	0.48
55:W:102:GLU:OE2	65:6:74:TYR:N	2.45	0.48
8:AH:155:VAL:HG21	28:A1:129:PHE:CB	2.43	0.48
35:A:2888:A:H3'	35:A:2889:C:C5'	2.44	0.48
47:O:64:LYS:NZ	47:O:100:GLN:O	2.47	0.48
35:A:2499:U:OP2	35:A:2504:A:N6	2.36	0.48
1:AA:1427:A:N7	101:AA:1873:HOH:O	2.35	0.48
66:7:156:ARG:HG3	66:7:156:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:z:133:LYS:HG2	88:z:134:LYS:N	2.29	0.48
1:AA:749:G:O3'	14:AN:78:LYS:NZ	2.40	0.47
15:AO:217:ARG:NH1	15:AO:227:GLU:OE2	2.46	0.47
22:AV:360:VAL:HG13	22:AV:364:LEU:HD22	1.96	0.47
1:AA:1479:C:OP1	101:AA:1820:HOH:O	2.20	0.47
22:AV:190:LEU:HD13	22:AV:226:TYR:CE2	2.49	0.47
35:A:1851:G:H2'	35:A:2693:A:N7	2.29	0.47
47:O:144:LEU:HD12	66:7:174:VAL:HG11	1.97	0.47
51:S:182:LYS:NZ	101:S:302:HOH:O	2.35	0.47
3:AC:115:ASN:ND2	25:AY:309:LYS:O	2.48	0.47
35:A:3201:A:H2'	35:A:3202:U:O4'	2.15	0.47
1:AA:875:U:O2'	1:AA:882:A:N1	2.45	0.47
3:AC:109:VAL:CG2	28:A1:103:LEU:HD11	2.45	0.47
4:AD:88:SER:N	101:AD:504:HOH:O	2.47	0.47
12:AL:126:GLU:HG2	12:AL:177:VAL:HG11	1.97	0.47
35:A:1697:A:N3	35:A:1703:C:O2'	2.48	0.47
41:I:197:LEU:HD12	41:I:198:PRO:HD2	1.97	0.47
20:AT:132:ARG:NH1	20:AT:136:LEU:O	2.48	0.47
35:A:2472:A:O2'	35:A:2478:G:N7	2.47	0.47
1:AA:1453:A:OP1	101:AA:1822:HOH:O	2.21	0.47
8:AH:125:HIS:CE1	8:AH:126:ILE:HG23	2.49	0.47
15:AO:221:GLN:NE2	22:AV:314:VAL:O	2.39	0.47
42:J:75:ASP:OD1	42:J:77:THR:HG22	2.15	0.47
35:A:1958:G:O2'	101:A:3518:HOH:O	2.18	0.47
35:A:2663:C:OP1	47:O:13:ARG:NH2	2.47	0.47
40:H:53:THR:N	40:H:86:THR:HG1	2.12	0.47
6:AF:176:ASP:OD2	6:AF:180:ARG:NH1	2.48	0.47
66:7:106:ALA:O	66:7:113:TRP:N	2.47	0.47
71:c:267:LEU:N	71:c:268:PRO:HD3	2.30	0.47
74:f:147:ASP:OD1	81:m:72:ARG:NH2	2.39	0.47
52:T:85:ALA:O	52:T:139:SER:OG	2.33	0.46
8:AH:155:VAL:HG21	28:A1:129:PHE:HB2	1.97	0.46
24:AX:153:LEU:HD21	24:AX:244:LEU:CD2	2.46	0.46
53:U:66:ALA:HB2	53:U:100:ALA:HA	1.98	0.46
54:V:127:ASP:O	54:V:129:LYS:N	2.49	0.46
59:0:133:GLU:OE2	59:0:160:TYR:OH	2.26	0.46
38:E:47:THR:OG1	38:E:51:GLU:OE1	2.22	0.46
22:AV:225:LEU:HD21	22:AV:280:LEU:HD23	1.97	0.46
40:H:107:VAL:HG12	40:H:108:ARG:N	2.30	0.46
88:z:250:GLU:O	88:z:250:GLU:HG2	2.16	0.46
22:AV:87:HIS:ND1	49:Q:60:PRO:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:2458:A:O2'	38:E:215:PHE:O	2.29	0.46
8:AH:184:ILE:O	8:AH:184:ILE:CG2	2.63	0.46
39:F:218:LEU:HD23	39:F:260:VAL:HB	1.98	0.46
7:AG:102:GLU:OE1	7:AG:102:GLU:N	2.44	0.46
27:A0:54:ALA:O	27:A0:58:VAL:HG23	2.16	0.46
35:A:2777:G:N3	40:H:179:ASN:ND2	2.63	0.46
66:7:257:ILE:O	66:7:257:ILE:HG13	2.15	0.46
8:AH:151:SER:O	8:AH:155:VAL:HG23	2.16	0.46
24:AX:81:HIS:ND1	24:AX:190:ASN:HB3	2.31	0.46
31:A4:305:ILE:HG22	31:A4:306:ASN:N	2.31	0.46
31:A4:493:MET:HE2	31:A4:493:MET:HA	1.98	0.46
35:A:1867:A:N1	35:A:2019:G:O2'	2.36	0.46
72:d:81:THR:HG22	72:d:82:ALA:H	1.80	0.46
35:A:2506:A:H1'	35:A:2601:A:N6	2.31	0.46
6:AF:193:ASP:OD1	6:AF:194:LYS:N	2.49	0.45
20:AT:92:THR:O	20:AT:92:THR:HG22	2.16	0.45
21:AU:56:LEU:HD11	21:AU:60:TYR:CZ	2.52	0.45
65:6:215:THR:OG1	65:6:275:GLN:OE1	2.31	0.45
27:A0:41:LEU:HD13	27:A0:55:TRP:CG	2.52	0.45
43:K:67:PHE:HB3	43:K:71:LYS:HB2	1.99	0.45
45:M:43:ARG:NH2	101:M:404:HOH:O	2.50	0.45
73:e:223:THR:HG22	73:e:224:GLU:N	2.31	0.45
88:z:77:TYR:HB2	88:z:97:TYR:OH	2.15	0.45
1:AA:1057:G:H4'	1:AA:1578:A:H4'	1.98	0.45
4:AD:312:TYR:N	4:AD:331:ASP:OD2	2.49	0.45
18:AR:169:GLU:OE1	27:A0:180:LYS:NZ	2.42	0.45
84:q:162:GLU:O	84:q:162:GLU:HG2	2.17	0.45
24:AX:265:ILE:CD1	24:AX:297:MET:HE2	2.45	0.45
65:6:224:HIS:HA	65:6:232:TYR:CE2	2.51	0.45
7:AG:198:ARG:NH1	7:AG:201:ILE:HG23	2.32	0.45
11:AK:70:VAL:HG11	25:AY:383:LYS:HE3	1.99	0.45
23:AW:92:MET:O	23:AW:98:LYS:NZ	2.49	0.45
31:A4:309:PHE:HB2	31:A4:345:PHE:CD1	2.52	0.45
38:E:111:THR:OG1	38:E:113:ASP:OD1	2.27	0.45
53:U:129:MET:HG3	72:d:82:ALA:HB2	1.98	0.45
75:g:108:THR:OG1	75:g:151:GLY:O	2.31	0.45
18:AR:317:ALA:O	18:AR:321:ALA:N	2.49	0.45
38:E:131:LYS:O	38:E:145:LEU:HD12	2.16	0.45
49:Q:251:GLU:OE1	49:Q:251:GLU:HA	2.16	0.45
54:V:147:SER:HG	54:V:152:ARG:H	1.63	0.45
58:Z:75:THR:HB	58:Z:83:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M:177:ALA:HA	45:M:222:TYR:CD1	2.52	0.45
86:s:174:LEU:HB3	86:s:175:PRO:HD3	1.99	0.44
18:AR:162:SER:O	18:AR:170:ARG:NH1	2.48	0.44
40:H:84:GLU:OE1	56:X:44:ARG:NH2	2.50	0.44
86:s:153:GLU:OE1	86:s:153:GLU:HA	2.18	0.44
19:AS:51:VAL:HG13	29:A2:117:LEU:HD11	1.99	0.44
35:A:3211:C:HO2'	35:A:3212:C:H5	1.59	0.44
49:Q:96:ARG:HA	49:Q:99:MET:HE3	1.99	0.44
64:5:105:TYR:CE1	64:5:262:ILE:HD12	2.53	0.44
76:h:87:GLN:OE1	76:h:124:ARG:NH1	2.51	0.44
39:F:98:GLN:NE2	101:F:406:HOH:O	2.51	0.44
58:Z:151:LEU:HD21	78:j:45:GLU:OE1	2.17	0.44
65:6:257:PRO:HB3	65:6:268:LEU:HD21	2.00	0.44
35:A:1822:U:O2	35:A:2707:A:O2'	2.33	0.44
35:A:2310:G:O2'	35:A:2675:G:O6	2.32	0.44
36:B:44:A:H2'	36:B:45:G:O4'	2.18	0.44
81:m:34:ASP:OD1	81:m:35:SER:N	2.51	0.44
88:z:123:LEU:HB3	88:z:257:ILE:HG12	2.00	0.44
88:z:125:LEU:HB3	88:z:127:LEU:HG	1.99	0.44
37:D:207:ILE:HG22	37:D:207:ILE:O	2.19	0.43
88:z:127:LEU:HD12	88:z:253:LEU:HD12	2.00	0.43
1:AA:1279:C:O2'	1:AA:1296:A:N1	2.49	0.43
7:AG:237:GLU:OE1	7:AG:237:GLU:N	2.50	0.43
35:A:2598:A:H3'	35:A:2625:C:H42	1.83	0.43
5:AE:65:LEU:HD11	16:AP:75:LYS:HD2	2.00	0.43
34:Az:-1:U:N3	34:Az:0:U:O4	2.51	0.43
1:AA:1080:A:O2'	1:AA:1082:A:N7	2.45	0.43
1:AA:1461:A:N6	101:AA:1898:HOH:O	2.41	0.43
5:AE:109:VAL:HG23	5:AE:109:VAL:O	2.19	0.43
40:H:223:VAL:N	40:H:231:VAL:O	2.46	0.43
88:z:139:PRO:HB2	88:z:245:VAL:HG21	1.99	0.43
7:AG:200:LEU:HD13	7:AG:246:ARG:CZ	2.49	0.43
35:A:1766:U:OP1	77:i:75:ARG:NH2	2.50	0.43
35:A:2259:C:O2'	35:A:2261:C:OP2	2.36	0.43
35:A:2135:A:N3	35:A:2135:A:H2'	2.34	0.43
66:7:51:GLU:OE1	66:7:51:GLU:HA	2.19	0.43
31:A4:58:VAL:O	31:A4:58:VAL:HG23	2.18	0.43
35:A:2293:A:N1	101:A:3603:HOH:O	2.37	0.43
35:A:2868:C:H2'	35:A:2869:A:O4'	2.19	0.43
5:AE:55:SER:O	5:AE:56:GLN:NE2	2.51	0.43
44:L:42:ASP:OD1	44:L:42:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:101:PRO:HB2	21:AU:60:TYR:CE1	2.53	0.43
35:A:1991:A:H5"	35:A:1992:C:OP1	2.18	0.43
35:A:2429:A:N1	35:A:2433:C:O2'	2.45	0.43
35:A:2116:C:O2'	35:A:2837:A:N3	2.47	0.42
35:A:2296:U:H5"	35:A:2297:A:OP1	2.19	0.42
49:Q:69:VAL:HG12	49:Q:71:PRO:HD3	2.00	0.42
28:A1:224:TYR:OH	81:m:115:HIS:ND1	2.15	0.42
31:A4:470:GLN:NE2	31:A4:472:ASP:OD2	2.52	0.42
35:A:3089:A:H3'	35:A:3090:G:H5'	2.01	0.42
46:N:135:SER:OG	46:N:138:HIS:CE1	2.72	0.42
71:c:161:THR:O	71:c:192:GLN:NE2	2.52	0.42
35:A:2882:U:O4'	48:P:173:ARG:NH2	2.52	0.42
51:S:152:ASP:OD1	51:S:153:LEU:N	2.53	0.42
31:A4:458:TYR:HB3	31:A4:486:TYR:CD1	2.54	0.42
35:A:1800:G:N1	35:A:1803:A:OP2	2.51	0.42
35:A:2039:A:N1	35:A:2932:G:O2'	2.48	0.42
24:AX:151:LEU:HD23	24:AX:247:LEU:HD22	2.00	0.42
35:A:2602:U:O4'	35:A:3078:C:O2'	2.27	0.42
54:V:165:ILE:HG21	68:9:76:TYR:CD2	2.54	0.42
54:V:181:ASP:O	57:Y:93:LYS:NZ	2.49	0.42
50:R:65:ARG:HA	50:R:68:TRP:CE3	2.55	0.42
67:8:202:VAL:O	67:8:203:GLU:HB3	2.19	0.42
76:h:69:ARG:NH2	76:h:107:ASP:OD1	2.53	0.42
1:AA:1199:G:N1	1:AA:1422:G:OP2	2.49	0.42
1:AA:1322:C:N3	4:AD:234:LYS:NZ	2.64	0.42
12:AL:213:VAL:O	12:AL:217:THR:HG23	2.20	0.42
35:A:2728:C:H4'	35:A:2815:OMG:HM22	2.01	0.42
70:b:41:ARG:NE	101:b:307:HOH:O	2.53	0.42
72:d:81:THR:HG1	72:d:209:TYR:HD2	1.64	0.42
3:AC:84:GLU:OE1	3:AC:84:GLU:N	2.44	0.42
28:A1:86:ARG:NH1	28:A1:96:PRO:O	2.50	0.42
52:T:206:LEU:HA	70:b:119:PHE:CE2	2.55	0.42
1:AA:1528:A:OP1	27:A0:101:ARG:NH2	2.51	0.42
4:AD:198:TRP:HA	4:AD:201:ILE:HD12	2.02	0.42
6:AF:114:THR:HG21	6:AF:205:LEU:HG	2.02	0.42
22:AV:241:ARG:HA	22:AV:244:TYR:CE2	2.55	0.42
27:A0:158:GLU:O	27:A0:158:GLU:HG2	2.20	0.42
35:A:3195:A:OP2	85:r:142:LYS:NZ	2.53	0.42
71:c:148:MET:HE2	71:c:307:PHE:CE2	2.54	0.42
81:m:96:ARG:O	81:m:99:GLN:HG3	2.20	0.42
85:r:37:GLU:OE1	85:r:52:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1265:C:H4'	8:AH:122:GLN:HG3	2.02	0.42
27:A0:110:ASP:OD1	27:A0:110:ASP:N	2.50	0.42
1:AA:948:U:O2'	101:AA:1823:HOH:O	2.21	0.41
3:AC:58:ALA:HB1	3:AC:59:PRO:CD	2.50	0.41
27:A0:13:GLU:OE2	27:A0:16:ARG:NH1	2.53	0.41
35:A:1787:G:N2	35:A:1790:A:OP2	2.51	0.41
35:A:2174:G:H4'	42:J:151:LEU:HD23	2.00	0.41
54:V:124:ASP:OD1	54:V:125:PRO:HD2	2.20	0.41
47:O:140:SER:O	47:O:146:ASN:ND2	2.50	0.41
64:5:56:GLU:O	64:5:56:GLU:HG3	2.19	0.41
66:7:114:ASP:OD1	66:7:268:LEU:N	2.53	0.41
12:AL:126:GLU:OE1	12:AL:126:GLU:N	2.41	0.41
22:AV:139:PRO:HD2	22:AV:144:PHE:CZ	2.55	0.41
35:A:2025:C:OP1	51:S:182:LYS:HD3	2.20	0.41
64:5:273:VAL:HG12	64:5:273:VAL:O	2.20	0.41
1:AA:1065:C:H2'	1:AA:1066:C:O4'	2.21	0.41
30:A3:173:LEU:HD12	30:A3:191:THR:HG23	2.02	0.41
35:A:1815:A:N1	101:A:3599:HOH:O	2.37	0.41
40:H:238:VAL:HG12	40:H:239:ASN:N	2.35	0.41
67:8:149:GLU:OE2	73:e:230:LYS:NZ	2.49	0.41
85:r:41:THR:HG23	85:r:41:THR:O	2.20	0.41
3:AC:75:ASN:ND2	11:AK:121:SER:O	2.53	0.41
18:AR:162:SER:O	18:AR:170:ARG:NH2	2.53	0.41
38:E:247:ASP:O	101:E:501:HOH:O	2.22	0.41
42:J:102:ARG:N	42:J:107:GLU:OE2	2.51	0.41
43:K:7:ALA:HB3	43:K:8:PRO:HD3	2.02	0.41
30:A3:159:GLU:OE2	35:A:2639:C:H5"	2.21	0.41
35:A:2015:G:O4'	45:M:56:GLU:HG3	2.21	0.41
38:E:69:ASP:OD1	38:E:154:ARG:NH1	2.54	0.41
52:T:49:ASN:ND2	52:T:68:TYR:O	2.53	0.41
53:U:146:GLY:O	72:d:179:LYS:NZ	2.54	0.41
88:z:311:LEU:HB2	88:z:312:PRO:HD3	2.02	0.41
1:AA:1046:A:O2'	1:AA:1048:C:OP2	2.34	0.41
2:AB:96:GLY:HA3	23:AW:159:ASP:OD2	2.21	0.41
2:AB:167:HIS:CD2	7:AG:153:THR:HA	2.56	0.41
14:AN:62:ASP:C	14:AN:62:ASP:OD1	2.64	0.41
35:A:1800:G:O6	54:V:34:LYS:NZ	2.52	0.41
70:b:44:ARG:NH2	82:o:99:LYS:O	2.53	0.41
72:d:109:THR:OG1	72:d:110:GLU:N	2.54	0.41
18:AR:162:SER:HB2	18:AR:165:ILE:HD12	2.02	0.41
25:AY:259:PHE:HB2	31:A4:363:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:2598:A:O2'	35:A:2599:U:H5'	2.21	0.41
52:T:94:ASP:OD2	66:7:97:GLU:N	2.38	0.41
69:a:44:ASN:OD1	69:a:44:ASN:C	2.63	0.41
1:AA:709:G:OP1	13:AM:13:ARG:NH2	2.53	0.41
1:AA:1001:C:N4	35:A:2558:A:O4'	2.54	0.41
1:AA:1289:G:O2'	1:AA:1297:G:OP2	2.32	0.41
2:AB:58:PHE:CD1	2:AB:58:PHE:C	2.98	0.41
14:AN:93:ASP:O	14:AN:97:GLY:N	2.48	0.41
25:AY:300:GLU:OE1	31:A4:87:TYR:OH	2.31	0.41
26:AZ:46:LYS:HA	26:AZ:49:TYR:CE1	2.55	0.41
35:A:2595:A:H2'	35:A:2596:G:O4'	2.21	0.41
46:N:87:PHE:HE1	46:N:169:PHE:HB2	1.85	0.41
74:f:48:TYR:N	101:f:304:HOH:O	2.54	0.41
87:u:60:TYR:HB2	87:u:61:PRO:HD3	2.02	0.41
1:AA:700:A:N1	1:AA:709:G:O2'	2.54	0.41
1:AA:1107:U:O4	30:A3:128:LYS:NZ	2.47	0.41
10:AJ:70:PRO:HB3	10:AJ:117:ASP:HB3	2.03	0.41
35:A:2343:G:H3'	35:A:2343:G:N3	2.36	0.41
45:M:14:ASP:OD1	45:M:15:LEU:N	2.54	0.41
55:W:103:VAL:HG11	65:6:61:ALA:HB1	2.03	0.41
84:q:169:ASP:N	84:q:170:PRO:HD2	2.35	0.41
1:AA:1066:C:O2'	9:AI:187:ARG:O	2.39	0.40
13:AM:19:ILE:HB	13:AM:83:LEU:HD23	2.03	0.40
42:J:110:GLY:C	42:J:111:LEU:HD12	2.46	0.40
65:6:324:ASP:OD1	65:6:324:ASP:C	2.64	0.40
88:z:78:MET:N	88:z:97:TYR:OH	2.54	0.40
88:z:97:TYR:HB3	88:z:306:LYS:HB2	2.03	0.40
31:A4:508:VAL:O	31:A4:508:VAL:HG12	2.20	0.40
35:A:2709:A:N3	59:0:98:GLN:OE1	2.53	0.40
40:H:193:PHE:O	40:H:198:GLY:N	2.54	0.40
54:V:130:PRO:O	54:V:149:ARG:NH1	2.54	0.40
66:7:36:SER:HB2	66:7:37:PRO:HD2	2.02	0.40
86:s:271:LEU:N	86:s:272:PRO:HA	2.35	0.40
5:AE:65:LEU:HD11	16:AP:75:LYS:HD3	2.03	0.40
22:AV:70:LEU:HD23	22:AV:393:GLU:OE1	2.22	0.40
35:A:2814:G:O2'	35:A:2983:G:OP1	2.39	0.40
41:I:144:LEU:N	41:I:145:PRO:HD2	2.37	0.40
47:O:36:LEU:O	47:O:40:GLU:N	2.50	0.40
1:AA:664:G:O2'	1:AA:1166:A:N1	2.50	0.40
1:AA:919:A:OP2	15:AO:96:ARG:NH2	2.49	0.40
35:A:2327:U:H2'	35:A:2328:C:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:A:3009:C:O2	35:A:3009:C:O5'	2.38	0.40
38:E:345:ILE:O	49:Q:172:GLN:NE2	2.51	0.40
42:J:69:LYS:HE3	42:J:69:LYS:HB2	1.96	0.40
47:O:86:ILE:HB	47:O:87:PRO:HD3	2.03	0.40
52:T:151:ARG:HB2	52:T:161:MET:HE2	2.03	0.40
83:p:108:ALA:O	83:p:116:ARG:NH1	2.55	0.40
16:AP:55:GLU:O	16:AP:56:ASN:C	2.64	0.40
35:A:2006:C:H2'	35:A:2007:U:C6	2.57	0.40
40:H:208:LEU:HB3	40:H:209:PRO:HD2	2.04	0.40
43:K:169:LEU:HD11	85:r:88:LEU:CD1	2.52	0.40
54:V:54:TRP:NE1	54:V:56:LEU:O	2.53	0.40

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	AB	223/296 (75%)	221 (99%)	2 (1%)	0	100 100
3	AC	130/167 (78%)	126 (97%)	4 (3%)	0	100 100
4	AD	341/430 (79%)	331 (97%)	10 (3%)	0	100 100
5	AE	120/125 (96%)	119 (99%)	1 (1%)	0	100 100
6	AF	206/242 (85%)	204 (99%)	2 (1%)	0	100 100
7	AG	323/396 (82%)	319 (99%)	4 (1%)	0	100 100
8	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18 18
9	AI	134/194 (69%)	132 (98%)	2 (2%)	0	100 100
10	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100 100
11	AK	99/128 (77%)	98 (99%)	1 (1%)	0	100 100
12	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AM	117/137 (85%)	117 (100%)	0	0	100	100
14	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
15	AO	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
16	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
17	AQ	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
18	AR	293/360 (81%)	284 (97%)	9 (3%)	0	100	100
19	AS	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
20	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	AU	174/205 (85%)	174 (100%)	0	0	100	100
22	AV	358/414 (86%)	353 (99%)	5 (1%)	0	100	100
23	AW	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
24	AX	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
25	AY	147/395 (37%)	146 (99%)	0	1 (1%)	18	18
26	AZ	98/106 (92%)	97 (99%)	1 (1%)	0	100	100
27	A0	213/217 (98%)	209 (98%)	4 (2%)	0	100	100
28	A1	277/323 (86%)	273 (99%)	4 (1%)	0	100	100
29	A2	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
30	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
31	A4	584/689 (85%)	577 (99%)	7 (1%)	0	100	100
37	D	236/305 (77%)	232 (98%)	4 (2%)	0	100	100
38	E	303/348 (87%)	296 (98%)	6 (2%)	1 (0%)	36	41
39	F	250/311 (80%)	247 (99%)	3 (1%)	0	100	100
40	H	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
41	I	210/261 (80%)	203 (97%)	7 (3%)	0	100	100
42	J	173/192 (90%)	173 (100%)	0	0	100	100
43	K	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
44	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
45	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
46	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
47	O	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
48	P	142/180 (79%)	142 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	Q	237/292 (81%)	237 (100%)	0	0	100	100
50	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
51	S	159/205 (78%)	156 (98%)	3 (2%)	0	100	100
52	T	164/206 (80%)	163 (99%)	1 (1%)	0	100	100
53	U	150/153 (98%)	147 (98%)	3 (2%)	0	100	100
54	V	203/216 (94%)	199 (98%)	4 (2%)	0	100	100
55	W	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
56	X	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
57	Y	179/250 (72%)	177 (99%)	2 (1%)	0	100	100
58	Z	120/161 (74%)	120 (100%)	0	0	100	100
59	0	108/188 (57%)	108 (100%)	0	0	100	100
60	1	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
61	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
62	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
63	4	36/103 (35%)	36 (100%)	0	0	100	100
64	5	392/423 (93%)	382 (97%)	10 (3%)	0	100	100
65	6	352/380 (93%)	344 (98%)	8 (2%)	0	100	100
66	7	292/338 (86%)	286 (98%)	6 (2%)	0	100	100
67	8	147/206 (71%)	144 (98%)	3 (2%)	0	100	100
68	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
69	a	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
70	b	148/215 (69%)	146 (99%)	2 (1%)	0	100	100
71	c	282/332 (85%)	279 (99%)	3 (1%)	0	100	100
72	d	235/306 (77%)	231 (98%)	4 (2%)	0	100	100
73	e	236/279 (85%)	229 (97%)	6 (2%)	1 (0%)	30	33
74	f	153/212 (72%)	152 (99%)	1 (1%)	0	100	100
75	g	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
76	h	108/158 (68%)	107 (99%)	1 (1%)	0	100	100
77	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
78	j	92/123 (75%)	90 (98%)	2 (2%)	0	100	100
79	k	99/112 (88%)	99 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	l	80/138 (58%)	80 (100%)	0	0	100	100
81	m	90/128 (70%)	89 (99%)	1 (1%)	0	100	100
82	o	92/102 (90%)	92 (100%)	0	0	100	100
83	p	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
84	q	153/222 (69%)	153 (100%)	0	0	100	100
85	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
86	s	382/439 (87%)	374 (98%)	8 (2%)	0	100	100
87	t	44/198 (22%)	44 (100%)	0	0	100	100
87	u	30/198 (15%)	30 (100%)	0	0	100	100
87	v	30/198 (15%)	30 (100%)	0	0	100	100
87	w	29/198 (15%)	29 (100%)	0	0	100	100
87	x	29/198 (15%)	29 (100%)	0	0	100	100
87	y	29/198 (15%)	29 (100%)	0	0	100	100
88	z	160/325 (49%)	151 (94%)	8 (5%)	1 (1%)	21	22
All	All	14595/19484 (75%)	14379 (98%)	211 (1%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	126	ILE
25	AY	323	ASP
88	z	128	ASP
38	E	150	LYS
73	e	197	GLU

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	AB	198/249 (80%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	115/143 (80%)	115 (100%)	0	100	100
4	AD	286/357 (80%)	286 (100%)	0	100	100
5	AE	104/107 (97%)	104 (100%)	0	100	100
6	AF	185/209 (88%)	185 (100%)	0	100	100
7	AG	285/342 (83%)	285 (100%)	0	100	100
8	AH	130/180 (72%)	130 (100%)	0	100	100
9	AI	104/146 (71%)	104 (100%)	0	100	100
10	AJ	93/118 (79%)	93 (100%)	0	100	100
11	AK	91/113 (80%)	91 (100%)	0	100	100
12	AL	158/226 (70%)	158 (100%)	0	100	100
13	AM	97/113 (86%)	97 (100%)	0	100	100
14	AN	96/115 (84%)	96 (100%)	0	100	100
15	AO	174/230 (76%)	174 (100%)	0	100	100
16	AP	88/123 (72%)	88 (100%)	0	100	100
17	AQ	78/79 (99%)	78 (100%)	0	100	100
18	AR	264/318 (83%)	264 (100%)	0	100	100
19	AS	116/164 (71%)	116 (100%)	0	100	100
20	AT	153/157 (98%)	153 (100%)	0	100	100
21	AU	152/174 (87%)	152 (100%)	0	100	100
22	AV	325/364 (89%)	325 (100%)	0	100	100
23	AW	87/158 (55%)	87 (100%)	0	100	100
24	AX	311/351 (89%)	311 (100%)	0	100	100
25	AY	137/357 (38%)	137 (100%)	0	100	100
26	AZ	90/95 (95%)	90 (100%)	0	100	100
27	A0	188/189 (100%)	188 (100%)	0	100	100
28	A1	257/291 (88%)	257 (100%)	0	100	100
29	A2	100/101 (99%)	100 (100%)	0	100	100
30	A3	65/166 (39%)	65 (100%)	0	100	100
31	A4	526/609 (86%)	526 (100%)	0	100	100
37	D	192/245 (78%)	192 (100%)	0	100	100
38	E	260/290 (90%)	260 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	F	219/262 (84%)	219 (100%)	0	100	100
40	H	182/228 (80%)	182 (100%)	0	100	100
41	I	194/232 (84%)	194 (100%)	0	100	100
42	J	138/150 (92%)	138 (100%)	0	100	100
43	K	154/155 (99%)	154 (100%)	0	100	100
44	L	98/124 (79%)	98 (100%)	0	100	100
45	M	246/249 (99%)	246 (100%)	0	100	100
46	N	189/211 (90%)	189 (100%)	0	100	100
47	O	134/150 (89%)	134 (100%)	0	100	100
48	P	126/155 (81%)	126 (100%)	0	100	100
49	Q	221/256 (86%)	221 (100%)	0	100	100
50	R	118/126 (94%)	118 (100%)	0	100	100
51	S	146/180 (81%)	146 (100%)	0	100	100
52	T	146/176 (83%)	146 (100%)	0	100	100
53	U	134/135 (99%)	134 (100%)	0	100	100
54	V	183/191 (96%)	183 (100%)	0	100	100
55	W	94/119 (79%)	94 (100%)	0	100	100
56	X	220/229 (96%)	220 (100%)	0	100	100
57	Y	163/223 (73%)	163 (100%)	0	100	100
58	Z	113/147 (77%)	113 (100%)	0	100	100
59	0	99/164 (60%)	99 (100%)	0	100	100
60	1	53/60 (88%)	53 (100%)	0	100	100
61	2	40/72 (56%)	40 (100%)	0	100	100
62	3	88/166 (53%)	88 (100%)	0	100	100
63	4	37/89 (42%)	37 (100%)	0	100	100
64	5	353/368 (96%)	353 (100%)	0	100	100
65	6	313/332 (94%)	313 (100%)	0	100	100
66	7	270/303 (89%)	270 (100%)	0	100	100
67	8	140/190 (74%)	140 (100%)	0	100	100
68	9	104/112 (93%)	104 (100%)	0	100	100
69	a	96/133 (72%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	b	131/185 (71%)	131 (100%)	0	100	100
71	c	251/288 (87%)	251 (100%)	0	100	100
72	d	223/274 (81%)	223 (100%)	0	100	100
73	e	207/236 (88%)	207 (100%)	0	100	100
74	f	139/188 (74%)	139 (100%)	0	100	100
75	g	124/148 (84%)	124 (100%)	0	100	100
76	h	104/148 (70%)	104 (100%)	0	100	100
77	i	86/110 (78%)	86 (100%)	0	100	100
78	j	74/97 (76%)	74 (100%)	0	100	100
79	k	83/90 (92%)	83 (100%)	0	100	100
80	l	76/116 (66%)	76 (100%)	0	100	100
81	m	85/113 (75%)	85 (100%)	0	100	100
82	o	80/87 (92%)	80 (100%)	0	100	100
83	p	135/181 (75%)	135 (100%)	0	100	100
84	q	132/178 (74%)	132 (100%)	0	100	100
85	r	147/169 (87%)	147 (100%)	0	100	100
86	s	340/381 (89%)	340 (100%)	0	100	100
87	t	40/158 (25%)	40 (100%)	0	100	100
87	u	31/158 (20%)	31 (100%)	0	100	100
87	v	31/158 (20%)	31 (100%)	0	100	100
87	w	30/158 (19%)	30 (100%)	0	100	100
87	x	30/158 (19%)	30 (100%)	0	100	100
87	y	30/158 (19%)	30 (100%)	0	100	100
88	z	150/287 (52%)	150 (100%)	0	100	100
All	All	13075/16790 (78%)	13075 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	113	HIS
2	AB	124	HIS

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Mol	Chain	Res	Type
2	AB	126	GLN
3	AC	154	HIS
3	AC	156	GLN
4	AD	356	GLN
4	AD	359	HIS
4	AD	415	GLN
5	AE	56	GLN
6	AF	127	HIS
6	AF	238	HIS
7	AG	176	GLN
7	AG	384	GLN
8	AH	133	GLN
8	AH	163	ASN
9	AI	96	GLN
9	AI	146	HIS
10	AJ	106	GLN
11	AK	28	HIS
13	AM	50	GLN
15	AO	166	HIS
15	AO	169	GLN
17	AQ	41	HIS
17	AQ	65	ASN
18	AR	288	GLN
18	AR	299	ASN
18	AR	320	GLN
19	AS	66	HIS
21	AU	188	ASN
22	AV	78	ASN
22	AV	141	ASN
22	AV	324	GLN
22	AV	380	GLN
23	AW	106	HIS
23	AW	110	ASN
23	AW	173	GLN
24	AX	69	ASN
24	AX	159	HIS
24	AX	257	HIS
24	AX	291	HIS
27	A0	111	HIS
27	A0	145	HIS
28	A1	122	HIS
28	A1	146	HIS

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Mol	Chain	Res	Type
28	A1	185	HIS
31	A4	175	GLN
31	A4	257	HIS
31	A4	470	GLN
31	A4	491	GLN
31	A4	495	HIS
31	A4	540	HIS
31	A4	602	HIS
31	A4	626	GLN
37	D	195	ASN
37	D	221	ASN
38	E	202	GLN
38	E	281	ASN
39	F	98	GLN
39	F	138	HIS
39	F	208	HIS
39	F	223	HIS
41	I	43	GLN
41	I	150	HIS
43	K	89	GLN
43	K	117	HIS
45	M	53	HIS
46	N	181	HIS
47	O	39	HIS
47	O	100	GLN
48	P	115	HIS
51	S	118	ASN
52	T	126	HIS
56	X	172	GLN
57	Y	99	HIS
58	Z	150	HIS
59	0	120	HIS
64	5	331	ASN
64	5	367	ASN
65	6	69	HIS
65	6	292	GLN
65	6	295	GLN
65	6	320	GLN
65	6	332	HIS
65	6	373	HIS
66	7	284	HIS
66	7	298	GLN

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Mol	Chain	Res	Type
66	7	305	HIS
67	8	143	GLN
67	8	158	HIS
71	c	77	HIS
72	d	77	HIS
72	d	193	HIS
73	e	75	GLN
73	e	144	ASN
73	e	252	HIS
77	i	124	HIS
80	l	135	ASN
82	o	21	HIS
82	o	94	HIS
84	q	107	GLN
85	r	96	HIS
86	s	107	GLN
86	s	423	HIS
88	z	104	HIS
88	z	241	HIS
88	z	266	GLN
88	z	272	GLN
88	z	276	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	953/954 (99%)	123 (12%)	0
32	Aw	20/22 (90%)	2 (10%)	0
33	Ax	68/70 (97%)	10 (14%)	0
34	Az	33/34 (97%)	13 (39%)	0
35	A	1556/1558 (99%)	220 (14%)	3 (0%)
36	B	71/72 (98%)	11 (15%)	0
89	Ay	48/52 (92%)	14 (29%)	0
All	All	2749/2762 (99%)	393 (14%)	3 (0%)

All (393) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	651	A
1	AA	680	U
1	AA	688	A

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Mol	Chain	Res	Type
1	AA	704	U
1	AA	721	U
1	AA	737	C
1	AA	738	A
1	AA	753	A
1	AA	761	A
1	AA	766	G
1	AA	773	U
1	AA	777	G
1	AA	786	G
1	AA	791	G
1	AA	794	U
1	AA	796	G
1	AA	830	U
1	AA	832	U
1	AA	835	C
1	AA	836	A
1	AA	860	A
1	AA	861	U
1	AA	868	C
1	AA	871	A
1	AA	890	C
1	AA	903	U
1	AA	904	C
1	AA	907	A
1	AA	919	A
1	AA	929	A
1	AA	932	C
1	AA	938	A
1	AA	939	A
1	AA	941	G
1	AA	942	A
1	AA	960	C
1	AA	962	C
1	AA	967	A
1	AA	1001	C
1	AA	1002	C
1	AA	1011	C
1	AA	1015	A
1	AA	1031	G
1	AA	1042	U
1	AA	1081	U

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Mol	Chain	Res	Type
1	AA	1082	A
1	AA	1103	A
1	AA	1105	C
1	AA	1106	C
1	AA	1107	U
1	AA	1109	A
1	AA	1113	G
1	AA	1118	A
1	AA	1121	A
1	AA	1126	A
1	AA	1137	A
1	AA	1151	C
1	AA	1153	C
1	AA	1160	A
1	AA	1167	A
1	AA	1179	G
1	AA	1187	U
1	AA	1189	U
1	AA	1190	C
1	AA	1193	U
1	AA	1199	G
1	AA	1200	G
1	AA	1220	A
1	AA	1223	C
1	AA	1225	C
1	AA	1229	U
1	AA	1247	G
1	AA	1248	C
1	AA	1250	C
1	AA	1251	A
1	AA	1271	C
1	AA	1273	G
1	AA	1284	U
1	AA	1285	G
1	AA	1290	C
1	AA	1291	U
1	AA	1292	A
1	AA	1326	A
1	AA	1327	G
1	AA	1343	A
1	AA	1354	A
1	AA	1356	A

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Mol	Chain	Res	Type
1	AA	1376	C
1	AA	1378	C
1	AA	1387	A
1	AA	1390	A
1	AA	1391	U
1	AA	1405	C
1	AA	1406	U
1	AA	1407	U
1	AA	1422	G
1	AA	1430	A
1	AA	1466	C
1	AA	1481	C
1	AA	1503	G
1	AA	1519	A
1	AA	1522	U
1	AA	1525	C
1	AA	1526	U
1	AA	1527	A
1	AA	1533	C
1	AA	1536	A
1	AA	1537	C
1	AA	1538	G
1	AA	1539	C
1	AA	1540	A
1	AA	1541	U
1	AA	1544	A
1	AA	1552	G
1	AA	1557	A
1	AA	1562	G
1	AA	1568	U
1	AA	1571	U
1	AA	1582	G
1	AA	1584	MA6
1	AA	1594	G
1	AA	1595	G
1	AA	1599	A
32	Aw	30	G
32	Aw	76	A
33	Ax	3	G
33	Ax	23	A
33	Ax	25	C
33	Ax	44	A

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Mol	Chain	Res	Type
33	Ax	45	G
33	Ax	46	A
33	Ax	48	U
33	Ax	49	G
33	Ax	59	U
33	Ax	62	C
34	Az	0	U
34	Az	4	A
34	Az	12	U
34	Az	13	U
34	Az	18	A
34	Az	21	A
34	Az	22	A
34	Az	23	U
34	Az	24	U
34	Az	25	U
34	Az	26	A
34	Az	27	C
34	Az	32	A
35	A	1678	C
35	A	1681	G
35	A	1689	C
35	A	1692	A
35	A	1700	U
35	A	1704	U
35	A	1708	A
35	A	1715	C
35	A	1724	A
35	A	1727	A
35	A	1728	U
35	A	1748	G
35	A	1765	C
35	A	1777	A
35	A	1805	A
35	A	1806	U
35	A	1807	U
35	A	1808	A
35	A	1810	A
35	A	1817	C
35	A	1821	A
35	A	1827	C
35	A	1828	A

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Mol	Chain	Res	Type
35	A	1829	A
35	A	1832	A
35	A	1836	A
35	A	1844	A
35	A	1854	U
35	A	1856	A
35	A	1869	A
35	A	1871	A
35	A	1882	A
35	A	1887	A
35	A	1893	A
35	A	1901	C
35	A	1903	C
35	A	1918	G
35	A	1937	A
35	A	1940	A
35	A	1958	G
35	A	1985	G
35	A	1992	C
35	A	1993	A
35	A	1994	A
35	A	2000	C
35	A	2003	A
35	A	2015	G
35	A	2022	G
35	A	2030	U
35	A	2032	G
35	A	2036	C
35	A	2037	U
35	A	2039	A
35	A	2054	U
35	A	2060	A
35	A	2069	U
35	A	2071	U
35	A	2079	C
35	A	2099	U
35	A	2113	G
35	A	2125	C
35	A	2126	U
35	A	2147	G
35	A	2160	A
35	A	2163	A

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Mol	Chain	Res	Type
35	A	2168	U
35	A	2181	A
35	A	2192	A
35	A	2198	A
35	A	2200	A
35	A	2207	A
35	A	2214	A
35	A	2219	C
35	A	2221	C
35	A	2222	U
35	A	2223	A
35	A	2224	C
35	A	2225	C
35	A	2226	U
35	A	2227	A
35	A	2230	A
35	A	2233	U
35	A	2237	A
35	A	2241	A
35	A	2243	A
35	A	2245	A
35	A	2246	A
35	A	2262	C
35	A	2263	C
35	A	2284	C
35	A	2285	U
35	A	2297	A
35	A	2300	G
35	A	2322	C
35	A	2331	C
35	A	2332	C
35	A	2345	G
35	A	2350	A
35	A	2353	A
35	A	2354	A
35	A	2357	C
35	A	2363	A
35	A	2372	U
35	A	2374	A
35	A	2390	A
35	A	2399	A
35	A	2401	A

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Mol	Chain	Res	Type
35	A	2404	U
35	A	2407	U
35	A	2415	C
35	A	2434	A
35	A	2446	A
35	A	2451	A
35	A	2478	G
35	A	2485	U
35	A	2493	C
35	A	2502	C
35	A	2520	C
35	A	2521	A
35	A	2527	A
35	A	2570	C
35	A	2592	G
35	A	2593	G
35	A	2594	U
35	A	2599	U
35	A	2600	A
35	A	2601	A
35	A	2603	C
35	A	2618	U
35	A	2627	G
35	A	2630	U
35	A	2633	A
35	A	2635	G
35	A	2654	U
35	A	2656	U
35	A	2683	C
35	A	2686	G
35	A	2694	A
35	A	2696	A
35	A	2706	A
35	A	2718	C
35	A	2719	G
35	A	2723	A
35	A	2724	G
35	A	2725	A
35	A	2732	G
35	A	2745	A
35	A	2757	A
35	A	2758	G

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Mol	Chain	Res	Type
35	A	2759	U
35	A	2762	C
35	A	2765	A
35	A	2767	A
35	A	2768	A
35	A	2775	A
35	A	2781	U
35	A	2782	A
35	A	2786	U
35	A	2788	C
35	A	2790	A
35	A	2791	A
35	A	2810	G
35	A	2832	A
35	A	2833	A
35	A	2847	C
35	A	2864	U
35	A	2865	C
35	A	2882	U
35	A	2883	A
35	A	2885	U
35	A	2888	A
35	A	2889	C
35	A	2893	A
35	A	2913	A
35	A	2917	G
35	A	2918	A
35	A	2922	A
35	A	2928	C
35	A	2932	G
35	A	2935	A
35	A	2956	A
35	A	2989	G
35	A	2990	A
35	A	2992	G
35	A	2993	U
35	A	3005	A
35	A	3016	G
35	A	3041	U
35	A	3053	A
35	A	3054	G
35	A	3060	C

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Mol	Chain	Res	Type
35	A	3072	U
35	A	3090	G
35	A	3100	U
35	A	3108	U
35	A	3109	U
35	A	3110	C
35	A	3111	A
35	A	3112	A
35	A	3113	A
35	A	3150	U
35	A	3157	C
35	A	3158	A
35	A	3162	C
35	A	3169	C
35	A	3172	C
35	A	3177	A
35	A	3183	U
35	A	3199	U
35	A	3200	U
35	A	3207	A
35	A	3209	A
35	A	3210	C
35	A	3212	C
35	A	3217	A
35	A	3218	A
35	A	3228	U
35	A	3229	U
35	A	3230	G
35	A	3231	U
36	B	8	U
36	B	16	C
36	B	21	A
36	B	45	G
36	B	48	U
36	B	54	C
36	B	55	U
36	B	56	U
36	B	64	A
36	B	69	U
36	B	76	A
89	Ay	3	G
89	Ay	4	G

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Mol	Chain	Res	Type
89	Ay	9	A
89	Ay	23	A
89	Ay	25	C
89	Ay	44	A
89	Ay	45	G
89	Ay	46	A
89	Ay	48	U
89	Ay	49	G
89	Ay	59	U
89	Ay	72	A
89	Ay	75	C
89	Ay	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	A	1691	C
35	A	2112	A
35	A	2245	A

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

20 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	$\#\|Z\| > 2$
35	OMG	A	3040	32,35	23,26,27	0.27	0	33,38,41	0.36	0
79	AYA	k	2	79	6,7,8	0.81	0	5,8,10	0.46	0
35	1MA	A	2617	35	21,25,26	0.75	1 (4%)	31,37,40	0.67	1 (3%)
1	MA6	AA	1583	1	23,26,27	0.29	0	34,38,41	0.57	1 (2%)
35	OMU	A	3039	35,94	19,22,23	0.27	0	26,31,34	0.44	0
9	5F0	AI	184	9	8,8,9	0.58	0	7,9,11	1.16	1 (14%)
1	5MU	AA	1076	1	19,22,23	0.62	0	28,32,35	1.21	3 (10%)
53	AYA	U	2	53	6,7,8	0.80	0	5,8,10	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	AYA	AQ	2	17	6,7,8	0.80	0	5,8,10	0.81	0
35	OMG	A	2815	33,35,94	23,26,27	0.29	0	33,38,41	0.40	0
29	AYA	A2	2	29	6,7,8	0.81	0	5,8,10	0.45	0
1	MA6	AA	1584	1	23,26,27	0.29	0	34,38,41	0.58	1 (2%)
36	PSU	B	39	36	18,21,22	0.76	0	22,30,33	2.54	4 (18%)
35	PSU	A	3067	35	18,21,22	0.78	0	22,30,33	2.56	5 (22%)
70	THC	b	2	70	8,9,10	0.28	0	9,11,13	0.48	0
1	5MC	AA	1488	1	18,22,23	0.32	0	26,32,35	0.42	0
43	SAC	K	2	43	7,8,9	0.22	0	8,9,11	0.61	0
36	1MA	B	9	36	21,25,26	0.76	1 (4%)	31,37,40	0.67	1 (3%)
1	B8T	AA	1486	93,1	19,22,23	0.29	0	26,31,34	0.34	0
36	2MG	B	10	36	23,26,27	0.49	0	32,38,41	0.51	0

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
35	OMG	A	3040	32,35	-	0/9/27/28	0/3/3/3
79	AYA	k	2	79	-	0/4/6/8	-
35	1MA	A	2617	35	-	0/7/25/26	0/3/3/3
1	MA6	AA	1583	1	-	0/11/29/30	0/3/3/3
35	OMU	A	3039	35,94	-	0/9/27/28	0/2/2/2
9	5F0	AI	184	9	-	0/9/9/10	-
1	5MU	AA	1076	1	-	0/7/25/26	0/2/2/2
53	AYA	U	2	53	-	1/4/6/8	-
17	AYA	AQ	2	17	-	1/4/6/8	-
35	OMG	A	2815	33,35,94	-	0/9/27/28	0/3/3/3
29	AYA	A2	2	29	-	0/4/6/8	-
1	MA6	AA	1584	1	-	2/11/29/30	0/3/3/3
36	PSU	B	39	36	-	0/7/25/26	0/2/2/2
35	PSU	A	3067	35	-	0/7/25/26	0/2/2/2
70	THC	b	2	70	-	0/8/10/12	-
1	5MC	AA	1488	1	-	0/7/25/26	0/2/2/2
43	SAC	K	2	43	-	0/7/8/10	-
36	1MA	B	9	36	-	0/7/25/26	0/3/3/3
1	B8T	AA	1486	93,1	-	0/7/27/28	0/2/2/2
36	2MG	B	10	36	-	0/9/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	2617	1MA	C6-N6	3.02	1.35	1.28
36	B	9	1MA	C6-N6	3.00	1.35	1.28

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B	39	PSU	N1-C2-N3	8.06	124.26	115.13
35	A	3067	PSU	N1-C2-N3	8.06	124.26	115.13
35	A	3067	PSU	C4-N3-C2	-6.55	116.90	126.34
36	B	39	PSU	C4-N3-C2	-6.50	116.97	126.34
1	AA	1076	5MU	C4-N3-C2	-4.77	121.18	127.35
36	B	39	PSU	O2-C2-N1	-3.68	118.74	122.79
35	A	3067	PSU	O2-C2-N1	-3.64	118.78	122.79
9	AI	184	5F0	O-C-CB	-2.69	117.58	125.43
1	AA	1076	5MU	C5-C4-N3	2.63	117.56	115.31
35	A	3067	PSU	O2-C2-N3	-2.58	116.96	121.82
36	B	39	PSU	O2-C2-N3	-2.56	117.00	121.82
1	AA	1584	MA6	C2-N1-C6	2.39	117.39	111.75
1	AA	1583	MA6	C2-N1-C6	2.35	117.31	111.75
1	AA	1076	5MU	N3-C2-N1	2.23	117.84	114.89
35	A	2617	1MA	N1-C6-N6	2.21	125.39	119.77
35	A	3067	PSU	O4'-C1'-C2'	2.15	108.17	105.14
36	B	9	1MA	N1-C6-N6	2.10	125.11	119.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AQ	2	AYA	C-CA-N-CT
1	AA	1584	MA6	C5-C6-N6-C9
53	U	2	AYA	C-CA-N-CT
1	AA	1584	MA6	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	2815	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 276 ligands modelled in this entry, 263 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
90	NAD	AA	1701	93	45,48,48	0.38	0	63,73,73	0.38	0
91	SPM	AA	1702	-	13,13,13	0.28	0	12,12,12	0.98	0
99	PUT	A	3304	-	5,5,5	0.25	0	4,4,4	0.53	0
96	FES	r	201	85,41	0,4,4	-	-	-		
92	SPD	A	3301	-	9,9,9	0.42	0	8,8,8	1.07	0
97	ATP	AX	501	93	29,33,33	0.50	0	44,52,52	0.49	0
100	VAL	B	101	36	4,6,7	0.51	0	6,7,9	0.95	0
96	FES	AT	201	20,13	0,4,4	-	-	-		
92	SPD	A	3302	-	9,9,9	0.33	0	8,8,8	1.22	0
92	SPD	AA	1703	-	9,9,9	0.28	0	8,8,8	1.31	2 (25%)
92	SPD	A	3303	-	9,9,9	0.38	0	8,8,8	1.14	0
98	GDP	AX	503	-	28,30,30	0.42	0	44,47,47	0.41	0
96	FES	AP	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
90	NAD	AA	1701	93	-	1/30/62/62	0/5/5/5
91	SPM	AA	1702	-	-	1/11/11/11	-
99	PUT	A	3304	-	-	0/3/3/3	-
96	FES	r	201	85,41	-	-	0/1/1/1
92	SPD	A	3301	-	-	2/7/7/7	-
97	ATP	AX	501	93	-	0/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
100	VAL	B	101	36	-	1/5/6/8	-
96	FES	AT	201	20,13	-	-	0/1/1/1
92	SPD	A	3302	-	-	0/7/7/7	-
92	SPD	AA	1703	-	-	0/7/7/7	-
92	SPD	A	3303	-	-	2/7/7/7	-
98	GDP	AX	503	-	-	0/16/32/32	0/3/3/3
96	FES	AP	201	5,16	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	AA	1703	SPD	C4-C5-N6	-2.24	106.09	112.14
92	AA	1703	SPD	C8-C7-N6	-2.13	106.38	112.14

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	A	3301	SPD	N6-C7-C8-C9
92	A	3301	SPD	C3-C4-C5-N6
92	A	3303	SPD	C4-C5-N6-C7
91	AA	1702	SPM	C12-C11-N10-C9
92	A	3303	SPD	C8-C7-N6-C5
100	B	101	VAL	O-C-CA-CB
90	AA	1701	NAD	C2B-C1B-N9A-C8A

There are no ring outliers.

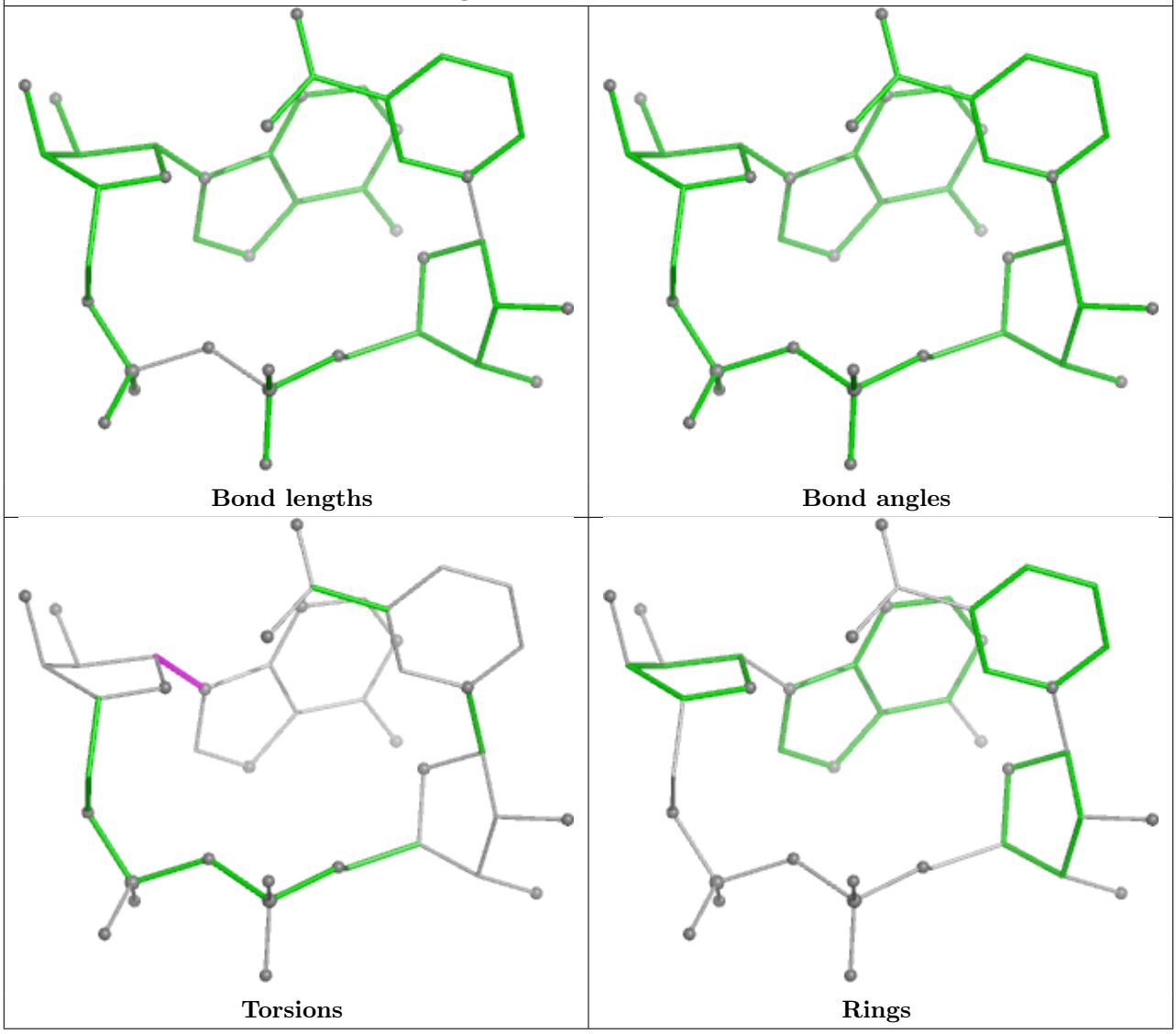
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AX	501	ATP	1	0

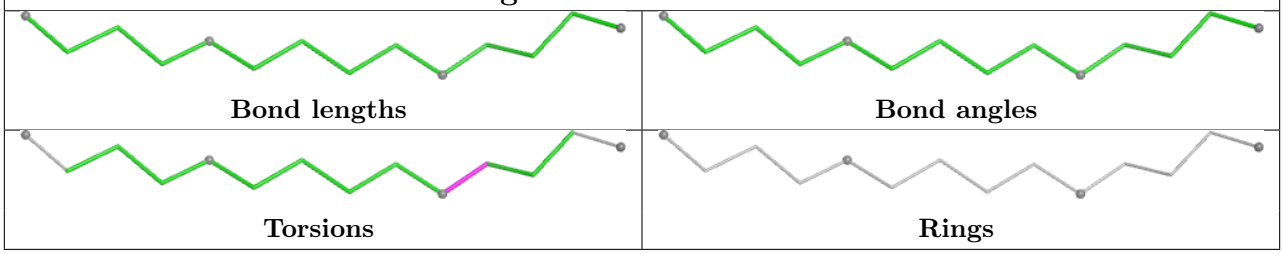
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

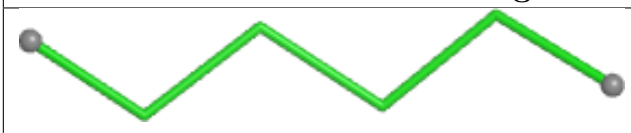
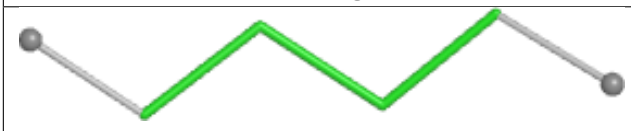
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

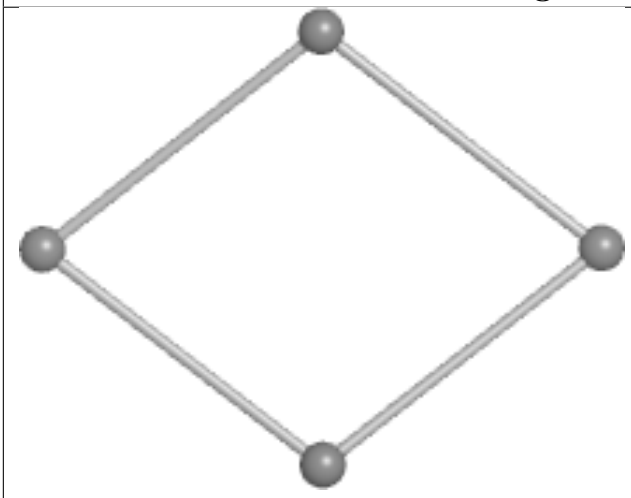
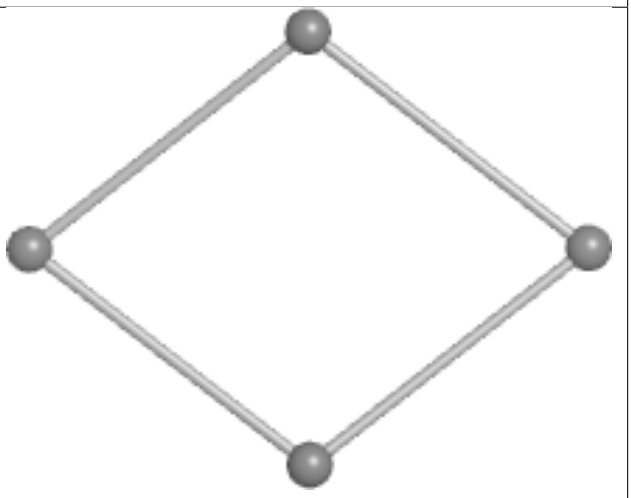
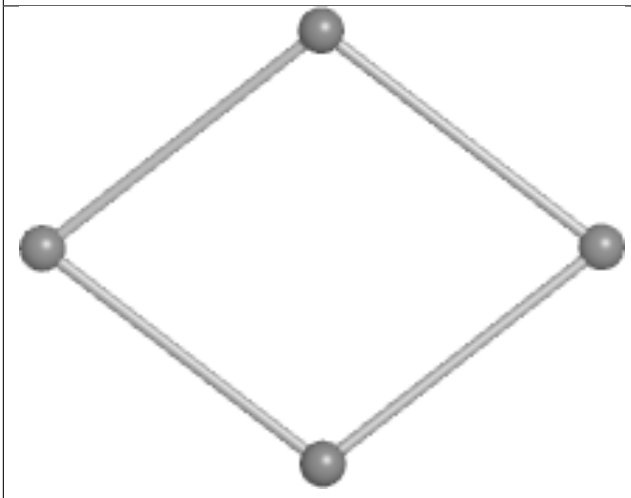
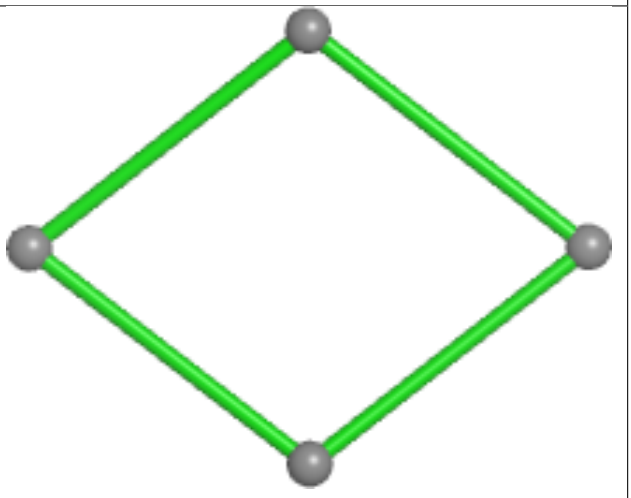
Ligand NAD AA 1701



Ligand SPM AA 1702



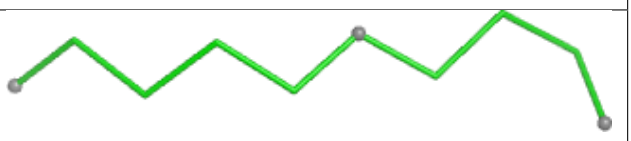
Ligand PUT A 3304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES r 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPD A 3301



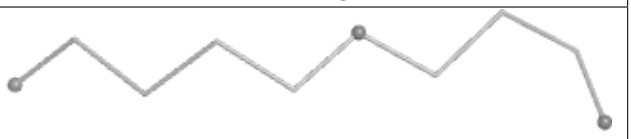
Bond lengths



Bond angles

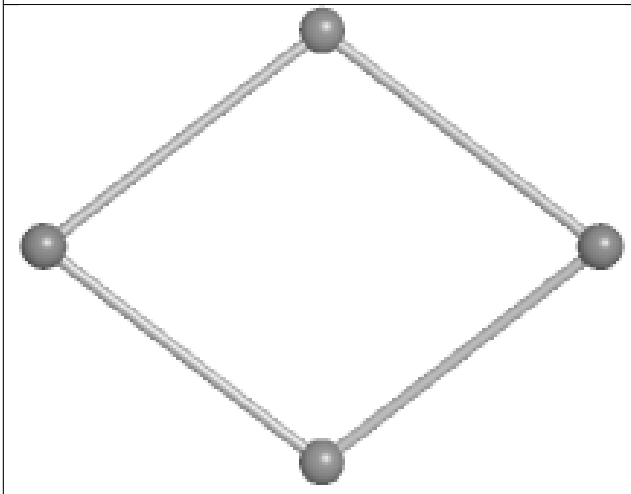


Torsions

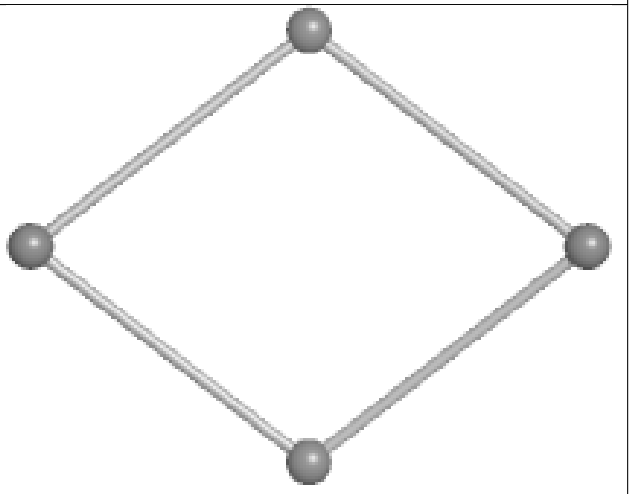


Rings

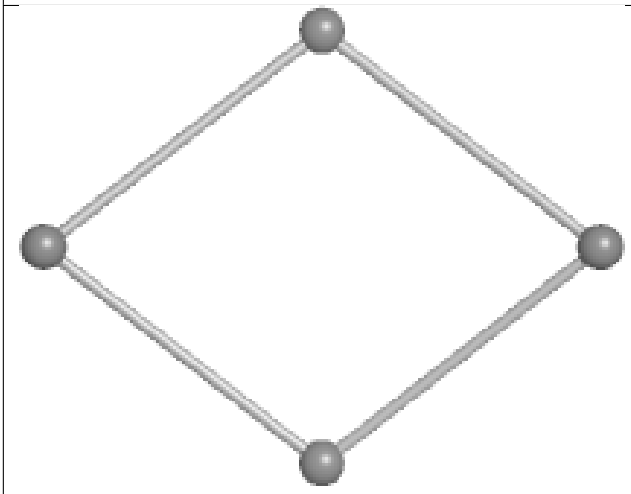
Ligand FES AT 201



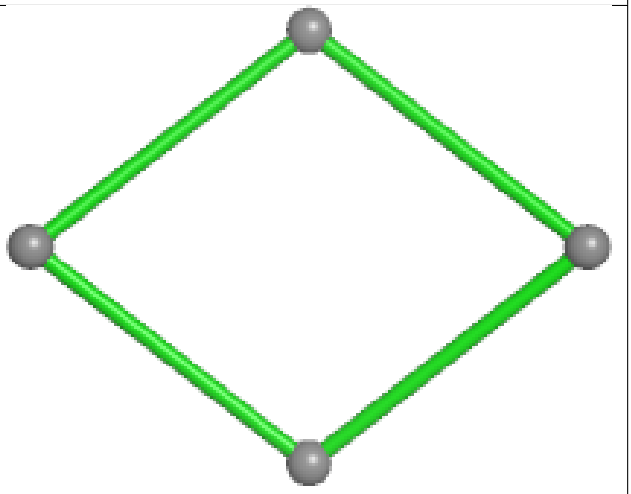
Bond lengths



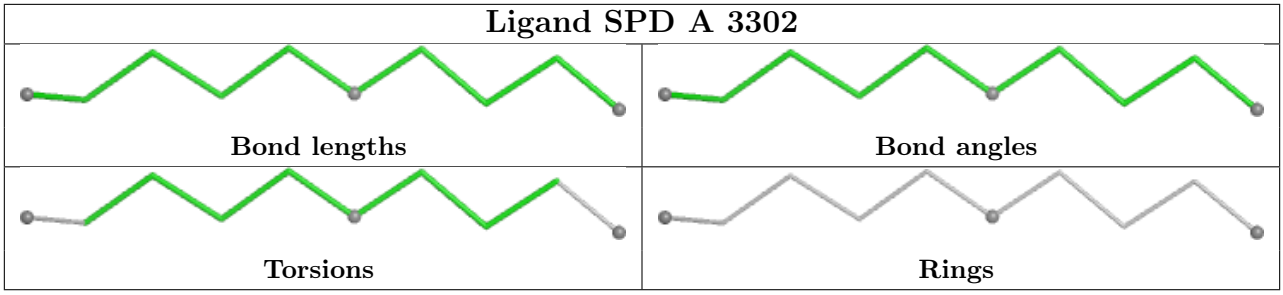
Bond angles

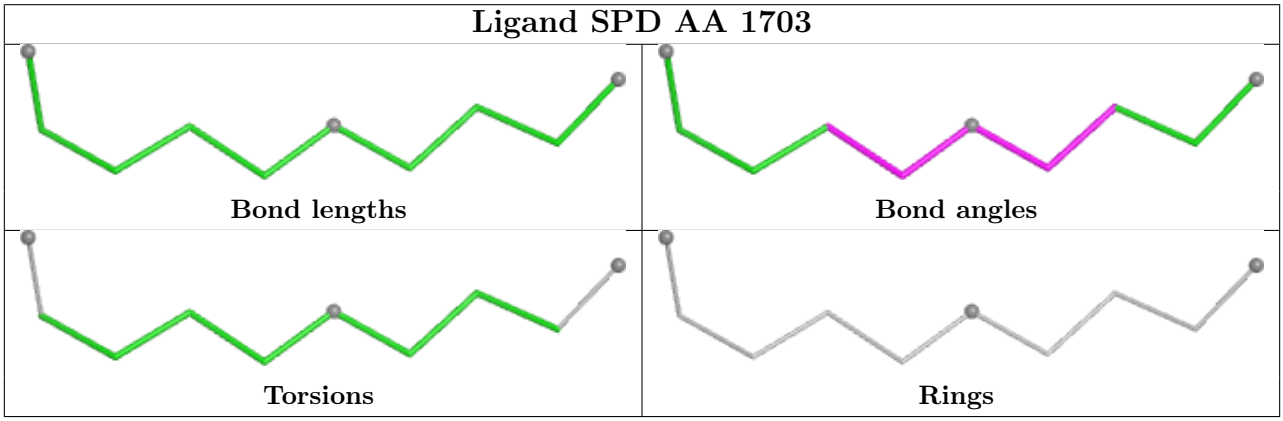


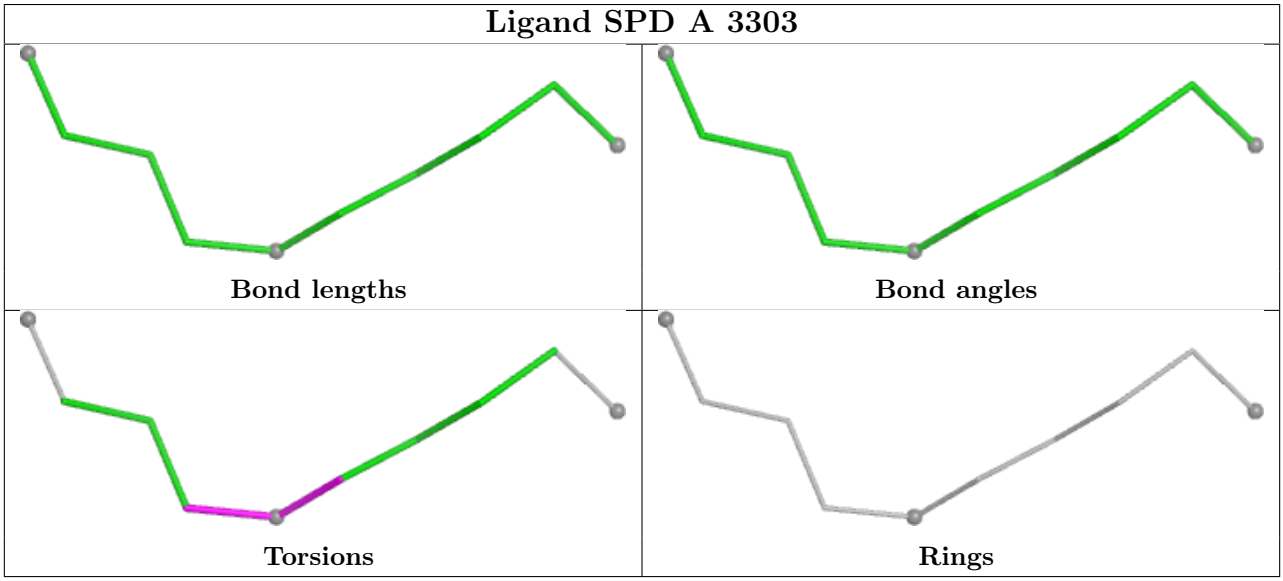
Torsions



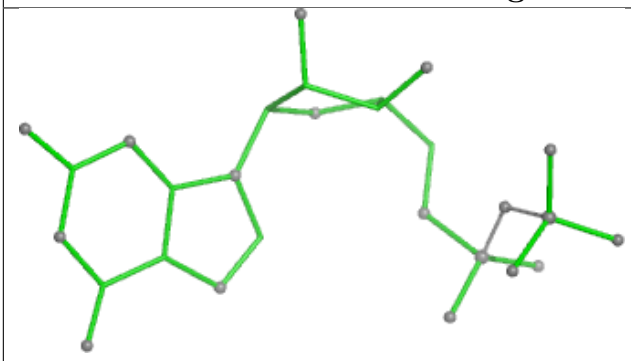
Rings


Ligand SPD A 3302
Bond lengths
Bond angles
Torsions
Rings

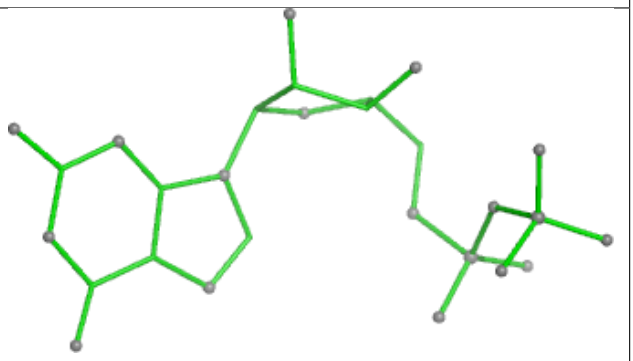

Ligand SPD AA 1703
Bond lengths
Bond angles
Torsions
Rings


Ligand SPD A 3303
Bond lengths
Bond angles
Torsions
Rings

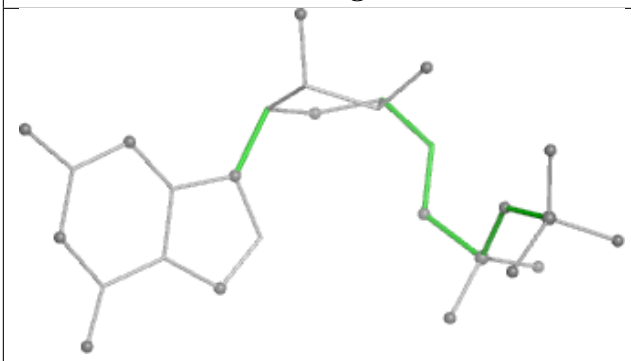
Ligand GDP AX 503



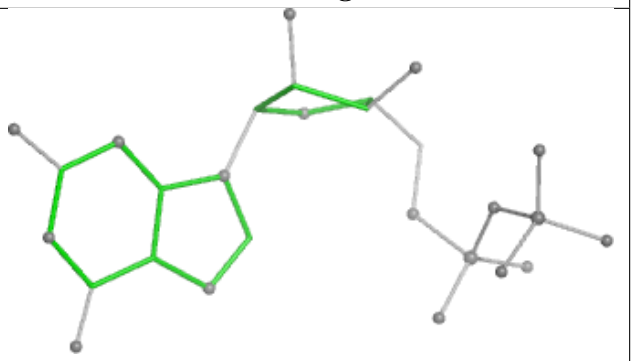
Bond lengths



Bond angles

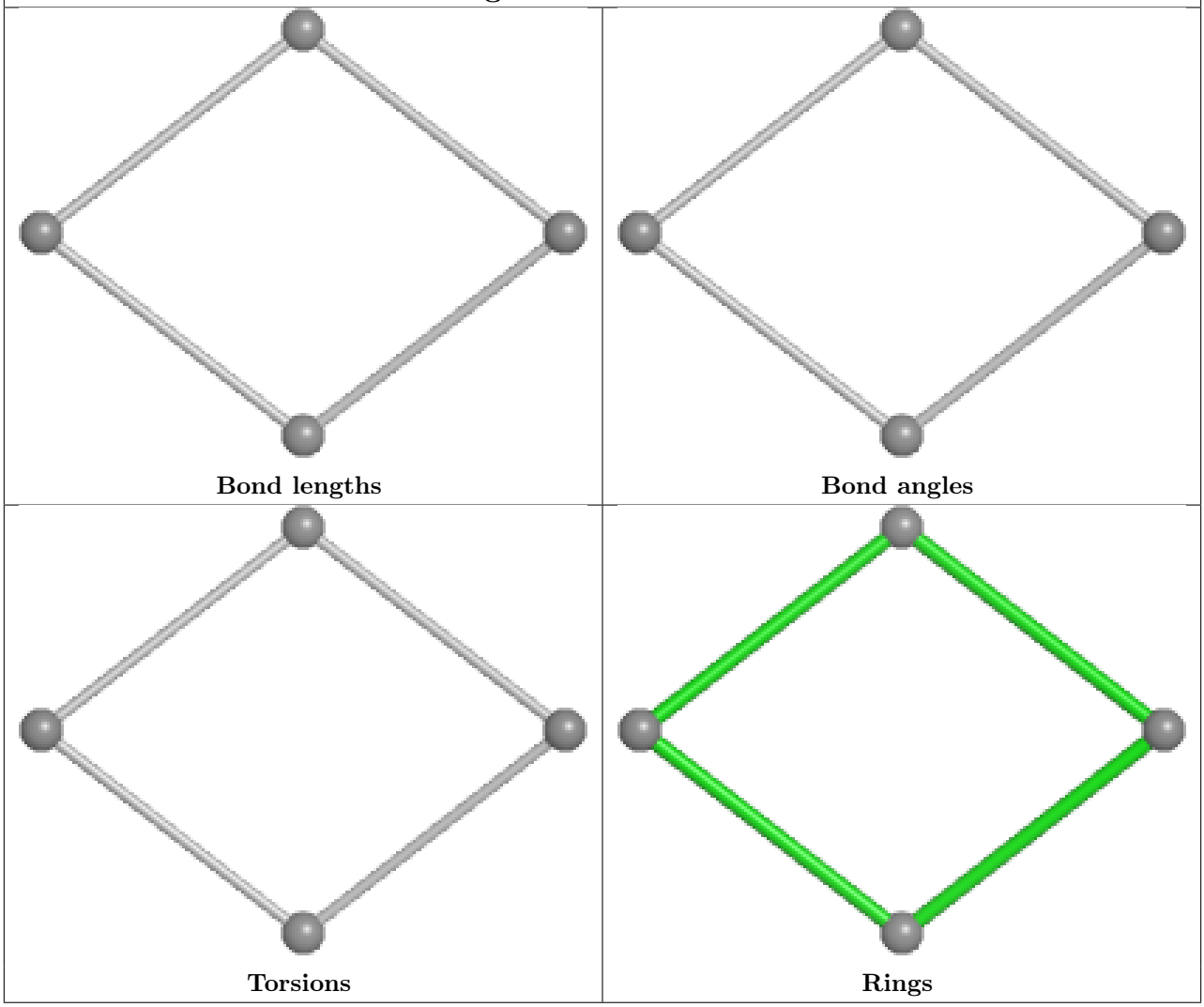


Torsions



Rings

Ligand FES AP 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
89	Ay	3
32	Aw	1
35	A	1
33	Ax	1
34	Az	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Aw	44:A	O3'	74:C	P	56.79
1	Ay	27:G	O3'	43:C	P	17.81
1	Ay	54:U	O3'	58:A	P	12.21
1	A	2357:C	O3'	2361:G	P	10.83
1	Ax	15:A	O3'	21:A	P	9.85
1	Ay	15:A	O3'	21:A	P	9.25
1	Az	3:A	O3'	4:A	P	3.05

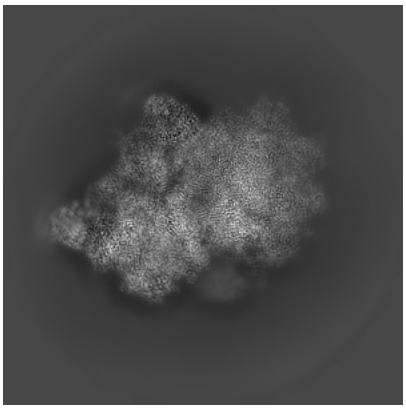
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13980. These allow visual inspection of the internal detail of the map and identification of artifacts.

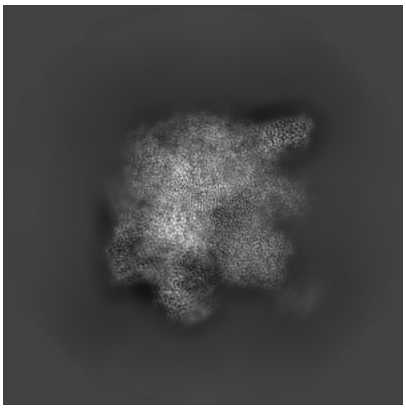
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

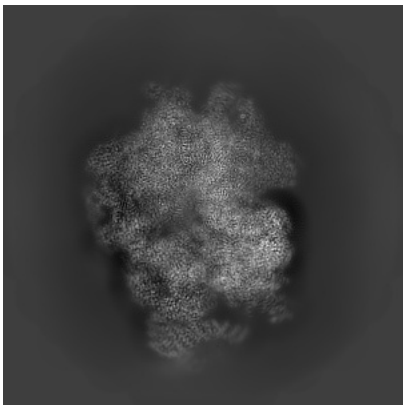
6.1.1 Primary map



X

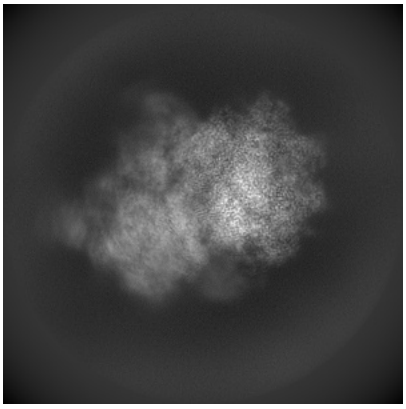


Y

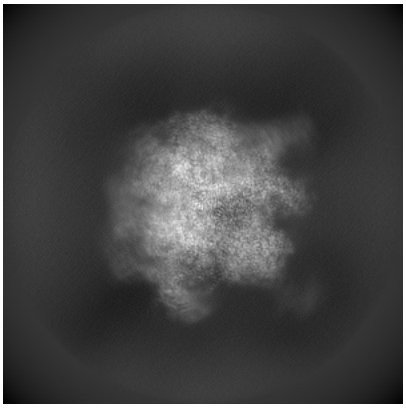


Z

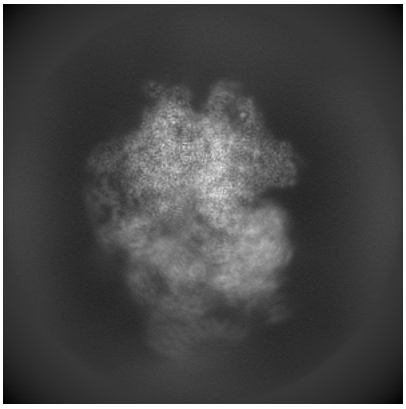
6.1.2 Raw map



X



Y

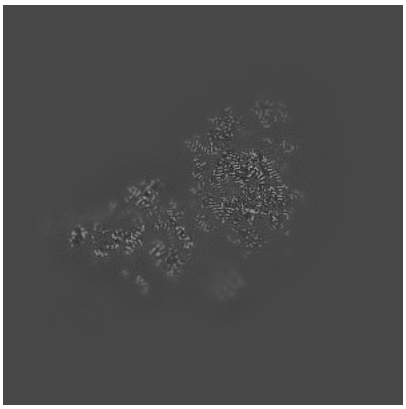


Z

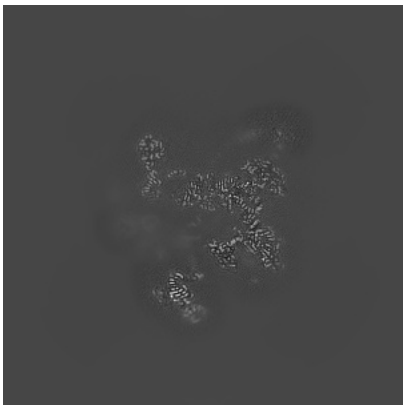
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

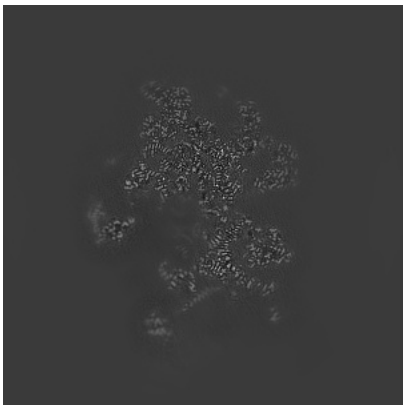
6.2.1 Primary map



X Index: 270

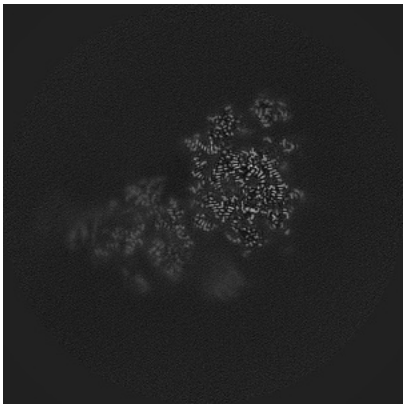


Y Index: 270

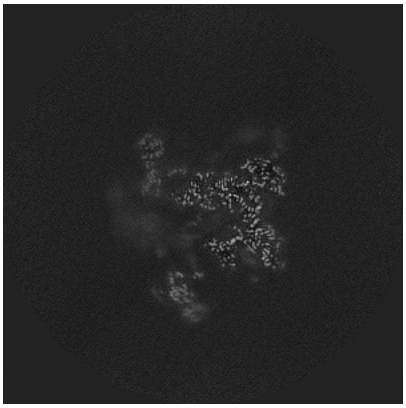


Z Index: 270

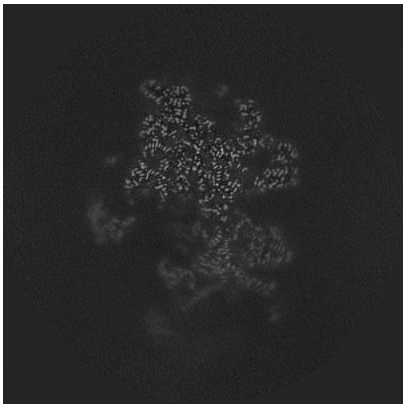
6.2.2 Raw map



X Index: 270



Y Index: 270

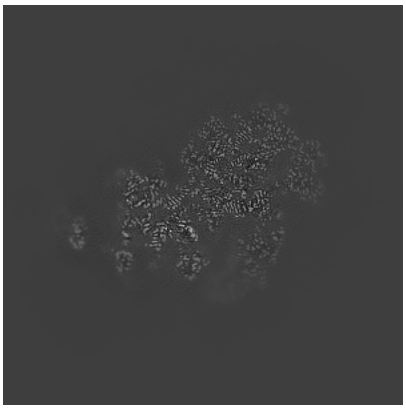


Z Index: 270

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

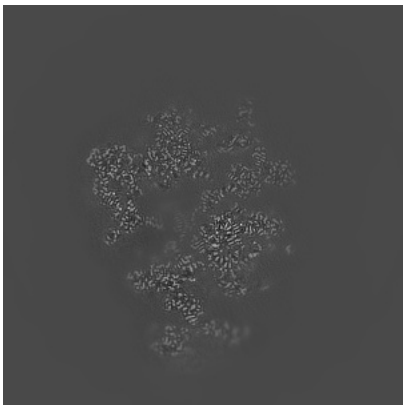
6.3.1 Primary map



X Index: 291

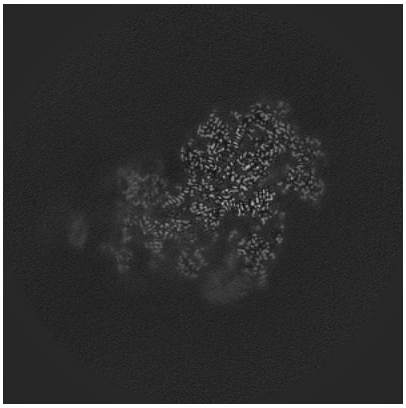


Y Index: 318

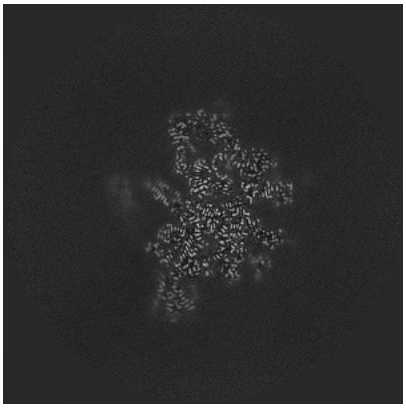


Z Index: 240

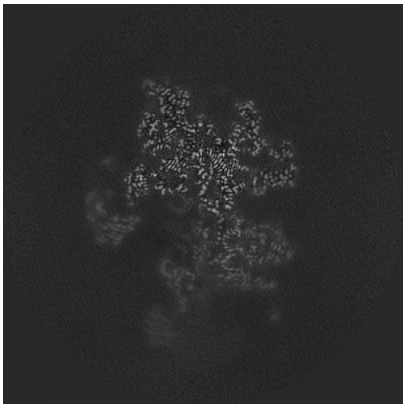
6.3.2 Raw map



X Index: 289



Y Index: 318

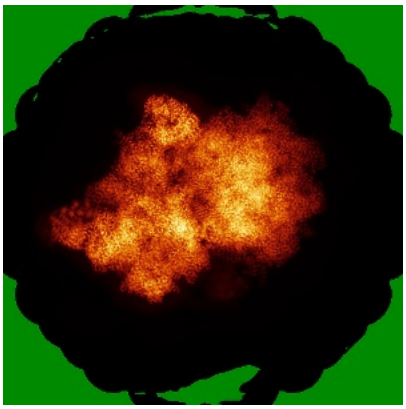


Z Index: 265

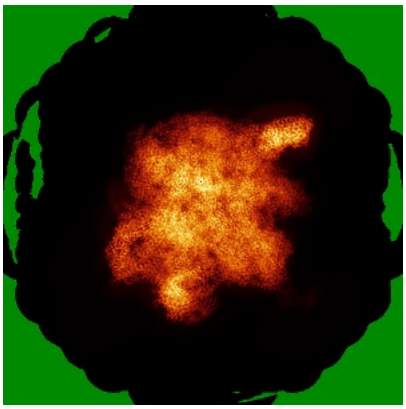
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

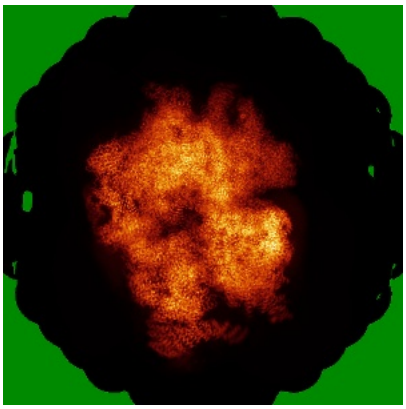
6.4.1 Primary map



X

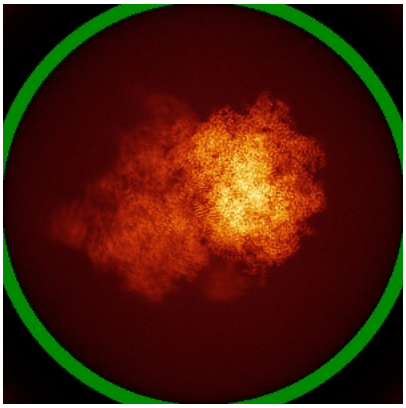


Y

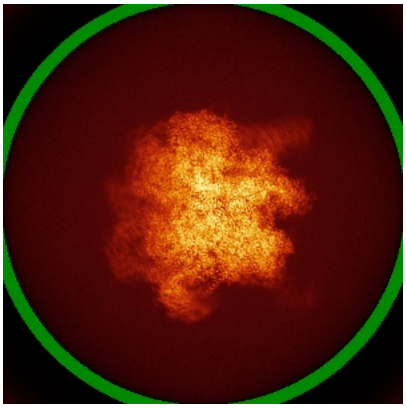


Z

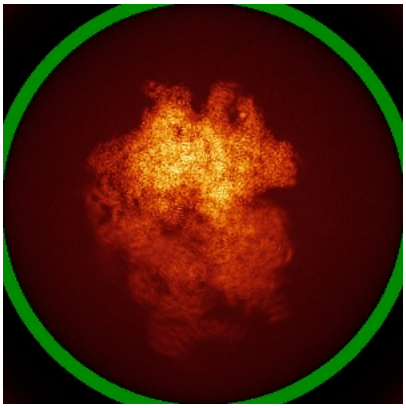
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

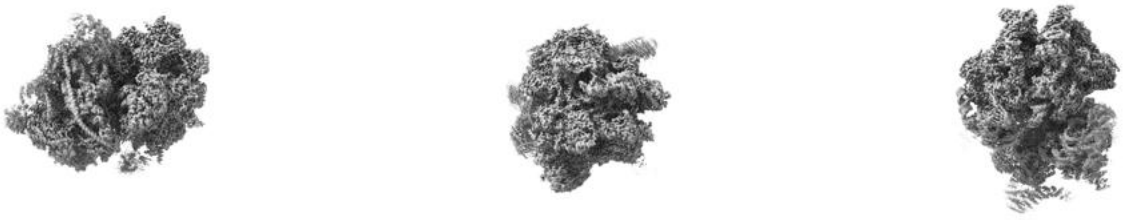
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

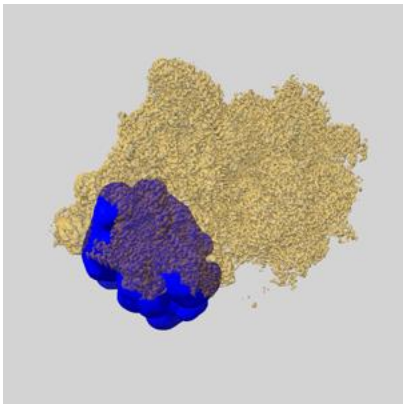
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

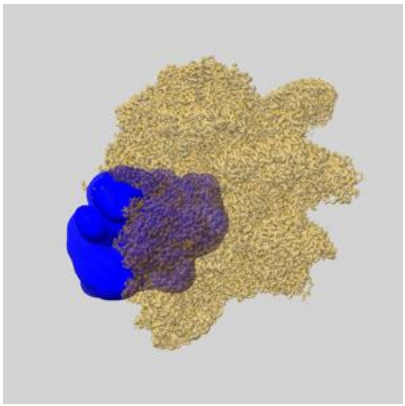
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

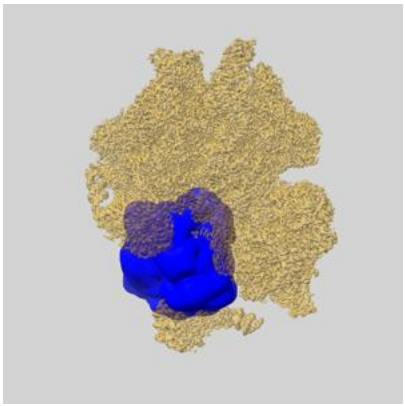
6.6.1 emd_13980_msk_1.map



X

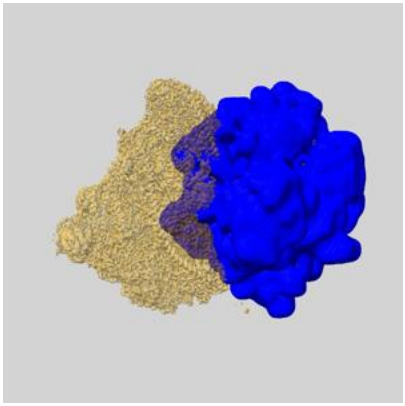


Y

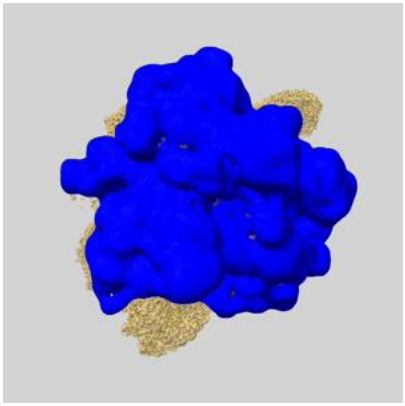


Z

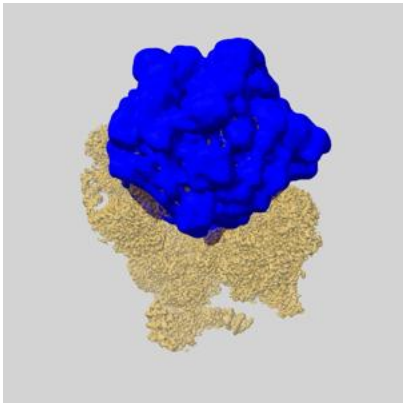
6.6.2 emd_13980_msk_2.map



X

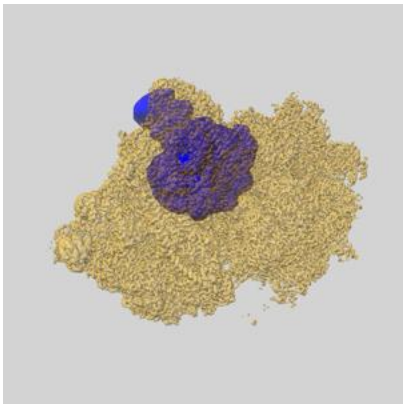


Y

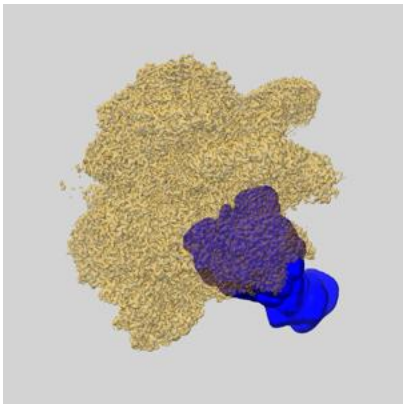


Z

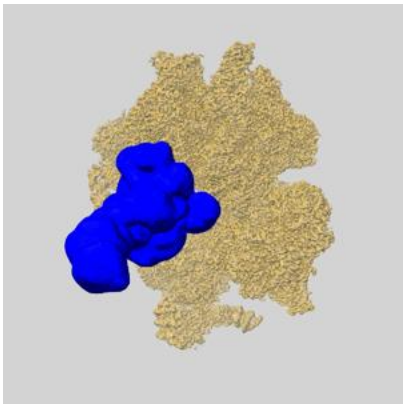
6.6.3 emd_13980_msk_3.map



X

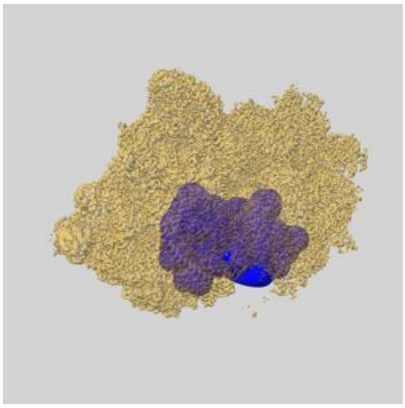


Y

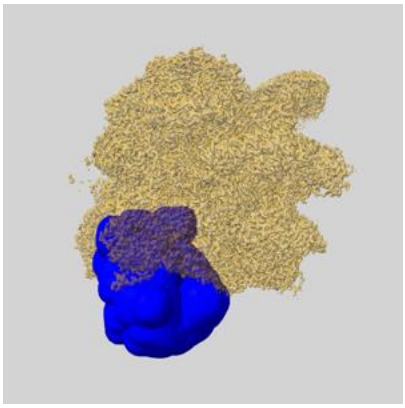


Z

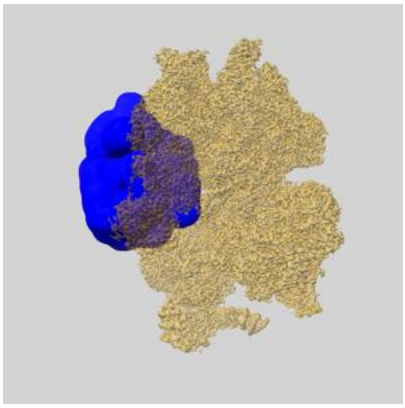
6.6.4 emd_13980_msk_4.map



X

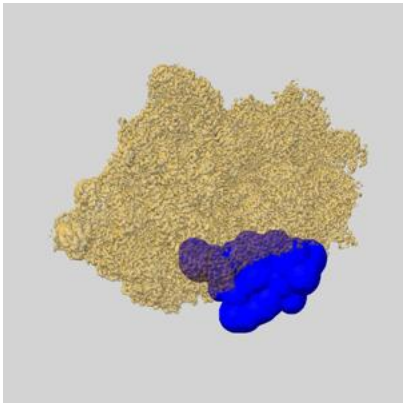


Y

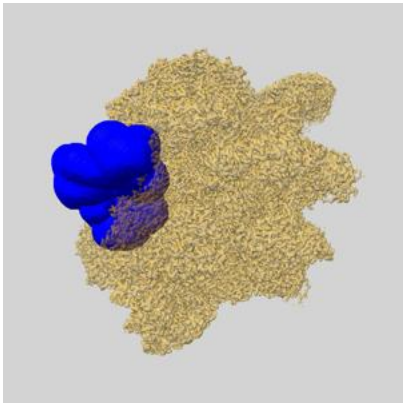


Z

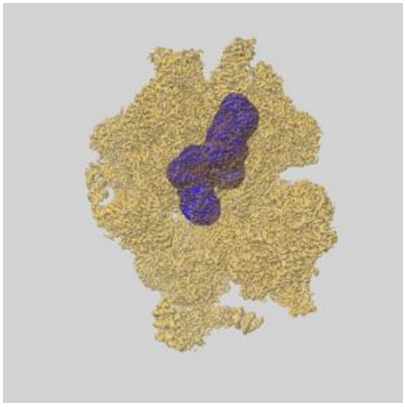
6.6.5 emd_13980_msk_5.map



X

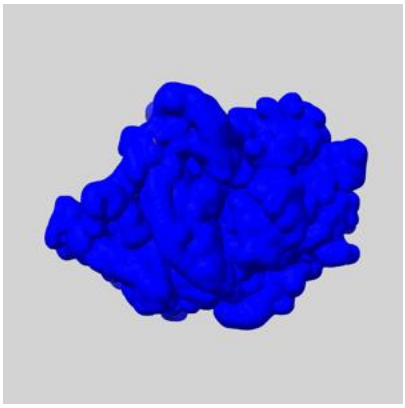


Y

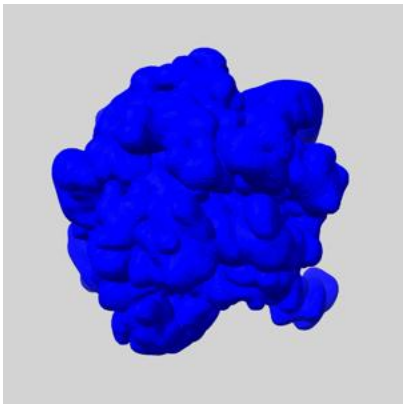


Z

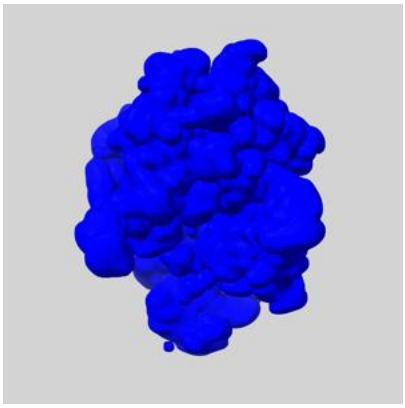
6.6.6 emd_13980_msk_6.map



X

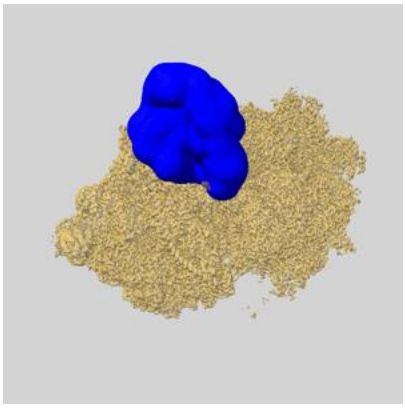


Y

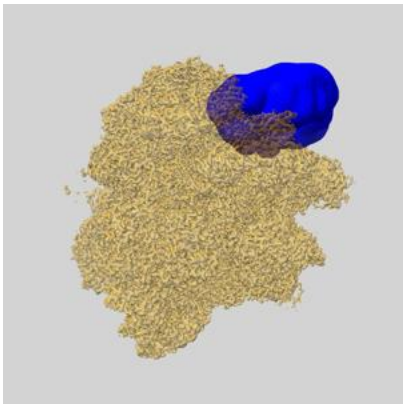


Z

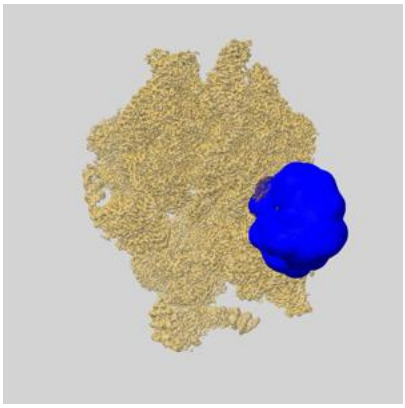
6.6.7 emd_13980_msk_7.map



X

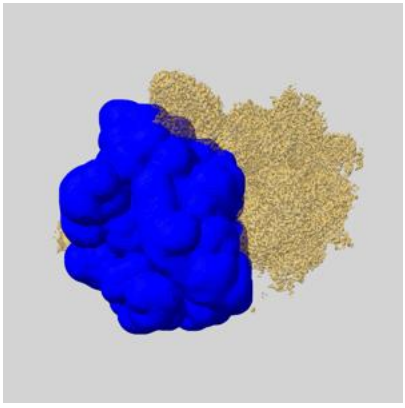


Y

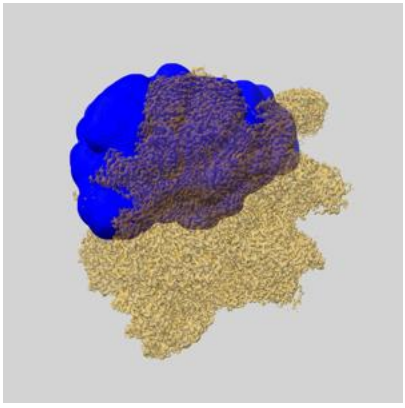


Z

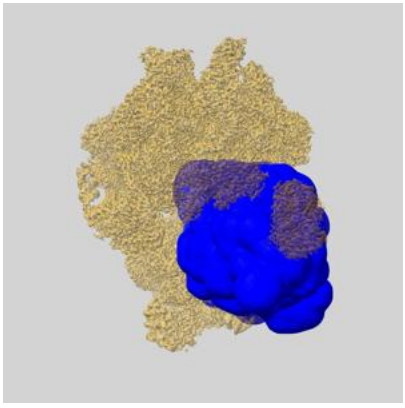
6.6.8 emd_13980_msk_8.map



X

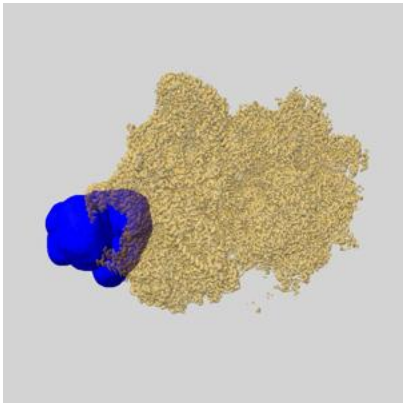


Y

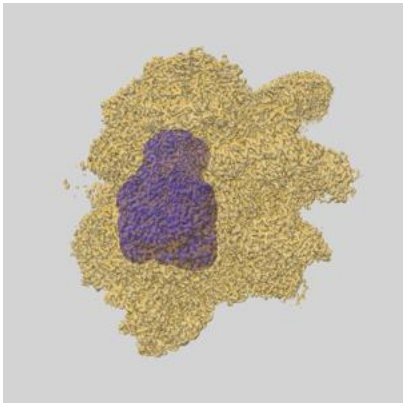


Z

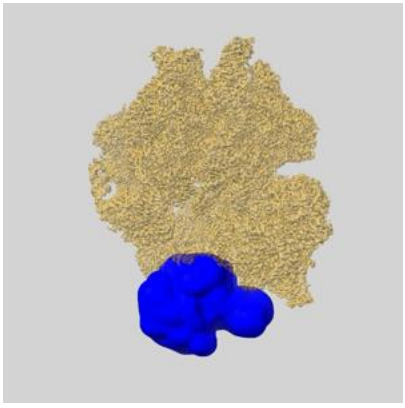
6.6.9 emd_13980_msk_9.map ⓘ



X



Y

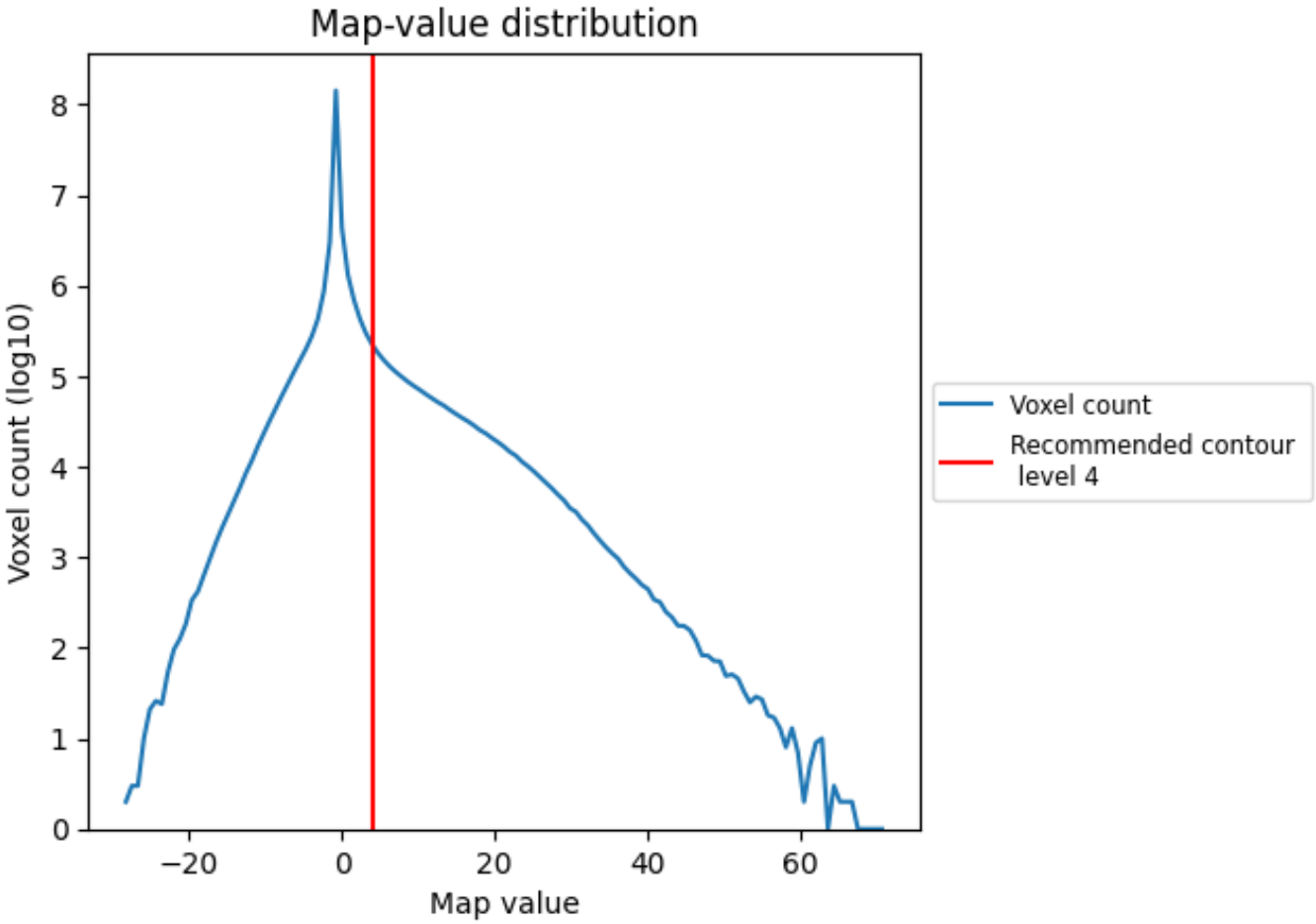


Z

7 Map analysis

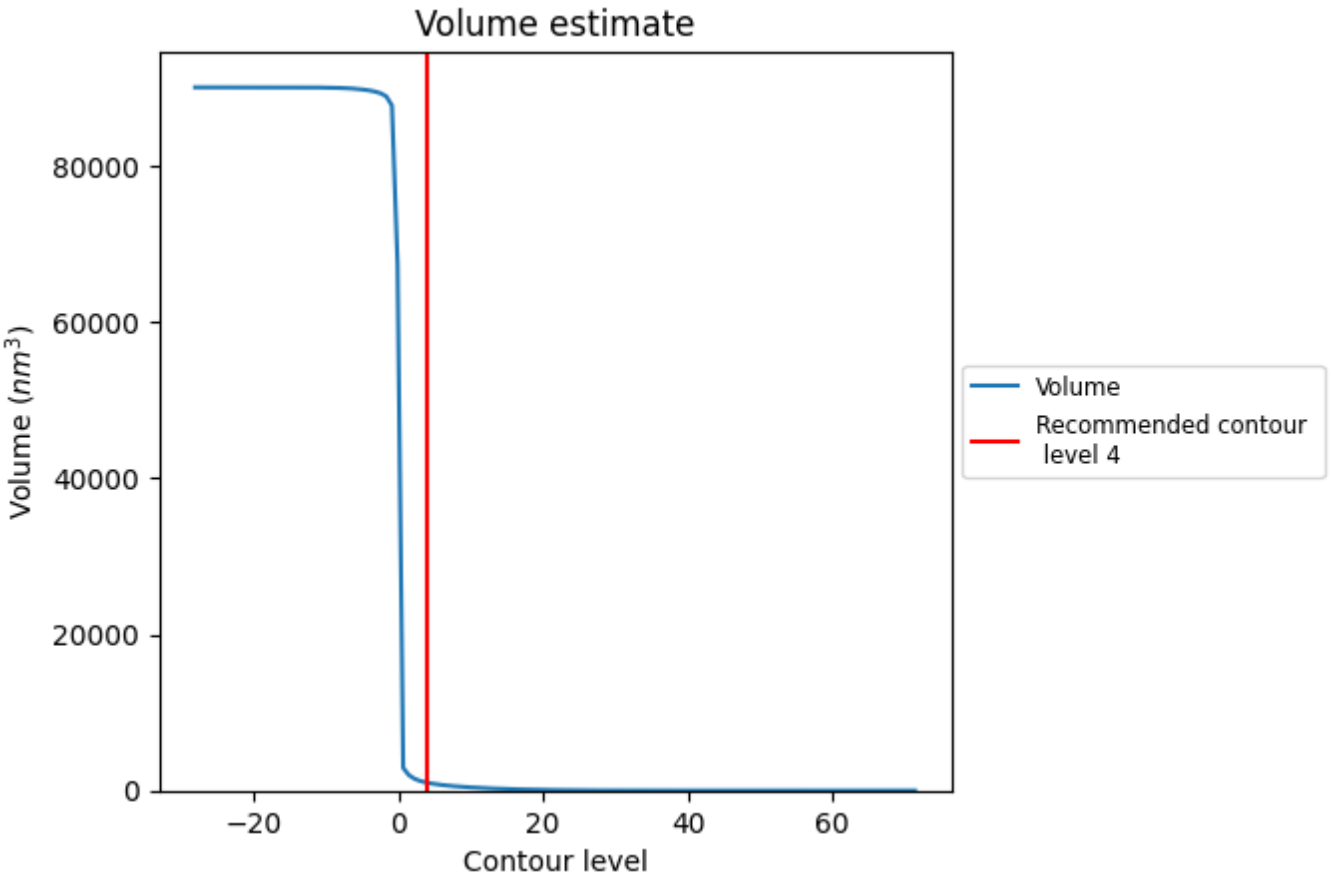
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

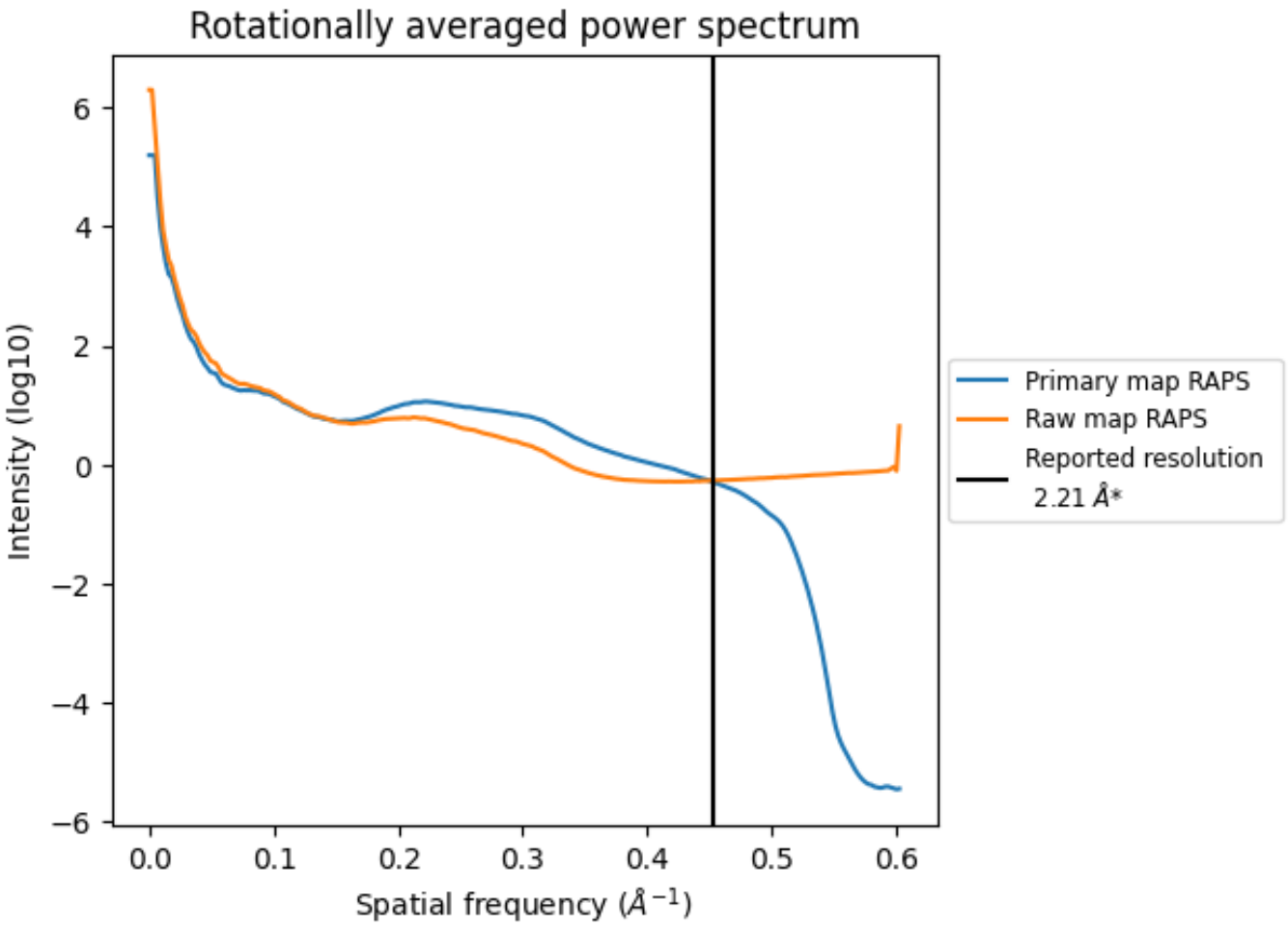
7.2 Volume estimate



The volume at the recommended contour level is 998 nm^3; this corresponds to an approximate mass of 902 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

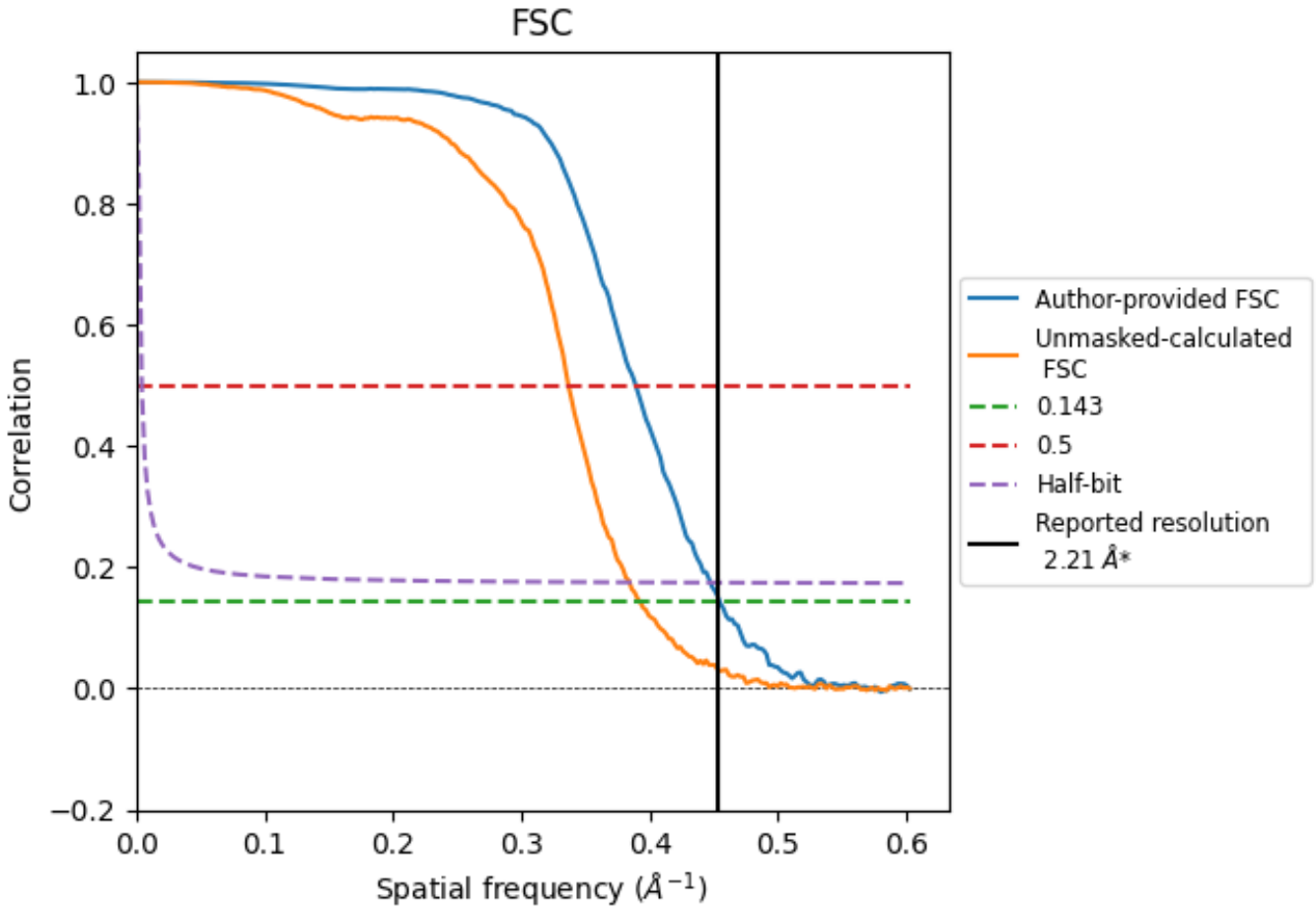


*Reported resolution corresponds to spatial frequency of 0.452 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.452 Å^{-1}

8.2 Resolution estimates (i)

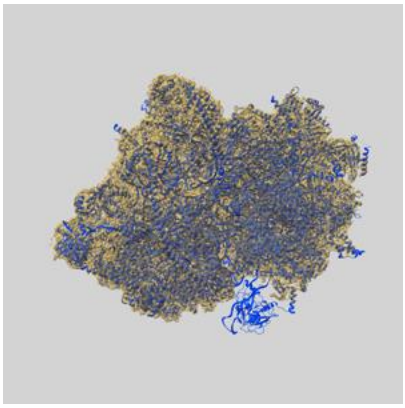
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.21	-	-
Author-provided FSC curve	2.20	2.57	2.24
Unmasked-calculated*	2.55	2.97	2.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.55 differs from the reported value 2.21 by more than 10 %

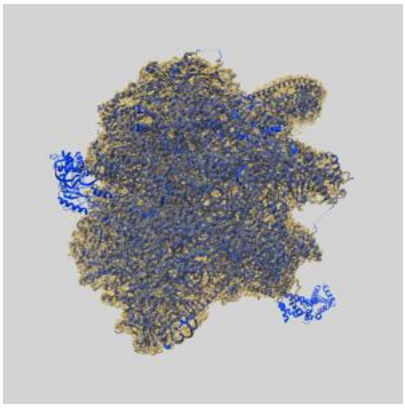
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13980 and PDB model 7QI4. Per-residue inclusion information can be found in section 3 on page 31.

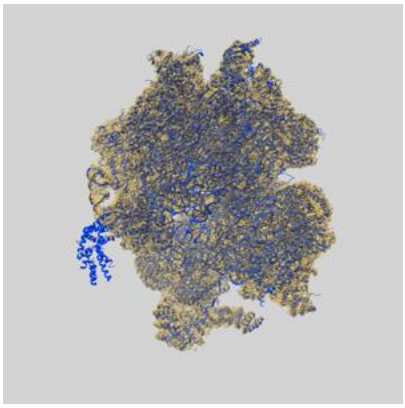
9.1 Map-model overlay



X



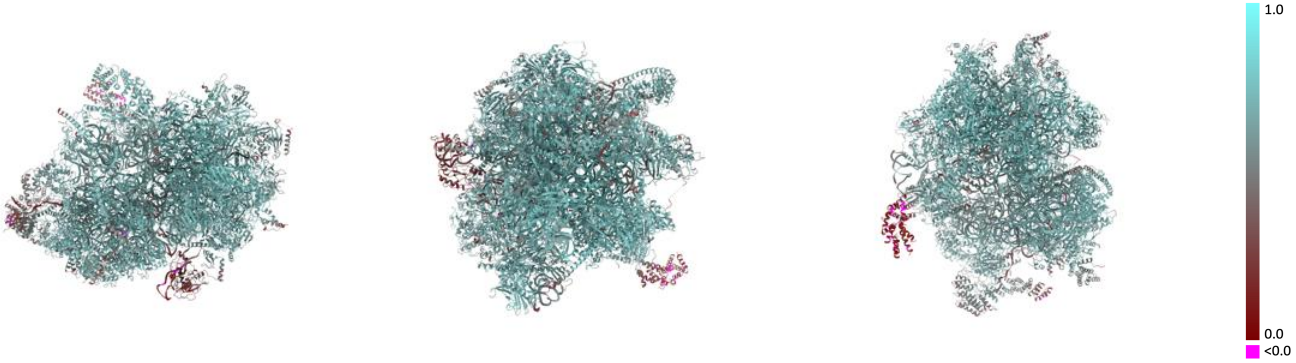
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

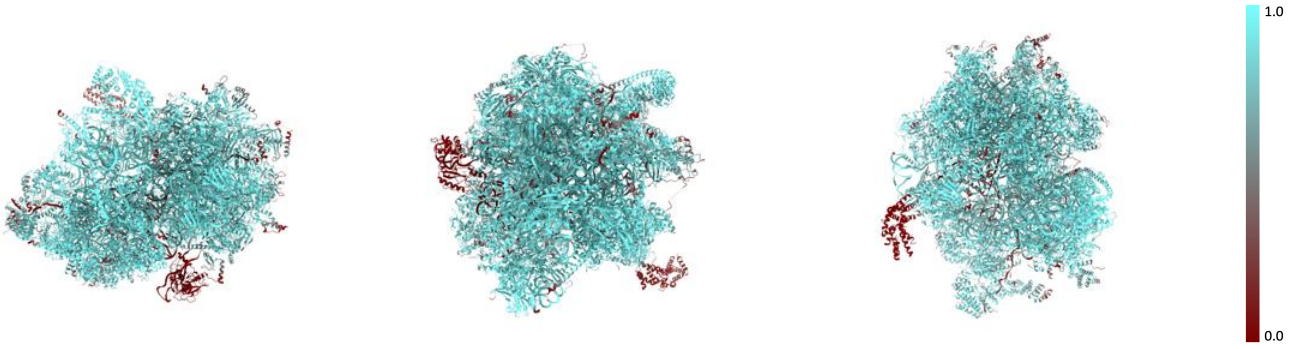
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

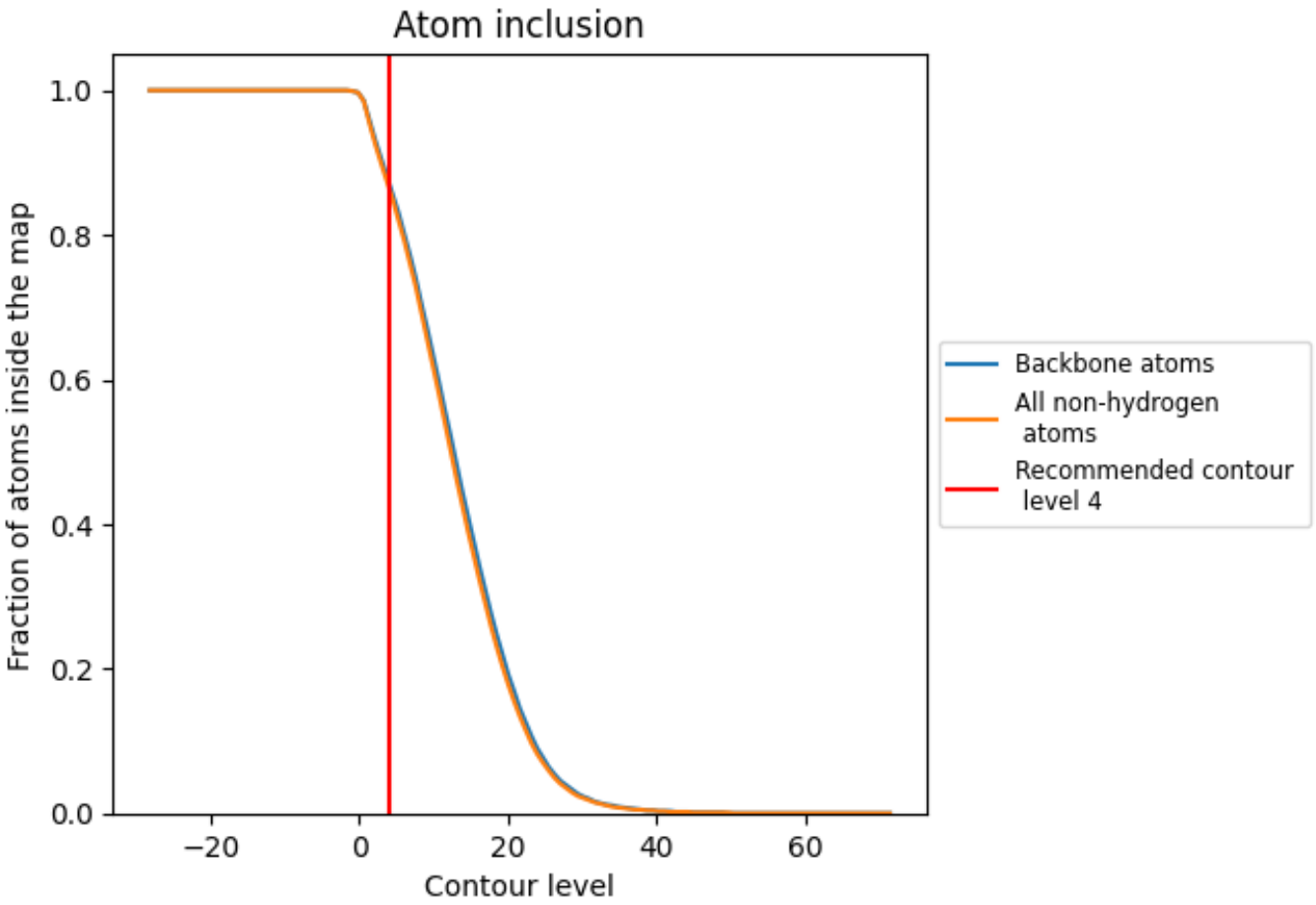
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8660	0.6580
0	0.8910	0.7120
1	0.8340	0.6530
2	0.9970	0.7990
3	0.9800	0.7760
4	0.9570	0.7280
5	0.8920	0.6790
6	0.9470	0.6840
7	0.7770	0.6380
8	0.7300	0.5620
9	0.8140	0.6560
A	0.9310	0.7150
A0	0.9350	0.6560
A1	0.9030	0.6410
A2	0.8240	0.6160
A3	0.9400	0.6960
A4	0.8330	0.5170
AA	0.9690	0.6790
AB	0.9370	0.6800
AC	0.9790	0.7080
AD	0.8780	0.6410
AE	0.9280	0.6750
AF	0.9240	0.6620
AG	0.8650	0.6250
AH	0.9420	0.6690
AI	0.9470	0.6810
AJ	0.9250	0.6580
AK	0.9770	0.7220
AL	0.8710	0.6390
AM	0.9230	0.6580
AN	0.9400	0.6820
AO	0.9200	0.6490
AP	0.9330	0.6880
AQ	0.9700	0.7130
AR	0.8420	0.5910



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Chain	Atom inclusion	Q-score
AS	0.8420	0.5980
AT	0.9180	0.6630
AU	0.8410	0.6050
AV	0.9450	0.6500
AW	0.9120	0.6420
AX	0.9440	0.6610
AY	0.8320	0.5840
AZ	0.9020	0.6580
Aw	0.4040	0.5580
Ax	0.3350	0.4630
Ay	0.0320	0.3360
Az	0.3840	0.3970
B	0.9290	0.6060
D	0.9450	0.7310
E	0.9310	0.7300
F	0.9500	0.7440
H	0.3380	0.4460
I	0.7310	0.5550
J	0.8260	0.5930
K	0.9680	0.7450
L	0.9410	0.7310
M	0.9400	0.7310
N	0.9210	0.6940
O	0.9380	0.7350
P	0.9700	0.7200
Q	0.8570	0.6850
R	0.9550	0.7670
S	0.9370	0.7330
T	0.9450	0.7360
U	0.8140	0.6740
V	0.7520	0.6230
W	0.9560	0.7350
X	0.8590	0.6760
Y	0.9190	0.7130
Z	0.9310	0.7310
a	0.8030	0.6550
b	0.9450	0.7370
c	0.8580	0.6730
d	0.6790	0.5740
e	0.8310	0.5750
f	0.8300	0.6020
g	0.8990	0.7070

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Chain	Atom inclusion	Q-score
h	0.7470	0.6260
i	0.9710	0.7750
j	0.8340	0.6530
k	0.9150	0.6390
l	0.8770	0.6230
m	0.6820	0.5220
o	0.9670	0.7590
p	0.7550	0.5880
q	0.6110	0.5270
r	0.9320	0.6980
s	0.9060	0.7060
t	0.1870	0.3060
u	0.1050	0.2870
v	0.0000	0.1330
w	0.0000	0.0340
x	0.0000	0.0990
y	0.0000	0.0580
z	0.0080	0.2250