



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:08 PM UTC

PDB ID : 7ODR / pdb_00007odr
EMDB ID : EMD-12845
Title : State A of the human mitoribosomal large subunit assembly intermediate
Authors : Lenarcic, T.; Jaskolowski, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Saurer, M.; Lee, R.G.; Rackham, O.; Filipovska, A.; Ban, N.
Deposited on : 2021-04-30
Resolution : 2.90 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:

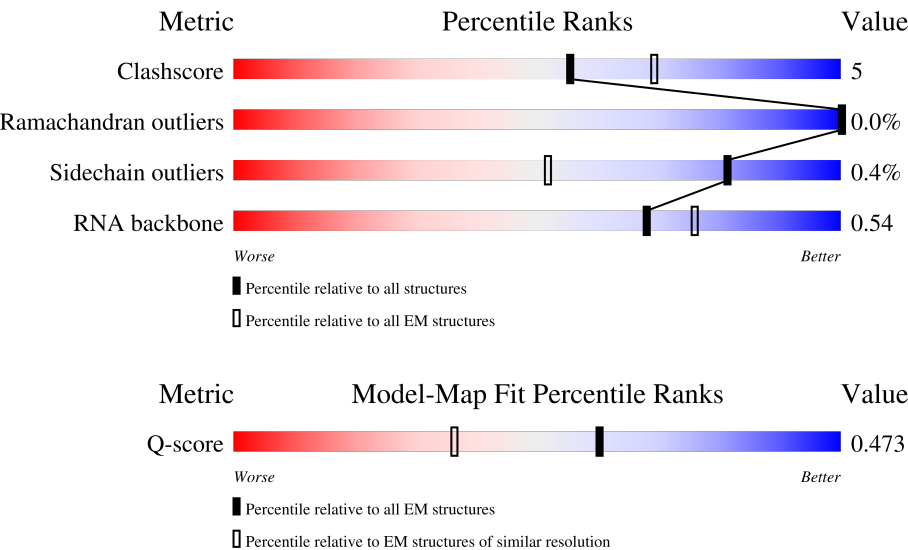
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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.



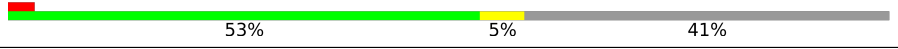
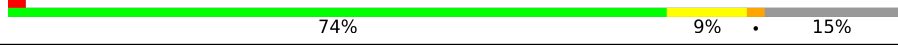
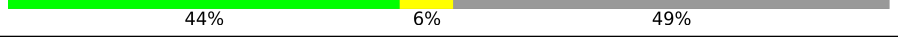
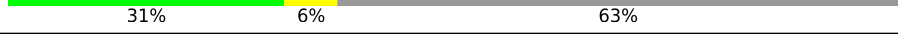
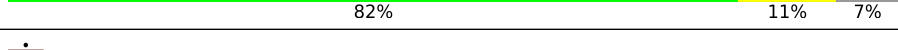
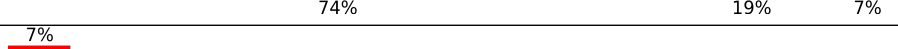
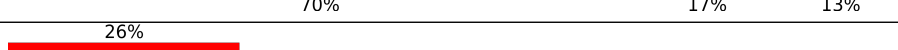
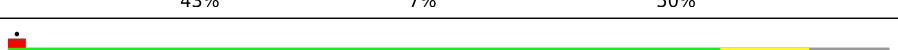
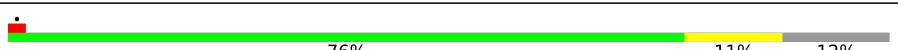
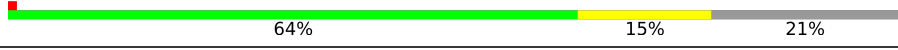
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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 $\leq 5\%$. 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	u	234	
2	v	70	
3	w	156	

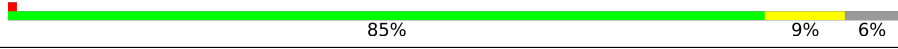
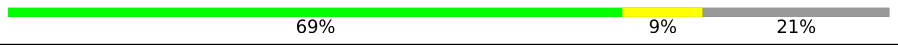
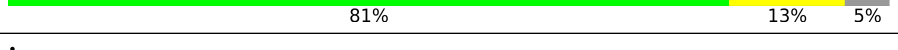
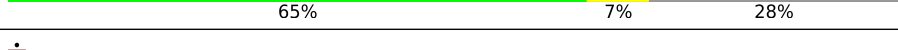
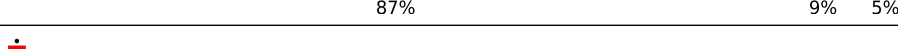
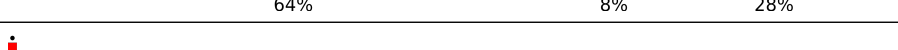
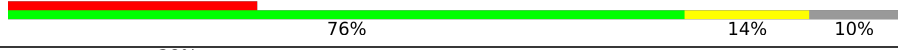
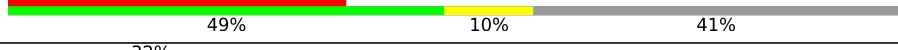
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Mol	Chain	Length	Quality of chain
4	x	384	
5	y	381	
6	0	188	
7	1	65	
8	2	92	
9	3	188	
10	4	103	
11	5	423	
12	6	380	
13	7	338	
14	8	206	
15	9	137	
16	A	1590	
17	B	72	
18	D	305	
19	E	348	
20	F	311	
21	H	267	
22	I	261	
23	J	192	
24	K	178	
25	L	145	
26	M	296	
27	N	251	
28	O	175	

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Mol	Chain	Length	Quality of chain
29	P	180	
30	Q	292	
31	R	149	
32	S	205	
33	T	206	
34	U	153	
35	V	216	
36	W	148	
37	X	256	
38	Y	250	
39	Z	161	
40	a	142	
41	b	215	
42	c	332	
43	d	306	
44	e	279	
45	f	212	
46	g	166	
47	h	158	
48	i	128	
49	j	123	
50	k	112	
51	l	138	
52	m	128	
53	o	102	

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Mol	Chain	Length	Quality of chain
54	p	206	11% 65% 6% 29%
55	q	222	5% 59% 5% 36%
56	r	196	5% 70% 12% 17%
57	s	439	75% 13% 12%

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 107464 atoms, of which 0 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 protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	110	Total	C	N	O	S	0	0
			919	591	154	164	10		

- Molecule 2 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	69	Total	C	N	O		0	0
			588	372	116	100			

- Molecule 3 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 4 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	x	336	Total	C	N	O	S	0	0
			2660	1694	465	484	17		

- Molecule 5 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	y	244	Total	C	N	O	S	0	0
			1980	1264	342	362	12		

- Molecule 6 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 7 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	55	Total	C	N	O	S	0	0
			455	290	87	76	2		

- Molecule 8 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 9 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 10 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 11 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 12 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 13 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 14 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	8	102	Total	C	N	O	S	0	0
			860	543	152	163	2		

- Molecule 15 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 16 is a RNA chain called 16S mitochondrial rRNA, DNA (31-MER),16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	1448	Total	C	N	O	P	0	0
			30460	13658	5442	9912	1448		

- Molecule 17 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	72	Total	C	N	O	P	0	0
			1522	683	269	498	72		

- Molecule 18 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	240	Total	C	N	O	S	0	0
			1872	1165	378	320	9		

- Molecule 19 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 20 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 21 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	H	97	Total	C	N	O		
			802	508	155	139	0	0

- Molecule 22 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	163	Total	C	N	O	S		
			1324	854	240	220	10	0	0

- Molecule 23 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	175	Total	C	N	O	S		
			1330	847	237	244	2	0	0

- Molecule 24 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	177	Total	C	N	O	S		
			1455	936	259	253	7	0	0

- Molecule 25 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	115	Total	C	N	O	S		
			890	559	171	155	5	0	0

- Molecule 26 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	291	Total	C	N	O	S		
			2327	1483	430	408	6	0	0

- Molecule 27 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	212	Total	C	N	O	S		
			1723	1107	310	297	9	0	0

- Molecule 28 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 29 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 30 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	221	Total	C	N	O	S	0	0
			1843	1179	327	328	9		

- Molecule 31 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 32 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 33 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 34 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	152	Total	C	N	O	S	0	0
			1251	788	234	226	3		

- Molecule 35 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 36 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	W	106	Total	C	N	O	S	0	0
			835	536	157	139	3		

- Molecule 37 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 38 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 40 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	a	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 41 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	b	149	Total	C	N	O	S	0	0
			1189	739	230	217	3		

- Molecule 42 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 43 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	259	Total	C	N	O	S	0	0
			2124	1357	369	384	14		

- Molecule 44 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	228	Total	C	N	O	S	0	0
			1848	1174	326	342	6		

- Molecule 45 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	f	150	Total	C	N	O	S	0	0
			1196	764	197	231	4		

- Molecule 46 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 47 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	h	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 48 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 49 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 50 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	k	101	Total	C	N	O	S	0	0
			774	479	148	142	5		

- Molecule 51 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 52 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	m	51	Total	C	N	O	S	0	0
			419	262	82	73	2		

- Molecule 53 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	o	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 54 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	p	147	Total	C	N	O	S	0	0
			1205	748	228	225	4		

- Molecule 55 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	q	141	Total	C	N	O	S	0	0
			1177	732	229	211	5		

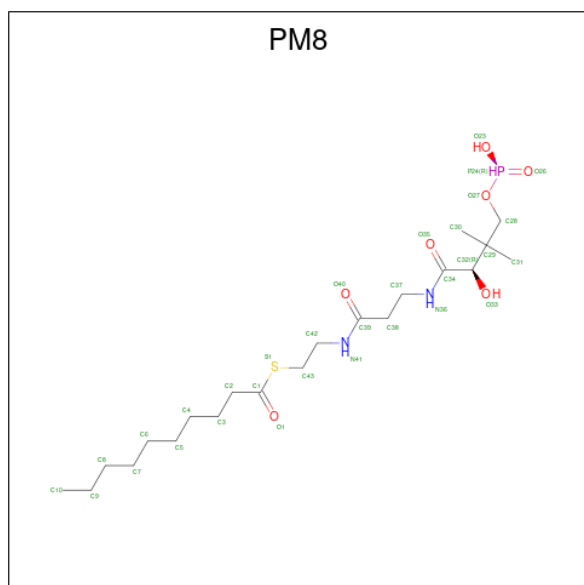
- Molecule 56 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 57 is a protein called 39S ribosomal protein S30, mitochondrial.

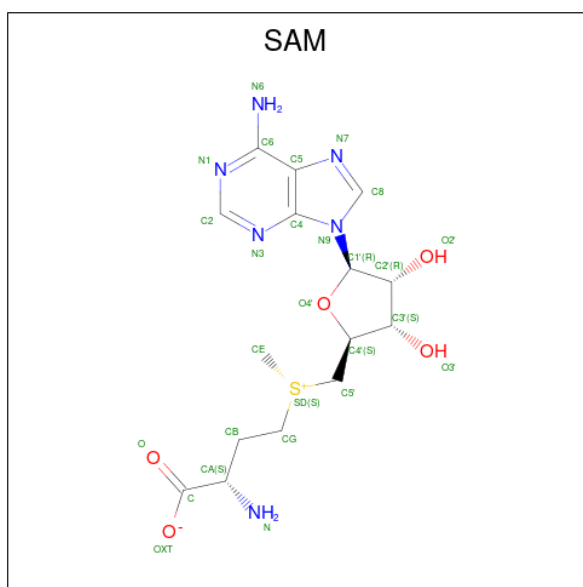
Mol	Chain	Residues	Atoms					AltConf	Trace
57	s	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

- Molecule 58 is S-(2-([N-(2-HYDROXY-4-([HYDROXY(OXIDO)PHOSPHINO]OXY)}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (CCD ID: PM8) (formula: $C_{21}H_{41}N_2O_7PS$).



Mol	Chain	Residues	Atoms						AltConf
58	w	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 59 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					AltConf
59	x	1	Total	C	N	O	S	0
			27	15	6	5	1	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Zn	0
			1	1	
60	4	1	Total	Zn	0
			1	1	

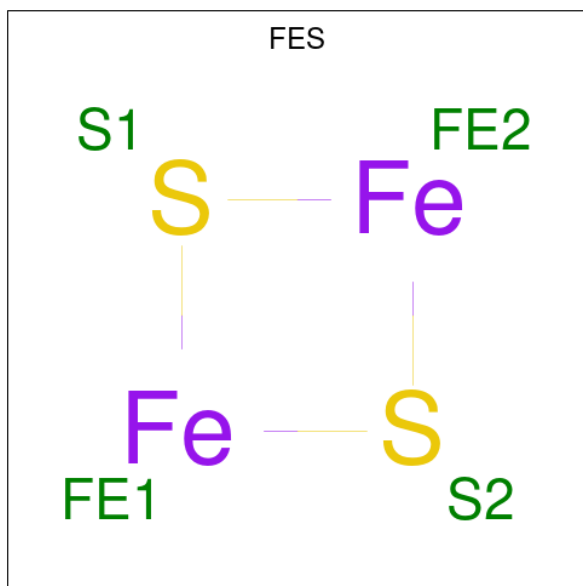
- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
61	9	1	Total	Mg	0
			1	1	
61	A	92	Total	Mg	0
			92	92	
61	D	1	Total	Mg	0
			1	1	
61	M	1	Total	Mg	0
			1	1	
61	O	1	Total	Mg	0
			1	1	
61	g	1	Total	Mg	0
			1	1	

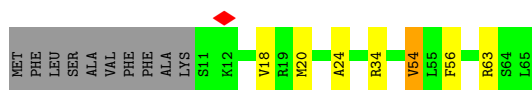
- Molecule 62 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
62	A	2	Total	K	0
			2	2	

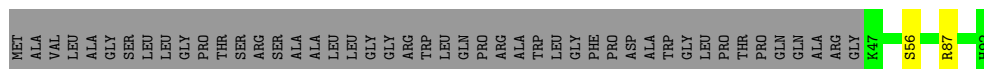
- Molecule 63 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



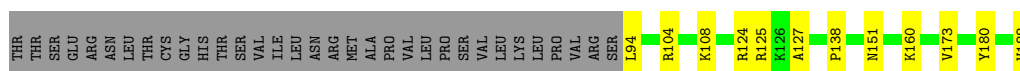
Mol	Chain	Residues	Atoms			AltConf
63	r	1	Total	Fe	S	0
			4	2	2	



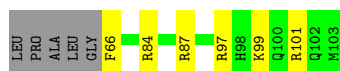
- Molecule 8: 39S ribosomal protein L34, mitochondrial



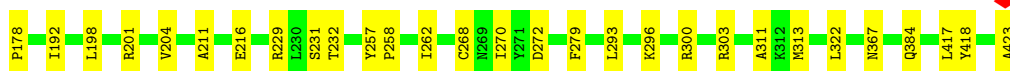
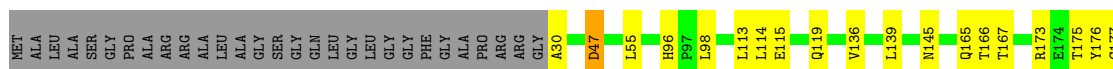
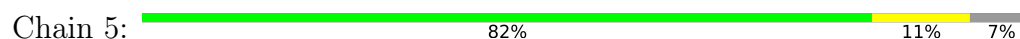
- Molecule 9: 39S ribosomal protein L35, mitochondrial



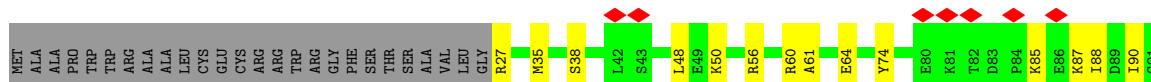
- Molecule 10: 39S ribosomal protein L36, mitochondrial

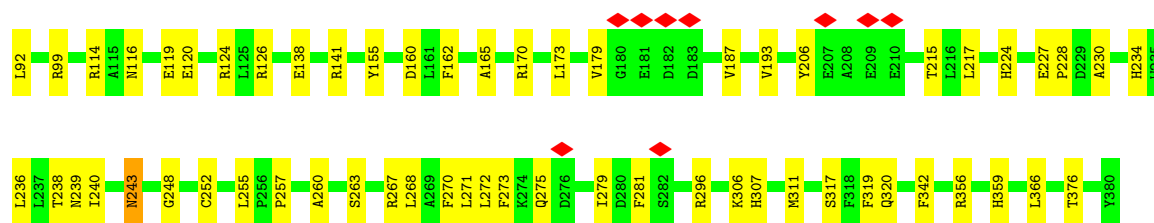


- Molecule 11: 39S ribosomal protein L37, mitochondrial



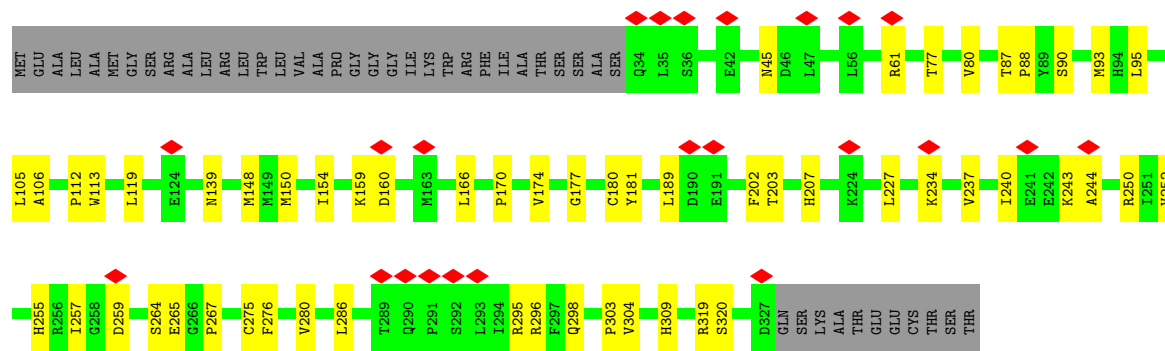
- Molecule 12: 39S ribosomal protein L38, mitochondrial





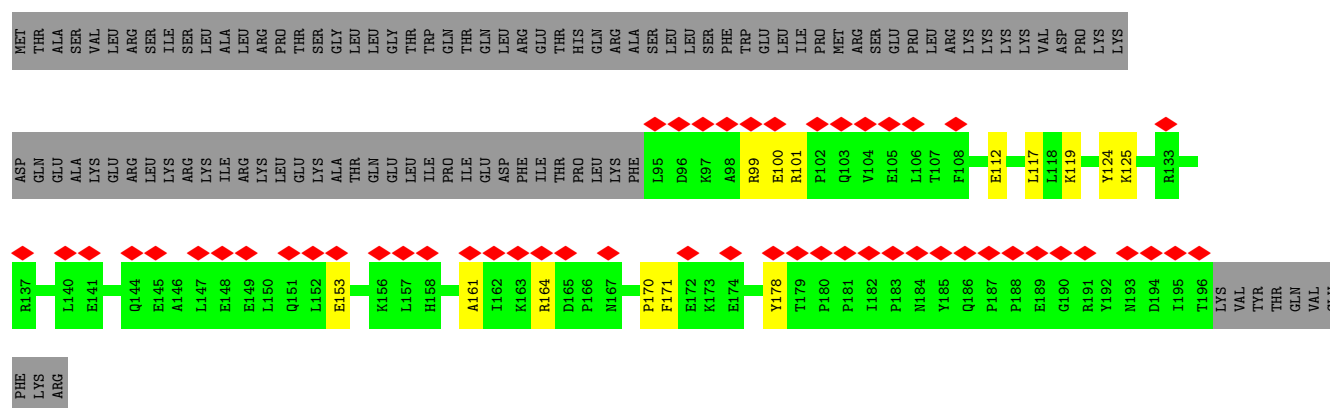
- Molecule 13: 39S ribosomal protein L39, mitochondrial

Chain 7:



- Molecule 14: 39S ribosomal protein L40, mitochondrial

Chain 8:



- Molecule 15: 39S ribosomal protein L41, mitochondrial

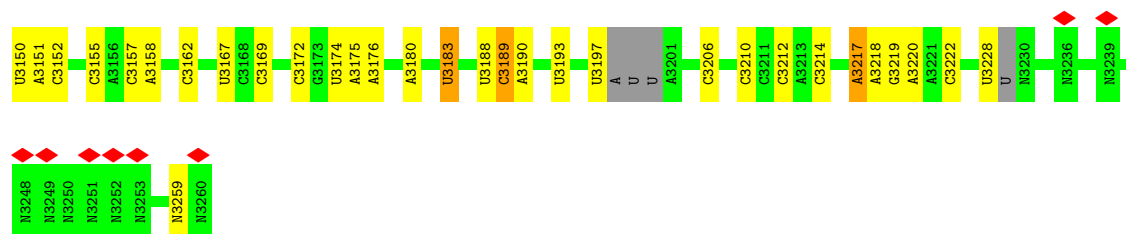
Chain 9:



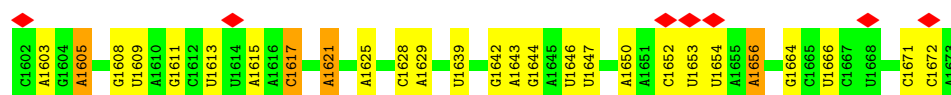
- Molecule 16: 16S mitochondrial rRNA, DNA (31-MER), 16S mitochondrial rRNA

Chain A:

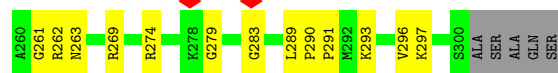
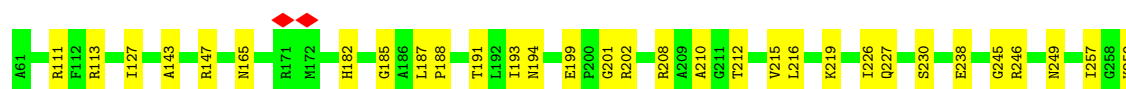
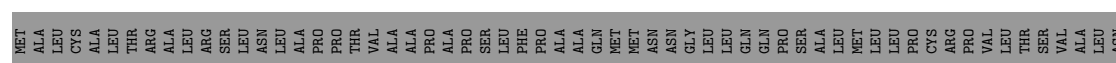
G3019	G2916	A	A2709	U2422	A2297	C2206	C2114	C1997	A1867	G1671
C3020	G2917	C	C2710	C2427	A2298	A2207	U2119	U1996	G1868	C1672
C3021	A2921	U	C2718	C	G2300	C2210	C2125	C2001	A1773	U1673
U3024	A2922	C	G2719	A2432	G2309	U2211	U2126	G2002	A1777	C1678
A3025	U2925	U	G2720	U2442	A2306	C2212	A2127	A2003	U1780	C1689
U3041	A2926	U	G2721	U2443	G2310	A2216	A2131	G2015	A1781	C1693
U3042	C2927	A	G2724	C2444	A2321	C2217	A2132	C2016	G1782	C1693
C3043	C2928	A	A2725	A2445	C2322	C	A2136	U2017	G1787	A1697
C3044	C2929	A	U2446	U2446	C2322	C	A2135	G2018	A1790	C1698
A3051	U2930	U	G2449	U2449	A2324	U	C2137	G2019	G1791	C1699
A3052	C2935	G	A2450	U2450	U2325	A	U2138	G2022	G1883	U1700
A3053	U	U	A2451	A2451	C2328	C	A2144	A2029	G1886	C1703
G3054	A	U	A2452	G2453	C	C	A2147	U2030	A1887	U1704
C3056	C2939	A	G2454	U2455	C2332	U	G2147	A2031	A1891	A1798
C3060	G2943	C	U2456	U2456	G2345	A2228	A2151	A2034	A1892	A1705
G3061	C2944	U	A2457	U2457	U2346	A2230	A2154	U2035	A1893	C1706
G3063	U2955	G	A2458	A2458	A2350	A2230	A2154	C2036	C1901	C1707
C3066	A2956	U	A2459	A2459	U2351	U2233	A2155	U2037	C1902	A1708
U3072	G2959	U	A2466	U2466	U2352	U2233	A2163	U2038	C1903	A1710
C3073	C2962	A	A2467	A2467	A2353	A2237	C2163	A2039	A1907	C1711
C3077	C2963	A	A2468	A2468	A2354	A2238	C2164	A2060	U1807	A1712
G3082	G2975	U	G2470	U2470	A2355	C2240	C2166	A2065	A1808	A1713
U3083	U2980	C	G2478	U2478	A2356	A2241	A2167	A1936	U1809	A1724
A3084	A2981	C	C2493	U2493	C2359	U2242	U2168	A1937	C1812	A1727
A3085	C2982	U	U2499	U2499	U2360	U2244	A2169	A1938	C1813	U1728
U3086	G2983	A	A2500	A2500	G2361	A2245	G2170	G1939	A1814	A1731
C3087	A2984	A	C2501	A2501	A2362	C2246	U2171	A1940	A1821	A1737
C3088	C2985	C	C2502	C2502	A2363	U2248	C2172	U1952	U1822	A1737
A3089	G2985	C	A2503	A2503	A2374	U2248	C2173	A1953	A1823	A1741
U3096	U2989	U	A2504	A2504	U2387	A2251	U2177	A1962	U1824	G1742
U3097	A	C	A2505	A2505	U2387	C2252	A2178	A1962	C1827	U1743
U3100	U2993	U	A2506	A2506	A2390	U2256	A2179	G1973	A1828	A1744
U3102	G2994	C	A2507	A2507	A2391	U2256	A2180	A1974	A1829	U1745
C3103	G2995	A	C2511	C2511	U2392	C2259	G2181	U1977	G1830	G1746
U3104	U2998	C	A2512	A2512	C2393	A2260	C2182	A1978	G1831	G1747
U3109	C2999	U	G2519	G2519	A2394	C2261	A2184	U1979	G1748	C1749
C3110	A3000	A	C2520	C2520	A2395	C2262	A2184	U1980	C1832	C1749
A3111	A3005	C	A2521	A2521	C2396	C2263	A2191	A1984	A1836	G1750
A3113	C3008	U	A2527	A2527	A2401	U2277	U2194	G1985	A1844	U1751
A3125	U2910	U	G2528	G2528	C2405	C2283	A2195	A1986	A1853	A1753
G3132	G3013	C	U2529	U2529	A2406	C2284	G2197	G1987	U1854	G1754
U3015	G3014	A	A2530	A2530	U2407	U2285	A2198	C2100	A1855	A1755
A3141	G3016	U	U2531	U2531	U2408	A2286	A2199	G2105	A1859	G1760
		C	U2540	U2540	U2410	U2287	G2201	A2186	A1860	A1761
		A	C2541	C2541	C2415	A2293	C2202	G2107	U1862	A1763
		C	C2541	C2541	A2294	U2294	U2204	A2109	A1863	C1765
		U			G2421		U2205	A2110	A1864	G1770



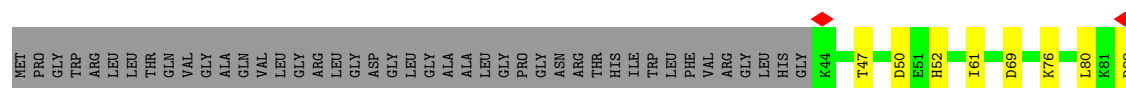
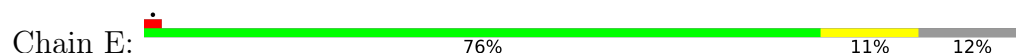
- Molecule 17: mitochondrial tRNA^{Val}



- Molecule 18: 39S ribosomal protein L2, mitochondrial

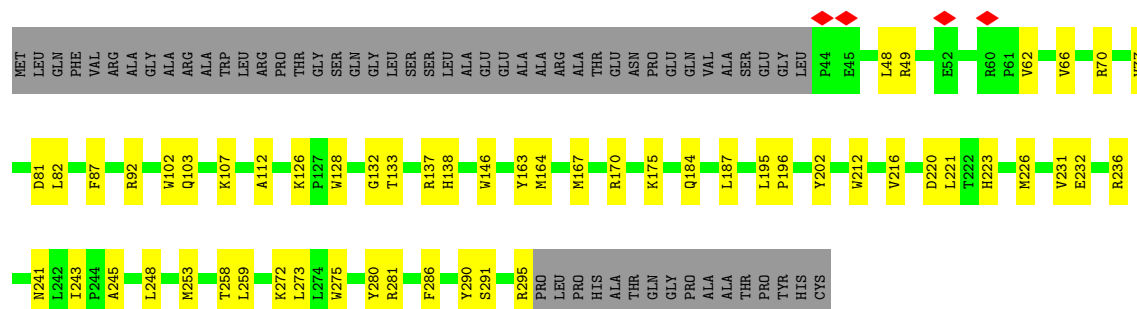


- Molecule 19: 39S ribosomal protein L3, mitochondrial

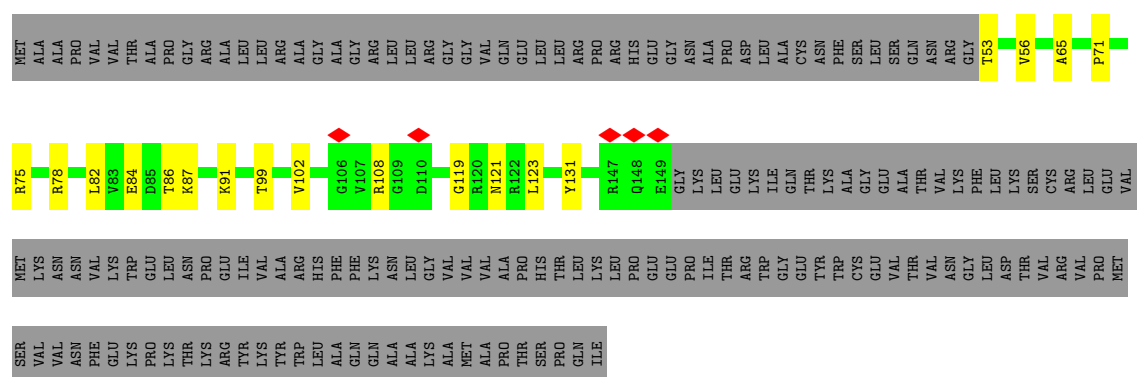


- Molecule 20: 39S ribosomal protein L4, mitochondrial

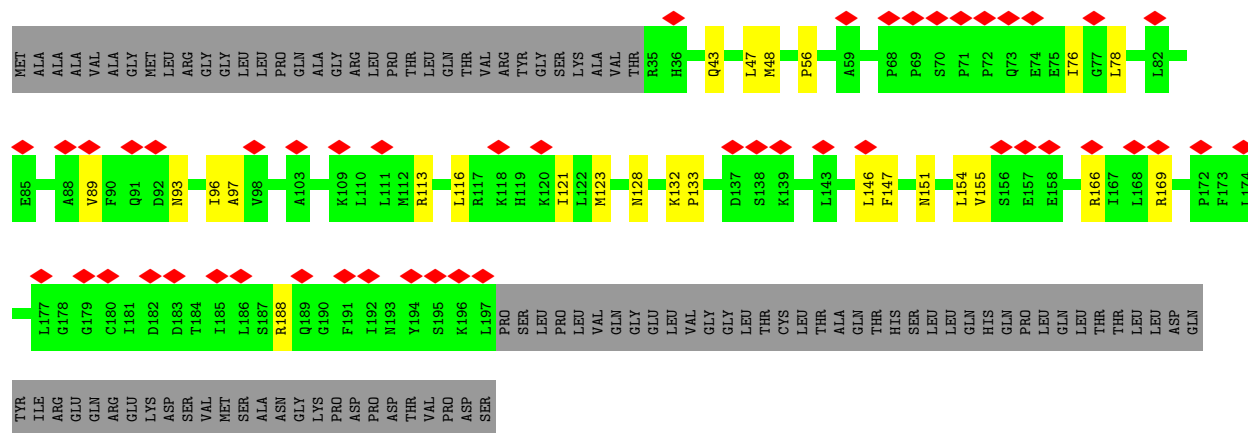




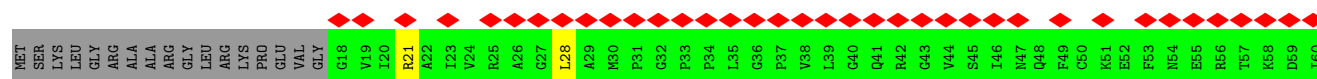
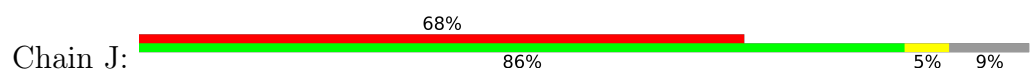
- Molecule 21: 39S ribosomal protein L9, mitochondrial

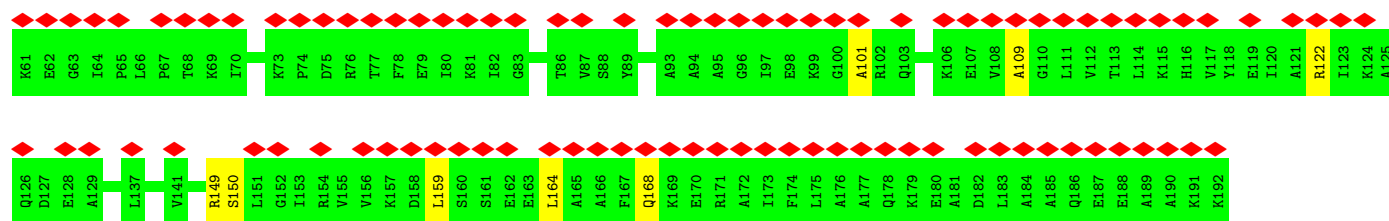


- Molecule 22: 39S ribosomal protein L10, mitochondrial



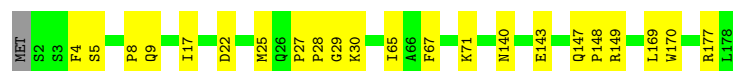
- Molecule 23: 39S ribosomal protein L11, mitochondrial





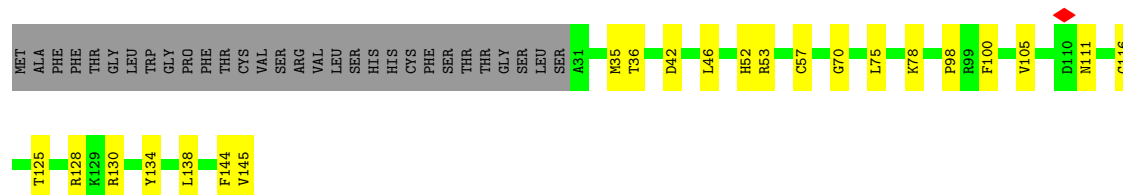
- Molecule 24: 39S ribosomal protein L13, mitochondrial

Chain K: 87% 12% .



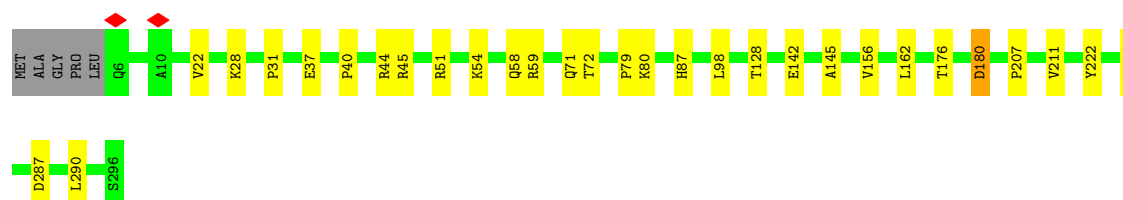
- Molecule 25: 39S ribosomal protein L14, mitochondrial

Chain L: 64% 15% 21%



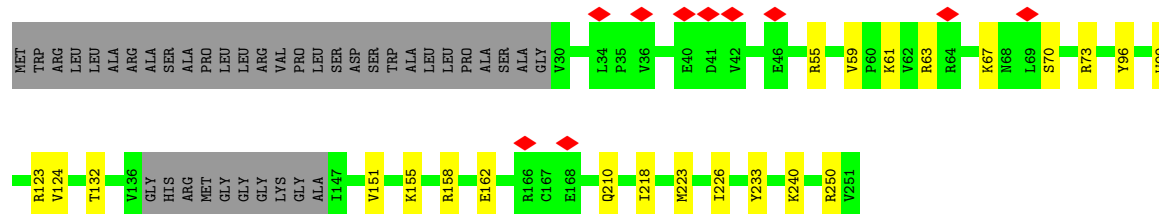
- Molecule 26: 39S ribosomal protein L15, mitochondrial

Chain M: 88% 10% .



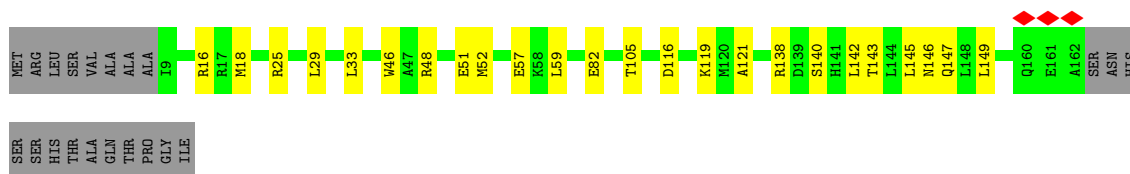
- Molecule 27: 39S ribosomal protein L16, mitochondrial

Chain N: 75% 9% 16%



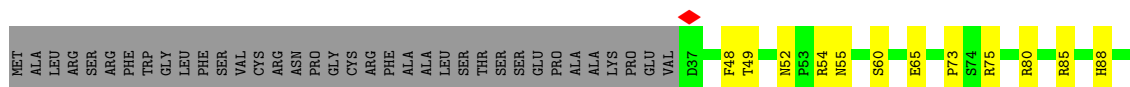
- Molecule 28: 39S ribosomal protein L17, mitochondrial

Chain O: 74% 14% 12%



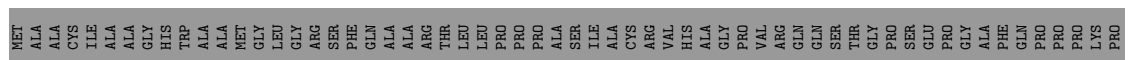
- Molecule 29: 39S ribosomal protein L18, mitochondrial

Chain P: 64% 16% 20%



- Molecule 30: 39S ribosomal protein L19, mitochondrial

Chain Q: 62% 13% 24%



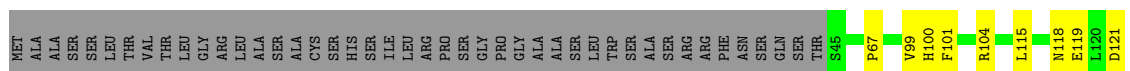
- Molecule 31: 39S ribosomal protein L20, mitochondrial

Chain R: 85% 9% 6%



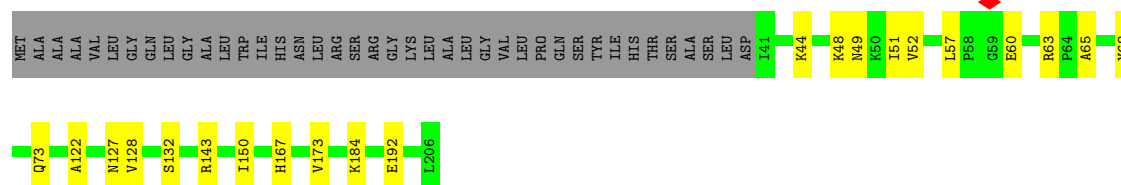
- Molecule 32: 39S ribosomal protein L21, mitochondrial

Chain S: 69% 9% 21%



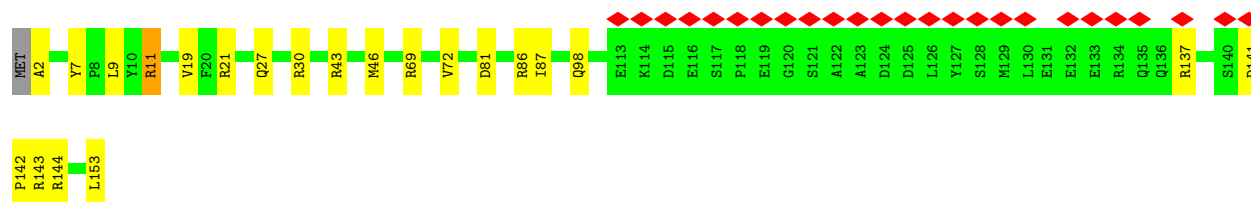
- Molecule 33: 39S ribosomal protein L22, mitochondrial

Chain T:  70% 10% 19%



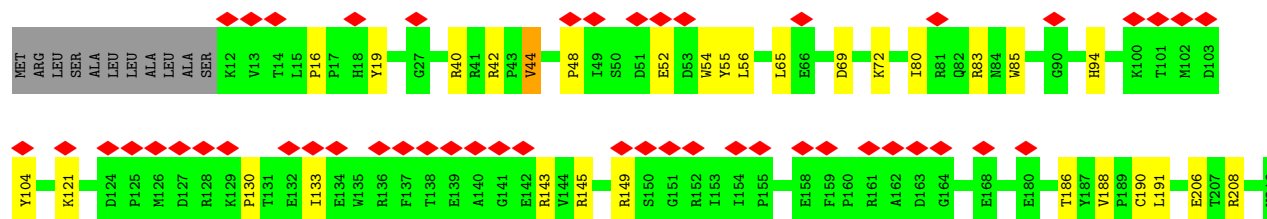
- Molecule 34: 39S ribosomal protein L23, mitochondrial

Chain U:  16% 85% 14% ..



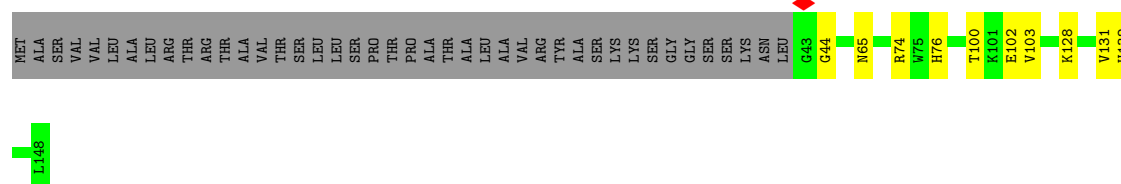
- Molecule 35: 39S ribosomal protein L24, mitochondrial

Chain V:  23% 81% 13% 5%



- Molecule 36: 39S ribosomal protein L27, mitochondrial

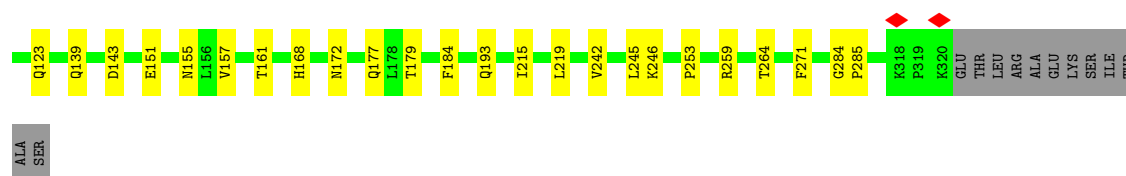
Chain W:  65% 7% 28%



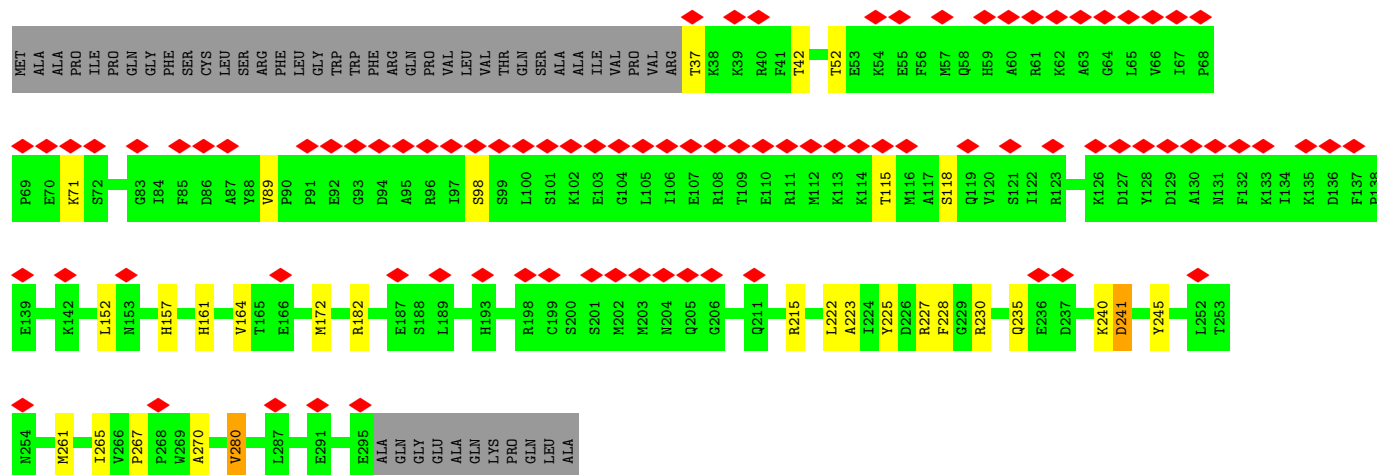
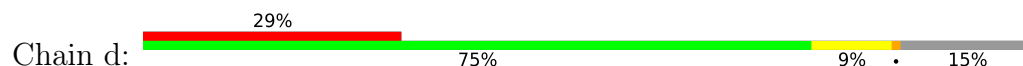
- Molecule 37: 39S ribosomal protein L28, mitochondrial

Chain X:  87% 9% 5%

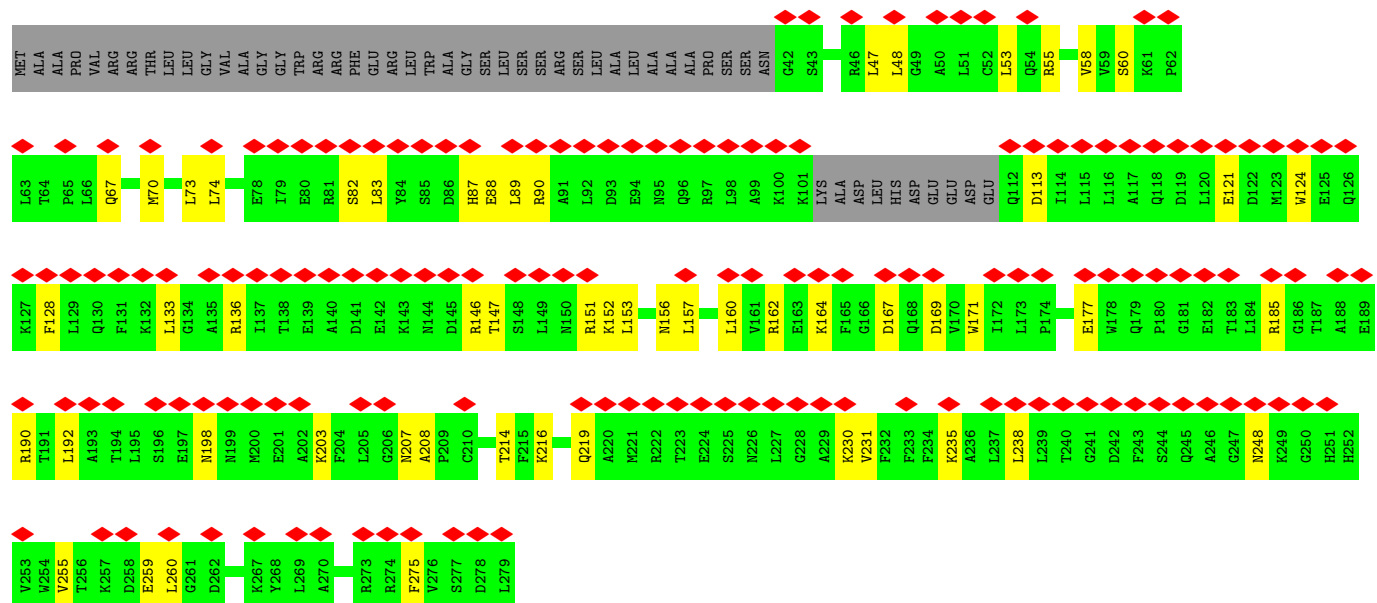




- Molecule 43: 39S ribosomal protein L45, mitochondrial

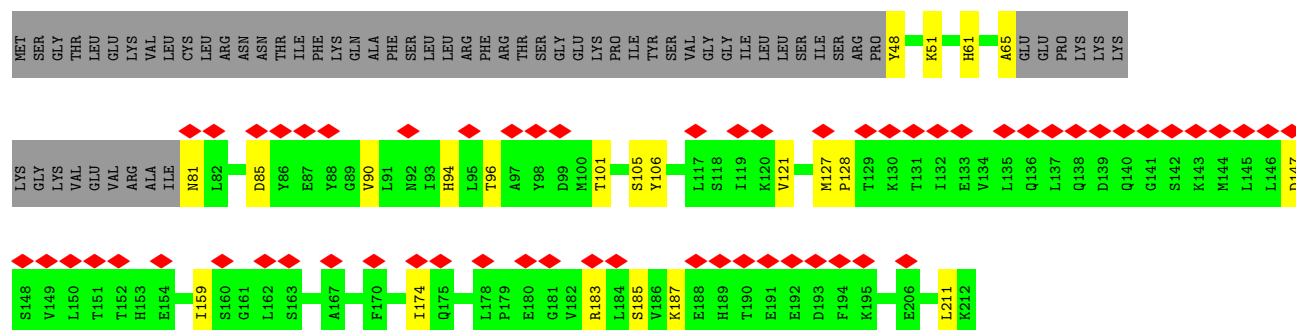


- Molecule 44: 39S ribosomal protein L46, mitochondrial

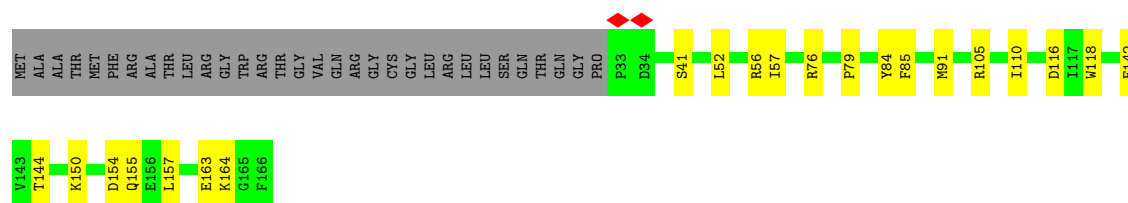


- Molecule 45: 39S ribosomal protein L48, mitochondrial

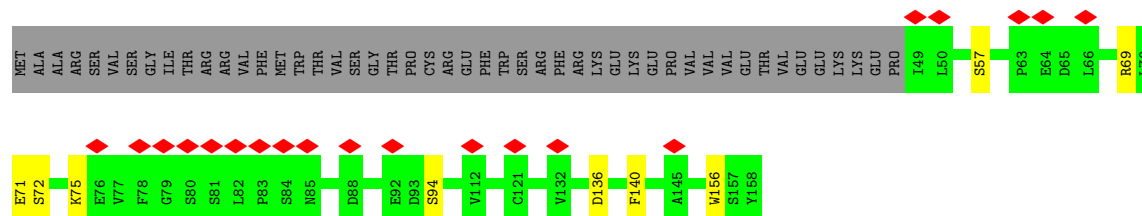




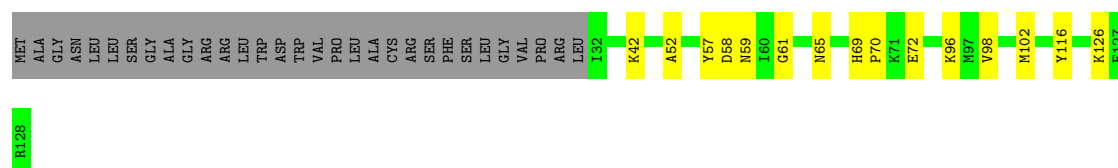
- Molecule 46: 39S ribosomal protein L49, mitochondrial



- Molecule 47: 39S ribosomal protein L50, mitochondrial



- Molecule 48: 39S ribosomal protein L51, mitochondrial



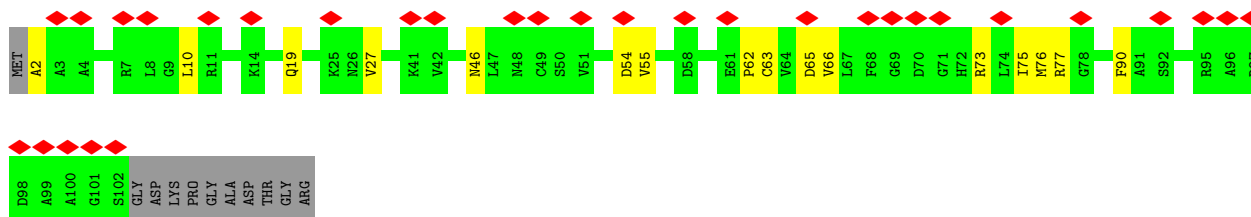
- Molecule 49: 39S ribosomal protein L52, mitochondrial



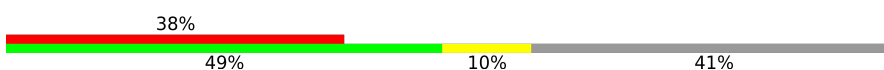
LEU
PRO
SER
GLN

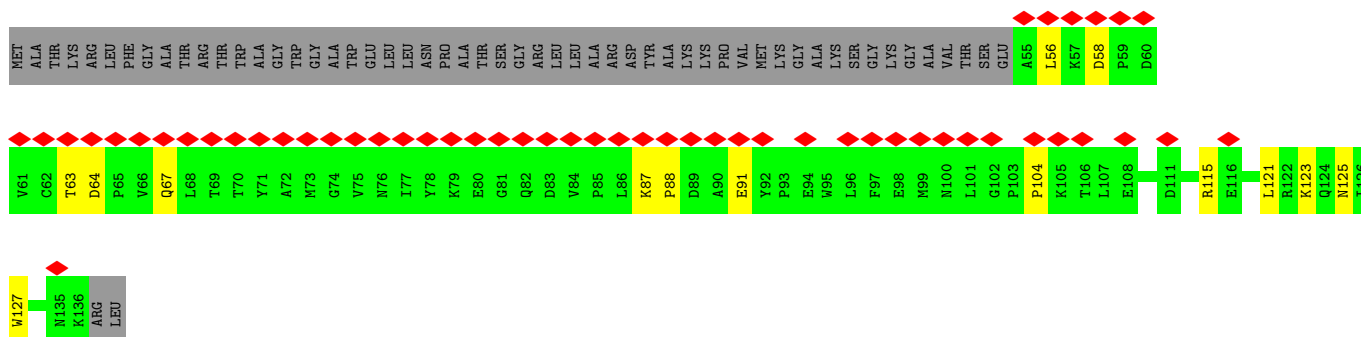
- Molecule 50: 39S ribosomal protein L53, mitochondrial

Chain k: 



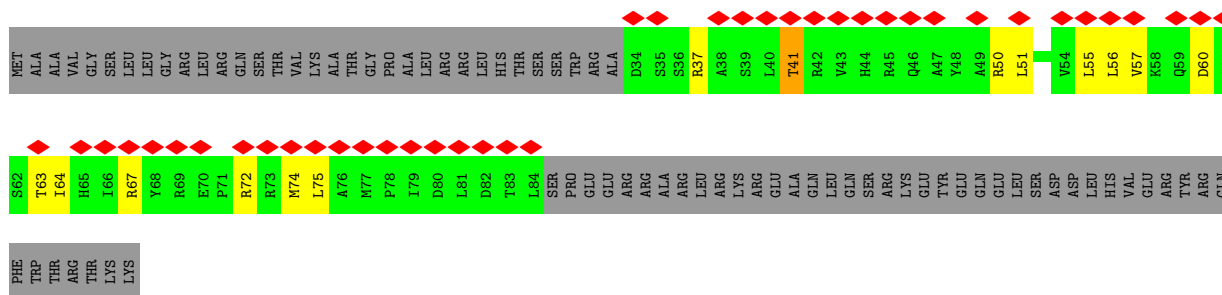
- Molecule 51: 39S ribosomal protein L54, mitochondrial

Chain l: 



- Molecule 52: 39S ribosomal protein L55, mitochondrial

Chain m: 

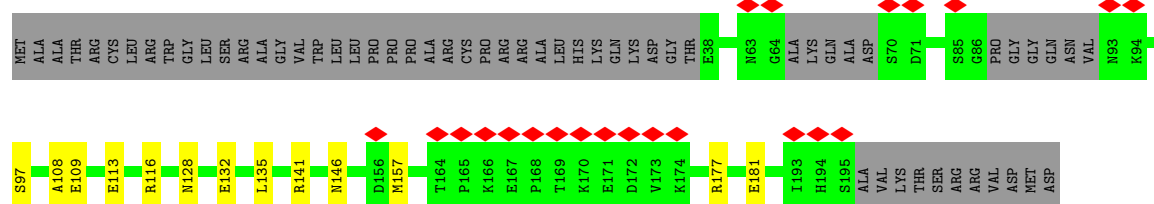


- Molecule 53: Ribosomal protein 63, mitochondrial

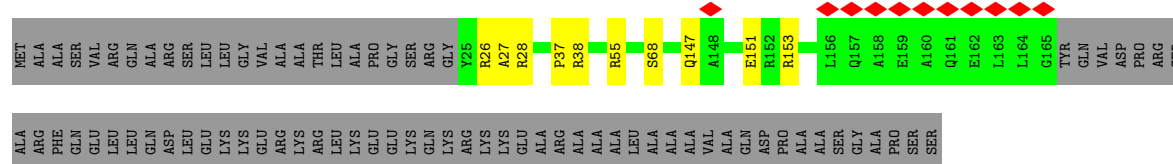
Chain o: 



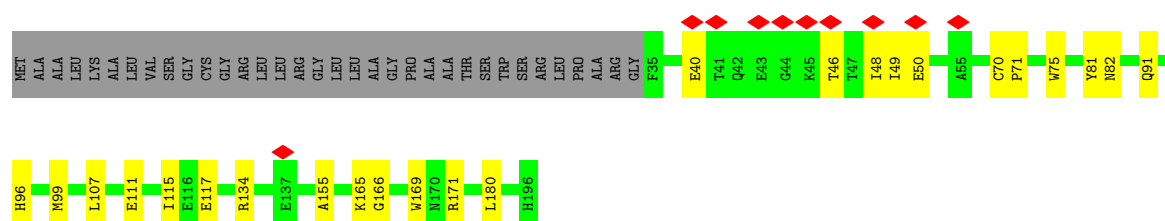
- Molecule 54: Peptidyl-tRNA hydrolase ICT1, mitochondrial



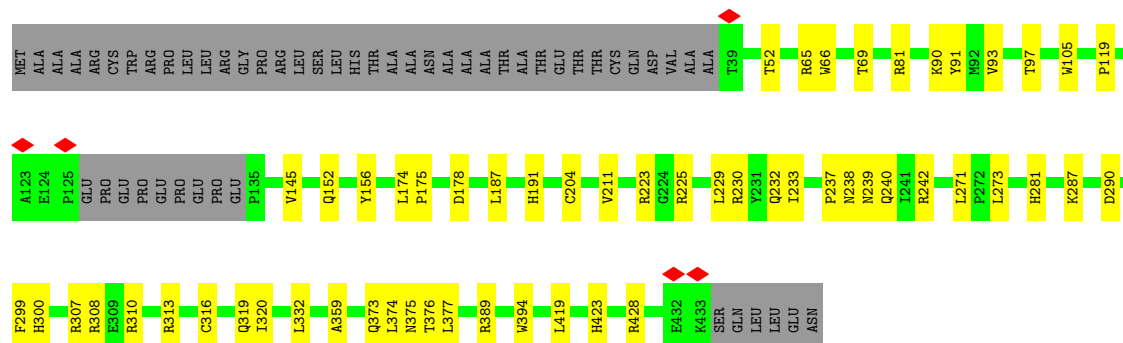
- Molecule 55: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 56: 39S ribosomal protein S18a, mitochondrial



- Molecule 57: 39S ribosomal protein S30, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123267	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.222	Depositor
Minimum map value	-1.532	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	474.87997, 474.87997, 474.87997	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAC, THC, K, SAM, FES, PM8, AYA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	u	0.10	0/941	0.28	0/1270
2	v	0.09	0/597	0.24	0/796
3	w	0.09	0/647	0.28	0/871
4	x	0.10	0/2721	0.28	0/3691
5	y	0.08	0/2011	0.22	0/2702
6	0	0.09	0/913	0.24	0/1224
7	1	0.08	0/460	0.23	0/610
8	2	0.11	0/383	0.24	0/507
9	3	0.11	0/853	0.25	0/1136
10	4	0.10	0/350	0.24	0/461
11	5	0.11	0/3305	0.27	0/4502
12	6	0.11	0/3043	0.27	0/4140
13	7	0.10	0/2447	0.25	0/3310
14	8	0.10	0/880	0.24	0/1188
15	9	0.12	0/1025	0.26	0/1379
16	A	0.09	0/33664	0.16	0/52392
17	B	0.05	0/1700	0.09	0/2641
18	D	0.11	0/1910	0.27	0/2569
19	E	0.11	0/2475	0.26	0/3355
20	F	0.11	0/2090	0.28	0/2842
21	H	0.11	0/816	0.27	0/1097
22	I	0.11	0/1354	0.30	0/1829
23	J	0.09	0/1348	0.28	0/1813
24	K	0.11	0/1490	0.28	0/2021
25	L	0.11	0/905	0.30	0/1218
26	M	0.11	0/2381	0.28	1/3212 (0.0%)
27	N	0.09	0/1768	0.24	0/2383
28	O	0.11	0/1283	0.27	0/1727
29	P	0.10	0/1199	0.27	0/1623
30	Q	0.10	0/1884	0.26	0/2535
31	R	0.10	0/1175	0.24	0/1572
32	S	0.12	0/1320	0.30	0/1789

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	T	0.11	0/1403	0.27	0/1886
34	U	0.11	0/1274	0.27	0/1723
35	V	0.10	0/1721	0.23	0/2333
36	W	0.12	0/857	0.27	0/1155
37	X	0.09	0/2099	0.24	0/2837
38	Y	0.09	0/1593	0.24	0/2136
39	Z	0.11	0/1021	0.27	0/1378
40	a	0.10	0/866	0.25	0/1174
41	b	0.12	0/1203	0.29	0/1627
42	c	0.09	0/2347	0.25	0/3171
43	d	0.10	0/2181	0.26	0/2949
44	e	0.08	0/1885	0.26	0/2542
45	f	0.09	0/1216	0.27	0/1638
46	g	0.12	0/1151	0.29	0/1569
47	h	0.09	0/918	0.23	0/1249
48	i	0.11	0/850	0.25	0/1135
49	j	0.10	0/760	0.24	0/1023
50	k	0.09	0/777	0.23	0/1048
51	l	0.10	0/707	0.27	0/960
52	m	0.08	0/426	0.24	0/575
53	o	0.08	0/819	0.22	0/1097
54	p	0.09	0/1223	0.23	0/1641
55	q	0.08	0/1208	0.20	0/1633
56	r	0.10	0/1362	0.26	0/1846
57	s	0.11	0/3239	0.27	0/4400
All	All	0.10	0/112444	0.23	1/159130 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	54	LYS	CB-CA-C	-5.03	109.80	115.79

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	u	919	0	917	13	0
2	v	588	0	604	13	0
3	w	638	0	636	8	0
4	x	2660	0	2640	43	0
5	y	1980	0	2066	33	0
6	0	898	0	916	9	0
7	1	455	0	498	4	0
8	2	377	0	406	2	0
9	3	832	0	883	10	0
10	4	342	0	361	6	0
11	5	3210	0	3206	34	0
12	6	2948	0	2841	56	0
13	7	2390	0	2397	32	0
14	8	860	0	852	15	0
15	9	997	0	987	13	0
16	A	30460	0	15537	256	0
17	B	1522	0	776	13	0
18	D	1872	0	1932	30	0
19	E	2406	0	2415	26	0
20	F	2031	0	2065	44	0
21	H	802	0	846	14	0
22	I	1324	0	1400	16	0
23	J	1330	0	1407	8	0
24	K	1455	0	1452	15	0
25	L	890	0	941	16	0
26	M	2327	0	2395	23	0
27	N	1723	0	1754	15	0
28	O	1259	0	1294	17	0
29	P	1173	0	1165	21	0
30	Q	1843	0	1878	25	0
31	R	1154	0	1214	12	0
32	S	1293	0	1365	15	0
33	T	1369	0	1410	15	0
34	U	1251	0	1232	15	0
35	V	1676	0	1687	20	0
36	W	835	0	858	7	0
37	X	2044	0	2060	15	0
38	Y	1556	0	1597	17	0
39	Z	996	0	1044	8	0
40	a	840	0	810	11	0
41	b	1189	0	1183	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	c	2299	0	2320	17	0
43	d	2124	0	2125	22	0
44	e	1848	0	1849	39	0
45	f	1196	0	1212	13	0
46	g	1113	0	1097	15	0
47	h	895	0	881	5	0
48	i	828	0	857	15	0
49	j	745	0	746	13	0
50	k	774	0	784	12	0
51	l	688	0	674	9	0
52	m	419	0	435	16	0
53	o	798	0	804	18	0
54	p	1205	0	1223	9	0
55	q	1177	0	1154	8	0
56	r	1322	0	1348	20	0
57	s	3155	0	3139	34	0
58	w	32	0	39	5	0
59	x	27	0	22	0	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
61	9	1	0	0	0	0
61	A	92	0	0	0	0
61	D	1	0	0	0	0
61	M	1	0	0	0	0
61	O	1	0	0	0	0
61	g	1	0	0	0	0
62	A	2	0	0	0	0
63	r	4	0	0	0	0
All	All	107464	0	92636	961	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (961) 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)
16:A:2499:U:OP2	16:A:2504:A:N6	2.18	0.76
40:a:41:ASP:HB3	40:a:46:ASN:HD22	1.51	0.75
5:y:162:ARG:NH1	5:y:186:ILE:O	2.19	0.74
4:x:258:CYS:SG	4:x:316:GLN:NE2	2.62	0.73
2:v:45:LEU:HD23	2:v:50:ALA:HB1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:2725:A:H4'	16:A:3072:U:H3	1.52	0.72
4:x:328:LEU:HB3	4:x:334:ILE:HB	1.72	0.72
16:A:2259:C:O2'	16:A:2261:C:OP2	2.08	0.72
16:A:1990:G:OP1	18:D:269:ARG:NH2	2.22	0.71
22:I:97:ALA:HB3	22:I:154:LEU:HB2	1.72	0.71
16:A:1777:A:N6	16:A:1780:U:OP2	2.22	0.71
34:U:21:ARG:HH12	38:Y:143:ASP:HA	1.53	0.71
16:A:2354:A:H61	16:A:2361:G:H1	1.37	0.71
16:A:2248:U:OP1	31:R:99:ARG:NH2	2.24	0.71
21:H:53:THR:N	21:H:86:THR:HG1	1.88	0.70
13:7:80:VAL:HG21	34:U:143:ARG:HG2	1.74	0.70
1:u:135:LEU:HD22	1:u:179:LEU:HB3	1.74	0.70
11:5:115:GLU:HB2	11:5:119:GLN:HB2	1.73	0.70
32:S:144:LEU:HB2	40:a:58:ILE:HB	1.75	0.69
16:A:2165:C:N4	16:A:2212:C:OP1	2.27	0.68
23:J:28:LEU:HB3	51:l:56:LEU:HD22	1.75	0.68
53:o:15:ARG:HB3	53:o:18:ILE:HG12	1.75	0.68
11:5:229:ARG:NH1	11:5:231:SER:OG	2.27	0.68
16:A:2360:U:H3'	16:A:2361:G:H4'	1.76	0.68
20:F:132:GLY:HA3	43:d:42:THR:HG21	1.75	0.67
28:O:142:LEU:HA	28:O:147:GLN:HE21	1.59	0.67
17:B:1605:A:H61	17:B:1666:U:H3	1.41	0.67
7:1:24:ALA:HB2	7:1:54:VAL:HG11	1.77	0.67
13:7:170:PRO:HG2	13:7:296:ARG:HH12	1.58	0.67
16:A:2442:U:OP1	57:s:81:ARG:NH2	2.25	0.67
44:e:255:VAL:HB	44:e:259:GLU:HG3	1.76	0.67
4:x:170:GLY:O	4:x:251:ARG:NH1	2.27	0.67
4:x:274:LYS:HE3	4:x:276:SER:HB3	1.77	0.67
14:8:153:GLU:HG2	44:e:47:LEU:HD21	1.77	0.66
22:I:128:ASN:HB3	22:I:132:LYS:HE3	1.78	0.66
13:7:112:PRO:HB2	13:7:267:PRO:HG2	1.78	0.66
57:s:191:HIS:O	57:s:428:ARG:NH2	2.28	0.66
12:6:88:ILE:HD13	49:j:109:LEU:HB3	1.78	0.66
13:7:180:CYS:SG	13:7:296:ARG:NH1	2.69	0.66
43:d:182:ARG:HB2	43:d:223:ALA:HB3	1.78	0.66
16:A:1853:A:OP2	32:S:177:ARG:NH1	2.29	0.65
4:x:42:ARG:NH1	4:x:46:GLN:OE1	2.29	0.65
24:K:27:PRO:HG2	24:K:30:LYS:HB2	1.77	0.65
12:6:90:ILE:HA	49:j:112:LYS:HB2	1.77	0.65
18:D:113:ARG:O	18:D:147:ARG:NH2	2.30	0.65
16:A:2167:A:N6	16:A:2212:C:OP2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:257:ILE:O	18:D:262:ARG:NH1	2.25	0.65
42:c:259:ARG:HB2	42:c:271:PHE:HB2	1.79	0.65
50:k:19:GLN:NE2	50:k:63:CYS:SG	2.71	0.64
50:k:73:ARG:HB2	56:r:46:THR:HG23	1.79	0.64
16:A:2110:A:N1	16:A:2980:U:O2'	2.28	0.64
19:E:82:ASP:O	19:E:188:LYS:NZ	2.30	0.63
20:F:164:MET:HE1	48:i:70:PRO:HB2	1.80	0.63
29:P:142:ASN:HD22	54:p:181:GLU:HG2	1.62	0.63
46:g:84:TYR:OH	46:g:164:LYS:NZ	2.28	0.63
6:0:139:ARG:NH1	16:A:2322:C:OP1	2.31	0.63
11:5:113:LEU:HD12	11:5:311:ALA:HB1	1.80	0.63
16:A:2191:A:N6	16:A:2198:A:OP1	2.31	0.63
29:P:104:SER:O	29:P:135:ARG:NH1	2.31	0.63
52:m:57:VAL:N	52:m:75:LEU:O	2.30	0.63
16:A:2531:U:O4	18:D:246:ARG:NH2	2.31	0.63
18:D:194:ASN:ND2	18:D:245:GLY:O	2.30	0.63
33:T:184:LYS:NZ	33:T:192:GLU:OE1	2.29	0.63
20:F:272:LYS:NZ	48:i:65:ASN:OD1	2.31	0.63
18:D:296:VAL:HG23	18:D:297:LYS:HG2	1.81	0.62
19:E:244:ALA:HB1	19:E:248:ILE:HD11	1.81	0.62
35:V:54:TRP:NE1	35:V:56:LEU:O	2.32	0.62
46:g:110:ILE:HD11	46:g:157:LEU:HD13	1.80	0.62
13:7:61:ARG:HD3	43:d:235:GLN:HE22	1.64	0.62
1:u:111:VAL:H	2:v:26:THR:HG22	1.62	0.62
19:E:69:ASP:OD1	19:E:154:ARG:NH1	2.32	0.62
30:Q:182:ARG:HG3	30:Q:187:LEU:HD11	1.81	0.62
12:6:60:ARG:HH12	12:6:64:GLU:HB2	1.64	0.62
13:7:244:ALA:HB1	13:7:250:ARG:HE	1.65	0.62
4:x:288:GLN:HE22	4:x:316:GLN:HE21	1.48	0.62
12:6:187:VAL:HG13	12:6:319:PHE:HB3	1.82	0.62
16:A:2137:C:H4'	22:I:43:GLN:HE21	1.65	0.62
33:T:63:ARG:NH1	43:d:228:PHE:O	2.33	0.62
16:A:1737:A:H5'	48:i:96:LYS:HE3	1.82	0.62
44:e:55:ARG:NH2	44:e:152:LYS:O	2.30	0.61
29:P:60:SER:OG	54:p:177:ARG:NH1	2.34	0.61
30:Q:183:LEU:HD21	30:Q:219:GLU:HG2	1.82	0.61
5:y:135:GLY:HA3	5:y:173:GLU:HB3	1.82	0.61
16:A:3082:G:N2	16:A:3085:A:OP2	2.28	0.61
34:U:9:LEU:O	34:U:11:ARG:NH1	2.33	0.61
45:f:94:HIS:HB2	45:f:185:SER:HB3	1.83	0.61
12:6:124:ARG:NH2	14:8:112:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4:66:PHE:N	16:A:3013:G:HO2'	1.98	0.61
16:A:2277:U:OP2	48:i:42:LYS:NZ	2.34	0.61
30:Q:121:THR:HG22	30:Q:171:VAL:HA	1.83	0.61
30:Q:127:SER:OG	30:Q:129:LYS:NZ	2.33	0.61
44:e:235:LYS:NZ	44:e:275:PHE:O	2.32	0.61
5:y:157:MET:SD	5:y:160:ARG:NH2	2.72	0.61
22:I:47:LEU:HD22	27:N:226:ILE:HG12	1.83	0.61
24:K:140:ASN:ND2	42:c:264:THR:OG1	2.33	0.61
3:w:138:LEU:HD13	3:w:144:ILE:HG12	1.83	0.60
5:y:116:ARG:HD3	5:y:124:LEU:HD22	1.83	0.60
41:b:28:ARG:NH1	41:b:78:GLU:OE1	2.33	0.60
45:f:61:HIS:HA	45:f:65:ALA:HB3	1.82	0.60
9:3:94:LEU:N	16:A:1752:U:OP1	2.34	0.60
51:l:121:LEU:O	51:l:125:ASN:ND2	2.34	0.60
16:A:2039:A:N7	16:A:2729:U:O2'	2.33	0.60
16:A:2119:U:O2'	39:Z:36:PHE:O	2.18	0.60
44:e:48:LEU:HB2	44:e:231:VAL:HG12	1.81	0.60
16:A:1994:A:H61	16:A:2736:C:H4'	1.67	0.60
16:A:3113:A:OP1	16:A:3167:U:O2'	2.18	0.60
29:P:52:ASN:HB3	29:P:55:ASN:HB2	1.82	0.60
12:6:252:CYS:SG	12:6:296:ARG:NH1	2.75	0.60
16:A:2795:U:O2	21:H:87:LYS:NZ	2.33	0.60
32:S:99:VAL:HG12	32:S:133:VAL:HG22	1.84	0.60
13:7:276:PHE:HB2	13:7:304:VAL:HG22	1.84	0.60
16:A:2003:A:OP2	16:A:2734:A:O2'	2.18	0.60
16:A:2015:G:H22	16:A:2037:U:H5''	1.65	0.60
17:B:1671:C:OP1	44:e:219:GLN:NE2	2.34	0.60
54:p:113:GLU:OE1	54:p:116:ARG:NH1	2.33	0.60
57:s:271:LEU:HD23	57:s:273:LEU:HD13	1.82	0.60
42:c:215:ILE:HG23	42:c:219:LEU:HD12	1.84	0.60
16:A:2740:A:N3	16:A:2921:A:O2'	2.29	0.60
57:s:178:ASP:OD1	57:s:238:ASN:ND2	2.35	0.60
26:M:44:ARG:HG3	26:M:45:ARG:HG3	1.84	0.59
28:O:140:SER:O	28:O:146:ASN:ND2	2.35	0.59
11:5:216:GLU:OE2	11:5:367:ASN:ND2	2.33	0.59
13:7:189:LEU:O	13:7:295:ARG:NH2	2.34	0.59
16:A:1749:C:OP2	16:A:2899:C:O2'	2.20	0.59
16:A:2195:A:OP1	51:l:115:ARG:NH1	2.34	0.59
16:A:3189:C:O2'	56:r:155:ALA:N	2.31	0.59
32:S:101:PHE:HE1	49:j:49:TRP:HB3	1.66	0.59
19:E:96:ARG:NH1	19:E:315:PRO:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:218:ILE:HG23	27:N:223:MET:HB2	1.84	0.59
31:R:78:GLU:OE1	41:b:135:ASN:ND2	2.35	0.59
43:d:98:SER:OG	43:d:215:ARG:NH2	2.35	0.59
12:6:138:GLU:OE1	12:6:141:ARG:NH2	2.36	0.59
14:8:170:PRO:HB3	45:f:187:LYS:HG2	1.84	0.59
11:5:178:PRO:HG3	11:5:296:LYS:HD3	1.85	0.59
16:A:2346:U:OP1	57:s:223:ARG:NH2	2.36	0.59
45:f:96:THR:HB	45:f:183:ARG:HB3	1.84	0.59
42:c:151:GLU:O	42:c:155:ASN:ND2	2.34	0.59
46:g:118:TRP:NE1	46:g:142:GLU:OE2	2.33	0.59
57:s:178:ASP:HA	57:s:239:ASN:HD21	1.67	0.59
13:7:286:LEU:HD21	13:7:296:ARG:HE	1.68	0.59
16:A:2456:U:OP1	28:O:16:ARG:NH1	2.35	0.58
16:A:3019:G:O2'	16:A:3125:A:N1	2.35	0.58
19:E:80:LEU:HD12	19:E:323:GLY:HA3	1.85	0.58
25:L:100:PHE:HB3	30:Q:158:GLN:HE21	1.69	0.58
44:e:185:ARG:NH1	44:e:207:ASN:OD1	2.31	0.58
6:0:98:GLN:NE2	16:A:2709:A:N3	2.52	0.58
30:Q:165:GLU:HB2	30:Q:168:ASN:HB2	1.85	0.58
56:r:71:PRO:HD2	56:r:107:LEU:HD23	1.84	0.58
1:u:128:SER:HB2	1:u:185:ARG:HE	1.68	0.58
16:A:2016:C:OP2	26:M:59:ARG:NH1	2.36	0.58
30:Q:233:TRP:HB3	30:Q:240:ILE:HD12	1.84	0.58
16:A:1747:G:OP2	16:A:1749:C:N4	2.37	0.58
16:A:3219:G:O2'	16:A:3222:C:N4	2.34	0.58
4:x:86:VAL:HG21	4:x:154:GLU:HB2	1.85	0.58
11:5:98:LEU:HD13	11:5:272:ASP:HB2	1.85	0.58
16:A:1706:C:OP1	38:Y:193:ARG:NH2	2.35	0.58
35:V:130:PRO:O	35:V:149:ARG:NH2	2.37	0.58
36:W:100:THR:HG1	36:W:132:HIS:HE2	1.52	0.58
12:6:215:THR:HB	12:6:273:PHE:HB2	1.86	0.58
20:F:253:MET:HE3	20:F:259:LEU:HD22	1.85	0.58
24:K:28:PRO:HG3	24:K:65:ILE:HD12	1.86	0.58
6:0:96:ASN:OD1	16:A:2708:C:O2'	2.18	0.58
16:A:1883:G:H5'	46:g:91:MET:HG3	1.86	0.58
20:F:281:ARG:NH2	26:M:128:THR:OG1	2.36	0.58
20:F:232:GLU:O	20:F:236:ARG:NH1	2.37	0.57
24:K:25:MET:O	24:K:149:ARG:NH1	2.37	0.57
56:r:81:TYR:OH	56:r:111:GLU:OE1	2.21	0.57
13:7:275:CYS:HA	13:7:303:PRO:HA	1.85	0.57
28:O:143:THR:OG1	28:O:146:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5:30:ALA:N	18:D:201:GLY:O	2.37	0.57
14:8:161:ALA:HB1	44:e:208:ALA:HA	1.87	0.57
16:A:1805:A:OP2	35:V:94:HIS:NE2	2.34	0.57
16:A:2180:A:O2'	16:A:2206:C:O3'	2.21	0.57
39:Z:105:SER:OG	53:o:59:GLU:OE2	2.20	0.57
9:3:104:ARG:NH2	16:A:1871:A:N3	2.52	0.57
20:F:70:ARG:HA	20:F:196:PRO:HD3	1.85	0.57
21:H:131:TYR:HB3	37:X:139:TYR:HD1	1.70	0.57
12:6:35:MET:HB2	12:6:38:SER:HB3	1.87	0.57
12:6:126:ARG:NH1	29:P:156:ASP:OD2	2.38	0.57
2:v:43:GLN:HG2	58:w:200:PM8:H431	1.87	0.57
16:A:2237:A:OP1	56:r:171:ARG:NH2	2.38	0.57
3:w:83:VAL:HG22	3:w:122:MET:HE1	1.88	0.56
13:7:243:LYS:NZ	13:7:265:GLU:OE1	2.38	0.56
16:A:1814:A:N3	16:A:1862:U:O2'	2.36	0.56
56:r:70:CYS:HB2	56:r:107:LEU:HA	1.86	0.56
1:u:120:TYR:O	25:L:128:ARG:NH1	2.39	0.56
16:A:1693:C:O2	38:Y:162:ARG:NH1	2.38	0.56
12:6:270:PHE:N	12:6:317:SER:O	2.34	0.56
35:V:55:TYR:HB2	35:V:133:ILE:HD11	1.87	0.56
16:A:2721:G:H1	16:A:3097:U:H3	1.51	0.56
41:b:72:VAL:HG13	41:b:90:HIS:HB2	1.88	0.56
4:x:272:ILE:HA	4:x:277:ARG:HE	1.69	0.56
9:3:188:VAL:O	12:6:356:ARG:NH2	2.39	0.56
11:5:201:ARG:NH1	11:5:418:TYR:O	2.35	0.56
16:A:2109:A:N6	27:N:61:LYS:O	2.38	0.56
16:A:2238:A:OP1	56:r:165:LYS:NZ	2.39	0.56
16:A:2310:G:O2'	16:A:2675:G:O6	2.22	0.56
16:A:1822:U:O2	16:A:2707:A:O2'	2.22	0.56
16:A:2943:G:H5''	53:o:20:LYS:HD2	1.88	0.56
31:R:112:THR:OG1	41:b:127:GLN:NE2	2.34	0.56
35:V:121:LYS:HD3	35:V:130:PRO:HB2	1.87	0.56
57:s:374:LEU:HD21	57:s:377:LEU:HD13	1.87	0.56
11:5:300:ARG:NH2	16:A:2394:A:O2'	2.39	0.56
33:T:52:VAL:HG22	43:d:227:ARG:HG3	1.87	0.56
35:V:48:PRO:HD3	38:Y:234:LEU:HD21	1.89	0.56
16:A:2107:G:H2'	16:A:2981:A:C8	2.42	0.55
35:V:16:PRO:HD2	35:V:19:TYR:HB2	1.87	0.55
35:V:80:ILE:HB	35:V:85:TRP:HB2	1.89	0.55
16:A:1763:A:N7	55:q:38:ARG:NH1	2.50	0.55
54:p:109:GLU:HA	54:p:116:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:240:ILE:HG12	12:6:248:GLY:HA3	1.88	0.55
16:A:2822:C:O2'	16:A:2915:C:OP2	2.23	0.55
20:F:241:ASN:HD21	48:i:52:ALA:HB1	1.70	0.55
5:y:130:GLU:HG2	5:y:159:MET:HG2	1.87	0.55
20:F:248:LEU:O	48:i:59:ASN:ND2	2.38	0.55
42:c:245:LEU:HD12	42:c:253:PRO:HD3	1.88	0.55
50:k:10:LEU:O	50:k:46:ASN:ND2	2.31	0.55
16:A:2299:U:H5''	16:A:2300:G:H5''	1.87	0.55
44:e:214:THR:HG22	44:e:230:LYS:HG2	1.89	0.55
20:F:220:ASP:OD1	20:F:221:LEU:N	2.40	0.55
4:x:180:LEU:HD13	4:x:254:VAL:HG22	1.87	0.55
16:A:1742:G:O2'	16:A:1754:G:O6	2.24	0.55
16:A:2354:A:N6	16:A:2361:G:H1	2.04	0.55
32:S:100:HIS:HB2	32:S:134:LEU:HD11	1.89	0.55
33:T:57:LEU:HB2	33:T:60:GLU:HG3	1.89	0.54
34:U:81:ASP:HB3	34:U:87:ILE:HD11	1.88	0.54
16:A:1709:G:H4'	38:Y:192:LYS:HG3	1.89	0.54
16:A:2182:G:O2'	16:A:2199:A:OP2	2.25	0.54
16:A:2830:A:H5''	16:A:2831:G:H5''	1.89	0.54
20:F:62:VAL:HG23	20:F:82:LEU:HB2	1.89	0.54
57:s:204:CYS:SG	57:s:240:GLN:NE2	2.80	0.54
8:2:87:ARG:NH2	16:A:1792:G:N7	2.50	0.54
16:A:2332:C:H42	16:A:2442:U:H3	1.54	0.54
20:F:49:ARG:NH1	20:F:81:ASP:O	2.35	0.54
27:N:63:ARG:HH22	27:N:67:LYS:HG2	1.72	0.54
45:f:147:ASP:O	52:m:72:ARG:NH1	2.41	0.54
9:3:108:LYS:NZ	16:A:1745:U:O4	2.41	0.54
18:D:127:ILE:HD11	18:D:143:ALA:HB2	1.90	0.54
5:y:302:LEU:HA	5:y:306:ALA:HB3	1.89	0.54
16:A:1803:A:H4'	16:A:1804:A:H3'	1.89	0.54
41:b:49:ARG:HG3	41:b:50:GLU:HG2	1.88	0.54
25:L:98:PRO:HA	30:Q:162:ILE:HG12	1.90	0.54
11:5:166:THR:O	57:s:287:LYS:NZ	2.38	0.54
16:A:2138:U:O2'	16:A:2151:A:N3	2.41	0.54
15:9:130:LEU:HD13	38:Y:154:ARG:HA	1.90	0.54
16:A:2392:U:H2'	16:A:2394:A:H62	1.73	0.54
16:A:2458:A:O2'	19:E:215:PHE:O	2.25	0.54
16:A:2459:A:N6	16:A:2668:A:O2'	2.40	0.54
19:E:274:TRP:HE1	19:E:286:ASN:HB2	1.73	0.54
20:F:164:MET:HE3	48:i:69:HIS:HE1	1.73	0.54
45:f:48:TYR:HB3	45:f:51:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5:270:ILE:O	16:A:2409:A:O2'	2.26	0.54
12:6:217:LEU:HD13	12:6:236:LEU:HD13	1.90	0.54
5:y:300:GLU:OE2	5:y:304:ARG:NH2	2.41	0.54
33:T:49:ASN:ND2	33:T:68:TYR:O	2.41	0.54
12:6:114:ARG:NH1	29:P:117:TYR:O	2.41	0.53
13:7:139:ASN:HB3	13:7:174:VAL:HG21	1.90	0.53
16:A:2093:U:H4'	48:i:126:LYS:HE2	1.89	0.53
16:A:2261:C:O2'	32:S:184:ARG:NH1	2.40	0.53
16:A:1760:G:N7	55:q:55:ARG:NH2	2.56	0.53
37:X:7:PRO:HD2	37:X:10:LEU:HD12	1.88	0.53
57:s:152:GLN:HA	57:s:156:TYR:HB2	1.90	0.53
16:A:1749:C:O2'	26:M:80:LYS:NZ	2.39	0.53
22:I:116:LEU:HB3	22:I:121:ILE:HB	1.91	0.53
22:I:188:ARG:HD3	50:k:55:VAL:HB	1.91	0.53
24:K:5:SER:HB2	24:K:8:PRO:HD2	1.90	0.53
32:S:142:THR:OG1	40:a:62:HIS:NE2	2.35	0.53
16:A:1787:G:N2	16:A:1790:A:OP2	2.29	0.53
15:9:24:LYS:NZ	16:A:2422:U:OP2	2.40	0.53
35:V:80:ILE:HD12	35:V:85:TRP:HE3	1.73	0.53
11:5:55:LEU:HD11	37:X:163:ARG:HE	1.72	0.53
14:8:101:ARG:NE	44:e:82:SER:O	2.36	0.53
17:B:1672:C:O2'	44:e:216:LYS:O	2.23	0.53
52:m:57:VAL:HG22	52:m:63:THR:HG22	1.90	0.53
5:y:178:ARG:HA	5:y:181:TYR:CZ	2.44	0.53
11:5:173:ARG:NH2	16:A:2395:A:OP1	2.26	0.53
13:7:177:GLY:HA3	13:7:319:ARG:HE	1.74	0.53
16:A:2107:G:H2'	16:A:2981:A:H8	1.72	0.53
42:c:139:GLN:NE2	42:c:143:ASP:OD2	2.42	0.53
16:A:1867:A:N1	16:A:2019:G:O2'	2.38	0.53
11:5:139:LEU:O	11:5:145:ASN:ND2	2.35	0.53
16:A:2519:G:N7	18:D:230:SER:OG	2.40	0.53
12:6:173:LEU:HD13	12:6:272:LEU:HD22	1.90	0.52
13:7:93:MET:O	33:T:132:SER:OG	2.26	0.52
27:N:123:ARG:NH1	27:N:162:GLU:OE1	2.42	0.52
57:s:373:GLN:NE2	57:s:375:ASN:OD1	2.39	0.52
20:F:223:HIS:HA	20:F:226:MET:HE3	1.91	0.52
32:S:119:GLU:HG2	32:S:121:ASP:H	1.74	0.52
39:Z:64:HIS:HE1	39:Z:67:HIS:CE1	2.26	0.52
4:x:252:VAL:HB	4:x:305:VAL:HG22	1.91	0.52
12:6:162:PHE:HB3	12:6:165:ALA:HB3	1.91	0.52
16:A:2071:U:H2'	16:A:2831:G:N2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:q:37:PRO:HG2	55:q:68:SER:HA	1.89	0.52
15:9:16:ASP:OD2	34:U:86:ARG:NH1	2.42	0.52
16:A:1831:G:O6	41:b:4:ARG:NH2	2.38	0.52
16:A:1859:A:OP1	16:A:2299:U:O2'	2.23	0.52
34:U:153:LEU:HD11	43:d:240:LYS:HB2	1.90	0.52
9:3:104:ARG:NH1	9:3:160:LYS:O	2.42	0.52
29:P:85:ARG:NH1	29:P:157:SER:OG	2.42	0.52
44:e:60:SER:O	44:e:136:ARG:NH2	2.41	0.52
33:T:51:ILE:O	43:d:227:ARG:NH1	2.43	0.52
10:4:84:ARG:NE	16:A:3188:U:OP2	2.40	0.52
13:7:202:PHE:HB2	13:7:280:VAL:HG21	1.92	0.52
16:A:2240:C:H5'	24:K:29:GLY:HA3	1.91	0.52
33:T:127:ASN:O	43:d:230:ARG:NH2	2.42	0.52
41:b:49:ARG:HH21	41:b:94:VAL:HG11	1.75	0.52
44:e:177:GLU:O	44:e:190:ARG:NH2	2.43	0.52
16:A:1737:A:H61	16:A:1760:G:H1'	1.75	0.52
42:c:57:PRO:HB2	42:c:184:PHE:HE2	1.74	0.52
44:e:162:ARG:HD2	44:e:169:ASP:HB3	1.92	0.52
5:y:131:PHE:HE2	5:y:145:LEU:HD21	1.73	0.52
5:y:215:ILE:HD11	5:y:249:VAL:HG22	1.92	0.52
12:6:217:LEU:HB3	12:6:271:LEU:HB2	1.92	0.52
14:8:124:TYR:OH	44:e:67:GLN:NE2	2.43	0.52
34:U:69:ARG:NH1	34:U:98:GLN:OE1	2.37	0.52
42:c:157:VAL:O	42:c:161:THR:OG1	2.22	0.52
45:f:127:MET:HE3	45:f:128:PRO:HD2	1.92	0.52
10:4:87:ARG:HH11	10:4:101:ARG:HD3	1.75	0.52
45:f:101:THR:OG1	52:m:67:ARG:NH1	2.42	0.52
12:6:56:ARG:NH1	17:B:1625:A:OP1	2.40	0.51
20:F:216:VAL:HG22	20:F:258:THR:HB	1.92	0.51
38:Y:126:MET:HB3	38:Y:129:PRO:HG3	1.92	0.51
44:e:128:PHE:HD1	52:m:74:MET:HB3	1.75	0.51
4:x:299:THR:O	4:x:382:ARG:NH1	2.43	0.51
57:s:419:LEU:O	57:s:423:HIS:ND1	2.41	0.51
9:3:138:PRO:HG2	16:A:2854:U:H4'	1.91	0.51
16:A:1868:G:H2'	26:M:40:PRO:HG3	1.91	0.51
48:i:57:TYR:OH	55:q:28:ARG:O	2.28	0.51
20:F:103:GLN:O	20:F:107:LYS:NZ	2.43	0.51
26:M:31:PRO:HG2	53:o:86:ARG:HH12	1.76	0.51
16:A:2710:C:O2'	16:A:3220:A:N1	2.39	0.51
32:S:127:ARG:NH1	32:S:157:GLU:OE1	2.43	0.51
39:Z:134:MET:HE1	49:j:78:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:x:82:ALA:HA	55:q:153:ARG:HE	1.76	0.51
11:5:268:CYS:SG	16:A:2409:A:O2'	2.62	0.51
16:A:3125:A:H62	16:A:3132:G:H21	1.58	0.51
23:J:149:ARG:HH12	51:l:104:PRO:HD3	1.75	0.51
25:L:70:GLY:O	25:L:134:TYR:OH	2.27	0.51
26:M:156:VAL:O	26:M:176:THR:HA	2.10	0.51
43:d:245:TYR:HB2	43:d:265:ILE:HB	1.91	0.51
11:5:384:GLN:NE2	16:A:2395:A:O2'	2.44	0.51
40:a:62:HIS:O	40:a:62:HIS:ND1	2.44	0.51
56:r:166:GLY:O	56:r:171:ARG:NH1	2.44	0.51
2:v:45:LEU:O	2:v:51:ARG:NE	2.34	0.51
20:F:128:TRP:HB2	20:F:133:THR:HG21	1.92	0.50
49:j:63:GLN:OE1	49:j:66:ARG:NH2	2.39	0.50
16:A:3109:U:H3'	16:A:3110:C:H4'	1.93	0.50
44:e:90:ARG:NH2	44:e:113:ASP:OD2	2.45	0.50
44:e:147:THR:HG21	44:e:248:ASN:HB3	1.92	0.50
5:y:236:TYR:CE1	5:y:240:ARG:HD3	2.46	0.50
11:5:47:ASP:OD1	11:5:47:ASP:N	2.44	0.50
16:A:1879:G:OP1	20:F:92:ARG:NH1	2.39	0.50
16:A:3152:C:OP1	30:Q:141:SER:OG	2.21	0.50
16:A:2998:U:H5''	19:E:225:LYS:HB2	1.93	0.50
57:s:239:ASN:HB2	57:s:299:PHE:HB2	1.92	0.50
13:7:77:THR:HG21	13:7:95:LEU:HD21	1.94	0.50
16:A:2470:G:HO2'	25:L:36:THR:HG1	1.58	0.50
44:e:70:MET:HE3	44:e:74:LEU:HD21	1.93	0.50
47:h:71:GLU:HG2	47:h:75:LYS:HE3	1.94	0.50
5:y:211:GLN:HB3	5:y:249:VAL:HG21	1.93	0.50
16:A:2943:G:O3'	53:o:20:LYS:NZ	2.38	0.50
17:B:1613:U:O2'	17:B:1615:A:OP1	2.29	0.50
47:h:69:ARG:O	47:h:72:SER:OG	2.25	0.50
11:5:211:ALA:HB1	11:5:322:LEU:HD23	1.94	0.50
16:A:1828:A:O2'	16:A:2684:C:N3	2.38	0.50
16:A:2245:A:H1'	16:A:2246:A:C8	2.46	0.50
4:x:72:LYS:H	4:x:371:ASN:HB3	1.76	0.50
16:A:3176:A:H61	16:A:3193:U:H3	1.60	0.50
28:O:18:MET:HE1	28:O:29:LEU:HD21	1.92	0.50
35:V:69:ASP:HB2	35:V:72:LYS:HD2	1.93	0.50
48:i:69:HIS:HB3	48:i:72:GLU:HG3	1.94	0.50
16:A:2917:G:N7	26:M:72:THR:OG1	2.45	0.50
19:E:221:ARG:HG3	19:E:261:MET:HB3	1.92	0.50
43:d:164:VAL:HG12	43:d:261:MET:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:j:91:TRP:CD2	53:o:58:GLN:HG2	2.47	0.50
12:6:74:TYR:N	36:W:102:GLU:OE2	2.45	0.49
13:7:159:LYS:HZ3	40:a:93:LYS:HA	1.78	0.49
16:A:1830:G:H5'	41:b:2:THC:HG21	1.94	0.49
17:B:1608:G:O2'	17:B:1647:U:OP2	2.27	0.49
20:F:102:TRP:NE1	20:F:163:TYR:O	2.43	0.49
35:V:52:GLU:HB3	35:V:143:ARG:HH12	1.77	0.49
35:V:65:LEU:HD11	35:V:121:LYS:HB2	1.93	0.49
45:f:81:ASN:HD22	45:f:90:VAL:HG23	1.77	0.49
38:Y:191:ASN:O	38:Y:195:ASN:ND2	2.32	0.49
12:6:27:ARG:N	16:A:2073:A:OP2	2.46	0.49
57:s:376:THR:HB	57:s:389:ARG:HG3	1.94	0.49
12:6:243:ASN:OD1	12:6:243:ASN:N	2.44	0.49
16:A:2127:A:H4'	16:A:2251:A:C5	2.47	0.49
20:F:175:LYS:HE2	20:F:273:LEU:HB3	1.94	0.49
27:N:124:VAL:HG12	27:N:158:ARG:HE	1.77	0.49
4:x:129:LEU:HD13	4:x:163:LEU:HD11	1.93	0.49
12:6:206:TYR:O	12:6:243:ASN:ND2	2.45	0.49
16:A:1878:U:H5'	46:g:144:THR:HG21	1.95	0.49
16:A:1886:G:N7	20:F:170:ARG:NH2	2.47	0.49
29:P:80:ARG:NH2	29:P:95:GLU:OE2	2.45	0.49
45:f:105:SER:HB2	52:m:41:THR:HG21	1.94	0.49
49:j:87:GLY:HA3	53:o:62:HIS:HB2	1.94	0.49
57:s:66:TRP:O	57:s:69:THR:OG1	2.25	0.49
12:6:306:LYS:HG3	12:6:307:HIS:ND1	2.27	0.49
16:A:1882:A:N1	16:A:1891:A:O2'	2.46	0.49
16:A:2860:G:O2'	36:W:65:ASN:OD1	2.22	0.49
16:A:3073:C:C2	43:d:37:THR:HG21	2.48	0.49
21:H:78:ARG:NH1	37:X:87:LEU:O	2.43	0.49
54:p:108:ALA:O	54:p:116:ARG:NE	2.43	0.49
56:r:40:GLU:HG2	56:r:49:ILE:HG12	1.94	0.49
1:u:115:PRO:HG2	1:u:118:MET:HG2	1.95	0.49
1:u:190:LEU:HD23	1:u:193:LEU:HD12	1.95	0.49
5:y:99:LEU:HD12	5:y:109:ILE:HG23	1.94	0.49
12:6:311:MET:O	49:j:112:LYS:NZ	2.46	0.49
23:J:101:ALA:HB2	23:J:109:ALA:HB2	1.93	0.49
16:A:2755:A:OP2	21:H:91:LYS:NZ	2.40	0.49
57:s:316:CYS:HB3	57:s:319:GLN:HB2	1.94	0.49
12:6:155:TYR:HE2	12:6:320:GLN:HE21	1.61	0.49
16:A:2328:C:N4	57:s:52:THR:O	2.41	0.49
21:H:53:THR:N	21:H:86:THR:OG1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:75:LEU:HD11	25:L:105:VAL:HG21	1.95	0.49
43:d:182:ARG:HD2	43:d:225:TYR:HE2	1.78	0.49
11:5:96:HIS:HD1	16:A:2410:U:HO2'	1.56	0.48
13:7:166:LEU:HB3	13:7:181:TYR:HE1	1.78	0.48
45:f:106:TYR:OH	45:f:174:ILE:O	2.28	0.48
52:m:56:LEU:HB3	52:m:64:ILE:HG13	1.93	0.48
4:x:66:SER:O	4:x:262:ARG:NH1	2.40	0.48
11:5:167:THR:HG21	57:s:281:HIS:CD2	2.48	0.48
12:6:85:LYS:HZ1	49:j:106:GLU:HG2	1.79	0.48
12:6:224:HIS:CE1	12:6:227:GLU:H	2.31	0.48
16:A:2204:U:N3	16:A:2207:A:OP2	2.46	0.48
16:A:2830:A:O4'	16:A:2837:A:N6	2.46	0.48
42:c:242:VAL:HG12	42:c:246:LYS:HE3	1.93	0.48
57:s:332:LEU:HD21	57:s:359:ALA:HB2	1.95	0.48
16:A:1886:G:H1	48:i:61:GLY:HA3	1.77	0.48
16:A:2737:U:O2'	16:A:3084:A:N3	2.43	0.48
22:I:146:LEU:O	22:I:151:ASN:ND2	2.46	0.48
6:0:82:LYS:NZ	16:A:2719:G:O3'	2.47	0.48
6:0:179:ARG:HH12	6:0:182:PRO:HG3	1.78	0.48
20:F:243:ILE:HG22	55:q:27:ALA:HB2	1.95	0.48
25:L:42:ASP:HB2	25:L:116:GLY:HA3	1.95	0.48
42:c:168:HIS:O	42:c:172:ASN:ND2	2.45	0.48
50:k:65:ASP:OD2	50:k:73:ARG:NH2	2.47	0.48
4:x:105:HIS:HB2	4:x:347:VAL:HG13	1.95	0.48
16:A:1672:C:O2'	33:T:143:ARG:O	2.24	0.48
16:A:1977:U:H2'	16:A:1978:A:C8	2.48	0.48
16:A:3008:C:O2'	16:A:3051:A:N3	2.43	0.48
20:F:66:VAL:O	20:F:77:VAL:N	2.46	0.48
20:F:164:MET:HE3	48:i:69:HIS:CE1	2.48	0.48
29:P:102:VAL:HG11	29:P:141:ILE:HG13	1.94	0.48
16:A:2361:G:H5'	16:A:2362:A:H5''	1.94	0.48
22:I:166:ARG:HA	22:I:169:ARG:HE	1.79	0.48
2:v:29:ASP:OD1	2:v:29:ASP:N	2.47	0.48
3:w:103:HIS:HE1	3:w:105:MET:HE2	1.78	0.48
3:w:108:LEU:HB3	3:w:110:LEU:HG	1.95	0.48
12:6:260:ALA:O	12:6:263:SER:OG	2.32	0.48
16:A:2256:U:O2'	32:S:118:ASN:ND2	2.46	0.48
25:L:145:VAL:HG11	30:Q:160:VAL:HG11	1.95	0.48
30:Q:103:ARG:HG2	30:Q:108:ILE:HD12	1.95	0.48
44:e:164:LYS:HE2	44:e:167:ASP:HA	1.96	0.48
2:v:12:LEU:HD21	2:v:59:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:8:100:GLU:HA	44:e:83:LEU:HD22	1.96	0.48
15:9:110:ASP:OD1	15:9:110:ASP:N	2.45	0.48
16:A:2137:C:OP2	39:Z:77:ARG:NH1	2.46	0.48
16:A:3151:A:H4'	30:Q:146:GLY:O	2.14	0.48
18:D:185:GLY:N	18:D:238:GLU:O	2.46	0.48
24:K:22:ASP:HB3	24:K:147:GLN:HE21	1.79	0.48
35:V:190:CYS:SG	35:V:191:LEU:N	2.85	0.48
44:e:87:HIS:NE2	44:e:121:GLU:OE2	2.43	0.48
13:7:87:THR:O	13:7:90:SER:OG	2.24	0.48
16:A:2147:G:OP1	32:S:104:ARG:NE	2.43	0.48
19:E:52:HIS:HB2	28:O:145:LEU:HD23	1.96	0.48
19:E:334:ASP:HB3	19:E:337:VAL:HG23	1.94	0.48
22:I:56:PRO:HB3	27:N:210:GLN:HE21	1.79	0.48
31:R:141:ILE:HG22	40:a:51:LEU:HD12	1.96	0.48
40:a:40:PRO:HG2	40:a:43:TYR:HE1	1.79	0.48
4:x:258:CYS:HA	4:x:284:LEU:HD21	1.95	0.48
11:5:201:ARG:HB3	11:5:232:THR:HG22	1.96	0.48
12:6:85:LYS:HZ3	49:j:109:LEU:HD12	1.79	0.48
44:e:88:GLU:OE2	52:m:50:ARG:NH1	2.42	0.48
11:5:173:ARG:HD2	11:5:303:ARG:HD3	1.96	0.47
30:Q:168:ASN:HD21	30:Q:170:ARG:HD3	1.79	0.47
41:b:26:LEU:HD22	41:b:105:ALA:HA	1.96	0.47
41:b:34:SER:O	41:b:44:ARG:NH1	2.40	0.47
40:a:104:GLU:HB2	40:a:107:PRO:HD2	1.96	0.47
11:5:192:ILE:HG12	11:5:198:LEU:HB2	1.95	0.47
13:7:255:HIS:CD2	13:7:264:SER:HB2	2.49	0.47
16:A:1871:A:N7	16:A:1902:C:N4	2.61	0.47
18:D:215:VAL:HB	18:D:227:GLN:HB3	1.95	0.47
18:D:216:LEU:HD21	18:D:219:LYS:HD3	1.97	0.47
20:F:286:PHE:HA	20:F:290:TYR:HE2	1.79	0.47
30:Q:153:ASN:OD1	30:Q:154:VAL:N	2.47	0.47
4:x:312:LEU:HD23	4:x:363:LEU:HD11	1.96	0.47
16:A:1874:A:HO2'	16:A:2090:A:HO2'	1.63	0.47
16:A:2198:A:N6	23:J:150:SER:HB2	2.29	0.47
20:F:275:TRP:HD1	20:F:295:ARG:HH21	1.62	0.47
26:M:287:ASP:HB3	26:M:290:LEU:HB2	1.95	0.47
29:P:122:VAL:HG13	29:P:157:SER:HA	1.94	0.47
12:6:376:THR:HG22	54:p:141:ARG:HH12	1.80	0.47
16:A:1869:A:N6	48:i:116:TYR:OH	2.46	0.47
16:A:1936:A:H1'	16:A:1938:A:C6	2.50	0.47
16:A:2107:G:H1	16:A:2114:C:H42	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:76:LYS:HG3	19:E:170:LEU:HD21	1.96	0.47
57:s:242:ARG:NH1	57:s:290:ASP:OD2	2.47	0.47
7:1:18:VAL:HG11	7:1:34:ARG:HE	1.79	0.47
13:7:298:GLN:NE2	13:7:320:SER:O	2.48	0.47
2:v:6:ARG:NH2	58:w:200:PM8:O23	2.47	0.47
12:6:61:ALA:HB1	36:W:103:VAL:HG11	1.97	0.47
12:6:92:LEU:HB2	12:6:170:ARG:HG3	1.95	0.47
16:A:2110:A:O2'	16:A:2981:A:N6	2.47	0.47
16:A:3083:U:OP1	18:D:297:LYS:NZ	2.33	0.47
41:b:27:GLN:NE2	42:c:177:GLN:OE1	2.36	0.47
42:c:92:PHE:HB3	42:c:179:THR:HA	1.96	0.47
54:p:128:ASN:HD21	54:p:132:GLU:HB2	1.79	0.47
5:y:214:LYS:HE3	5:y:249:VAL:HG11	1.96	0.47
14:8:117:LEU:HD23	44:e:73:LEU:HD22	1.97	0.47
50:k:54:ASP:OD1	50:k:54:ASP:N	2.47	0.47
7:1:63:ARG:NH1	16:A:2909:G:OP1	2.39	0.47
12:6:215:THR:HG23	12:6:238:THR:HG22	1.96	0.47
16:A:2682:A:OP1	31:R:34:ARG:NH2	2.42	0.47
26:M:28:LYS:HD3	53:o:94:HIS:CD2	2.49	0.47
50:k:75:ILE:HD12	56:r:48:ILE:HG12	1.97	0.47
2:v:43:GLN:HB3	58:w:200:PM8:H36	1.80	0.47
4:x:192:LEU:HD13	4:x:221:VAL:HG21	1.97	0.47
13:7:106:ALA:O	13:7:113:TRP:N	2.48	0.47
16:A:2072:A:H62	16:A:2831:G:H2'	1.80	0.47
39:Z:66:LEU:HD12	39:Z:122:LEU:HD23	1.97	0.47
50:k:27:VAL:HG12	50:k:62:PRO:HG3	1.97	0.47
2:v:3:PRO:HB3	58:w:200:PM8:H371	1.96	0.46
11:5:204:VAL:HG11	11:5:279:PHE:HZ	1.80	0.46
14:8:178:TYR:O	44:e:136:ARG:NH1	2.48	0.46
47:h:57:SER:OG	47:h:136:ASP:OD2	2.32	0.46
4:x:342:THR:HG22	4:x:346:ARG:HE	1.80	0.46
5:y:104:PHE:HE2	5:y:132:ILE:HD11	1.80	0.46
5:y:243:ILE:HD13	5:y:290:LEU:HD22	1.98	0.46
16:A:1800:G:N1	16:A:1803:A:OP2	2.49	0.46
20:F:291:SER:OG	46:g:52:LEU:O	2.33	0.46
56:r:96:HIS:CE1	56:r:134:ARG:HB2	2.50	0.46
5:y:237:ALA:HB2	5:y:253:TYR:CZ	2.50	0.46
16:A:1974:A:H5'	18:D:261:GLY:HA2	1.98	0.46
16:A:2693:A:H4'	16:A:2694:A:H8	1.80	0.46
23:J:159:LEU:HD21	23:J:164:LEU:HD13	1.96	0.46
28:O:33:LEU:HD21	28:O:59:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:y:186:ILE:O	5:y:189:MET:HG2	2.16	0.46
12:6:239:ASN:OD1	12:6:275:GLN:NE2	2.44	0.46
20:F:184:GLN:HE22	26:M:22:VAL:HG23	1.81	0.46
22:I:76:ILE:HG22	22:I:78:LEU:H	1.81	0.46
50:k:76:MET:HG2	56:r:49:ILE:HD12	1.97	0.46
52:m:55:LEU:O	52:m:75:LEU:N	2.47	0.46
16:A:1812:C:O2'	42:c:48:GLN:OE1	2.32	0.46
17:B:1617:C:OP2	17:B:1656:A:N6	2.34	0.46
27:N:70:SER:O	27:N:155:LYS:NZ	2.49	0.46
29:P:65:GLU:OE1	29:P:97:GLN:NE2	2.49	0.46
4:x:45:LEU:HD21	4:x:64:ARG:HH21	1.81	0.46
17:B:1644:G:O6	29:P:88:HIS:NE2	2.47	0.46
42:c:44:GLU:OE2	42:c:48:GLN:NE2	2.49	0.46
16:A:2034:A:O2'	26:M:71:GLN:OE1	2.24	0.46
16:A:2795:U:H2'	16:A:2796:G:H8	1.81	0.46
26:M:51:ARG:HB3	26:M:58:GLN:HA	1.98	0.46
57:s:145:VAL:HG21	57:s:187:LEU:HD11	1.96	0.46
11:5:165:GLN:NE2	11:5:175:THR:HG22	2.30	0.46
13:7:148:MET:HE2	13:7:257:ILE:HG13	1.98	0.46
13:7:150:MET:O	13:7:154:ILE:HG12	2.16	0.46
16:A:2071:U:H2'	16:A:2831:G:H22	1.81	0.46
16:A:2529:U:H2'	18:D:208:ARG:HB2	1.98	0.46
16:A:3024:U:H2'	16:A:3025:A:C8	2.50	0.46
44:e:146:ARG:HD3	44:e:255:VAL:HG12	1.97	0.46
1:u:119:ARG:HD2	25:L:125:THR:HG21	1.98	0.46
1:u:164:THR:HG22	25:L:111:ASN:HB2	1.98	0.46
4:x:177:VAL:HG11	4:x:191:LEU:HD13	1.98	0.46
4:x:368:LEU:HD12	5:y:312:GLU:HB3	1.97	0.46
12:6:215:THR:OG1	12:6:275:GLN:OE1	2.34	0.46
16:A:1995:A:H4'	16:A:2499:U:H4'	1.98	0.46
16:A:2030:U:H4'	16:A:2031:A:O5'	2.16	0.46
44:e:156:ASN:OD1	44:e:157:LEU:N	2.48	0.46
5:y:112:LEU:HD13	5:y:128:ILE:HD13	1.99	0.45
16:A:2468:A:H61	16:A:2659:C:H42	1.63	0.45
29:P:54:ARG:HH12	29:P:140:GLY:C	2.24	0.45
4:x:187:LYS:HD3	4:x:253:LEU:HD21	1.97	0.45
12:6:99:ARG:NH2	17:B:1621:A:O5'	2.49	0.45
16:A:1798:A:N3	35:V:42:ARG:NH2	2.64	0.45
16:A:1992:C:C4	18:D:274:ARG:HB2	2.52	0.45
16:A:2131:A:OP1	53:o:23:ARG:NH1	2.49	0.45
16:A:2293:A:N6	26:M:37:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:91:LYS:HA	30:Q:94:ILE:HD12	1.98	0.45
30:Q:210:GLU:HB2	30:Q:213:GLN:HG3	1.97	0.45
37:X:156:LYS:NZ	37:X:205:GLY:O	2.48	0.45
53:o:17:TRP:HZ3	53:o:25:ARG:HB2	1.81	0.45
57:s:211:VAL:HG22	57:s:230:ARG:HG2	1.97	0.45
1:u:127:VAL:HG11	1:u:138:MET:HE1	1.99	0.45
5:y:181:TYR:CE1	16:A:3259:N:H4'	2.51	0.45
16:A:2230:A:H62	16:A:2975:G:H1'	1.82	0.45
16:A:2959:G:H2'	16:A:2962:C:H42	1.81	0.45
17:B:1642:G:H2'	17:B:1643:A:C8	2.51	0.45
1:u:113:GLN:N	2:v:68:ARG:O	2.41	0.45
5:y:252:GLU:O	5:y:255:GLN:HG2	2.16	0.45
19:E:99:LEU:HD22	19:E:193:LEU:HB3	1.99	0.45
21:H:75:ARG:NH2	37:X:100:ARG:HH22	2.15	0.45
24:K:67:PHE:HB3	24:K:71:LYS:HB2	1.97	0.45
29:P:102:VAL:HG12	29:P:103:VAL:HG13	1.98	0.45
31:R:26:LYS:HE3	31:R:27:HIS:CE1	2.52	0.45
44:e:151:ARG:NH2	44:e:259:GLU:OE2	2.47	0.45
7:l:20:MET:HB3	7:l:56:PHE:HB3	1.98	0.45
12:6:217:LEU:HD23	12:6:271:LEU:HD12	1.99	0.45
16:A:1761:A:H2'	16:A:1762:A:C8	2.51	0.45
31:R:83:TYR:CZ	31:R:87:ILE:HG13	2.52	0.45
35:V:69:ASP:OD1	35:V:69:ASP:N	2.49	0.45
3:w:90:TYR:HE1	3:w:92:LYS:HB3	1.80	0.45
4:x:200:LEU:N	4:x:230:GLN:O	2.43	0.45
15:9:136:LEU:HD21	34:U:7:TYR:HA	1.97	0.45
16:A:3063:G:N2	16:A:3063:G:OP1	2.50	0.45
19:E:50:ASP:O	28:O:138:ARG:NH2	2.50	0.45
24:K:169:LEU:HD22	56:r:75:TRP:CD1	2.52	0.45
36:W:76:HIS:NE2	36:W:128:LYS:HD3	2.32	0.45
41:b:30:SER:HB2	41:b:76:VAL:HB	1.99	0.45
4:x:65:VAL:HG12	4:x:368:LEU:HD21	1.99	0.45
6:0:96:ASN:HD22	6:0:98:GLN:HB3	1.81	0.45
16:A:2634:U:H2'	16:A:2635:G:H8	1.82	0.45
17:B:1628:C:H2'	17:B:1629:A:H8	1.82	0.45
45:f:121:VAL:HG22	45:f:159:ILE:HG22	1.97	0.45
3:w:90:TYR:HB3	3:w:93:ILE:HG12	1.99	0.45
5:y:302:LEU:O	5:y:307:CYS:N	2.42	0.45
11:5:136:VAL:HG11	11:5:417:LEU:HD23	1.98	0.45
14:8:178:TYR:N	52:m:63:THR:O	2.44	0.45
20:F:295:ARG:HH22	46:g:56:ARG:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:240:LYS:NZ	27:N:250:ARG:O	2.50	0.45
14:8:99:ARG:HG2	44:e:89:LEU:HD11	1.98	0.45
15:9:86:LEU:N	38:Y:148:GLU:OE2	2.49	0.45
16:A:2944:C:C6	53:o:20:LYS:HE3	2.52	0.45
22:I:48:MET:O	27:N:250:ARG:NH1	2.47	0.45
46:g:105:ARG:NH2	53:o:83:PRO:HD3	2.31	0.45
16:A:1697:A:N3	16:A:1703:C:O2'	2.50	0.45
43:d:267:PRO:HG2	43:d:270:ALA:HB2	1.99	0.45
4:x:288:GLN:NE2	4:x:316:GLN:HE21	2.13	0.44
15:9:68:PHE:CE2	15:9:70:LEU:HB2	2.52	0.44
16:A:2240:C:O2'	24:K:30:LYS:NZ	2.49	0.44
16:A:2795:U:H2'	16:A:2796:G:C8	2.52	0.44
16:A:2926:A:O2'	16:A:3087:C:OP1	2.23	0.44
18:D:111:ARG:NH2	18:D:165:ASN:OD1	2.42	0.44
50:k:77:ARG:HD2	56:r:50:GLU:HG2	1.98	0.44
54:p:97:SER:O	54:p:146:ASN:ND2	2.50	0.44
13:7:227:LEU:HD22	13:7:237:VAL:HG13	1.98	0.44
16:A:1744:A:OP1	26:M:87:HIS:NE2	2.39	0.44
16:A:2168:U:O2'	16:A:2169:A:O4'	2.33	0.44
16:A:2847:C:H2'	16:A:2848:A:O4'	2.17	0.44
20:F:220:ASP:O	20:F:245:ALA:N	2.51	0.44
55:q:147:GLN:NE2	55:q:151:GLU:OE2	2.49	0.44
5:y:98:SER:O	5:y:102:MET:HG2	2.17	0.44
12:6:48:LEU:O	12:6:50:LYS:NZ	2.44	0.44
12:6:257:PRO:HB3	12:6:268:LEU:HD21	1.97	0.44
16:A:1984:A:N1	16:A:1997:C:O2'	2.38	0.44
16:A:2361:G:H5''	16:A:2362:A:H8	1.81	0.44
20:F:231:VAL:HG13	55:q:26:ARG:HD2	1.99	0.44
24:K:4:PHE:HB2	24:K:9:GLN:HB2	1.99	0.44
33:T:122:ALA:HB1	33:T:128:VAL:HG21	1.99	0.44
51:l:64:ASP:HB3	51:l:67:GLN:HB3	1.99	0.44
4:x:141:ARG:HH22	5:y:322:ARG:HD3	1.81	0.44
16:A:1886:G:OP1	20:F:167:MET:N	2.48	0.44
16:A:1907:A:N3	16:A:2930:U:O2'	2.47	0.44
22:I:132:LYS:HB2	22:I:133:PRO:HD3	1.99	0.44
42:c:123:GLN:OE1	42:c:193:GLN:NE2	2.50	0.44
44:e:160:LEU:HD11	44:e:260:LEU:HD12	1.98	0.44
11:5:139:LEU:HD22	11:5:423:ALA:HB3	2.00	0.44
16:A:1770:G:H4'	20:F:112:ALA:HB2	1.99	0.44
16:A:1939:G:C5	18:D:259:LYS:HB2	2.53	0.44
28:O:46:TRP:HD1	28:O:121:ALA:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Y:128:SER:HB2	38:Y:131:ARG:NE	2.33	0.44
56:r:117:GLU:HG3	56:r:180:LEU:HD12	1.99	0.44
1:u:140:PHE:HA	1:u:143:VAL:HG12	2.00	0.44
12:6:228:PRO:HB3	29:P:49:THR:HB	2.00	0.44
16:A:2449:G:OP2	57:s:225:ARG:NH2	2.48	0.44
27:N:55:ARG:HG2	27:N:99:TRP:CD1	2.53	0.44
50:k:75:ILE:HB	56:r:48:ILE:HA	2.00	0.44
3:w:103:HIS:ND1	3:w:106:LYS:HG2	2.32	0.44
14:8:125:LYS:NZ	52:m:37:ARG:O	2.51	0.44
16:A:2754:A:N3	37:X:108:GLN:NE2	2.65	0.44
18:D:199:GLU:HG2	18:D:202:ARG:HB2	2.00	0.44
21:H:119:GLY:HA2	21:H:123:LEU:HB2	2.00	0.44
31:R:112:THR:HG23	32:S:142:THR:HG21	1.99	0.44
35:V:44:VAL:HG21	35:V:83:ARG:HH21	1.82	0.44
1:u:121:THR:HG21	1:u:176:VAL:HG12	2.00	0.44
3:w:80:GLN:HG2	3:w:145:VAL:HG11	1.98	0.44
16:A:1998:U:OP1	16:A:2001:C:N4	2.35	0.44
16:A:2454:G:OP1	28:O:48:ARG:NH2	2.48	0.44
16:A:3214:C:OP1	28:O:119:LYS:NZ	2.48	0.44
26:M:180:ASP:OD1	26:M:180:ASP:N	2.40	0.44
32:S:67:PRO:HG3	40:a:36:TYR:HB3	2.00	0.44
34:U:141:ASP:HB3	34:U:144:ARG:HG2	1.98	0.44
12:6:234:HIS:ND1	12:6:255:LEU:O	2.50	0.44
13:7:45:ASN:HD21	13:7:259:ASP:HA	1.83	0.44
15:9:24:LYS:HG2	16:A:2421:G:H5'	1.99	0.44
16:A:1861:U:H2'	16:A:1862:U:C6	2.52	0.44
16:A:2065:A:H5'	36:W:74:ARG:HE	1.83	0.44
16:A:3141:A:H4'	25:L:130:ARG:HH22	1.82	0.44
21:H:84:GLU:OE1	37:X:44:ARG:NH2	2.50	0.44
13:7:203:THR:O	13:7:207:HIS:ND1	2.34	0.43
16:A:2724:G:H2'	16:A:2725:A:H8	1.83	0.43
34:U:142:PRO:O	43:d:280:VAL:HG11	2.18	0.43
44:e:53:LEU:HD21	44:e:238:LEU:HD13	1.99	0.43
52:m:51:LEU:HB3	52:m:67:ARG:HB3	1.99	0.43
57:s:91:TYR:HE1	57:s:229:LEU:HD22	1.82	0.43
4:x:136:ARG:NH1	4:x:350:ASP:O	2.46	0.43
20:F:138:HIS:CD2	20:F:146:TRP:HE1	2.36	0.43
25:L:46:LEU:HD12	25:L:78:LYS:HD3	2.00	0.43
27:N:73:ARG:O	27:N:155:LYS:NZ	2.51	0.43
43:d:241:ASP:OD1	43:d:241:ASP:N	2.52	0.43
57:s:105:TRP:CG	57:s:271:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1741:A:N1	16:A:1755:A:H5''	2.34	0.43
16:A:2512:A:O2'	16:A:2541:C:OP1	2.29	0.43
18:D:188:PRO:HG2	18:D:191:THR:OG1	2.18	0.43
28:O:116:ASP:OD1	28:O:116:ASP:N	2.50	0.43
43:d:152:LEU:HD21	43:d:172:MET:HE2	1.99	0.43
47:h:140:PHE:HB2	47:h:156:TRP:CE3	2.54	0.43
57:s:237:PRO:HB3	57:s:300:HIS:CE1	2.53	0.43
12:6:279:ILE:HG21	12:6:307:HIS:HD2	1.82	0.43
16:A:2017:U:O2	20:F:137:ARG:NH2	2.52	0.43
16:A:2180:A:H4'	16:A:2181:A:C8	2.54	0.43
16:A:2685:U:O2'	16:A:3104:U:H5'	2.19	0.43
4:x:154:GLU:HG3	4:x:155:TYR:CD2	2.54	0.43
4:x:355:PHE:CE2	4:x:357:SER:HB2	2.53	0.43
5:y:139:GLU:HB3	5:y:140:PRO:HD3	2.01	0.43
9:3:127:ALA:HA	26:M:79:PRO:HD3	2.00	0.43
16:A:2100:C:H1'	16:A:2135:A:C8	2.53	0.43
16:A:2724:G:H2'	16:A:2725:A:C8	2.53	0.43
19:E:106:MET:HE2	19:E:118:VAL:HG22	1.99	0.43
27:N:96:TYR:HB3	27:N:151:VAL:HB	2.01	0.43
5:y:102:MET:HG3	5:y:132:ILE:HD13	2.00	0.43
5:y:235:GLN:HE22	18:D:289:LEU:H	1.65	0.43
12:6:120:GLU:OE2	14:8:119:LYS:NZ	2.37	0.43
30:Q:113:VAL:HG11	30:Q:186:SER:HA	1.99	0.43
33:T:73:GLN:H	33:T:167:HIS:CE1	2.36	0.43
54:p:135:LEU:HD21	54:p:157:MET:HE1	2.00	0.43
57:s:174:LEU:HB3	57:s:175:PRO:HD3	2.00	0.43
6:0:84:ARG:NH2	16:A:2306:A:O2'	2.43	0.43
16:A:2072:A:N6	16:A:2831:G:H2'	2.34	0.43
16:A:2294:A:H1'	31:R:20:ARG:HH12	1.84	0.43
17:B:1643:A:H62	29:P:120:ARG:HH12	1.65	0.43
18:D:193:ILE:HD11	18:D:226:ILE:HG23	2.01	0.43
21:H:56:VAL:HG12	21:H:82:LEU:HA	2.00	0.43
31:R:108:TYR:HD1	41:b:125:SER:HB2	1.84	0.43
33:T:44:LYS:O	33:T:48:LYS:HG3	2.19	0.43
35:V:206:GLU:OE2	35:V:208:ARG:NE	2.40	0.43
11:5:177:CYS:HB3	11:5:178:PRO:HD3	2.01	0.43
15:9:131:TYR:HA	15:9:132:PRO:HA	1.90	0.43
16:A:2197:G:O2'	16:A:2199:A:H5'	2.19	0.43
18:D:210:ALA:HB1	18:D:249:ASN:HB2	2.00	0.43
23:J:122:ARG:HH12	51:l:87:LYS:NZ	2.16	0.43
10:4:97:ARG:HH21	16:A:3015:U:H5''	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:2757:A:OP2	21:H:121:ASN:ND2	2.46	0.43
44:e:162:ARG:HB2	44:e:171:TRP:CD2	2.53	0.43
4:x:135:ASP:OD1	4:x:136:ARG:N	2.48	0.43
16:A:2925:U:O2'	16:A:2927:C:OP1	2.29	0.43
18:D:182:HIS:HB2	18:D:187:LEU:HD21	2.01	0.43
34:U:153:LEU:HD23	43:d:222:LEU:HB3	2.01	0.43
43:d:157:HIS:O	43:d:161:HIS:ND1	2.50	0.43
46:g:84:TYR:HB3	46:g:116:ASP:O	2.19	0.43
5:y:310:VAL:O	5:y:314:GLN:HG2	2.19	0.42
11:5:262:ILE:H	11:5:262:ILE:HG13	1.68	0.42
12:6:74:TYR:OH	29:P:65:GLU:OE1	2.35	0.42
16:A:2332:C:N4	16:A:2442:U:H3	2.15	0.42
16:A:2693:A:H4'	16:A:2694:A:C8	2.54	0.42
19:E:304:LEU:HD12	19:E:307:TYR:HE2	1.84	0.42
23:J:168:GLN:HE22	51:l:63:THR:HB	1.84	0.42
26:M:142:GLU:HB2	26:M:162:LEU:HD23	2.01	0.42
38:Y:202:LEU:HB2	38:Y:204:TYR:CE2	2.54	0.42
4:x:82:ALA:HB1	4:x:85:HIS:HD2	1.84	0.42
13:7:160:ASP:OD1	13:7:160:ASP:N	2.52	0.42
16:A:1977:U:H2'	16:A:1978:A:H8	1.83	0.42
19:E:236:THR:HG23	19:E:239:ARG:HD3	2.02	0.42
20:F:187:LEU:HD13	20:F:259:LEU:HD23	2.01	0.42
4:x:328:LEU:O	4:x:333:SER:N	2.52	0.42
16:A:1710:A:H5''	16:A:1711:C:H5'	2.00	0.42
16:A:1901:C:OP1	26:M:37:GLU:HG3	2.19	0.42
16:A:2105:G:OP1	27:N:233:TYR:OH	2.30	0.42
19:E:148:GLY:HA3	19:E:173:LYS:HG3	2.01	0.42
24:K:143:GLU:OE1	41:b:136:LYS:NZ	2.43	0.42
32:S:159:THR:OG1	32:S:196:ASN:OD1	2.30	0.42
35:V:133:ILE:HD12	35:V:145:ARG:HB2	2.01	0.42
37:X:20:ILE:HG21	37:X:212:ILE:HG23	2.01	0.42
44:e:58:VAL:HB	44:e:153:LEU:HB3	2.00	0.42
57:s:307:ARG:HG3	57:s:310:ARG:H	1.84	0.42
4:x:296:LEU:O	4:x:299:THR:HG22	2.20	0.42
15:9:126:LYS:HE2	15:9:126:LYS:HB3	1.83	0.42
16:A:1782:G:O2'	16:A:1793:G:O6	2.31	0.42
48:i:98:VAL:O	48:i:102:MET:HG3	2.20	0.42
53:o:17:TRP:CZ3	53:o:25:ARG:HB2	2.54	0.42
4:x:345:ARG:HG3	4:x:354:PHE:CG	2.55	0.42
11:5:257:TYR:CG	11:5:258:PRO:HA	2.54	0.42
16:A:1762:A:H2'	16:A:1763:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1803:A:H2	16:A:1806:U:H5'	1.85	0.42
16:A:2135:A:N3	16:A:2135:A:H2'	2.33	0.42
16:A:2155:A:N6	56:r:169:TRP:O	2.52	0.42
16:A:2466:A:OP1	30:Q:235:ARG:NH1	2.49	0.42
16:A:2511:C:O5'	18:D:263:ASN:ND2	2.52	0.42
16:A:2655:G:N2	16:A:2659:C:O2'	2.53	0.42
16:A:3063:G:O2'	16:A:3066:C:OP2	2.36	0.42
25:L:35:MET:N	25:L:57:CYS:O	2.47	0.42
38:Y:226:LEU:O	38:Y:230:LYS:HG2	2.19	0.42
16:A:1939:G:O2'	16:A:1973:G:H4'	2.19	0.42
16:A:3072:U:H1'	16:A:3073:C:O4'	2.19	0.42
37:X:190:LYS:HE3	37:X:191:TYR:CZ	2.55	0.42
42:c:284:GLY:HA2	42:c:285:PRO:HD3	1.93	0.42
14:8:171:PHE:HD1	44:e:203:LYS:HE2	1.84	0.42
16:A:1678:C:N4	16:A:1773:A:OP2	2.35	0.42
16:A:2144:A:OP1	31:R:57:ARG:NH1	2.53	0.42
20:F:195:LEU:HD22	20:F:202:TYR:HE2	1.85	0.42
22:I:147:PHE:HA	22:I:151:ASN:ND2	2.35	0.42
29:P:73:PRO:O	29:P:75:ARG:NH1	2.53	0.42
38:Y:191:ASN:HB3	38:Y:194:TYR:HB3	2.01	0.42
5:y:240:ARG:HG2	5:y:265:HIS:HE1	1.84	0.42
10:4:99:LYS:NZ	16:A:3175:A:OP1	2.48	0.42
11:5:257:TYR:CD1	11:5:258:PRO:HA	2.55	0.42
13:7:240:ILE:HG23	13:7:252:VAL:HG21	2.00	0.42
16:A:2171:U:C2	16:A:2173:G:H4'	2.55	0.42
16:A:3183:U:H3	24:K:177:ARG:HB3	1.84	0.42
27:N:218:ILE:HG22	27:N:226:ILE:HG21	2.02	0.42
34:U:27:GLN:HG3	34:U:43:ARG:HB2	2.00	0.42
39:Z:36:PHE:HE2	39:Z:79:PRO:HG3	1.85	0.42
49:j:100:GLU:HG2	49:j:104:LYS:HE3	2.01	0.42
17:B:1639:U:H5''	29:P:155:SER:HB3	2.02	0.42
22:I:96:ILE:HG12	22:I:155:VAL:HG12	2.01	0.42
24:K:30:LYS:HD3	24:K:148:PRO:HB2	2.01	0.42
33:T:150:ILE:HB	43:d:52:THR:HG21	2.01	0.42
37:X:226:LEU:HD23	37:X:229:ILE:HD12	2.00	0.42
44:e:124:TRP:CD2	52:m:72:ARG:HG2	2.55	0.42
50:k:66:VAL:HG11	50:k:90:PHE:HE1	1.85	0.42
10:4:66:PHE:CE2	16:A:3174:U:H5'	2.55	0.42
11:5:114:LEU:HD11	18:D:127:ILE:HD13	2.02	0.42
13:7:88:PRO:HG3	13:7:119:LEU:HD21	2.01	0.42
16:A:3217:A:H2'	19:E:292:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:82:LEU:HB3	20:F:87:PHE:CD2	2.55	0.42
21:H:99:THR:HA	21:H:108:ARG:HG3	2.01	0.42
37:X:222:ASP:OD1	37:X:222:ASP:N	2.53	0.42
11:5:293:LEU:HD12	11:5:313:MET:HG2	2.02	0.41
13:7:309:HIS:CE1	19:E:155:PHE:HA	2.55	0.41
16:A:2182:G:H1'	16:A:2199:A:C8	2.55	0.41
44:e:192:LEU:O	44:e:198:ASN:ND2	2.53	0.41
2:v:54:GLN:O	2:v:57:LYS:HG2	2.19	0.41
4:x:69:SER:O	4:x:262:ARG:NH1	2.53	0.41
16:A:2829:C:OP2	16:A:2829:C:H3'	2.20	0.41
20:F:212:TRP:O	20:F:258:THR:OG1	2.38	0.41
26:M:98:LEU:HD12	26:M:145:ALA:HA	2.02	0.41
26:M:284:LYS:NZ	46:g:41:SER:HB3	2.35	0.41
30:Q:175:GLN:NE2	30:Q:206:PRO:HG3	2.35	0.41
39:Z:53:HIS:ND1	53:o:47:TYR:OH	2.35	0.41
56:r:99:MET:HE1	56:r:115:ILE:HG22	2.00	0.41
57:s:90:LYS:HD2	57:s:232:GLN:HB2	2.02	0.41
57:s:93:VAL:HB	57:s:233:ILE:HG12	2.01	0.41
1:u:119:ARG:HD3	30:Q:123:ASP:OD2	2.19	0.41
2:v:63:ASN:O	2:v:68:ARG:NH2	2.51	0.41
12:6:342:PHE:CE1	29:P:48:PHE:HB2	2.55	0.41
40:a:45:CYS:HA	40:a:65:VAL:HG13	2.02	0.41
51:l:88:PRO:HG2	51:l:91:GLU:HG3	2.03	0.41
4:x:58:ASP:O	4:x:61:PRO:HD2	2.20	0.41
4:x:223:GLU:O	4:x:227:ASP:N	2.53	0.41
16:A:1673:U:O2'	33:T:143:ARG:NH1	2.53	0.41
16:A:2530:A:H5''	18:D:212:THR:HG21	2.02	0.41
20:F:280:TYR:CD1	46:g:57:ILE:HG12	2.55	0.41
25:L:138:LEU:HD22	25:L:144:PHE:HE1	1.85	0.41
26:M:207:PRO:O	26:M:211:VAL:HG23	2.20	0.41
34:U:46:MET:HE1	34:U:72:VAL:HG13	2.01	0.41
51:l:123:LYS:HE2	51:l:127:TRP:CZ2	2.55	0.41
57:s:119:PRO:HG3	57:s:394:TRP:CE3	2.55	0.41
16:A:1952:U:H2'	16:A:1953:A:C8	2.56	0.41
29:P:152:GLU:O	29:P:155:SER:OG	2.34	0.41
32:S:115:LEU:HB2	41:b:11:LEU:HD22	2.01	0.41
37:X:92:ALA:O	37:X:98:SER:OG	2.39	0.41
44:e:133:LEU:HD22	52:m:63:THR:HG21	2.02	0.41
46:g:150:LYS:NZ	53:o:79:THR:O	2.51	0.41
57:s:308:ARG:HG3	57:s:320:ILE:HD13	2.02	0.41
9:3:180:TYR:HD1	12:6:366:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6:160:ASP:OD2	12:6:267:ARG:NH2	2.54	0.41
14:8:164:ARG:N	45:f:85:ASP:O	2.50	0.41
16:A:1868:G:N7	26:M:51:ARG:NH1	2.66	0.41
16:A:2446:A:OP1	57:s:65:ARG:NH2	2.51	0.41
16:A:2796:G:H1'	21:H:87:LYS:HD2	2.02	0.41
43:d:115:THR:HG22	43:d:118:SER:H	1.86	0.41
5:y:123:GLN:O	5:y:127:ILE:HG12	2.21	0.41
5:y:256:TYR:OH	5:y:295:ARG:HG2	2.20	0.41
6:0:166:SER:H	6:0:169:ASP:HB2	1.85	0.41
12:6:173:LEU:HD22	12:6:272:LEU:HB2	2.03	0.41
12:6:234:HIS:CE1	12:6:257:PRO:HA	2.55	0.41
16:A:2081:U:H2'	16:A:2082:G:C8	2.55	0.41
16:A:2182:G:N3	16:A:2199:A:O2'	2.38	0.41
16:A:2387:U:O2'	16:A:2406:A:N7	2.48	0.41
18:D:279:GLY:H	18:D:283:GLY:H	1.68	0.41
28:O:25:ARG:NH2	28:O:51:GLU:OE2	2.35	0.41
30:Q:177:VAL:HG11	30:Q:204:MET:HG3	2.02	0.41
41:b:35:ARG:HG3	53:o:101:TRP:HB2	2.03	0.41
8:2:56:SER:OG	16:A:1980:A:OP1	2.33	0.41
12:6:87:LYS:HE2	12:6:87:LYS:HB3	1.87	0.41
16:A:2325:U:O2'	28:O:82:GLU:OE2	2.39	0.41
16:A:2739:U:H1'	18:D:293:LYS:NZ	2.35	0.41
19:E:170:LEU:HD11	19:E:190:GLY:HA2	2.03	0.41
19:E:274:TRP:NE1	19:E:286:ASN:HB2	2.34	0.41
38:Y:128:SER:HB2	38:Y:131:ARG:HE	1.86	0.41
4:x:70:GLU:O	4:x:371:ASN:ND2	2.54	0.41
4:x:176:ILE:HG22	4:x:249:TYR:HD2	1.85	0.41
4:x:210:ILE:HD13	4:x:210:ILE:HA	1.92	0.41
9:3:124:ARG:NH1	9:3:125:ARG:O	2.54	0.41
9:3:151:ASN:HB3	12:6:359:HIS:CD2	2.56	0.41
12:6:116:ASN:HD22	12:6:119:GLU:HG2	1.86	0.41
13:7:105:LEU:HD11	13:7:267:PRO:HB2	2.02	0.41
16:A:2030:U:H1'	16:A:2031:A:OP2	2.20	0.41
16:A:2080:U:O2'	53:o:60:ARG:HA	2.21	0.41
16:A:2286:A:H2'	16:A:2287:U:C6	2.56	0.41
16:A:2674:U:H2'	16:A:2675:G:O4'	2.21	0.41
16:A:2825:G:O6	36:W:44:GLY:HA3	2.20	0.41
19:E:61:ILE:HD11	28:O:149:LEU:HD13	2.02	0.41
22:I:89:VAL:O	22:I:93:ASN:ND2	2.54	0.41
22:I:113:ARG:HD2	22:I:123:MET:HE2	2.02	0.41
25:L:52:HIS:HD2	25:L:53:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:O:52:MET:HE3	28:O:52:MET:HB3	1.94	0.41
30:Q:221:LYS:HB3	30:Q:244:ARG:HG3	2.02	0.41
40:a:51:LEU:HD21	40:a:58:ILE:HG12	2.02	0.41
44:e:128:PHE:CD1	52:m:74:MET:HB3	2.55	0.41
44:e:235:LYS:HD2	44:e:275:PHE:HD1	1.86	0.41
49:j:45:GLU:OE2	49:j:70:ARG:NH2	2.54	0.41
4:x:171:LEU:HD12	4:x:171:LEU:HA	1.91	0.41
12:6:227:GLU:HB2	12:6:230:ALA:HB3	2.02	0.41
12:6:279:ILE:HB	12:6:281:PHE:CE1	2.56	0.41
16:A:2169:A:OP2	23:J:21:ARG:NH1	2.54	0.41
16:A:3210:C:O2'	19:E:47:THR:O	2.34	0.41
18:D:290:PRO:N	18:D:291:PRO:HD2	2.36	0.41
19:E:345:ILE:HG12	30:Q:169:PRO:HB2	2.02	0.41
20:F:107:LYS:NZ	48:i:58:ASP:OD2	2.42	0.41
24:K:170:TRP:NE1	56:r:91:GLN:O	2.54	0.41
30:Q:90:LEU:HG	30:Q:94:ILE:HD11	2.03	0.41
41:b:28:ARG:HH21	42:c:71:GLU:CD	2.29	0.41
6:0:138:ARG:NH1	16:A:2321:A:OP1	2.49	0.40
11:5:173:ARG:HA	11:5:176:TYR:CE2	2.56	0.40
15:9:72:PRO:HG3	38:Y:104:VAL:HG12	2.02	0.40
16:A:2868:C:H2'	16:A:2869:A:O4'	2.21	0.40
20:F:48:LEU:HD22	47:h:94:SER:HB3	2.03	0.40
28:O:57:GLU:OE2	28:O:105:THR:OG1	2.30	0.40
37:X:42:HIS:CG	37:X:86:ILE:HD11	2.56	0.40
53:o:17:TRP:CH2	53:o:25:ARG:HD3	2.55	0.40
58:w:200:PM8:O40	58:w:200:PM8:N36	2.54	0.40
16:A:2241:A:H61	56:r:82:ASN:CG	2.28	0.40
34:U:30:ARG:O	38:Y:121:ARG:NH1	2.49	0.40
38:Y:130:GLU:OE1	43:d:71:LYS:NZ	2.41	0.40
46:g:79:PRO:HB3	46:g:85:PHE:HE1	1.87	0.40
52:m:60:ASP:OD1	52:m:60:ASP:N	2.52	0.40
15:9:119:PHE:HB2	37:X:227:PHE:CE1	2.56	0.40
16:A:1864:A:OP1	31:R:17:ARG:NH1	2.52	0.40
41:b:42:GLY:HA3	41:b:92:LYS:O	2.21	0.40
2:v:13:TYR:OH	2:v:36:ARG:HG2	2.21	0.40
5:y:197:THR:HG21	5:y:223:LEU:HD23	2.03	0.40
15:9:110:ASP:OD1	15:9:113:ASN:ND2	2.55	0.40
16:A:1797:G:O2'	35:V:40:ARG:O	2.38	0.40
16:A:1907:A:OP1	20:F:126:LYS:NZ	2.53	0.40
16:A:2652:G:H2'	16:A:2653:C:O4'	2.21	0.40
20:F:138:HIS:CG	20:F:146:TRP:HE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:65:ALA:HB2	21:H:71:PRO:HA	2.04	0.40
34:U:137:ARG:NH1	35:V:104:TYR:OH	2.52	0.40
49:j:27:TRP:O	49:j:31:GLN:HG2	2.22	0.40
12:6:193:VAL:HB	12:6:319:PHE:CD2	2.57	0.40
16:A:2502:C:H1'	16:A:3096:U:H5'	2.04	0.40
16:A:2896:G:C6	16:A:2915:C:H1'	2.57	0.40
16:A:3110:C:H42	19:E:265:TYR:HB2	1.86	0.40
25:L:100:PHE:HB3	30:Q:158:GLN:NE2	2.35	0.40
33:T:65:ALA:O	33:T:173:VAL:HA	2.21	0.40
41:b:34:SER:OG	41:b:36:ASP:O	2.39	0.40
46:g:76:ARG:NH2	46:g:163:GLU:O	2.54	0.40
46:g:154:ASP:OD2	46:g:155:GLN:NE2	2.54	0.40
57:s:310:ARG:HG3	57:s:313:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	u	108/234 (46%)	104 (96%)	4 (4%)	0	100	100
2	v	67/70 (96%)	67 (100%)	0	0	100	100
3	w	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
4	x	332/384 (86%)	328 (99%)	4 (1%)	0	100	100
5	y	242/381 (64%)	240 (99%)	2 (1%)	0	100	100
6	0	108/188 (57%)	108 (100%)	0	0	100	100
7	1	53/65 (82%)	52 (98%)	1 (2%)	0	100	100
8	2	44/92 (48%)	42 (96%)	2 (4%)	0	100	100
9	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
10	4	36/103 (35%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	5	392/423 (93%)	389 (99%)	3 (1%)	0	100	100
12	6	352/380 (93%)	346 (98%)	6 (2%)	0	100	100
13	7	292/338 (86%)	287 (98%)	5 (2%)	0	100	100
14	8	100/206 (48%)	100 (100%)	0	0	100	100
15	9	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
18	D	238/305 (78%)	234 (98%)	4 (2%)	0	100	100
19	E	303/348 (87%)	298 (98%)	4 (1%)	1 (0%)	36	65
20	F	250/311 (80%)	248 (99%)	2 (1%)	0	100	100
21	H	95/267 (36%)	94 (99%)	1 (1%)	0	100	100
22	I	161/261 (62%)	159 (99%)	2 (1%)	0	100	100
23	J	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
24	K	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
25	L	113/145 (78%)	113 (100%)	0	0	100	100
26	M	289/296 (98%)	287 (99%)	2 (1%)	0	100	100
27	N	208/251 (83%)	206 (99%)	2 (1%)	0	100	100
28	O	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
29	P	142/180 (79%)	138 (97%)	4 (3%)	0	100	100
30	Q	219/292 (75%)	219 (100%)	0	0	100	100
31	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
32	S	159/205 (78%)	159 (100%)	0	0	100	100
33	T	164/206 (80%)	164 (100%)	0	0	100	100
34	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
35	V	203/216 (94%)	202 (100%)	1 (0%)	0	100	100
36	W	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
37	X	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
38	Y	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
39	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
40	a	96/142 (68%)	95 (99%)	1 (1%)	0	100	100
41	b	147/215 (68%)	145 (99%)	2 (1%)	0	100	100
42	c	282/332 (85%)	280 (99%)	2 (1%)	0	100	100
43	d	257/306 (84%)	255 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	e	224/279 (80%)	219 (98%)	5 (2%)	0	100	100
45	f	146/212 (69%)	143 (98%)	3 (2%)	0	100	100
46	g	132/166 (80%)	131 (99%)	1 (1%)	0	100	100
47	h	108/158 (68%)	106 (98%)	2 (2%)	0	100	100
48	i	95/128 (74%)	95 (100%)	0	0	100	100
49	j	92/123 (75%)	92 (100%)	0	0	100	100
50	k	99/112 (88%)	97 (98%)	2 (2%)	0	100	100
51	l	80/138 (58%)	80 (100%)	0	0	100	100
52	m	49/128 (38%)	49 (100%)	0	0	100	100
53	o	92/102 (90%)	92 (100%)	0	0	100	100
54	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100
55	q	139/222 (63%)	139 (100%)	0	0	100	100
56	r	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
57	s	382/439 (87%)	374 (98%)	8 (2%)	0	100	100
All	All	9116/11894 (77%)	9015 (99%)	100 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	E	150	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	u	104/200 (52%)	101 (97%)	3 (3%)	37	71
2	v	59/60 (98%)	59 (100%)	0	100	100
3	w	73/136 (54%)	73 (100%)	0	100	100
4	x	291/328 (89%)	288 (99%)	3 (1%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	y	226/350 (65%)	225 (100%)	1 (0%)	84	94
6	0	99/164 (60%)	99 (100%)	0	100	100
7	1	52/60 (87%)	51 (98%)	1 (2%)	50	79
8	2	40/72 (56%)	40 (100%)	0	100	100
9	3	88/166 (53%)	87 (99%)	1 (1%)	65	88
10	4	37/89 (42%)	37 (100%)	0	100	100
11	5	353/368 (96%)	352 (100%)	1 (0%)	86	96
12	6	313/332 (94%)	311 (99%)	2 (1%)	78	93
13	7	270/303 (89%)	269 (100%)	1 (0%)	84	94
14	8	93/190 (49%)	93 (100%)	0	100	100
15	9	104/112 (93%)	104 (100%)	0	100	100
18	D	194/245 (79%)	194 (100%)	0	100	100
19	E	260/290 (90%)	260 (100%)	0	100	100
20	F	219/262 (84%)	219 (100%)	0	100	100
21	H	88/228 (39%)	87 (99%)	1 (1%)	65	88
22	I	151/232 (65%)	151 (100%)	0	100	100
23	J	138/150 (92%)	138 (100%)	0	100	100
24	K	154/155 (99%)	153 (99%)	1 (1%)	78	93
25	L	98/124 (79%)	98 (100%)	0	100	100
26	M	246/249 (99%)	244 (99%)	2 (1%)	73	90
27	N	185/211 (88%)	183 (99%)	2 (1%)	65	88
28	O	134/150 (89%)	134 (100%)	0	100	100
29	P	126/155 (81%)	125 (99%)	1 (1%)	73	90
30	Q	203/256 (79%)	202 (100%)	1 (0%)	81	93
31	R	118/126 (94%)	118 (100%)	0	100	100
32	S	146/180 (81%)	146 (100%)	0	100	100
33	T	146/176 (83%)	146 (100%)	0	100	100
34	U	134/135 (99%)	132 (98%)	2 (2%)	57	84
35	V	183/191 (96%)	180 (98%)	3 (2%)	55	83
36	W	86/119 (72%)	85 (99%)	1 (1%)	63	86
37	X	220/229 (96%)	220 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Y	163/223 (73%)	163 (100%)	0	100	100
39	Z	113/147 (77%)	112 (99%)	1 (1%)	70	90
40	a	96/133 (72%)	96 (100%)	0	100	100
41	b	130/185 (70%)	129 (99%)	1 (1%)	73	90
42	c	251/288 (87%)	251 (100%)	0	100	100
43	d	237/274 (86%)	234 (99%)	3 (1%)	61	86
44	e	198/236 (84%)	198 (100%)	0	100	100
45	f	133/188 (71%)	132 (99%)	1 (1%)	73	90
46	g	124/148 (84%)	124 (100%)	0	100	100
47	h	104/148 (70%)	104 (100%)	0	100	100
48	i	86/110 (78%)	86 (100%)	0	100	100
49	j	74/97 (76%)	74 (100%)	0	100	100
50	k	83/90 (92%)	83 (100%)	0	100	100
51	l	76/116 (66%)	75 (99%)	1 (1%)	61	86
52	m	46/113 (41%)	45 (98%)	1 (2%)	45	77
53	o	80/87 (92%)	80 (100%)	0	100	100
54	p	135/181 (75%)	135 (100%)	0	100	100
55	q	119/178 (67%)	119 (100%)	0	100	100
56	r	147/169 (87%)	147 (100%)	0	100	100
57	s	340/381 (89%)	339 (100%)	1 (0%)	86	96
All	All	8166/10285 (79%)	8130 (100%)	36 (0%)	81	94

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	u	176	VAL
1	u	186	GLU
1	u	191	GLU
4	x	282	GLN
4	x	326	GLU
4	x	360	VAL
5	y	326	GLU
7	1	54	VAL
9	3	173	VAL
11	5	47	ASP

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Mol	Chain	Res	Type
12	6	179	VAL
12	6	243	ASN
13	7	234	LYS
21	H	102	VAL
24	K	17	ILE
26	M	180	ASP
26	M	222	TYR
27	N	59	VAL
27	N	132	THR
29	P	161	LEU
30	Q	125	TYR
34	U	11	ARG
34	U	19	VAL
35	V	44	VAL
35	V	186	THR
35	V	188	VAL
36	W	131	VAL
39	Z	99	VAL
41	b	75	VAL
43	d	89	VAL
43	d	241	ASP
43	d	280	VAL
45	f	211	LEU
51	l	58	ASP
52	m	41	THR
57	s	97	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	u	136	HIS
2	v	19	GLN
2	v	63	ASN
3	w	103	HIS
4	x	47	ASN
4	x	85	HIS
4	x	172	GLN
4	x	214	GLN
4	x	230	GLN
4	x	316	GLN
4	x	322	GLN
4	x	371	ASN

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Mol	Chain	Res	Type
5	y	122	GLN
5	y	123	GLN
5	y	192	GLN
5	y	195	ASN
5	y	210	GLN
5	y	235	GLN
5	y	255	GLN
5	y	284	GLN
6	0	115	HIS
7	1	31	ASN
7	1	52	GLN
11	5	160	HIS
11	5	165	GLN
11	5	191	GLN
11	5	214	ASN
11	5	266	HIS
11	5	384	GLN
12	6	174	HIS
12	6	320	GLN
12	6	359	HIS
13	7	45	ASN
13	7	255	HIS
13	7	290	GLN
18	D	195	ASN
20	F	223	HIS
20	F	241	ASN
22	I	43	GLN
22	I	114	HIS
23	J	168	GLN
24	K	94	GLN
25	L	52	HIS
27	N	202	GLN
27	N	210	GLN
27	N	237	HIS
28	O	146	ASN
28	O	147	GLN
29	P	79	HIS
29	P	134	GLN
29	P	142	ASN
30	Q	107	HIS
31	R	27	HIS
31	R	77	GLN

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Mol	Chain	Res	Type
32	S	75	HIS
32	S	84	ASN
32	S	118	ASN
35	V	73	GLN
36	W	80	HIS
37	X	89	GLN
37	X	93	ASN
38	Y	99	HIS
38	Y	179	HIS
38	Y	189	HIS
39	Z	64	HIS
40	a	46	ASN
40	a	102	HIS
40	a	126	HIS
41	b	25	GLN
42	c	139	GLN
43	d	153	ASN
43	d	157	HIS
43	d	235	GLN
44	e	54	GLN
44	e	67	GLN
44	e	75	GLN
44	e	212	HIS
44	e	251	HIS
45	f	138	GLN
46	g	93	ASN
46	g	155	GLN
48	i	111	ASN
48	i	120	HIS
48	i	124	HIS
51	l	82	GLN
52	m	65	HIS
53	o	94	HIS
54	p	194	HIS
55	q	51	GLN
56	r	96	HIS
56	r	112	HIS
56	r	130	ASN
57	s	107	GLN
57	s	239	ASN
57	s	240	GLN
57	s	343	GLN

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Mol	Chain	Res	Type
57	s	358	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	A	1409/1590 (88%)	246 (17%)	1 (0%)
17	B	71/72 (98%)	13 (18%)	0
All	All	1480/1662 (89%)	259 (17%)	1 (0%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	A	1689	C
16	A	1693	C
16	A	1699	C
16	A	1700	U
16	A	1704	U
16	A	1707	C
16	A	1708	A
16	A	1711	C
16	A	1713	A
16	A	1724	A
16	A	1727	A
16	A	1728	U
16	A	1731	A
16	A	1737	A
16	A	1748	G
16	A	1750	G
16	A	1765	C
16	A	1770	G
16	A	1780	U
16	A	1805	A
16	A	1806	U
16	A	1807	U
16	A	1809	U
16	A	1821	A
16	A	1824	U
16	A	1827	C
16	A	1828	A
16	A	1829	A
16	A	1832	A

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Mol	Chain	Res	Type
16	A	1836	A
16	A	1844	A
16	A	1853	A
16	A	1854	U
16	A	1855	A
16	A	1867	A
16	A	1869	A
16	A	1882	A
16	A	1883	G
16	A	1887	A
16	A	1892	A
16	A	1893	A
16	A	1901	C
16	A	1903	C
16	A	1918	G
16	A	1937	A
16	A	1940	A
16	A	1962	A
16	A	1974	A
16	A	1984	A
16	A	1985	G
16	A	1986	A
16	A	1987	G
16	A	1992	C
16	A	1993	A
16	A	1994	A
16	A	2002	G
16	A	2015	G
16	A	2022	G
16	A	2029	A
16	A	2030	U
16	A	2031	A
16	A	2036	C
16	A	2039	A
16	A	2060	A
16	A	2065	A
16	A	2068	C
16	A	2069	U
16	A	2074	A
16	A	2079	C
16	A	2083	U
16	A	2092	C

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Mol	Chain	Res	Type
16	A	2098	G
16	A	2108	G
16	A	2109	A
16	A	2110	A
16	A	2125	C
16	A	2126	U
16	A	2132	A
16	A	2147	G
16	A	2154	A
16	A	2163	A
16	A	2167	A
16	A	2168	U
16	A	2169	A
16	A	2170	G
16	A	2171	U
16	A	2172	A
16	A	2181	A
16	A	2182	G
16	A	2183	C
16	A	2184	A
16	A	2194	U
16	A	2195	A
16	A	2197	G
16	A	2198	A
16	A	2199	A
16	A	2200	A
16	A	2202	C
16	A	2203	G
16	A	2210	C
16	A	2216	A
16	A	2228	A
16	A	2233	U
16	A	2237	A
16	A	2239	A
16	A	2241	A
16	A	2243	A
16	A	2245	A
16	A	2252	C
16	A	2262	C
16	A	2263	C
16	A	2283	C
16	A	2284	C

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Mol	Chain	Res	Type
16	A	2285	U
16	A	2293	A
16	A	2297	A
16	A	2300	G
16	A	2322	C
16	A	2324	U
16	A	2332	C
16	A	2345	G
16	A	2350	A
16	A	2351	U
16	A	2352	U
16	A	2353	A
16	A	2354	A
16	A	2355	A
16	A	2356	A
16	A	2359	C
16	A	2360	U
16	A	2361	G
16	A	2362	A
16	A	2363	A
16	A	2374	A
16	A	2390	A
16	A	2393	C
16	A	2396	C
16	A	2401	A
16	A	2405	C
16	A	2406	A
16	A	2407	U
16	A	2415	C
16	A	2427	C
16	A	2432	A
16	A	2444	A
16	A	2446	A
16	A	2451	A
16	A	2452	A
16	A	2478	G
16	A	2493	C
16	A	2500	A
16	A	2506	A
16	A	2507	A
16	A	2511	C
16	A	2520	C

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Mol	Chain	Res	Type
16	A	2521	A
16	A	2527	A
16	A	2540	C
16	A	2641	A
16	A	2654	U
16	A	2656	U
16	A	2660	U
16	A	2683	C
16	A	2684	C
16	A	2686	G
16	A	2693	A
16	A	2694	A
16	A	2695	G
16	A	2696	A
16	A	2706	A
16	A	2709	A
16	A	2718	C
16	A	2719	G
16	A	2727	C
16	A	2732	G
16	A	2745	A
16	A	2809	C
16	A	2810	G
16	A	2814	G
16	A	2829	C
16	A	2831	G
16	A	2832	A
16	A	2833	A
16	A	2847	C
16	A	2854	U
16	A	2864	U
16	A	2865	C
16	A	2889	C
16	A	2895	U
16	A	2910	A
16	A	2911	C
16	A	2913	A
16	A	2917	G
16	A	2922	A
16	A	2926	A
16	A	2928	C
16	A	2944	C

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Mol	Chain	Res	Type
16	A	2955	U
16	A	2956	A
16	A	2963	A
16	A	2982	C
16	A	2984	A
16	A	2985	C
16	A	2995	G
16	A	3000	A
16	A	3005	A
16	A	3016	G
16	A	3021	C
16	A	3041	U
16	A	3042	U
16	A	3043	C
16	A	3053	A
16	A	3054	G
16	A	3056	C
16	A	3060	C
16	A	3061	G
16	A	3072	U
16	A	3073	C
16	A	3077	C
16	A	3086	U
16	A	3089	A
16	A	3097	U
16	A	3100	U
16	A	3101	A
16	A	3102	U
16	A	3109	U
16	A	3110	C
16	A	3111	A
16	A	3112	A
16	A	3150	U
16	A	3155	C
16	A	3157	C
16	A	3158	A
16	A	3162	C
16	A	3169	C
16	A	3172	C
16	A	3180	A
16	A	3183	U
16	A	3189	C

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Mol	Chain	Res	Type
16	A	3190	A
16	A	3197	U
16	A	3206	C
16	A	3212	C
16	A	3217	A
16	A	3218	A
16	A	3228	U
17	B	1603	A
17	B	1605	A
17	B	1609	U
17	B	1611	G
17	B	1617	C
17	B	1621	A
17	B	1646	U
17	B	1650	A
17	B	1652	C
17	B	1653	U
17	B	1654	U
17	B	1656	A
17	B	1664	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	A	2030	U

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

4 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	$\# Z > 2$
24	SAC	K	2	24	7,8,9	1.04	0	7,9,11	0.90	0
50	AYA	k	2	50	6,7,8	1.24	1 (16%)	6,8,10	1.18	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	THC	b	2	41	8,9,10	1.10	1 (12%)	10,11,13	1.28	2 (20%)
34	AYA	U	2	34	6,7,8	1.30	1 (16%)	6,8,10	1.09	1 (16%)

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
24	SAC	K	2	24	-	2/7/8/10	-
50	AYA	k	2	50	-	1/5/6/8	-
41	THC	b	2	41	-	0/9/10/12	-
34	AYA	U	2	34	-	0/5/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	U	2	AYA	CA-N	-2.50	1.43	1.46
41	b	2	THC	CA-N1	-2.22	1.43	1.46
50	k	2	AYA	CA-N	-2.20	1.44	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	k	2	AYA	CB-CA-N	2.61	112.63	109.68
34	U	2	AYA	CB-CA-N	2.48	112.48	109.68
41	b	2	THC	CB-CA-C	-2.44	107.51	111.55
41	b	2	THC	C-CA-N1	2.41	113.60	109.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	K	2	SAC	N-CA-CB-OG
24	K	2	SAC	C-CA-CB-OG
50	k	2	AYA	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	b	2	THC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 101 are monoatomic - leaving 3 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	$\# Z > 2$
59	SAM	x	401	-	27,29,29	1.11	4 (14%)	34,42,42	2.01	8 (23%)
63	FES	r	201	56,22	0,4,4	-	-	-		
58	PM8	w	200	3	26,31,31	0.25	0	30,38,38	0.43	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
59	SAM	x	401	-	-	8/17/33/33	0/3/3/3
63	FES	r	201	56,22	-	-	0/1/1/1
58	PM8	w	200	3	-	13/36/38/38	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	x	401	SAM	C2-N3	2.60	1.38	1.33
59	x	401	SAM	C2-N1	2.56	1.38	1.33
59	x	401	SAM	OXT-C	-2.26	1.23	1.30
59	x	401	SAM	C8-N7	2.11	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	x	401	SAM	N3-C2-N1	-5.57	120.16	128.58
59	x	401	SAM	C5-C4-N3	-4.68	120.27	126.72
59	x	401	SAM	N9-C8-N7	-3.82	108.51	113.94
59	x	401	SAM	C2-N3-C4	3.48	120.34	111.83
59	x	401	SAM	C5-N7-C8	3.38	108.76	103.45
59	x	401	SAM	N3-C4-N9	3.13	132.50	127.17
59	x	401	SAM	OXT-C-O	-2.84	117.63	124.08
59	x	401	SAM	C4-C5-N7	-2.31	107.94	110.58

There are no chirality outliers.

All (21) torsion outliers are listed below:

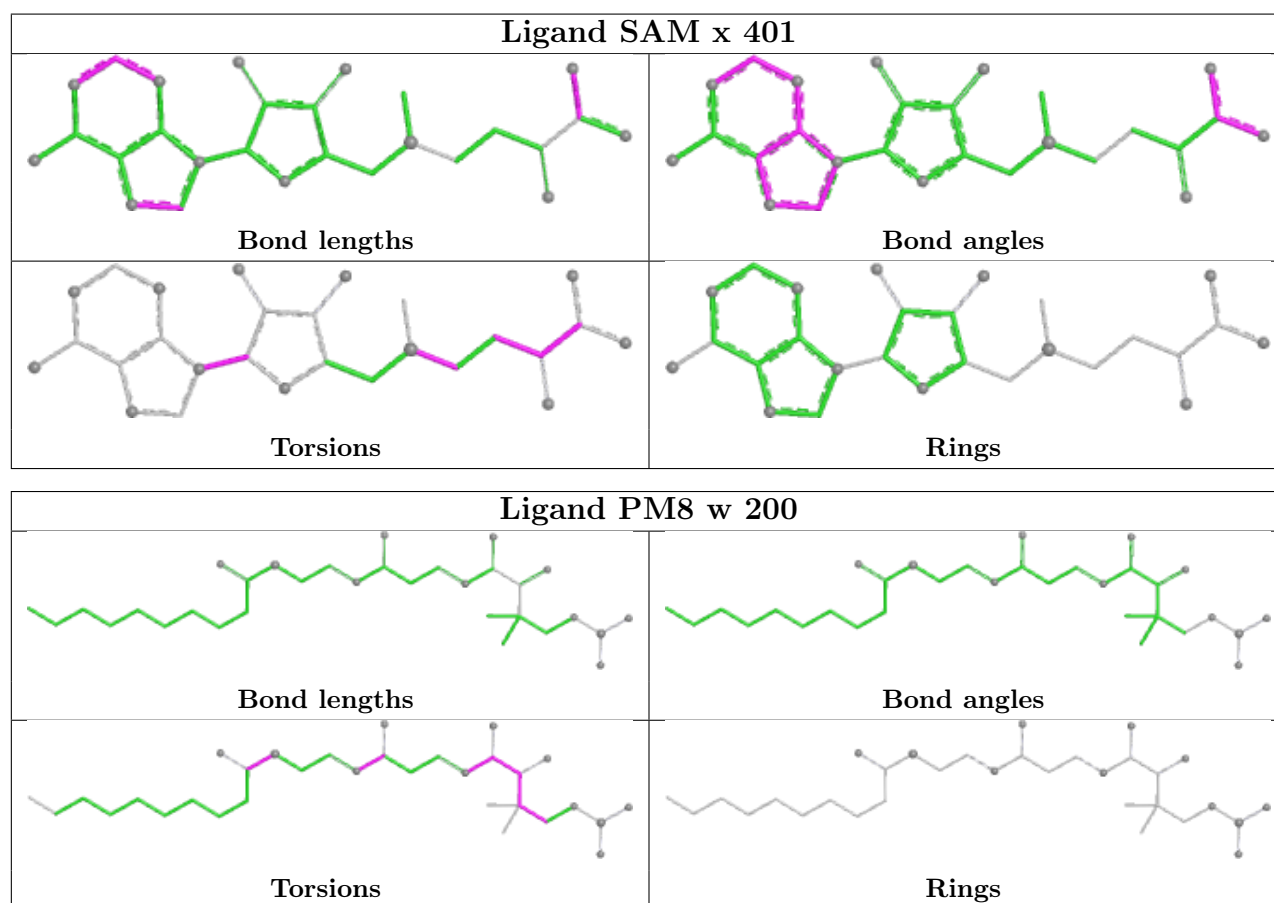
Mol	Chain	Res	Type	Atoms
58	w	200	PM8	O27-C28-C29-C30
58	w	200	PM8	O27-C28-C29-C31
58	w	200	PM8	O27-C28-C29-C32
58	w	200	PM8	C32-C34-N36-C37
58	w	200	PM8	O1-C1-S1-C43
58	w	200	PM8	C2-C1-S1-C43
59	x	401	SAM	N-CA-CB-CG
59	x	401	SAM	C-CA-CB-CG
59	x	401	SAM	CB-CG-SD-C5'
58	w	200	PM8	C38-C39-N41-C42
58	w	200	PM8	O35-C34-N36-C37
58	w	200	PM8	O40-C39-N41-C42
58	w	200	PM8	O33-C32-C34-O35
59	x	401	SAM	CB-CG-SD-CE
58	w	200	PM8	O33-C32-C34-N36
59	x	401	SAM	C2'-C1'-N9-C8
59	x	401	SAM	O4'-C1'-N9-C8
58	w	200	PM8	C31-C29-C32-C34
59	x	401	SAM	OXT-C-CA-N
59	x	401	SAM	C2'-C1'-N9-C4
58	w	200	PM8	C28-C29-C32-C34

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	w	200	PM8	5	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 than 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.



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
16	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3251:N	O3'	3252:N	P	17.10
1	A	3236:N	O3'	3237:N	P	13.81

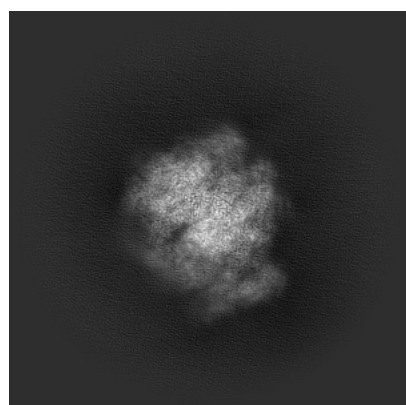
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12845. These allow visual inspection of the internal detail of the map and identification of artifacts.

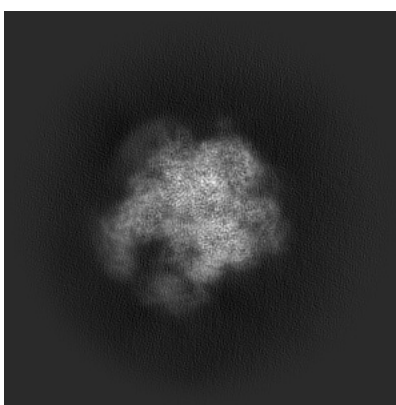
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

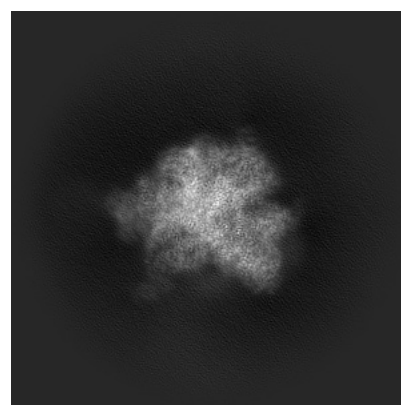
6.1.1 Primary map



X



Y

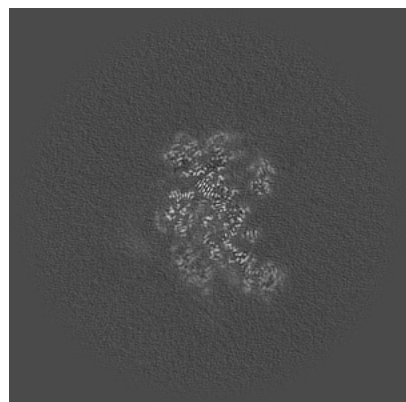


Z

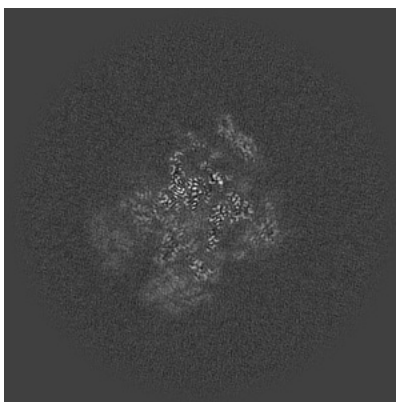
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

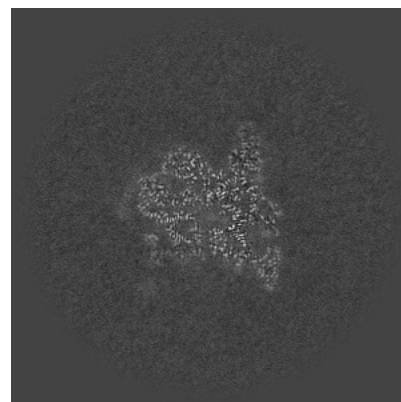
6.2.1 Primary map



X Index: 224



Y Index: 224

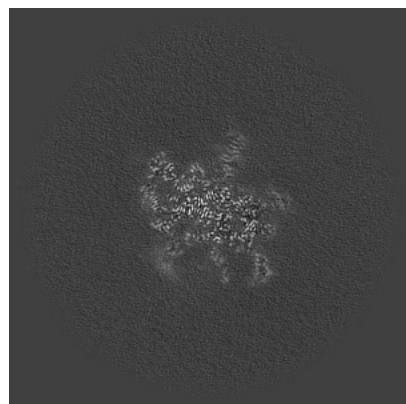


Z Index: 224

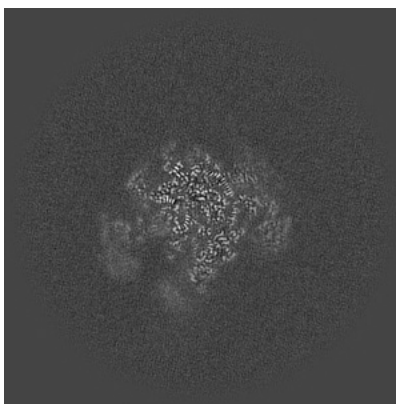
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

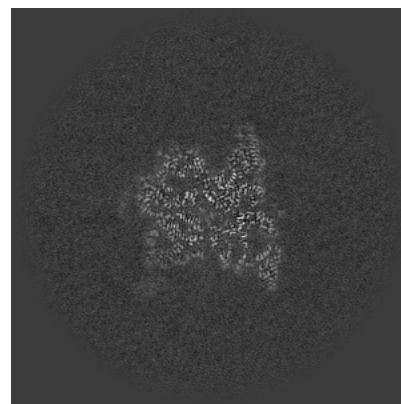
6.3.1 Primary map



X Index: 256



Y Index: 242

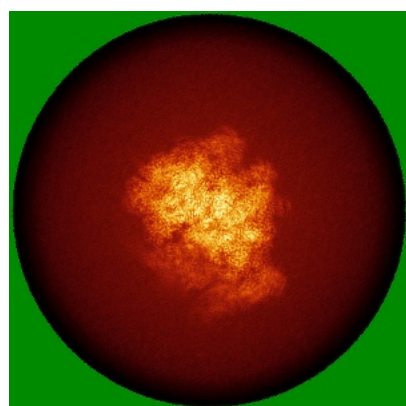


Z Index: 227

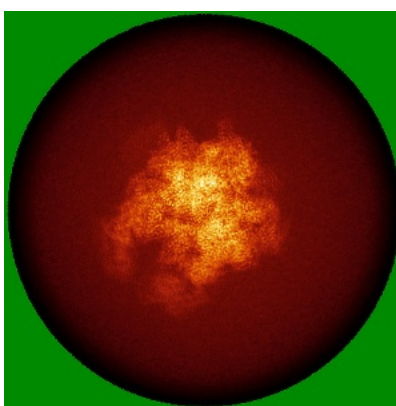
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

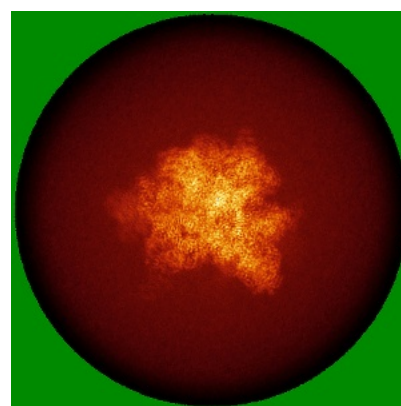
6.4.1 Primary map



X



Y

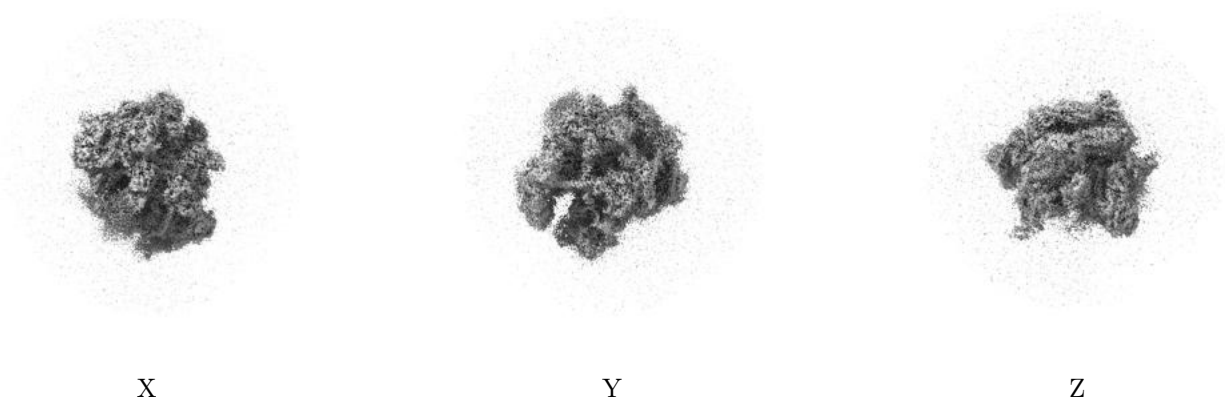


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

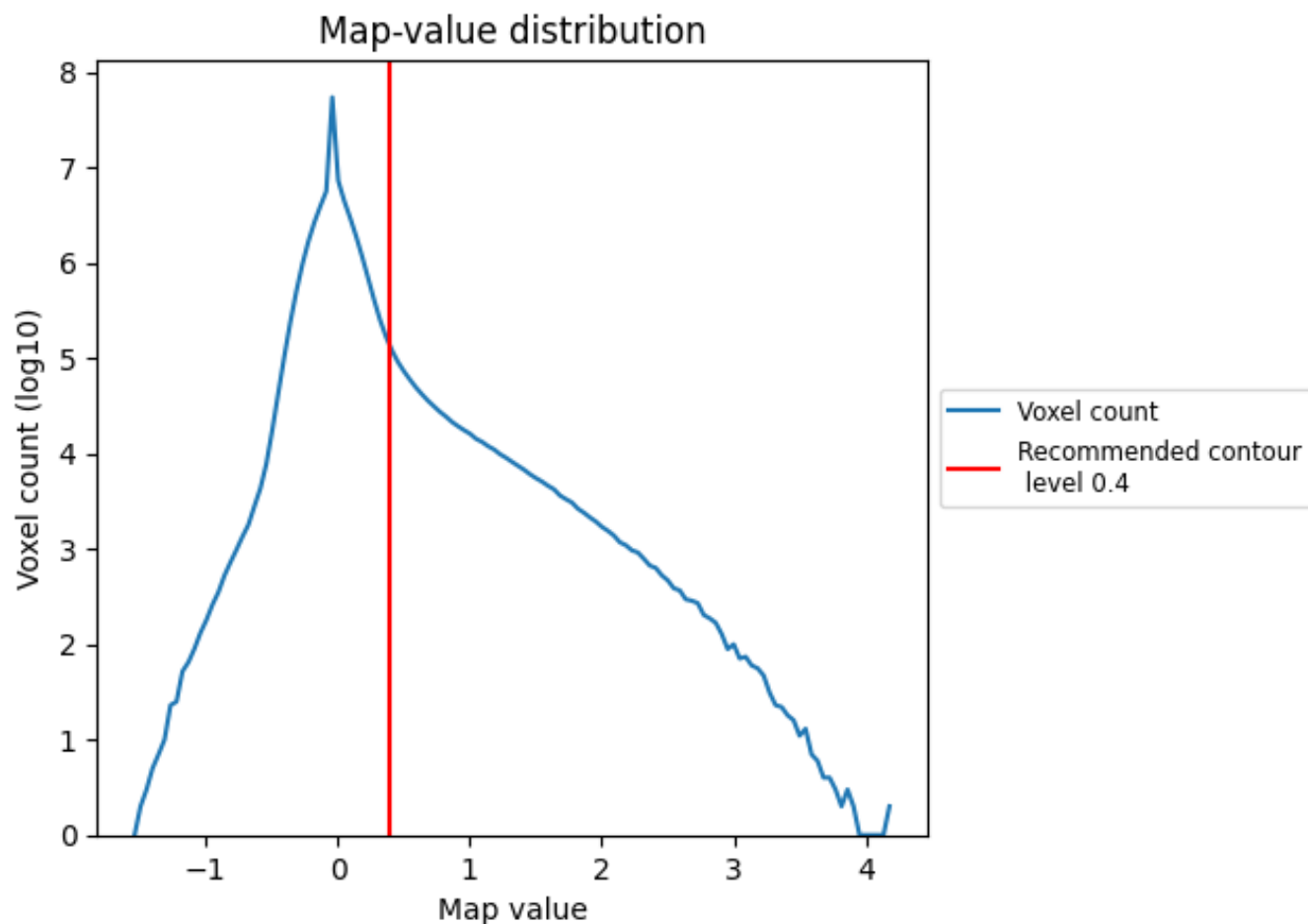
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

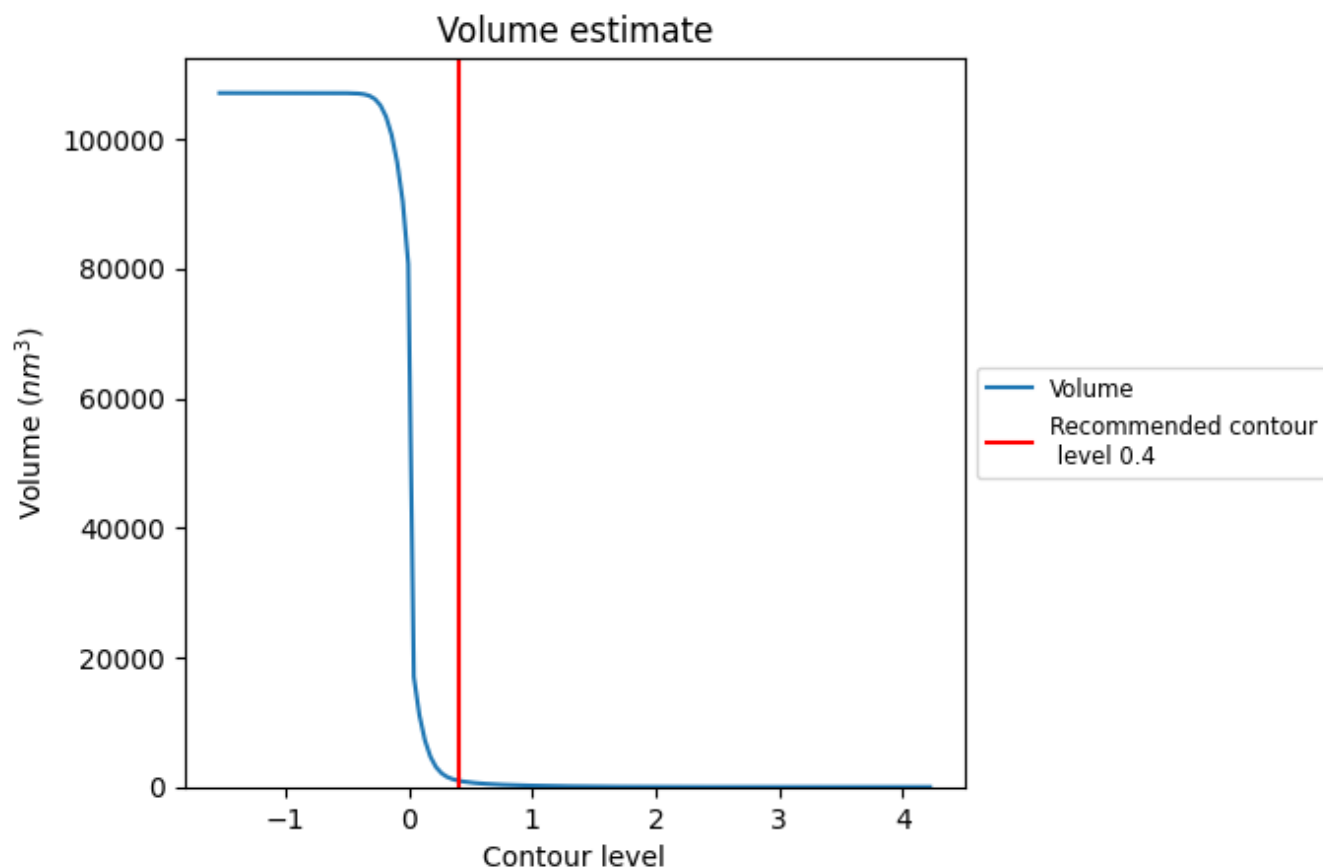
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

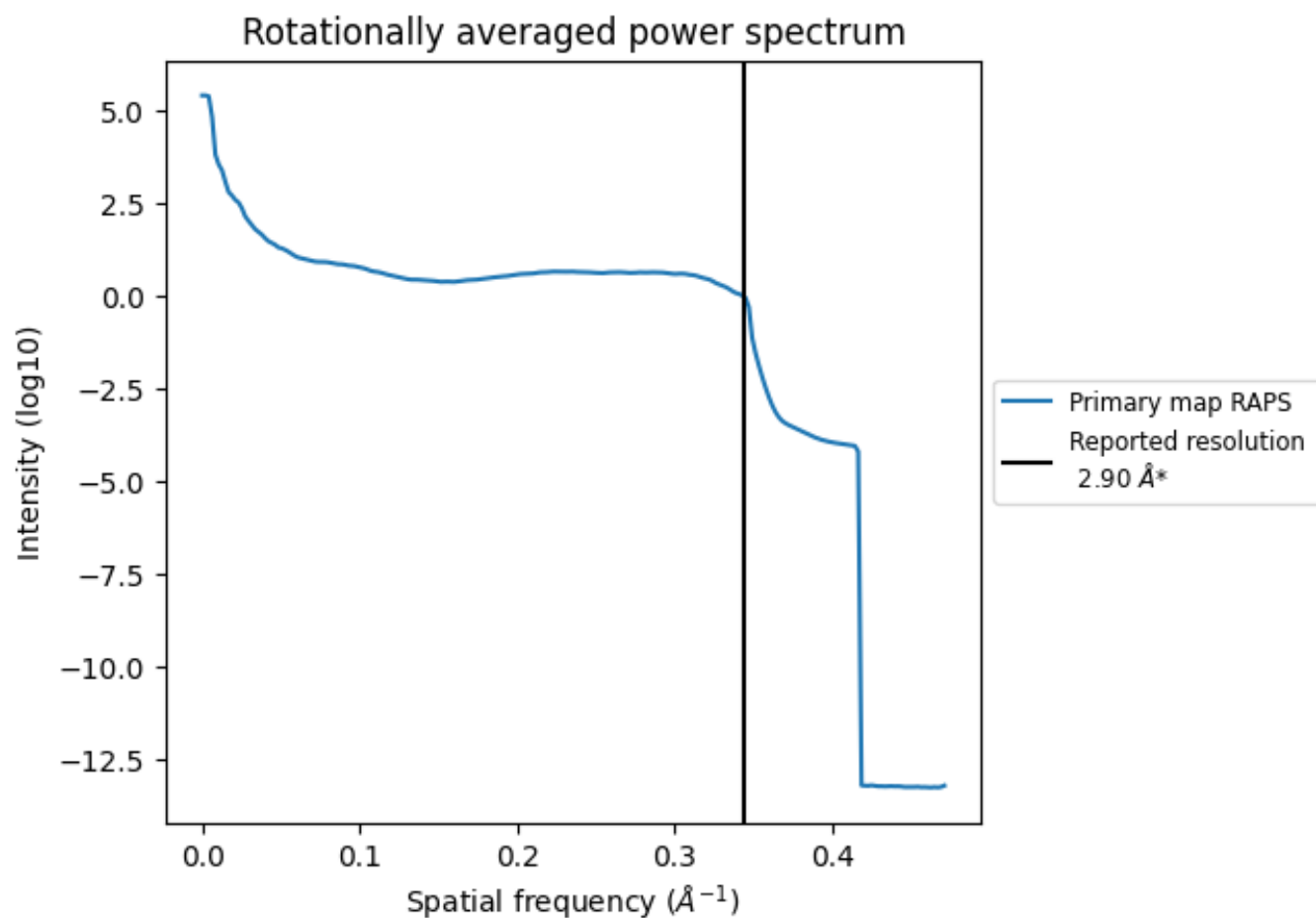
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 985 nm^3 ; this corresponds to an approximate mass of 890 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

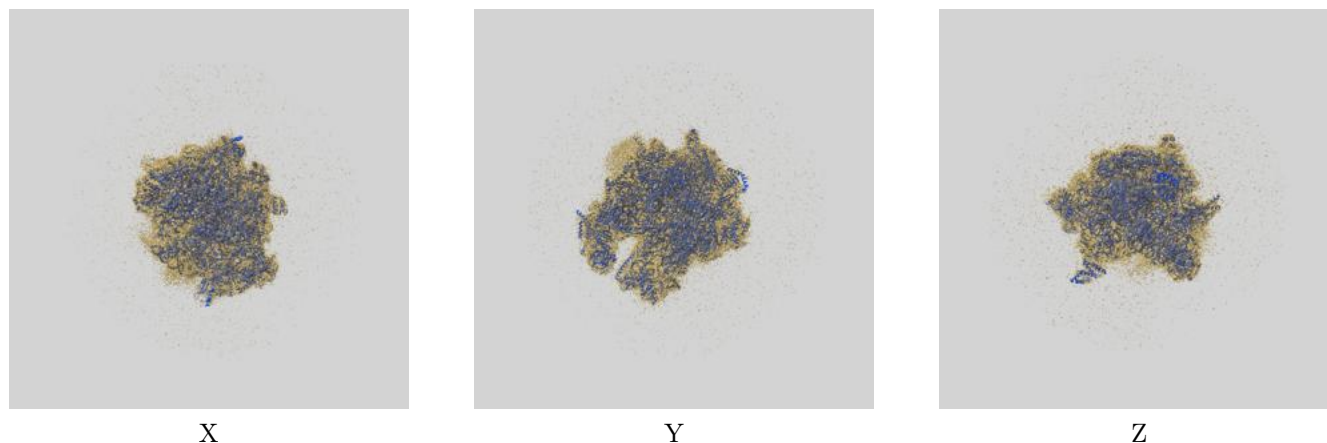
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

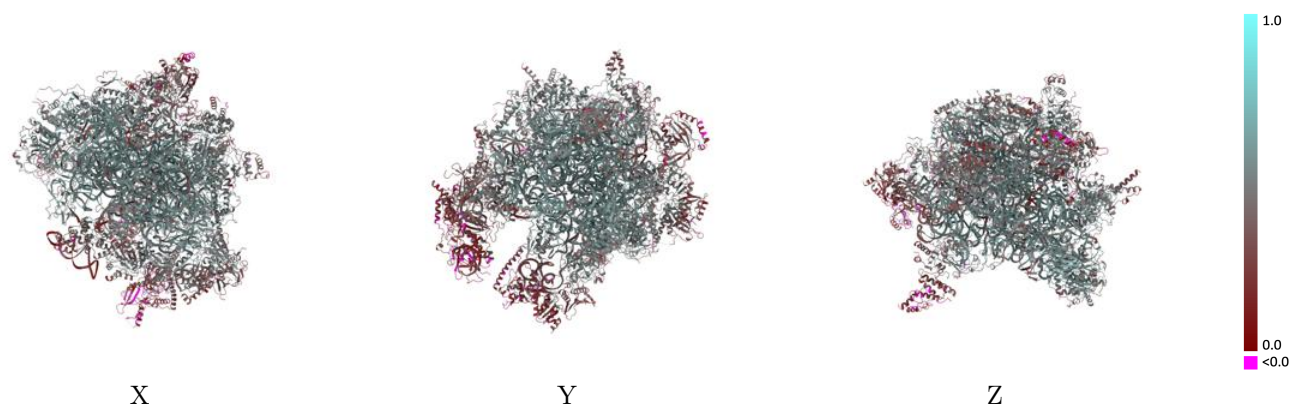
This section contains information regarding the fit between EMDB map EMD-12845 and PDB model 7ODR. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



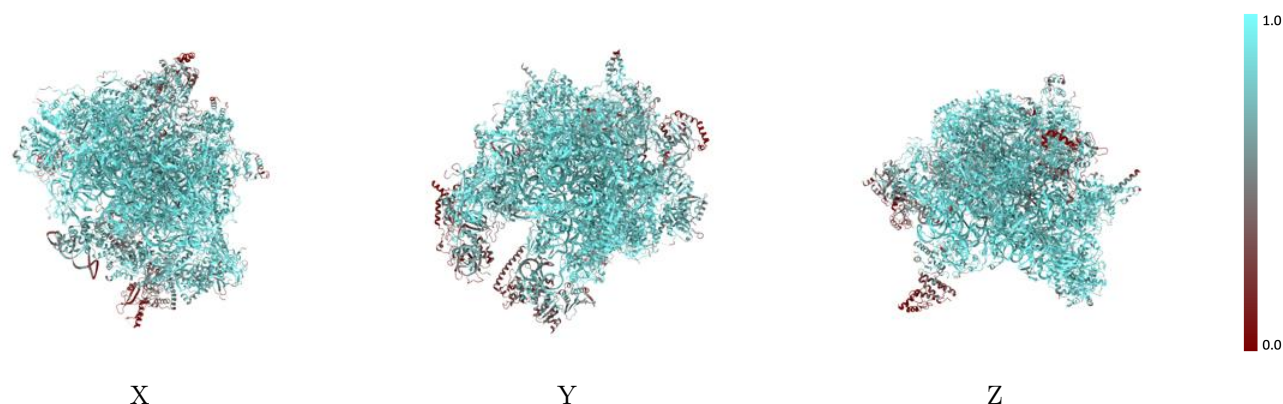
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



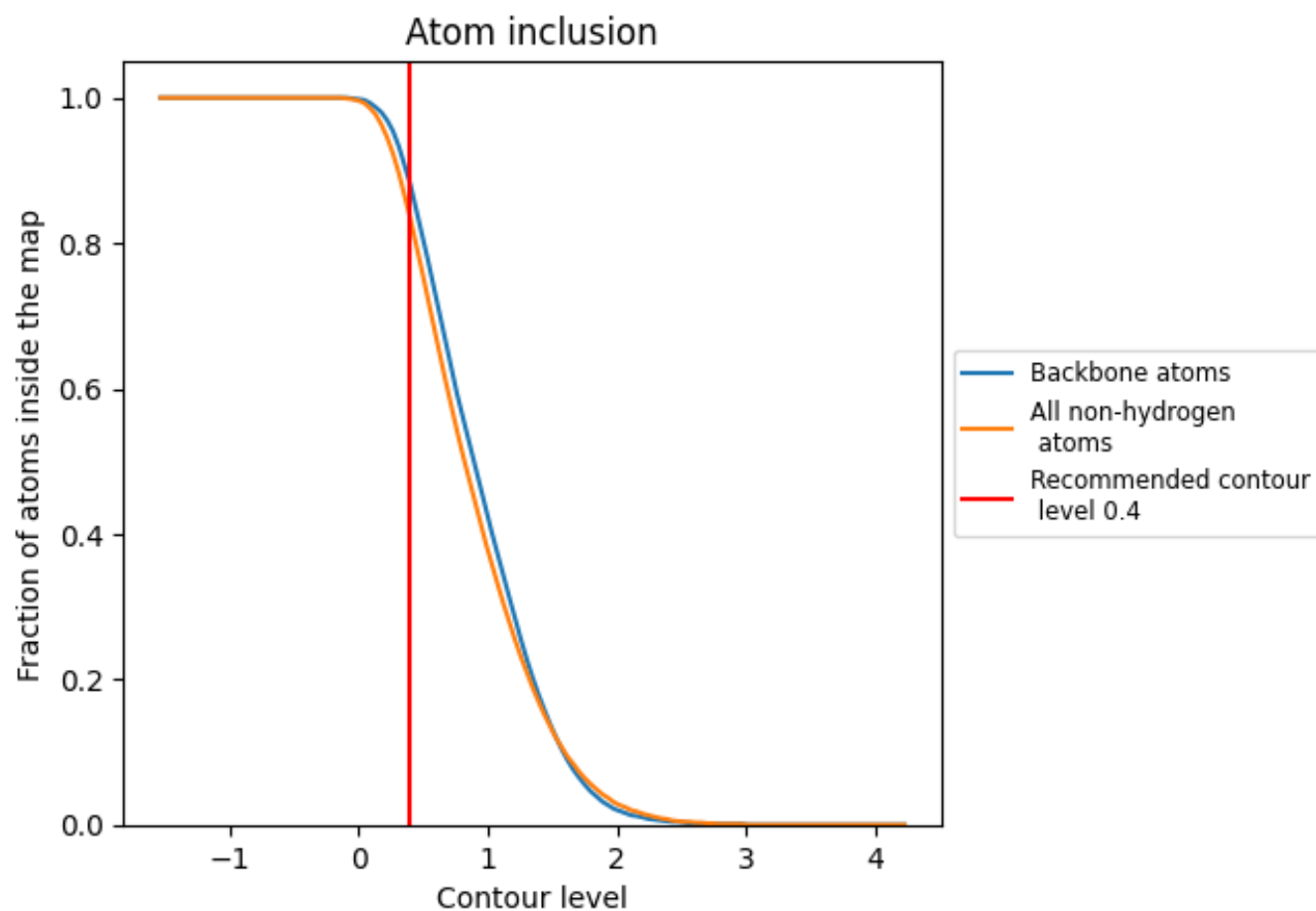
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.4730
0	 0.8600	 0.5060
1	 0.8620	 0.5230
2	 0.9780	 0.6110
3	 0.9700	 0.5930
4	 0.9330	 0.5280
5	 0.8930	 0.5110
6	 0.8300	 0.4200
7	 0.7720	 0.3860
8	 0.4000	 0.2120
9	 0.8600	 0.4840
A	 0.9540	 0.5400
B	 0.7920	 0.2830
D	 0.8960	 0.5290
E	 0.9100	 0.5170
F	 0.8970	 0.5250
H	 0.8210	 0.4780
I	 0.5630	 0.2770
J	 0.2810	 0.1600
K	 0.9310	 0.5430
L	 0.8760	 0.4930
M	 0.9180	 0.5410
N	 0.8220	 0.4720
O	 0.9140	 0.5310
P	 0.8920	 0.4850
Q	 0.8820	 0.4920
R	 0.9320	 0.5610
S	 0.9160	 0.5270
T	 0.9100	 0.5450
U	 0.8100	 0.4800
V	 0.6370	 0.3980
W	 0.9300	 0.5690
X	 0.8610	 0.5120
Y	 0.8860	 0.5180
Z	 0.9070	 0.5550



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Chain	Atom inclusion	Q-score
a	 0.8070	 0.4750
b	 0.9100	 0.5330
c	 0.8340	 0.4610
d	 0.5190	 0.3270
e	 0.2960	 0.1340
f	 0.4860	 0.2730
g	 0.8990	 0.5160
h	 0.6780	 0.3880
i	 0.9490	 0.5720
j	 0.8660	 0.4880
k	 0.5290	 0.2690
l	 0.3600	 0.1960
m	 0.2680	 0.1890
o	 0.8910	 0.5140
p	 0.7180	 0.4100
q	 0.7890	 0.4370
r	 0.8510	 0.4860
s	 0.9060	 0.5320
u	 0.6770	 0.3790
v	 0.2930	 0.2360
w	 0.0680	 0.1330
x	 0.8160	 0.4410
y	 0.7570	 0.4190