Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 09:38 am GMT

PDB ID	:	6HIX
EMDB ID	:	EMD-0231
Title	:	Cryo-EM structure of the Trypanosoma brucei mitochondrial ribosome - This entry contains the large mitoribosomal subunit
Authors	:	Ramrath, D.J.F.; Niemann, M.; Leibundgut, M.; Bieri, P.; Prange, C.; Horn, K.; Leitner, A.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on	:	2018-08-31
Resolution	:	3.39 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 (i) symbol.

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

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

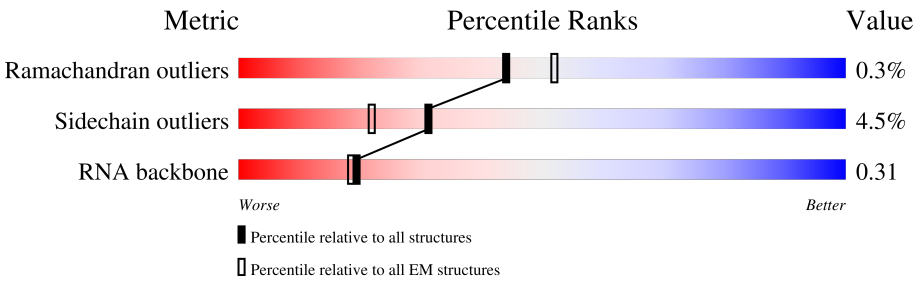
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.39 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	A0	185	79% • 18%
2	A1	241	5% 85% 5% • 10%
3	A2	471	92% • 5%
4	A3	218	66% • 31%
5	A4	183	13% 89% • 8%
6	A5	80	62% 6% 31%
7	A6	114	15% 57% 6% 37%
8	A8	181	9% 75% • 22%

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Mol	Chain	Length	Quality of chain
9	A9	184	25% 71%
10	AE	473	59% 38%
11	AF	459	91% 5%
12	AI	263	77% 19%
13	AJ	177	14% 68% 29%
14	AK	342	89% 6% 6%
15	AN	202	8% 86% 11%
16	AP	374	90% 6%
17	AQ	167	6% 72% 25%
18	AR	301	73% 25%
19	AT	144	22% 76%
20	AU	213	78% 18%
21	AV	188	95%
22	AW	278	95%
23	AX	246	67% 32%
24	AY	378	8% 84% 5% 10%
25	Ab	507	9% 88% 11%
26	Ad	289	6% 87% 11%
27	Ae	197	55% 41%
28	Af	189	62% 33%
29	Ag	260	97%
30	Aj	296	9% 92% 6%
31	Al	218	6% 94%
32	Ao	259	5% 67% 29%
33	Ap	309	5% 80% 16%

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Mol	Chain	Length	Quality of chain
34	At	154	16% 88% 10%
35	Av	242	9% 82% 5% 12%
36	AB	56	54% 100%
37	AC	28	36% 100%
37	AD	28	100% 100%
38	AG	27	100% 100%
39	AA	1178	11% 25% 24% 50%
40	BA	831	78% 18%
41	BB	541	13% 65% 7% 28%
42	BC	523	88% 9%
43	BD	547	17% 72% 24%
44	BE	449	84% 13%
45	BF	426	79% 19%
46	BG	378	6% 79% 5% 16%
47	BH	349	55% 5% 40%
48	BI	343	89% 7%
49	BJ	333	8% 47% 50%
50	BK	386	28% 63% 33%
51	BL	312	72% 25%
52	BM	283	82% 5% 13%
53	BN	302	16% 67% 29%
54	BO	262	8% 52% 44%
55	BP	266	12% 71% 5% 24%
56	BQ	231	90% 6%
57	BR	205	90% 5% 5%

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Mol	Chain	Length	Quality of chain
58	BS	198	47% 51%
59	BT	191	84% 12%
60	BU	185	43% 56%
61	BV	190	8% 77% 18%
62	BW	188	97%
63	BX	190	33% 49% 7% 44%
64	BY	172	58% 41%
65	BZ	190	11% 99%
66	Ba	153	89% 9%
67	Bb	162	5% 57% 39%
68	Bc	146	7% 58% 38%
69	Bd	144	94%
70	Be	113	7% 86% 11%
71	Bf	113	6% 42% 56%
72	Bg	105	6% 73% 5% 22%
73	Bh	92	35% 90% 7%
74	UA	46	28% 100%
75	UB	40	25% 100%
76	UC	12	50% 100%
76	UH	12	17% 100%
77	UD	177	51% 99%
78	UE	22	5% 100%
79	UF	24	100%
79	UG	24	17% 100%
79	UN	24	88% 100%

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Mol	Chain	Length	Quality of chain
80	UI	17	35% 100%
81	UK	10	10% 100%
82	UL	15	13% 100%
83	UM	6	100% 100%
84	UU	11	27% 91% 9%
85	UV	8	12% 100%
85	UX	8	12% 100%
86	UW	7	71% 100%

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 133849 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 bl27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A0	151	1269	801	236	227	5	0	0

- Molecule 2 is a protein called bl28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A1	217	1788	1138	324	317	9	0	0

- Molecule 3 is a protein called ul29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A2	449	3638	2324	631	670	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	238	GLY	ALA	conflict	UNP Q38EM7

- Molecule 4 is a protein called ul30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A3	150	1215	776	234	199	6	0	0

- Molecule 5 is a protein called bl31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A4	168	1387	880	262	240	5	0	0

- Molecule 6 is a protein called bl32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A5	55	483	311	90	76	6	0	0

- Molecule 7 is a protein called bl33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A6	72	568	361	102	101	4	0	0

- Molecule 8 is a protein called bl35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A8	142	1203	753	243	198	9	0	0

- Molecule 9 is a protein called bl36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A9	53	459	288	85	78	8	0	0

- Molecule 10 is a protein called Ribosomal protein L3 mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AE	293	2390	1543	395	440	12	0	0

- Molecule 11 is a protein called Ribosomal protein L4/L1 family, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AF	442	3597	2294	624	654	25	0	0

- Molecule 12 is a protein called bl9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AI	212	1790	1153	316	312	9	0	0

- Molecule 13 is a protein called ul10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AJ	126	965	606	191	165	3	0	0

- Molecule 14 is a protein called Ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AK	323	2676	1703	485	469	19	0	0

- Molecule 15 is a protein called 50S ribosomal protein L13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AN	179	1508	973	275	251	9	0	0

- Molecule 16 is a protein called ul15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AP	352	2904	1846	538	507	13	0	0

- Molecule 17 is a protein called 50S ribosomal protein L16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AQ	125	1020	658	183	175	4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	AR	227	1912	1211	356	332	13	0	0

- Molecule 19 is a protein called bl19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	AT	35	287	180	61	45	1	0	0

- Molecule 20 is a protein called bl20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AU	175	1423	895	280	243	5	0	0

- Molecule 21 is a protein called bl21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AV	181	1424	909	257	252	6	0	0

- Molecule 22 is a protein called ul22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	AW	276	2235	1416	415	391	13	0	0

- Molecule 23 is a protein called ul23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	AX	168	1416	913	253	245	5	0	0

- Molecule 24 is a protein called ul24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	AY	340	2712	1689	493	517	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	345	GLU	VAL	conflict	UNP C9ZK52

- Molecule 25 is a protein called ml38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Ab	453	3545	2252	621	657	15	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ab	290	SER	PHE	conflict	UNP Q381T7

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Chain	Residue	Modelled	Actual	Comment	Reference
Ab	299	GLU	LYS	conflict	UNP Q381T7
Ab	471	ASN	ILE	conflict	UNP Q381T7

- Molecule 26 is a protein called ml40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Ad	257	2122	1319	386	405	12	0	0

- Molecule 27 is a protein called ml41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Ae	116	927	594	170	158	5	0	0

- Molecule 28 is a protein called ml42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Af	126	1013	630	196	183	4	0	0

- Molecule 29 is a protein called ml43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ag	259	2193	1368	422	392	11	0	0

- Molecule 30 is a protein called ml46.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Aj	279	2246	1408	414	416	8	0	0

- Molecule 31 is a protein called ml49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Al	209	1618	1051	281	279	7	0	0

- Molecule 32 is a protein called ml52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Ao	183	1475	936	272	264	3	0	0

- Molecule 33 is a protein called ml53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Ap	261	2143	1391	372	368	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ap	2	LEU	SER	conflict	UNP Q57YA9

- Molecule 34 is a protein called ml63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	At	138	1100	690	210	196	4	0	0

- Molecule 35 is a protein called ml64.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Av	213	1792	1138	333	308	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Av	164	ARG	GLN	conflict	UNP Q383B7

- Molecule 36 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	AB	56	280	168	56	56	0	0

- Molecule 37 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	AC	28	140	84	28	28	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	AD	28	140	84	28	28	0	0

- Molecule 38 is a protein called bL12m.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	AG	27	135	81	27	27	0	0

- Molecule 39 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	AA	591	12491	5628	2125	4147	591	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	448	A	U	conflict	GB 343546
AA	622	A	U	conflict	GB 343546
AA	636	A	G	conflict	GB 343546
AA	702	G	A	conflict	GB 343546
AA	706	C	U	conflict	GB 343546
AA	743	C	G	conflict	GB 343546
AA	752	G	A	conflict	GB 343546
AA	757	U	A	conflict	GB 343546
AA	760	U	G	conflict	GB 343546
AA	762	U	G	conflict	GB 343546
AA	789	G	C	conflict	GB 343546
AA	793	G	U	conflict	GB 343546
AA	875	A	G	conflict	GB 343546
AA	876	G	A	conflict	GB 343546
AA	877	A	G	conflict	GB 343546

- Molecule 40 is a protein called ml67.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BA	679	5384	3422	948	981	33	0	0

- Molecule 41 is a protein called ml68.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BB	389	2966	1879	535	539	13	0	0

- Molecule 42 is a protein called ml69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BC	478	3821	2451	670	680	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	29	PRO	SER	conflict	UNP Q584V5
BC	42	GLY	SER	conflict	UNP Q584V5

- Molecule 43 is a protein called mL70.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	BD	417	2063	1229	417	417	0	0

- Molecule 44 is a protein called ml71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BE	392	3105	1970	540	582	13	0	0

- Molecule 45 is a protein called ml72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BF	345	2838	1797	517	511	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	296	ILE	THR	conflict	UNP C9ZR63

- Molecule 46 is a protein called ml73.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BG	319	2503	1578	449	459	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	185	PHE	LEU	conflict	UNP Q57Y49

- Molecule 47 is a protein called ml74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BH	211	1729	1110	301	315	3	0	0

- Molecule 48 is a protein called ml75.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BI	319	2609	1664	473	456	16	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	227	ASN	ASP	conflict	UNP Q38CK0
BI	319	ARG	GLN	conflict	UNP Q38CK0
BI	343	ALA	-	expression tag	UNP Q38CK0

- Molecule 49 is a protein called ml76.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BJ	166	1339	832	262	239	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	329	GLU	ALA	conflict	UNP Q383M2

- Molecule 50 is a protein called Chaperone protein DNAj, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BK	258	1996	1237	383	368	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	348	VAL	LEU	conflict	UNP C9ZQR6

- Molecule 51 is a protein called ml78.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BL	234	1887	1158	370	349	10	0	0

- Molecule 52 is a protein called ml79.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	BM	245	2015	1280	370	356	9	0	0

- Molecule 53 is a protein called ml80.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	BN	214	1714	1077	320	312	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	145	THR	ALA	conflict	UNP Q585A3

- Molecule 54 is a protein called ml81.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	BO	147	1146	719	202	213	12	0	0

- Molecule 55 is a protein called ml82.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	BP	202	1550	973	292	276	9	0	0

- Molecule 56 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	BQ	216	1675	1061	291	315	8	0	0

- Molecule 57 is a protein called ml84.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	BR	195	1650	1059	298	284	9	0	0

- Molecule 58 is a protein called ml85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	BS	97	784	493	141	144	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	45	ILE	VAL	conflict	UNP Q38FG8
BS	173	UNK	LEU	conflict	UNP Q38FG8

- Molecule 59 is a protein called ml86.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	BT	168	1389	853	270	260	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	70	ARG	GLN	conflict	UNP C9ZPU8

- Molecule 60 is a protein called ml87.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	BU	82	694	436	139	115	4	0	0

- Molecule 61 is a protein called ml88.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	BV	155	1307	832	233	236	6	0	0

- Molecule 62 is a protein called ml89.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	BW	187	1557	987	298	264	8	0	0

- Molecule 63 is a protein called ml90.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	BX	107	867	552	160	147	8	0	0

- Molecule 64 is a protein called ml91.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	BY	102	877	549	171	154	3	0	0

- Molecule 65 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	BZ	190	1390	878	242	263	7	0	0

- Molecule 66 is a protein called ml93.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Ba	139	1224	785	223	209	7	0	0

- Molecule 67 is a protein called ml94.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Bb	99	770	482	144	143	1	0	0

- Molecule 68 is a protein called ml95.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
68	Bc	90	781	495	148	138	0	0

- Molecule 69 is a protein called ml96.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Bd	140	1113	689	209	204	11	0	0

- Molecule 70 is a protein called ml97.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	Be	101	822	517	152	144	9	0	0

- Molecule 71 is a protein called ml98.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
71	Bf	50	434	279	80	75	0	0

- Molecule 72 is a protein called ml99.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	Bg	82	656	412	126	116	2	0	0

- Molecule 73 is a protein called ml100.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Bh	91	730	466	129	125	10	0	0

- Molecule 74 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
74	UA	46	276	184	46	46	0	0

- Molecule 75 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
75	UB	40	240	160	40	40	0	0

- Molecule 76 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
76	UC	12	72	48	12	12	0	0
76	UH	12	72	48	12	12	0	0

- Molecule 77 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
77	UD	177	1062	708	177	177	0	0

- Molecule 78 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
78	UE	22	132	88	22	22	0	0

- Molecule 79 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
79	UF	24	144	96	24	24	0	0
79	UG	24	144	96	24	24	0	0
79	UN	24	144	96	24	24	0	0

- Molecule 80 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
80	UI	17	102	68	17	17	0	0

- Molecule 81 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
81	UK	10	60	40	10	10	0	0

- Molecule 82 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
82	UL	15	90	60	15	15	0	0

- Molecule 83 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
83	UM	6	36	24	6	6	0	0

- Molecule 84 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
84	UU	11	66	44	11	11	0	0

- Molecule 85 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
85	UV	8	48	32	8	8	0	0
85	UX	8	48	32	8	8	0	0

- Molecule 86 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
86	UW	7	42	28	7	7	0	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
87	A5	1	1	1	0
87	A9	1	1	1	0

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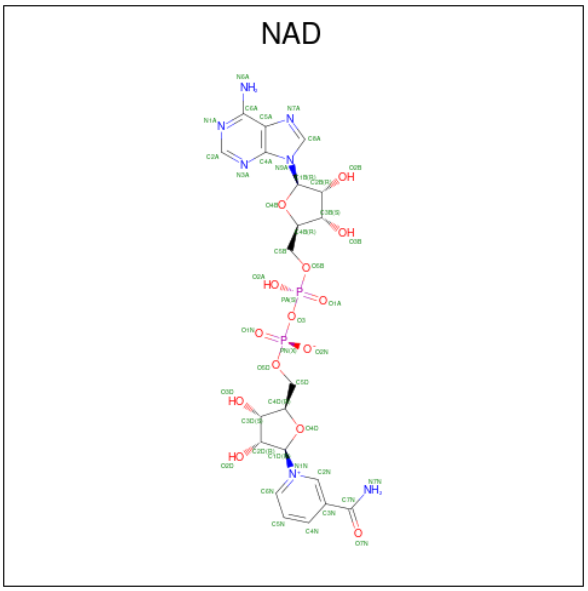
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
87	BX	2	2	2	0
			Total	Zn	
87	Be	1	1	1	0
			Total	Zn	
87	Bh	1	1	1	0

- Molecule 88 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
88	Av	1	44	21	7	14	2	0

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

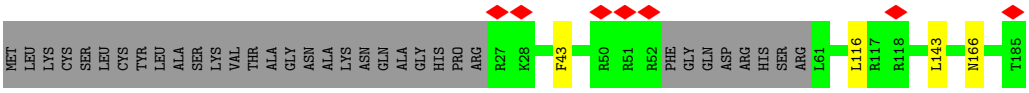
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
89	AA	7	7	7	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

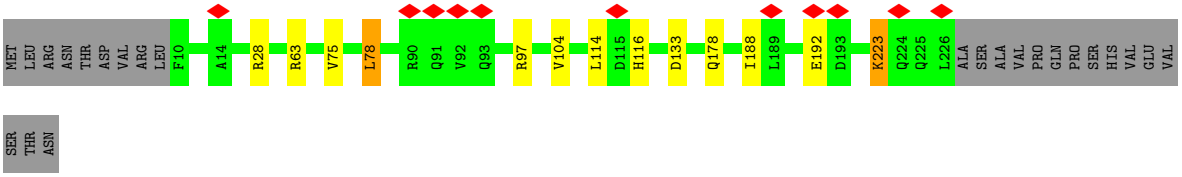
- Molecule 1: bl27m

Chain A0:



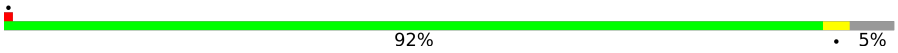
- Molecule 2: bl28m

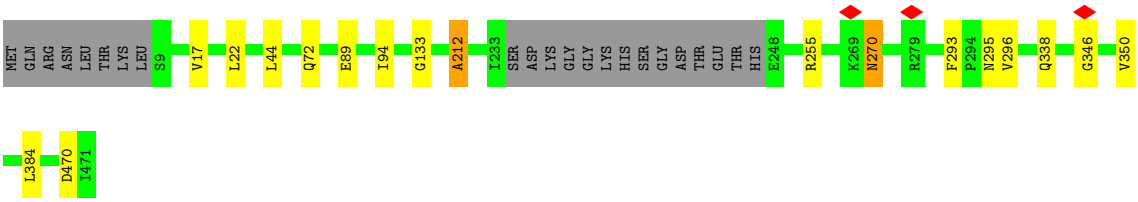
Chain A1:



- Molecule 3: ul29m

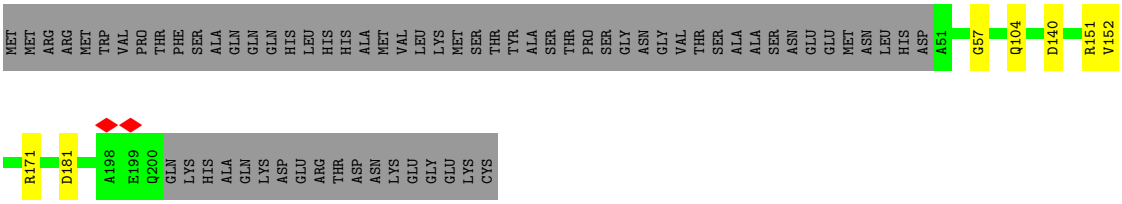
Chain A2:





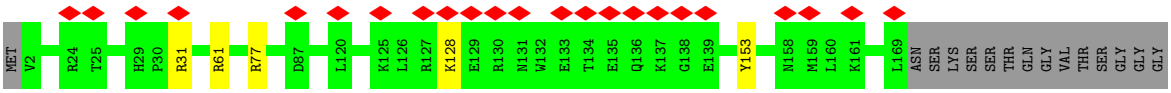
- Molecule 4: ul30m

Chain A3:



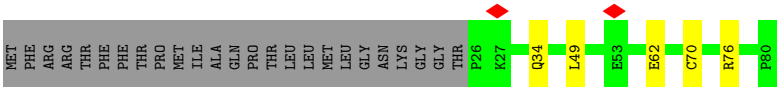
- Molecule 5: bl31m

Chain A4:



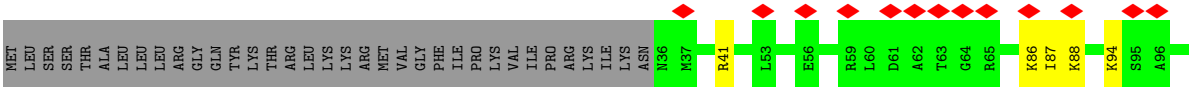
- Molecule 6: bl32m

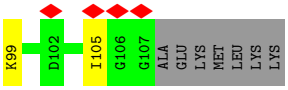
Chain A5:



- Molecule 7: bl33m

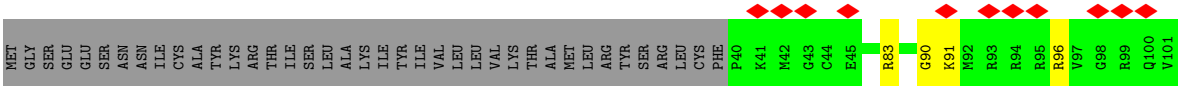
Chain A6:

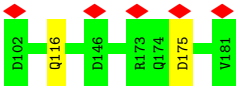




- Molecule 8: bl35m

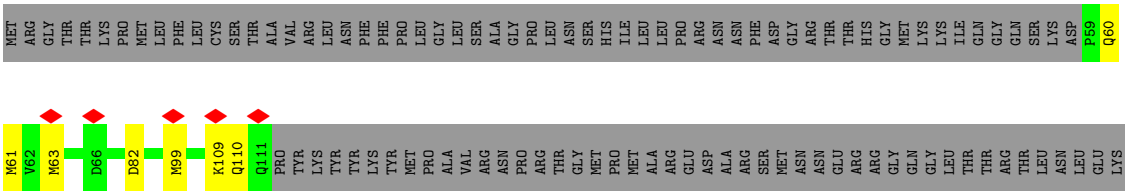
Chain A8:





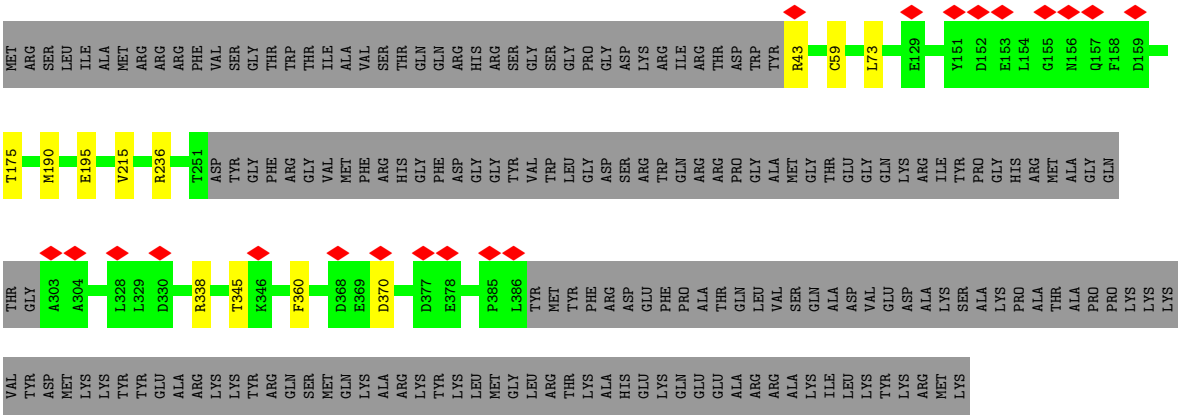
- Molecule 9: bl36m

Chain A9:



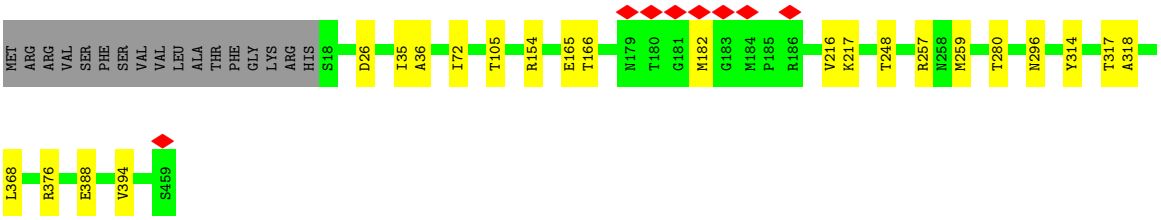
- Molecule 10: Ribosomal protein L3 mitochondrial, putative

Chain AE:



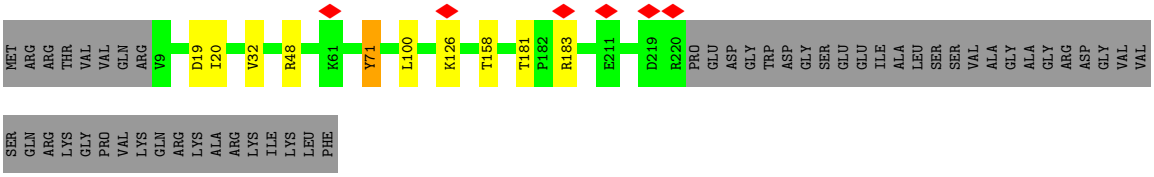
- Molecule 11: Ribosomal protein L4/L1 family, putative

Chain AF:



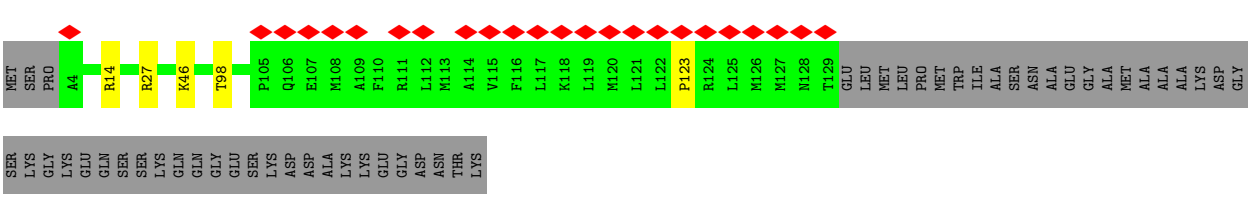
- Molecule 12: bl9m

Chain AI:



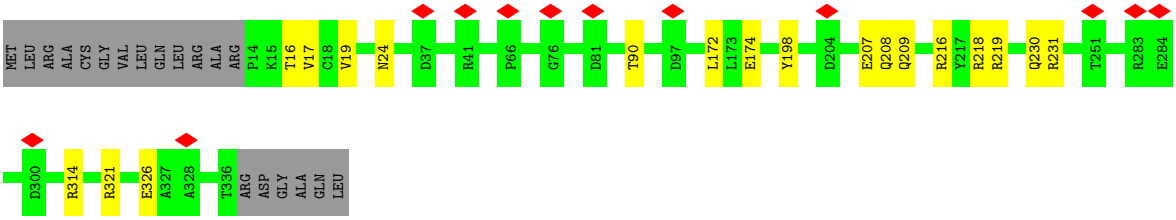
- Molecule 13: ul10m

Chain AJ:



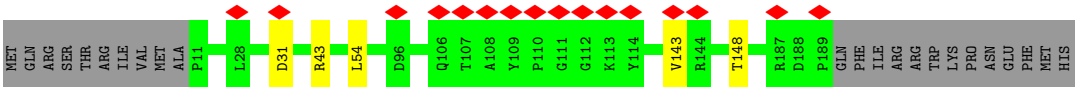
- Molecule 14: Ribosomal protein L11, putative

Chain AK:



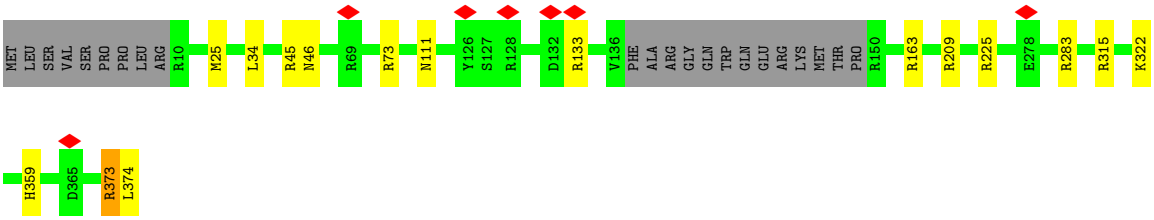
- Molecule 15: 50S ribosomal protein L13, putative

Chain AN:



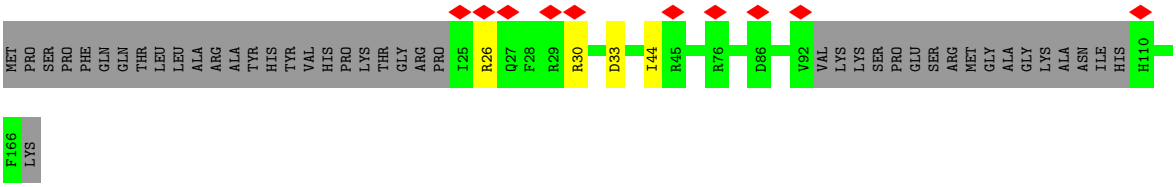
- Molecule 16: ul15m

Chain AP:



- Molecule 17: 50S ribosomal protein L16, putative

Chain AQ:

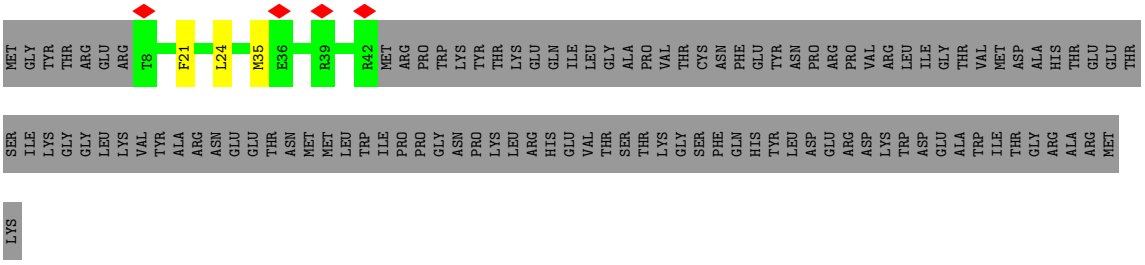


- Molecule 18: 50S ribosomal protein L17, putative

Chain AR:

- Molecule 19: bl19m

Chain AT:

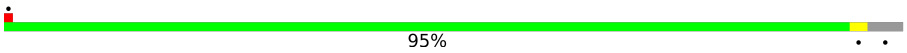


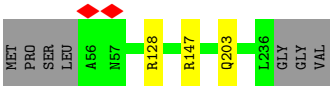
- Molecule 20: bl20m

Chain AU:

- Molecule 21: bl21m

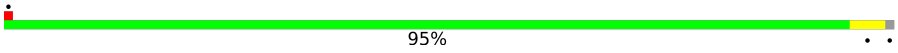
Chain AV:

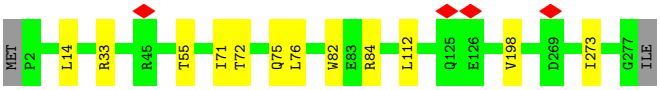




- Molecule 22: ul22m

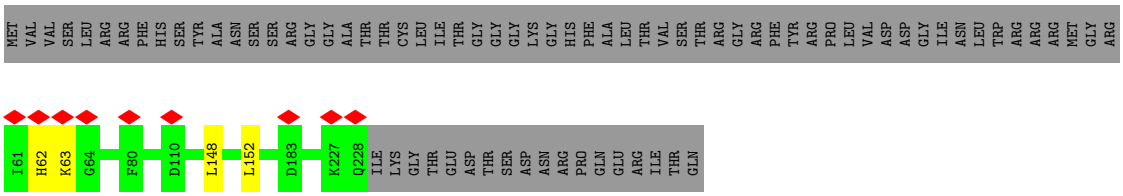
Chain AW:





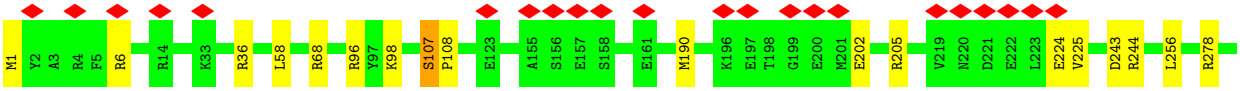
- Molecule 23: ul23m

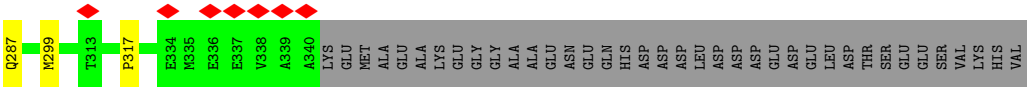
Chain AX:



- Molecule 24: ul24m

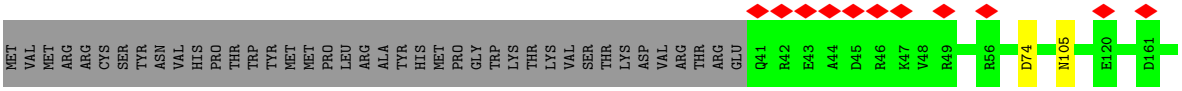
Chain AY:





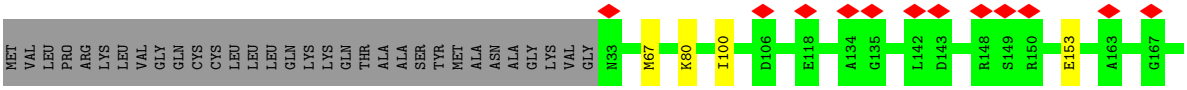
• Molecule 25: ml38

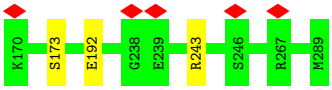
Chain Ab:



• Molecule 26: ml40

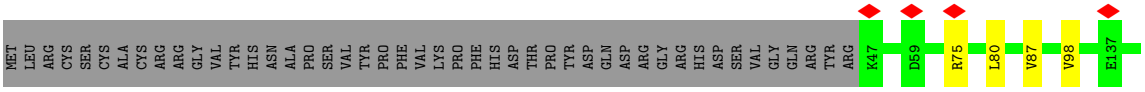
Chain Ad:

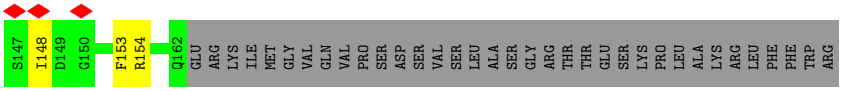




• Molecule 27: ml41

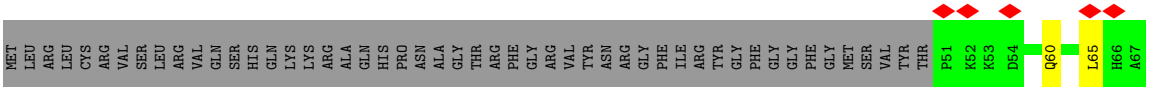
Chain Ae:

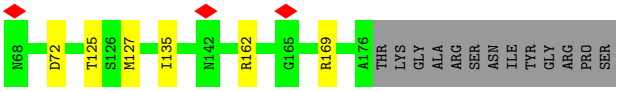




• Molecule 28: ml42

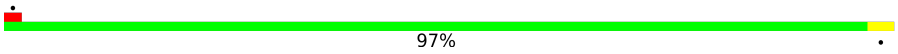
Chain Af:

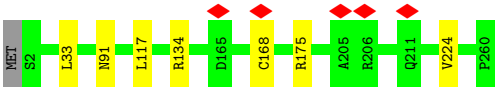




• Molecule 29: ml43

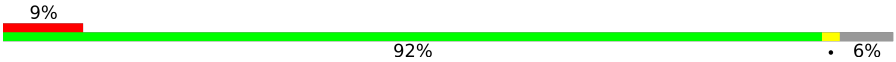
Chain Ag:

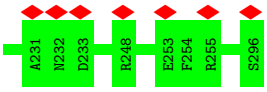




• Molecule 30: ml46

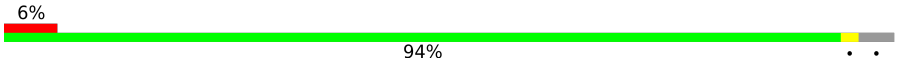
Chain Aj:

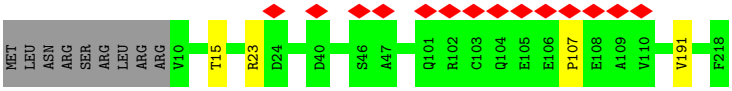




• Molecule 31: ml49

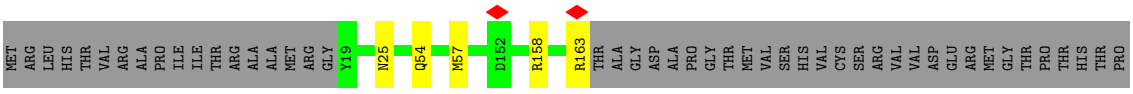
Chain Al:





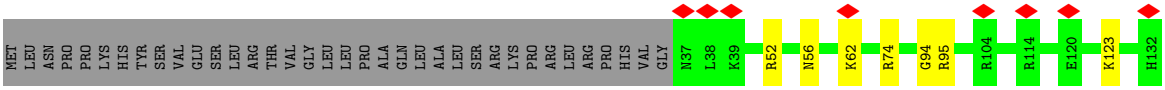
• Molecule 32: ml52

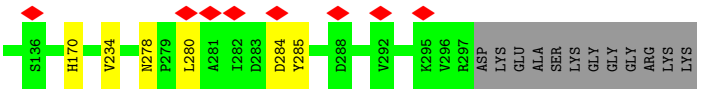
Chain Ao:



• Molecule 33: ml53

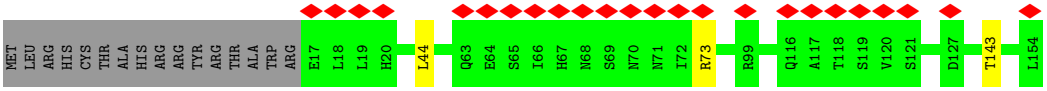
Chain Ap:





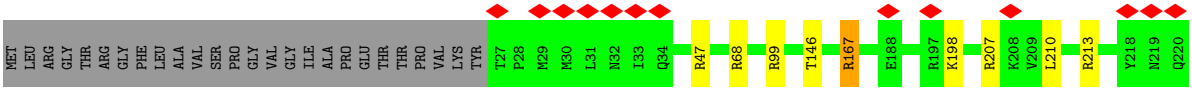
- Molecule 34: ml63

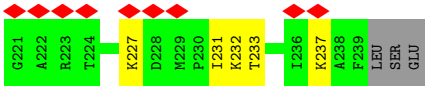
Chain At:



- Molecule 35: ml64

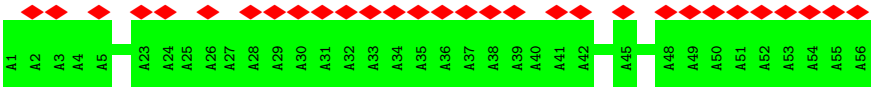
Chain Av:





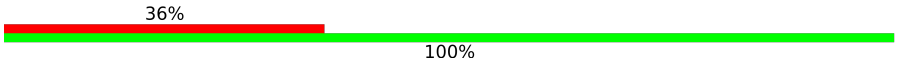
- Molecule 36: bL12m

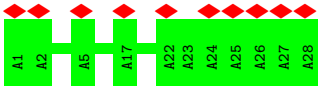
Chain AB:



- Molecule 37: bL12m

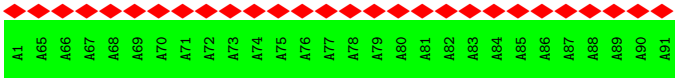
Chain AC:





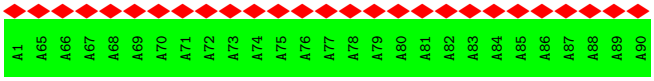
- Molecule 37: bL12m

Chain AD:



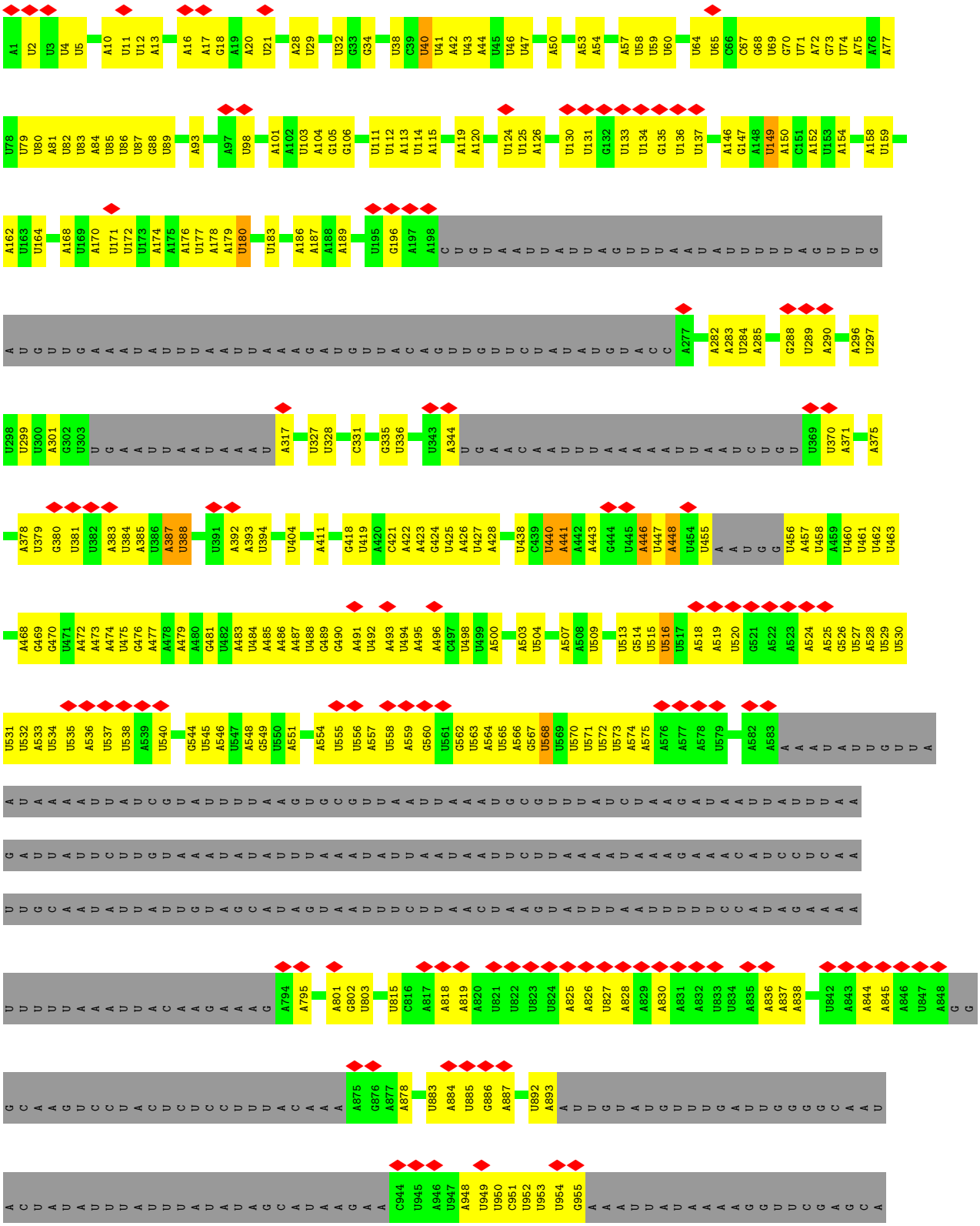
- Molecule 38: bL12m

Chain AG:



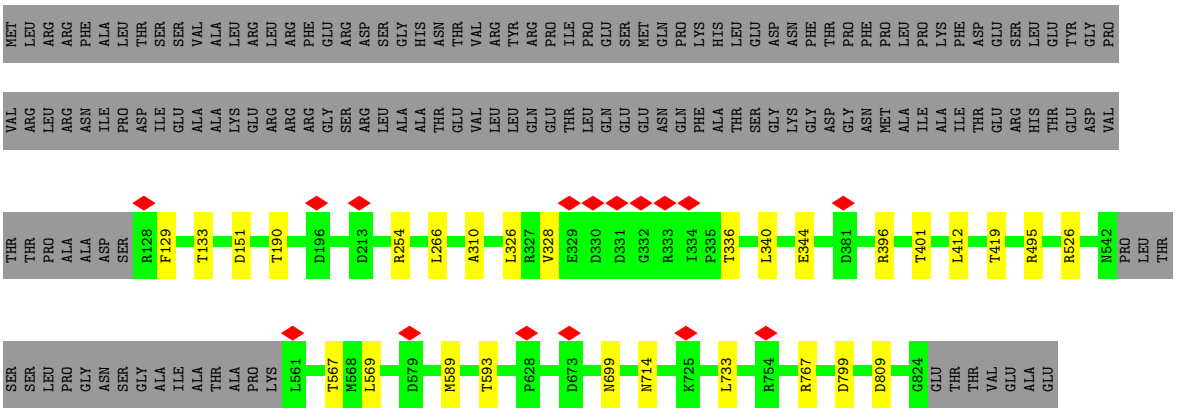
- Molecule 39: 12S rRNA

Chain AA: 11% 25% 24% • 50%



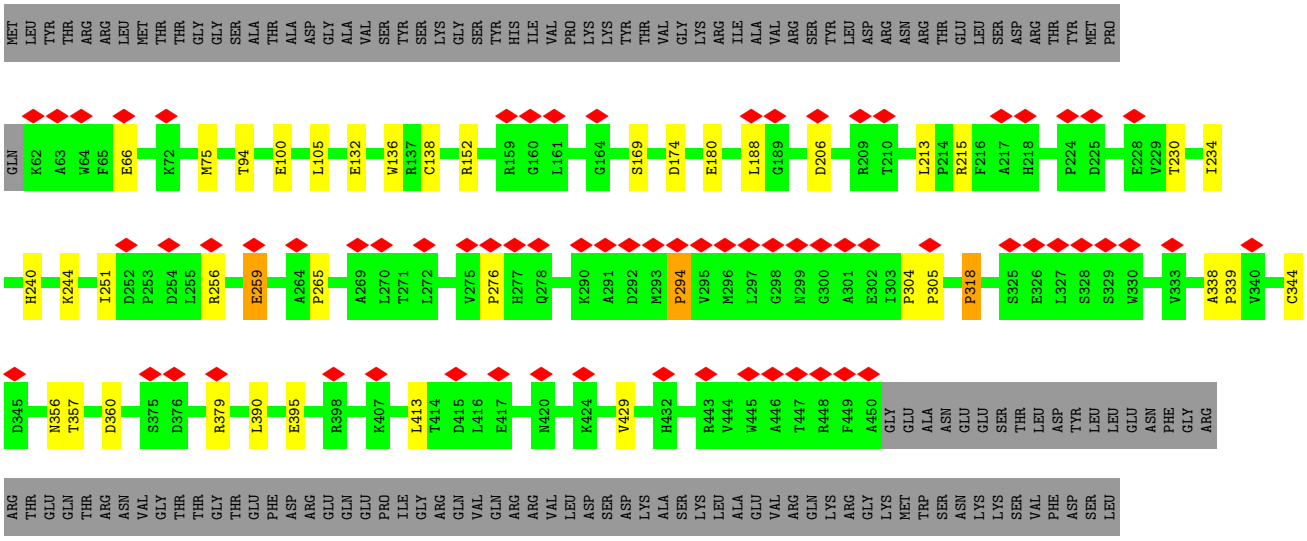
• Molecule 40: ml67

Chain BA: 78% 18%



• Molecule 41: ml68

Chain BB: 13% 65% 7% 28%



HIS GLN LYS GLN LEU GLN ASN VAL THR TYR GLY VAL HIS

- Molecule 42: ml69

Chain BC:

MET LEU ARG ARG LEU ALA GLY CYS VAL ALA PHE ARG LYS ASN VAL VAL ARG PRO PHE MET ASN SER THR ALA LEU LEU LEU SER SER PRO PRO ALA ALA VAL SER ALA PRO VAL ILE PRO LYS SER GLY ASN GLU GLY K46 R116 M230 G234 L268 M301 G302 I339

F344 V362 E400 K413 L427 L490 L494 C501 R512 G513 L522 Y523

- Molecule 43: mL70

Chain BD:

MET CYS LEU LYS ARG LYS ALA PRO HIS LEU PHE CYS PHE CYS LEU TRP SER ILE PHE LEU SER PHE ARG CYS PHE CYS PHE ARG SER TYR ALA ILE MET LEU PRO LEU LEU SER PHE PRO THR ILE GLN ILE SER ILE PHE LEU SER PHE LYS LEU PRO ILE THR THR PHE LEU LEU SER

PRO CYS PHE VAL PHE VAL PHE VAL PHE A105 I106 L112 T113 F121 L122 L123 Q128 T129 Q130 P133 M139 P143 P153 F154 R155 V156 P162 L171 P176 Y181 V187 F194 D198 L199 A200 S201 C202 D203 A204 E205 L206 L207 L208 S211 H212

I213 V216 Q219 T230 S234 P238 K239 M240 A241 E242 P243 S244 Q247 C252 T255 A270 K271 R272 P277 P284 R298 E301 E302 D303 A304 G305 A306 V307 M312 P319 L351 N352 R353 M354 I355 P356 P357 P370 F371 F379 V389

Y392 F393 K394 R395 A396 P409 T433 M434 P435 Q436 E437 V438 A439 V440 A441 V442 C443 F449 P450 A451 Q457 P463 W470 R471 T472 D473 A474 A475 V476 P477 R480 L481 F482 P483 L493 G496 V497 D500 A501 M504 H505 L506 E512 D517 L521

LYS VAL ARG ARG PHE VAL ASP GLU VAL GLY ASP MET TYR GLU THR ASN ILE ASP SER VAL LEU LYS ARG VAL ASP ASP ASN PHE LYS GLN VAL VAL PRO GLN LEU LYS ALA GLU ASP LEU GLN VAL ASP ALA PRO LEU GLN ASP GLY GLU GLY GLU ASP THR VAL ARG GLU THR VAL ALA

ALA

- Molecule 44: ml71

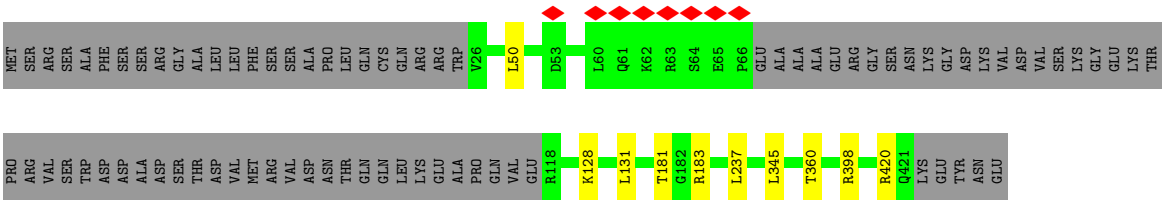
Chain BE:

MET LEU PHE ARG SER VAL SER CYS LYS ASN Y11 Q12 R13 G19 L28 N29 L32 G42 M61 E62 R88 E116 I128 E140 V144 R190 F191 GLU GLY SER LEU SER VAL LEU GLY GLU CYS GLU LYS CYS LEU PRO GLU GLN HIS GLN VAL GLU ILE

SER GLU SER LEU GLY THR PHE ILE GLY ALA THR VAL SER PRO A228 L266 D291 E296 D332 K335 V348 E354 N358 K359 R364 GLU GLU GLN PRO SER VAL TYR LYS GLN VAL P375 R376 R379 E380 H384 M412 T442 R448 LEU

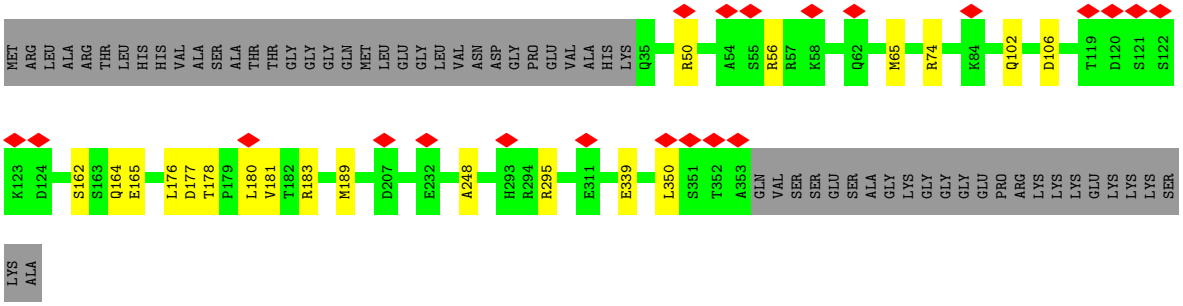
- Molecule 45: ml72

Chain BF:



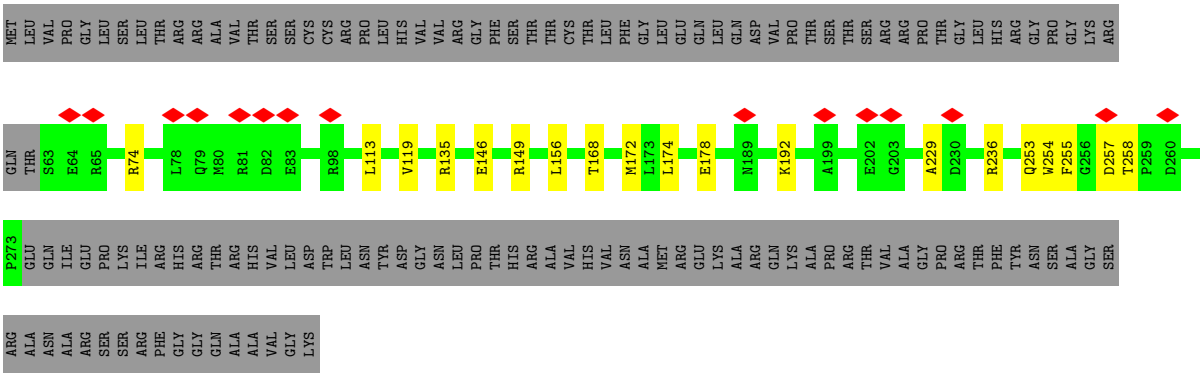
• Molecule 46: ml73

Chain BG:



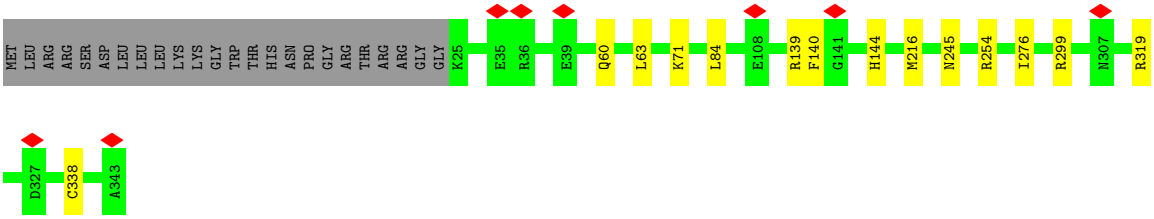
• Molecule 47: ml74

Chain BH:



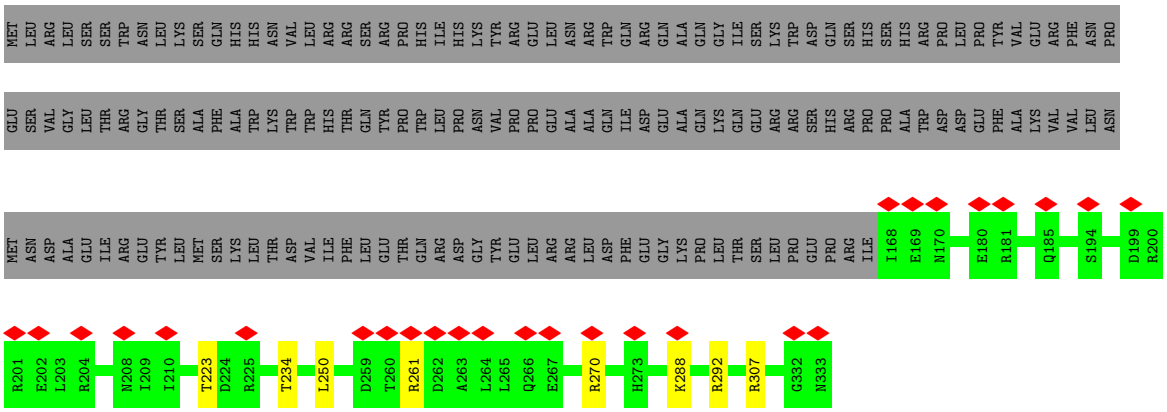
• Molecule 48: ml75

Chain BI:



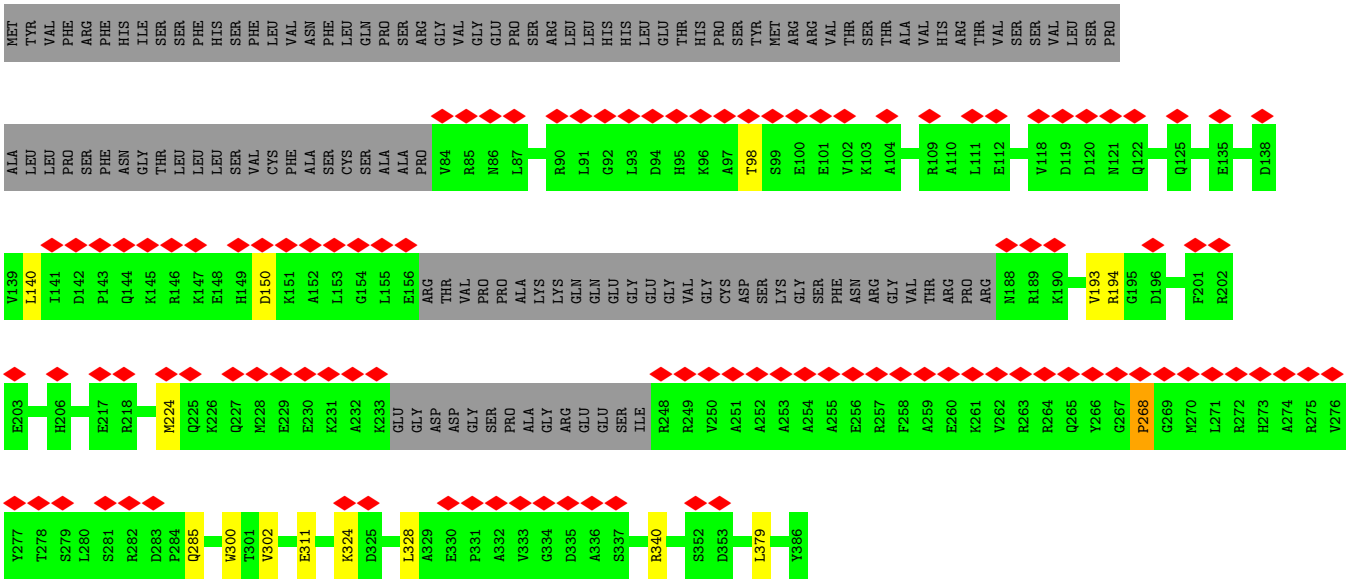
• Molecule 49: ml76

Chain BJ:



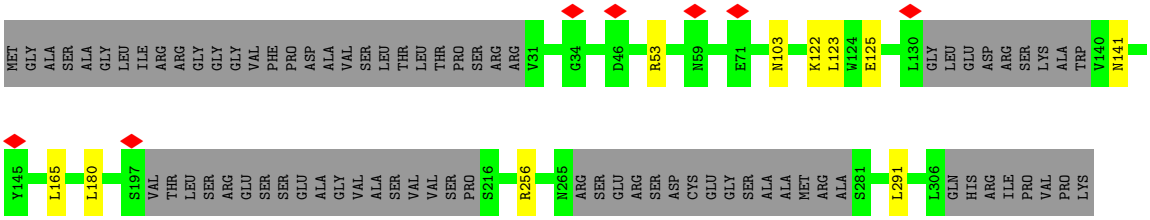
• Molecule 50: Chaperone protein DNAj, putative

Chain BK: 28% 63% • 33%



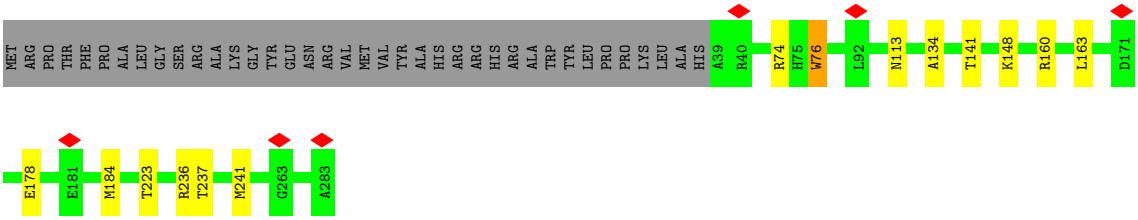
• Molecule 51: ml78

Chain BL: • 72% • 25%



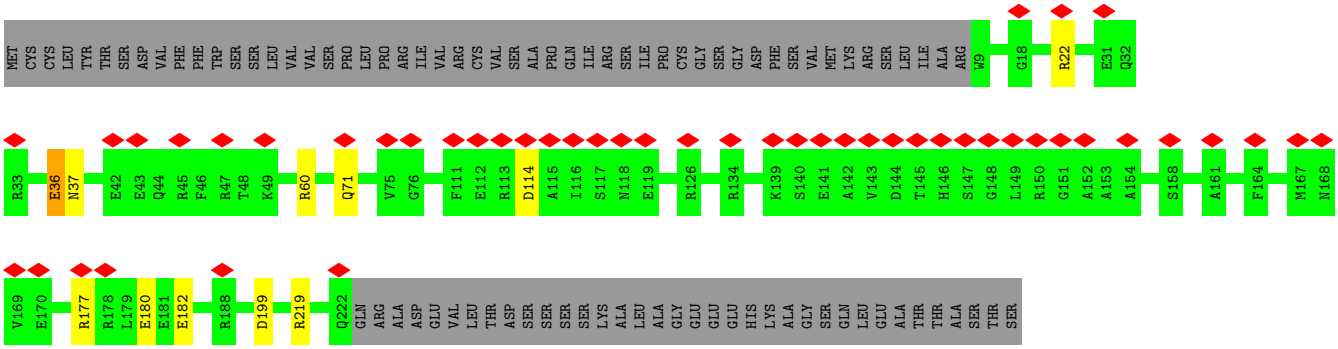
• Molecule 52: ml79

Chain BM: • 82% 5% 13%



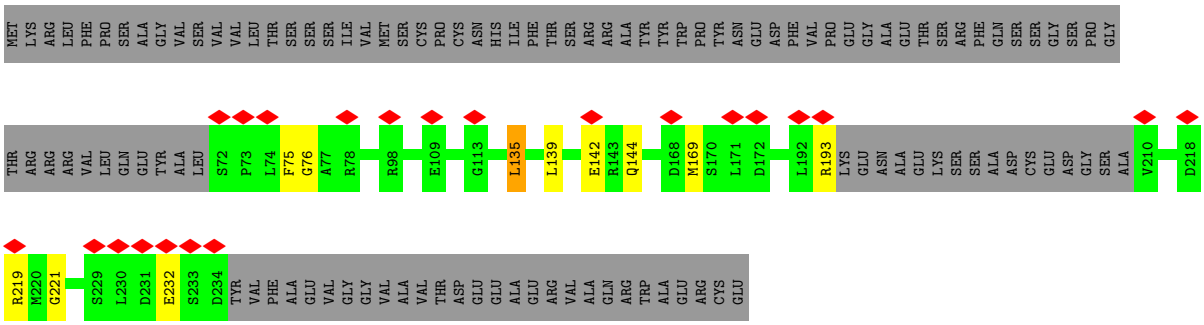
• Molecule 53: ml80

Chain BN:



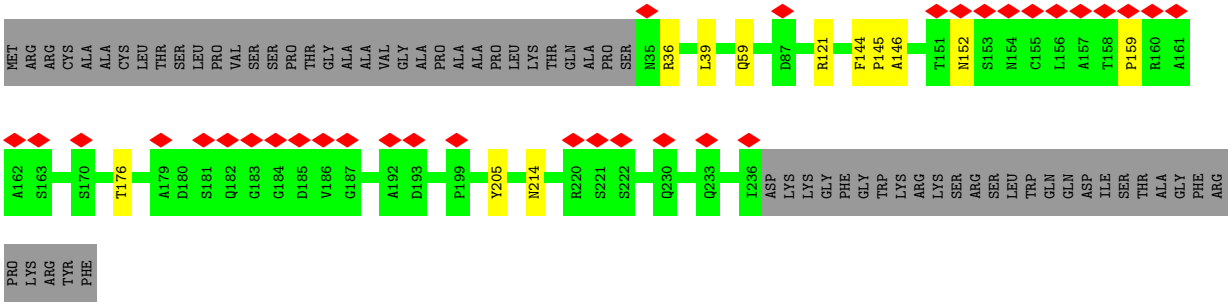
• Molecule 54: ml81

Chain BO:



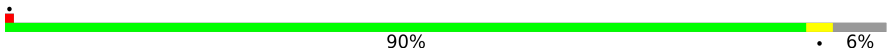
• Molecule 55: ml82

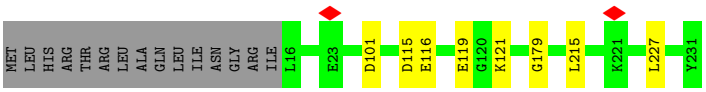
Chain BP:



• Molecule 56: Peptidyl-prolyl cis-trans isomerase

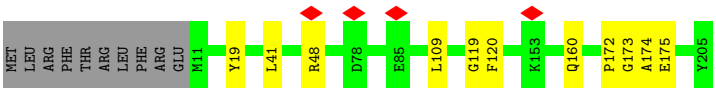
Chain BQ:





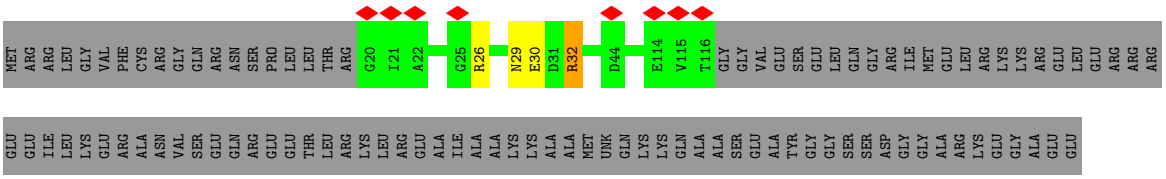
- Molecule 57: ml84

Chain BR:



- Molecule 58: ml85

Chain BS:

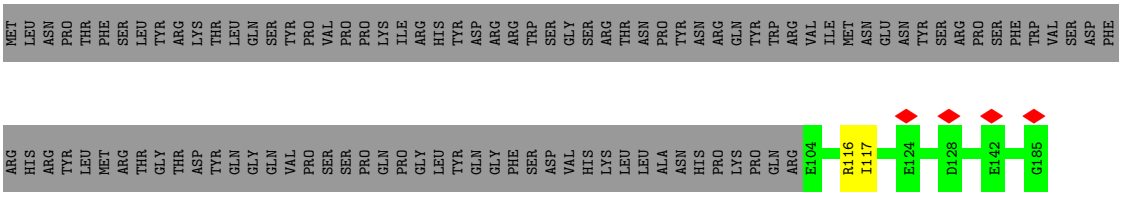


- Molecule 59: ml86

Chain BT:

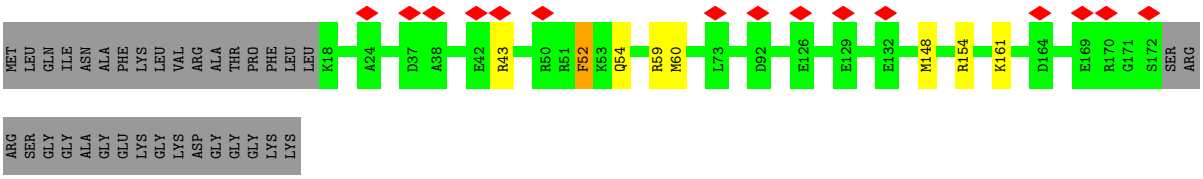
- Molecule 60: ml87

Chain BU:



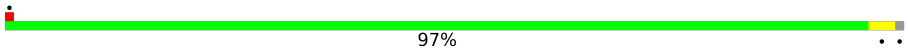
- Molecule 61: ml88

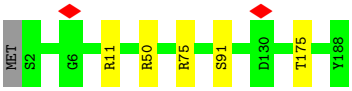
Chain BV:



- Molecule 62: ml89

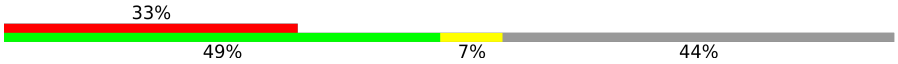
Chain BW:

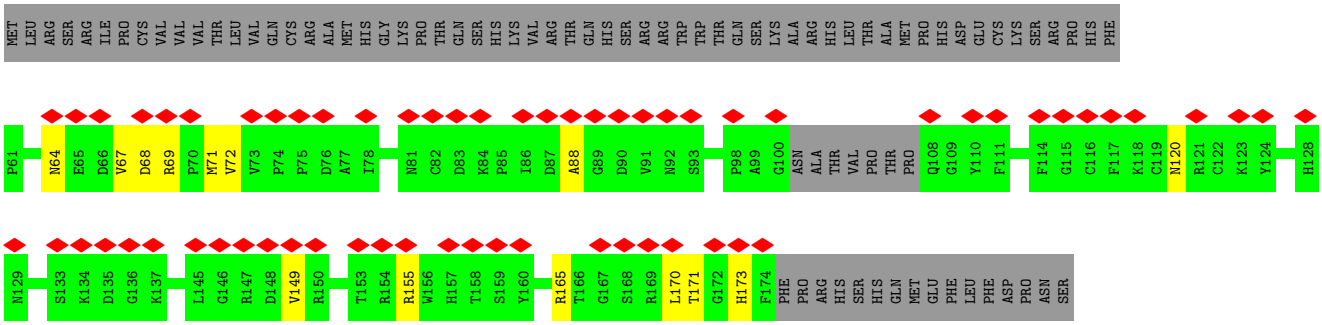




- Molecule 63: ml90

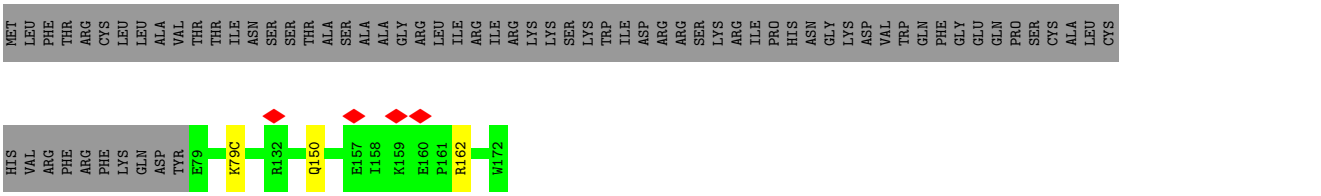
Chain BX:





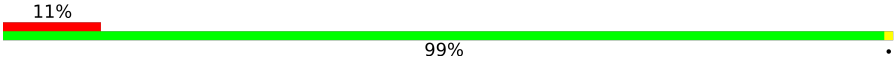
- Molecule 64: ml91

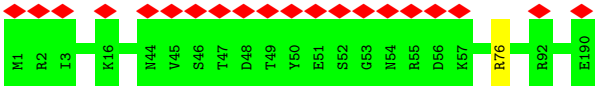
Chain BY:



- Molecule 65: Peptidyl-prolyl cis-trans isomerase

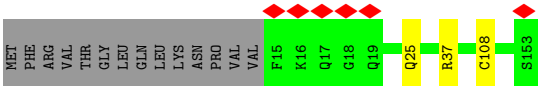
Chain BZ:





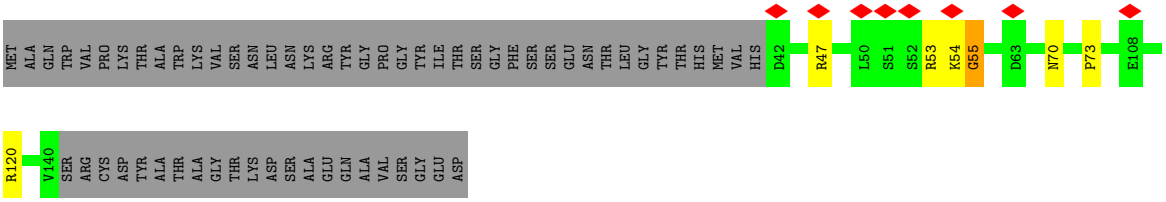
- Molecule 66: ml93

Chain Ba:



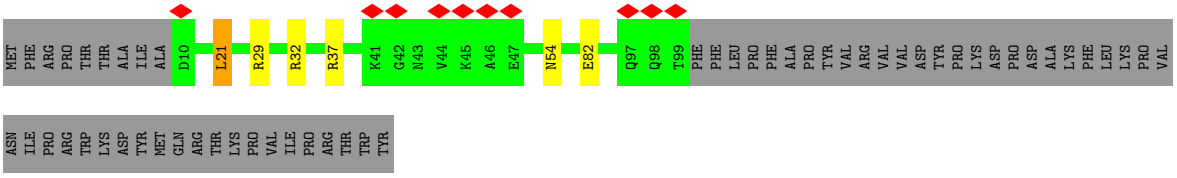
- Molecule 67: ml94

Chain Bb:



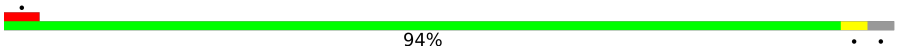
- Molecule 68: ml95

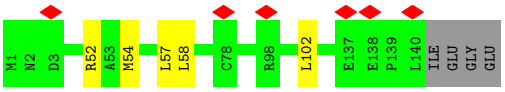
Chain Bc:



- Molecule 69: ml96

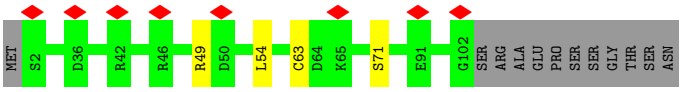
Chain Bd:





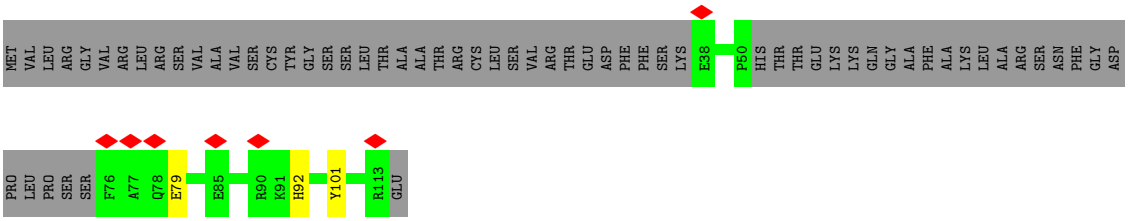
- Molecule 70: ml97

Chain Be:



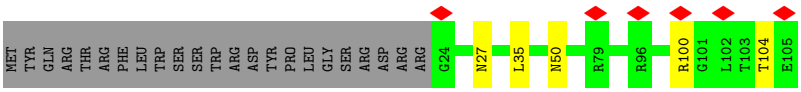
- Molecule 71: ml98

Chain Bf:



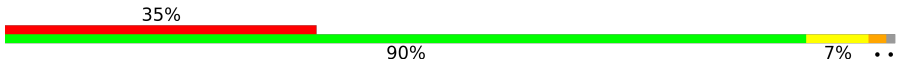
- Molecule 72: ml99

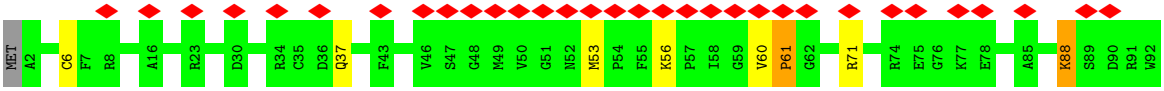
Chain Bg:



• Molecule 73: ml100

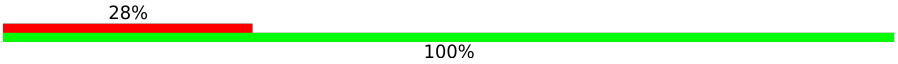
Chain Bh:

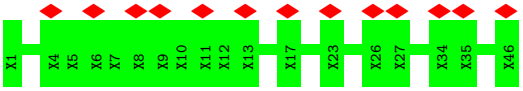




• Molecule 74: UNK

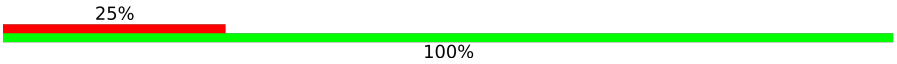
Chain UA:

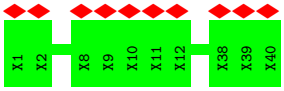




• Molecule 75: UNK

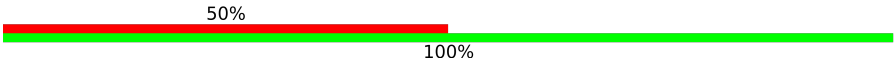
Chain UB:

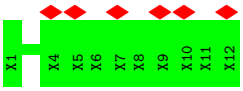




• Molecule 76: UNK

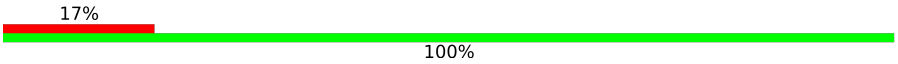
Chain UC:





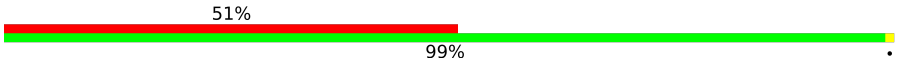
• Molecule 76: UNK

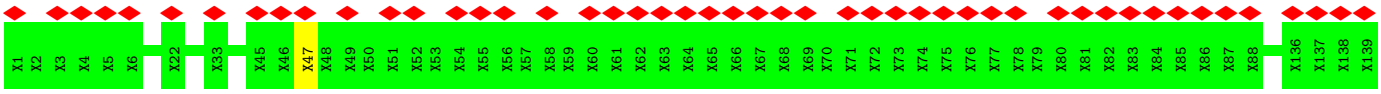
Chain UH:

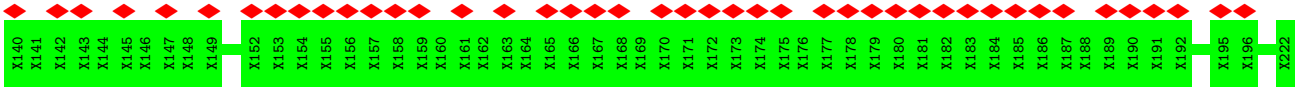


• Molecule 77: UNK

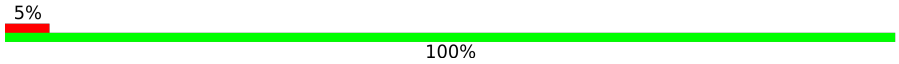
Chain UD:



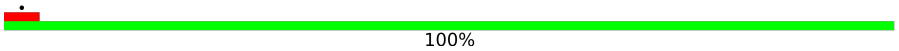




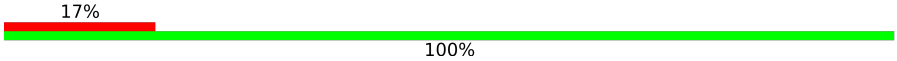
• Molecule 78: UNK

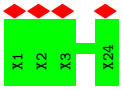
Chain UE: 

• Molecule 79: UNK

Chain UF: 

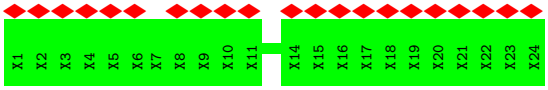
• Molecule 79: UNK

Chain UG: 

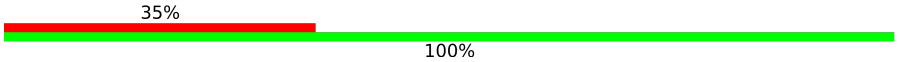


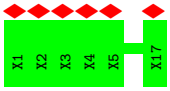
• Molecule 79: UNK

Chain UN:

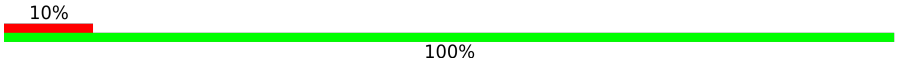


• Molecule 80: UNK

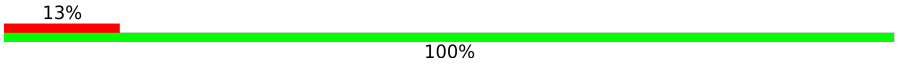
Chain UI: 

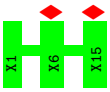


• Molecule 81: UNK

Chain UK: 

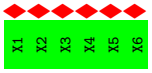
• Molecule 82: UNK

Chain UL: 



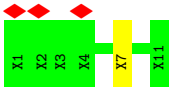
- Molecule 83: UNK

Chain UM: 100% 100%



- Molecule 84: UNK

Chain UU: 27% 91% 9%



- Molecule 85: UNK

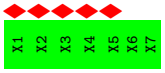
Chain UV: 12% 100%

- Molecule 85: UNK

Chain UX: 12% 100%

- Molecule 86: UNK

Chain UW: 71% 100%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.536	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, MG, ZN

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	A0	0.32	0/1297	0.53	0/1750
2	A1	0.47	0/1828	0.66	2/2466 (0.1%)
3	A2	0.35	0/3740	0.57	1/5094 (0.0%)
4	A3	0.35	0/1241	0.53	0/1674
5	A4	0.33	0/1423	0.60	1/1924 (0.1%)
6	A5	0.34	0/498	0.56	0/663
7	A6	0.37	0/578	0.58	0/774
8	A8	0.40	0/1230	0.61	0/1645
9	A9	0.37	0/474	0.60	0/639
10	AE	0.42	0/2469	0.61	1/3364 (0.0%)
11	AF	0.37	0/3706	0.57	0/5029
12	AI	0.38	0/1850	0.65	2/2515 (0.1%)
13	AJ	0.32	0/986	0.55	1/1339 (0.1%)
14	AK	0.46	2/2745 (0.1%)	0.66	2/3705 (0.1%)
15	AN	0.39	0/1561	0.56	0/2123
16	AP	0.38	0/2993	0.61	1/4060 (0.0%)
17	AQ	0.36	0/1046	0.54	0/1415
18	AR	0.38	0/1969	0.59	0/2656
19	AT	0.34	0/292	0.54	0/390
20	AU	0.34	0/1456	0.55	1/1971 (0.1%)
21	AV	0.37	0/1453	0.59	0/1970
22	AW	0.36	0/2291	0.56	0/3097
23	AX	0.40	0/1462	0.60	1/1986 (0.1%)
24	AY	0.38	0/2763	0.60	1/3739 (0.0%)
25	Ab	0.34	0/3651	0.56	0/4988
26	Ad	0.32	0/2171	0.52	0/2930
27	Ae	0.37	0/960	0.60	0/1304
28	Af	0.34	0/1037	0.61	0/1406
29	Ag	0.33	0/2253	0.54	0/3046
30	Aj	0.35	0/2306	0.56	0/3136
31	Al	0.38	0/1665	0.60	1/2270 (0.0%)
32	Ao	0.35	0/1523	0.56	0/2070

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ap	0.41	0/2213	0.64	1/3007 (0.0%)
34	At	0.36	0/1128	0.59	0/1532
35	Av	0.38	0/1839	0.59	2/2478 (0.1%)
36	AB	0.26	0/279	0.43	0/389
37	AC	0.24	0/139	0.36	0/193
37	AD	0.30	0/139	0.35	0/193
38	AG	0.29	0/134	0.36	0/186
39	AA	0.42	1/13972 (0.0%)	0.95	51/21705 (0.2%)
40	BA	0.37	0/5501	0.61	1/7463 (0.0%)
41	BB	0.33	0/3038	0.58	7/4134 (0.2%)
42	BC	0.36	0/3919	0.59	1/5318 (0.0%)
43	BD	0.35	0/2062	0.66	18/2872 (0.6%)
44	BE	0.37	0/3184	0.59	2/4308 (0.0%)
45	BF	0.36	0/2900	0.57	0/3909
46	BG	0.35	0/2561	0.61	0/3469
47	BH	0.40	0/1778	0.61	0/2423
48	BI	0.34	0/2685	0.60	0/3633
49	BJ	0.32	0/1366	0.58	0/1846
50	BK	0.33	0/2038	0.51	1/2753 (0.0%)
51	BL	0.35	0/1924	0.60	1/2596 (0.0%)
52	BM	0.42	0/2082	0.63	0/2830
53	BN	0.33	0/1755	0.51	0/2381
54	BO	0.43	0/1160	0.62	1/1565 (0.1%)
55	BP	0.34	0/1593	0.58	1/2166 (0.0%)
56	BQ	0.41	0/1716	0.67	1/2324 (0.0%)
57	BR	0.38	0/1693	0.65	1/2284 (0.0%)
58	BS	0.44	0/801	0.72	1/1090 (0.1%)
59	BT	0.35	0/1417	0.60	1/1907 (0.1%)
60	BU	0.35	0/711	0.57	0/955
61	BV	0.62	3/1340 (0.2%)	0.68	2/1802 (0.1%)
62	BW	0.37	0/1604	0.56	0/2167
63	BX	0.35	0/897	0.73	3/1215 (0.2%)
64	BY	0.34	0/908	0.56	0/1231
65	BZ	0.35	0/1416	0.58	0/1919
66	Ba	0.42	1/1267 (0.1%)	0.58	0/1711
67	Bb	0.36	0/785	0.70	1/1063 (0.1%)
68	Bc	0.39	0/805	0.63	1/1091 (0.1%)
69	Bd	0.36	0/1133	0.59	0/1528
70	Be	0.36	0/844	0.62	0/1139
71	Bf	0.36	0/450	0.60	0/609
72	Bg	0.34	0/671	0.58	0/905
73	Bh	0.37	0/752	0.62	0/1015
All	All	0.38	7/135516 (0.0%)	0.65	113/186442 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A1	0	1
3	A2	0	2
4	A3	0	1
8	A8	0	2
11	AF	0	3
18	AR	0	2
21	AV	0	1
22	AW	0	1
23	AX	0	1
24	AY	0	2
25	Ab	0	1
33	Ap	0	1
35	Av	0	1
41	BB	0	1
42	BC	0	2
44	BE	0	1
46	BG	0	1
47	BH	0	1
50	BK	0	2
52	BM	0	2
53	BN	0	3
54	BO	0	3
55	BP	0	2
57	BR	0	3
67	Bb	0	4
71	Bf	0	1
73	Bh	0	3
77	UD	0	1
84	UU	0	1
All	All	0	50

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BV	52	PHE	CE2-CZ	8.42	1.53	1.37
61	BV	52	PHE	CD1-CE1	8.27	1.55	1.39
14	AK	198	TYR	CB-CG	7.87	1.63	1.51
66	Ba	108	CYS	CB-SG	-5.99	1.72	1.81
14	AK	198	TYR	CD1-CE1	5.77	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	AA	446	A	C6-N6	-5.40	1.29	1.33
61	BV	52	PHE	CD2-CE2	5.32	1.49	1.39

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	BX	69	ARG	NE-CZ-NH2	12.13	126.36	120.30
39	AA	40	U	C6-N1-C2	-11.67	114.00	121.00
39	AA	40	U	C5-C6-N1	11.29	128.35	122.70
39	AA	317	A	O5'-P-OP2	11.12	124.04	110.70
39	AA	40	U	N3-C4-C5	-9.58	108.85	114.60
39	AA	388	U	C5-C4-O4	-8.91	120.55	125.90
39	AA	424	G	C8-N9-C4	8.74	109.90	106.40
58	BS	32	ARG	NE-CZ-NH2	8.57	124.58	120.30
12	AI	71	TYR	C-N-CD	8.44	146.13	128.40
68	Bc	21	LEU	CA-CB-CG	8.19	134.13	115.30
39	AA	446	A	C8-N9-C4	-8.01	102.60	105.80
39	AA	180	U	N1-C2-O2	7.86	128.30	122.80
35	Av	167	ARG	NE-CZ-NH1	-7.82	116.39	120.30
39	AA	446	A	N7-C8-N9	7.62	117.61	113.80
39	AA	180	U	N3-C2-O2	-7.37	117.04	122.20
39	AA	1111	A	C6-N1-C2	-7.36	114.18	118.60
39	AA	40	U	C2-N3-C4	7.30	131.38	127.00
39	AA	1112	U	N1-C2-O2	7.28	127.89	122.80
39	AA	1112	U	N3-C2-O2	-7.28	117.11	122.20
39	AA	424	G	N1-C6-O6	-7.27	115.54	119.90
39	AA	388	U	N1-C2-O2	-7.19	117.77	122.80
39	AA	1112	U	C2-N1-C1'	7.07	126.18	117.70
39	AA	1110	A	N1-C6-N6	-7.07	114.36	118.60
39	AA	424	G	C5-C6-N1	6.98	114.99	111.50
39	AA	440	U	C5-C6-N1	6.98	126.19	122.70
39	AA	424	G	N9-C4-C5	-6.94	102.62	105.40
39	AA	388	U	N3-C4-O4	6.92	124.24	119.40
41	BB	276	PRO	N-CA-CB	6.71	111.36	103.30
41	BB	305	PRO	N-CA-CB	6.66	111.29	103.30
63	BX	69	ARG	CG-CD-NE	6.63	125.71	111.80
43	BD	356	PRO	N-CA-CB	6.58	111.19	103.30
39	AA	40	U	C2-N1-C1'	6.54	125.54	117.70
39	AA	180	U	C2-N1-C1'	6.54	125.54	117.70
39	AA	387	A	C8-N9-C4	-6.50	103.20	105.80
14	AK	198	TYR	CZ-CE2-CD2	6.49	125.64	119.80
43	BD	143	PRO	N-CA-CB	6.48	111.08	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	BD	435	PRO	N-CA-CB	6.34	110.90	103.30
43	BD	370	PRO	N-CA-CB	6.26	110.82	103.30
61	BV	52	PHE	CG-CD1-CE1	6.23	127.65	120.80
39	AA	440	U	C2-N1-C1'	6.20	125.14	117.70
43	BD	176	PRO	N-CA-CB	6.19	110.72	103.30
41	BB	318	PRO	N-CA-CB	6.18	110.72	103.30
61	BV	52	PHE	CD1-CE1-CZ	-6.17	112.69	120.10
39	AA	440	U	C6-N1-C2	-6.16	117.31	121.00
39	AA	1110	A	N3-C4-C5	-6.15	122.50	126.80
39	AA	568	U	C2-N1-C1'	6.13	125.06	117.70
67	Bb	55	GLY	N-CA-C	6.11	128.38	113.10
41	BB	304	PRO	N-CA-CB	6.09	110.61	103.30
63	BX	69	ARG	NE-CZ-NH1	-6.06	117.27	120.30
39	AA	568	U	N1-C2-O2	6.05	127.04	122.80
42	BC	302	GLY	N-CA-C	-6.04	98.01	113.10
39	AA	446	A	C5-N7-C8	-6.02	100.89	103.90
39	AA	387	A	N7-C8-N9	6.02	116.81	113.80
39	AA	40	U	P-O3'-C3'	6.00	126.90	119.70
39	AA	1111	A	N1-C2-N3	5.98	132.29	129.30
41	BB	265	PRO	N-CA-CB	5.98	110.47	103.30
14	AK	198	TYR	CB-CG-CD1	5.91	124.55	121.00
43	BD	477	PRO	N-CA-CB	5.91	110.39	103.30
56	BQ	179	GLY	N-CA-C	5.89	127.83	113.10
43	BD	409	PRO	N-CA-CB	5.88	110.36	103.30
43	BD	162	PRO	N-CA-CB	5.86	110.33	103.30
43	BD	284	PRO	N-CA-CB	5.85	110.31	103.30
33	Ap	170	HIS	ND1-CG-CD2	-5.83	97.83	106.00
54	BO	135	LEU	CA-CB-CG	-5.83	101.90	115.30
43	BD	153	PRO	N-CA-CB	5.81	110.27	103.30
39	AA	67	C	C2-N1-C1'	5.79	125.16	118.80
43	BD	483	PRO	N-CA-CB	5.77	110.23	103.30
43	BD	133	PRO	N-CA-CB	5.75	110.20	103.30
43	BD	463	PRO	N-CA-CB	5.74	110.19	103.30
40	BA	733	LEU	CA-CB-CG	5.71	128.44	115.30
35	Av	167	ARG	NE-CZ-NH2	5.71	123.16	120.30
43	BD	357	PRO	N-CA-CB	5.69	110.13	103.30
43	BD	238	PRO	N-CA-CB	5.68	110.12	103.30
39	AA	568	U	N3-C2-O2	-5.67	118.23	122.20
24	AY	317	PRO	N-CA-CB	5.66	110.10	103.30
31	Al	107	PRO	N-CA-CB	5.66	110.09	103.30
13	AJ	123	PRO	N-CA-CB	5.66	110.09	103.30
41	BB	294	PRO	N-CA-CB	5.66	110.09	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	AA	440	U	P-O3'-C3'	5.65	126.48	119.70
43	BD	277	PRO	N-CA-CB	5.63	110.05	103.30
55	BP	159	PRO	N-CA-CB	5.62	110.05	103.30
59	BT	131	LEU	CA-CB-CG	5.61	128.20	115.30
50	BK	268	PRO	N-CA-CB	5.61	110.03	103.30
43	BD	319	PRO	N-CA-CB	5.60	110.02	103.30
39	AA	196	G	N3-C4-N9	-5.60	122.64	126.00
39	AA	441	A	O5'-P-OP1	-5.56	100.70	105.70
39	AA	424	G	C4-C5-C6	-5.52	115.49	118.80
2	A1	223	LYS	CD-CE-NZ	-5.50	99.04	111.70
20	AU	48	ARG	NE-CZ-NH2	5.50	123.05	120.30
43	BD	243	PRO	N-CA-CB	5.50	109.90	103.30
39	AA	67	C	N1-C2-O2	5.46	122.18	118.90
44	BE	266	LEU	CA-CB-CG	5.44	127.81	115.30
39	AA	878	A	O5'-P-OP2	-5.43	100.81	105.70
12	AI	71	TYR	C-N-CA	-5.40	99.33	122.00
39	AA	196	G	C4-N9-C1'	-5.40	119.48	126.50
3	A2	212	ALA	C-N-CD	5.34	139.62	128.40
39	AA	424	G	C4-C5-N7	5.33	112.93	110.80
39	AA	448	A	C4-C5-C6	5.29	119.64	117.00
16	AP	373	ARG	NE-CZ-NH2	5.28	122.94	120.30
5	A4	77	ARG	NE-CZ-NH1	5.27	122.94	120.30
23	AX	148	LEU	CB-CG-CD1	-5.27	102.04	111.00
41	BB	339	PRO	N-CA-CB	5.27	109.62	103.30
57	BR	109	LEU	CA-CB-CG	5.21	127.29	115.30
2	A1	78	LEU	CA-CB-CG	5.20	127.27	115.30
39	AA	446	A	C5-C6-N6	-5.17	119.56	123.70
39	AA	149	U	C2-N1-C1'	5.14	123.87	117.70
10	AE	360	PHE	C-N-CD	5.13	139.18	128.40
39	AA	516	U	C2-N1-C1'	5.11	123.83	117.70
51	BL	165	LEU	CA-CB-CG	5.10	127.02	115.30
39	AA	196	G	C8-N9-C1'	5.07	133.60	127.00
39	AA	1110	A	N3-C4-N9	5.05	131.44	127.40
39	AA	149	U	N1-C2-O2	5.04	126.33	122.80
44	BE	42	GLY	N-CA-C	5.03	125.67	113.10

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A1	78	LEU	Peptide
3	A2	133	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	A2	346	GLY	Peptide
4	A3	57	GLY	Peptide
8	A8	90	GLY	Peptide
8	A8	91	LYS	Peptide
11	AF	314	TYR	Peptide
11	AF	317	THR	Peptide
11	AF	318	ALA	Peptide
18	AR	166	LYS	Peptide
18	AR	235	TRP	Peptide
21	AV	128	ARG	Peptide
22	AW	71	ILE	Peptide
23	AX	152	LEU	Peptide
24	AY	107	SER	Peptide
24	AY	243	ASP	Peptide
25	Ab	288	GLY	Peptide
33	Ap	94	GLY	Peptide
35	Av	231	ILE	Peptide
41	BB	259	GLU	Peptide
42	BC	301	MET	Peptide
42	BC	400	GLU	Peptide
44	BE	42	GLY	Peptide
46	BG	248	ALA	Peptide
47	BH	229	ALA	Peptide
50	BK	311	GLU	Peptide
50	BK	324	LYS	Peptide
52	BM	134	ALA	Peptide
52	BM	76	TRP	Peptide
53	BN	114	ASP	Peptide
53	BN	36	GLU	Peptide
53	BN	37	ASN	Peptide
54	BO	221	GLY	Peptide
54	BO	232	GLU	Peptide
54	BO	75	PHE	Peptide
55	BP	144	PHE	Peptide
55	BP	59	GLN	Peptide
57	BR	119	GLY	Peptide
57	BR	173	GLY	Peptide
57	BR	174	ALA	Peptide
67	Bb	54	LYS	Peptide
67	Bb	55	GLY	Peptide
67	Bb	70	ASN	Peptide
67	Bb	73	PRO	Peptide

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Mol	Chain	Res	Type	Group
71	Bf	92	HIS	Peptide
73	Bh	60	VAL	Peptide
73	Bh	61	PRO	Peptide
73	Bh	88	LYS	Peptide
77	UD	47	UNK	Peptide
84	UU	7	UNK	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	147/185 (80%)	143 (97%)	4 (3%)	0	100	100
2	A1	215/241 (89%)	209 (97%)	5 (2%)	1 (0%)	29	61
3	A2	445/471 (94%)	432 (97%)	10 (2%)	3 (1%)	22	55
4	A3	148/218 (68%)	143 (97%)	5 (3%)	0	100	100
5	A4	166/183 (91%)	156 (94%)	10 (6%)	0	100	100
6	A5	53/80 (66%)	51 (96%)	2 (4%)	0	100	100
7	A6	70/114 (61%)	70 (100%)	0	0	100	100
8	A8	139/181 (77%)	128 (92%)	11 (8%)	0	100	100
9	A9	51/184 (28%)	49 (96%)	2 (4%)	0	100	100
10	AE	289/473 (61%)	277 (96%)	12 (4%)	0	100	100
11	AF	440/459 (96%)	415 (94%)	24 (6%)	1 (0%)	47	78
12	AI	210/263 (80%)	201 (96%)	7 (3%)	2 (1%)	15	46
13	AJ	124/177 (70%)	116 (94%)	8 (6%)	0	100	100
14	AK	319/342 (93%)	307 (96%)	11 (3%)	1 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AN	177/202 (88%)	169 (96%)	8 (4%)	0	100	100
16	AP	348/374 (93%)	327 (94%)	20 (6%)	1 (0%)	41	72
17	AQ	121/167 (72%)	117 (97%)	4 (3%)	0	100	100
18	AR	225/301 (75%)	211 (94%)	13 (6%)	1 (0%)	34	67
19	AT	33/144 (23%)	33 (100%)	0	0	100	100
20	AU	171/213 (80%)	168 (98%)	3 (2%)	0	100	100
21	AV	178/188 (95%)	174 (98%)	4 (2%)	0	100	100
22	AW	274/278 (99%)	267 (97%)	6 (2%)	1 (0%)	34	67
23	AX	166/246 (68%)	160 (96%)	6 (4%)	0	100	100
24	AY	338/378 (89%)	325 (96%)	9 (3%)	4 (1%)	13	41
25	Ab	449/507 (89%)	425 (95%)	24 (5%)	0	100	100
26	Ad	255/289 (88%)	249 (98%)	6 (2%)	0	100	100
27	Ae	114/197 (58%)	109 (96%)	5 (4%)	0	100	100
28	Af	124/189 (66%)	117 (94%)	7 (6%)	0	100	100
29	Ag	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
30	Aj	277/296 (94%)	259 (94%)	18 (6%)	0	100	100
31	Al	207/218 (95%)	197 (95%)	10 (5%)	0	100	100
32	Ao	179/259 (69%)	169 (94%)	10 (6%)	0	100	100
33	Ap	259/309 (84%)	247 (95%)	11 (4%)	1 (0%)	34	67
34	At	136/154 (88%)	130 (96%)	5 (4%)	1 (1%)	22	55
35	Av	211/242 (87%)	205 (97%)	4 (2%)	2 (1%)	17	49
36	AB	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
37	AC	26/28 (93%)	26 (100%)	0	0	100	100
37	AD	26/28 (93%)	25 (96%)	1 (4%)	0	100	100
38	AG	25/27 (93%)	25 (100%)	0	0	100	100
40	BA	675/831 (81%)	647 (96%)	27 (4%)	1 (0%)	51	82
41	BB	387/541 (72%)	361 (93%)	22 (6%)	4 (1%)	15	46
42	BC	476/523 (91%)	448 (94%)	24 (5%)	4 (1%)	19	51
43	BD	415/547 (76%)	386 (93%)	23 (6%)	6 (1%)	11	37
44	BE	386/449 (86%)	361 (94%)	23 (6%)	2 (0%)	29	61
45	BF	341/426 (80%)	328 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	BG	317/378 (84%)	290 (92%)	27 (8%)	0	100	100
47	BH	209/349 (60%)	202 (97%)	7 (3%)	0	100	100
48	BI	317/343 (92%)	300 (95%)	16 (5%)	1 (0%)	41	72
49	BJ	164/333 (49%)	157 (96%)	7 (4%)	0	100	100
50	BK	252/386 (65%)	241 (96%)	10 (4%)	1 (0%)	34	67
51	BL	226/312 (72%)	220 (97%)	6 (3%)	0	100	100
52	BM	243/283 (86%)	220 (90%)	22 (9%)	1 (0%)	34	67
53	BN	212/302 (70%)	204 (96%)	8 (4%)	0	100	100
54	BO	143/262 (55%)	136 (95%)	6 (4%)	1 (1%)	22	55
55	BP	200/266 (75%)	192 (96%)	6 (3%)	2 (1%)	15	46
56	BQ	214/231 (93%)	201 (94%)	13 (6%)	0	100	100
57	BR	193/205 (94%)	180 (93%)	11 (6%)	2 (1%)	15	46
58	BS	95/198 (48%)	93 (98%)	2 (2%)	0	100	100
59	BT	166/191 (87%)	160 (96%)	6 (4%)	0	100	100
60	BU	80/185 (43%)	79 (99%)	1 (1%)	0	100	100
61	BV	153/190 (80%)	147 (96%)	6 (4%)	0	100	100
62	BW	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
63	BX	103/190 (54%)	94 (91%)	8 (8%)	1 (1%)	15	46
64	BY	100/172 (58%)	90 (90%)	9 (9%)	1 (1%)	15	46
65	BZ	188/190 (99%)	176 (94%)	12 (6%)	0	100	100
66	Ba	137/153 (90%)	130 (95%)	7 (5%)	0	100	100
67	Bb	97/162 (60%)	88 (91%)	9 (9%)	0	100	100
68	Bc	88/146 (60%)	85 (97%)	3 (3%)	0	100	100
69	Bd	138/144 (96%)	132 (96%)	6 (4%)	0	100	100
70	Be	99/113 (88%)	97 (98%)	2 (2%)	0	100	100
71	Bf	46/113 (41%)	41 (89%)	4 (9%)	1 (2%)	6	29
72	Bg	80/105 (76%)	72 (90%)	8 (10%)	0	100	100
73	Bh	89/92 (97%)	84 (94%)	3 (3%)	2 (2%)	6	29
All	All	14660/18620 (79%)	13953 (95%)	658 (4%)	49 (0%)	44	72

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	AW	72	THR
35	Av	232	LYS
41	BB	294	PRO
43	BD	356	PRO
43	BD	389	VAL
3	A2	270	ASN
3	A2	293	PHE
18	AR	141	ALA
24	AY	244	ARG
33	Ap	95	ARG
44	BE	384	HIS
50	BK	268	PRO
54	BO	76	GLY
71	Bf	101	TYR
24	AY	98	LYS
24	AY	108	PRO
34	At	73	ARG
40	BA	310	ALA
42	BC	268	LEU
42	BC	344	PHE
42	BC	513	GLY
48	BI	216	MET
52	BM	76	TRP
57	BR	172	PRO
63	BX	88	ALA
12	AI	19	ASP
12	AI	71	TYR
16	AP	359	HIS
43	BD	162	PRO
44	BE	348	VAL
55	BP	145	PRO
64	BY	162	ARG
73	Bh	61	PRO
2	A1	116	HIS
35	Av	68	ARG
41	BB	318	PRO
41	BB	338	ALA
43	BD	153	PRO
57	BR	120	PHE
3	A2	212	ALA
11	AF	36	ALA
24	AY	107	SER
43	BD	449	PHE

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Mol	Chain	Res	Type
55	BP	146	ALA
73	Bh	37	GLN
43	BD	139	MET
14	AK	17	VAL
41	BB	429	VAL
42	BC	339	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	140/167 (84%)	136 (97%)	4 (3%)	42	69
2	A1	195/217 (90%)	184 (94%)	11 (6%)	21	51
3	A2	394/413 (95%)	380 (96%)	14 (4%)	35	63
4	A3	131/193 (68%)	125 (95%)	6 (5%)	27	57
5	A4	153/164 (93%)	149 (97%)	4 (3%)	46	72
6	A5	52/73 (71%)	47 (90%)	5 (10%)	8	29
7	A6	61/99 (62%)	54 (88%)	7 (12%)	5	20
8	A8	126/161 (78%)	122 (97%)	4 (3%)	39	67
9	A9	51/166 (31%)	44 (86%)	7 (14%)	3	14
10	AE	258/406 (64%)	247 (96%)	11 (4%)	29	59
11	AF	394/409 (96%)	375 (95%)	19 (5%)	25	56
12	AI	192/233 (82%)	184 (96%)	8 (4%)	30	59
13	AJ	90/151 (60%)	86 (96%)	4 (4%)	28	58
14	AK	287/301 (95%)	270 (94%)	17 (6%)	19	49
15	AN	160/182 (88%)	155 (97%)	5 (3%)	40	68
16	AP	310/330 (94%)	295 (95%)	15 (5%)	25	56
17	AQ	106/141 (75%)	102 (96%)	4 (4%)	33	61
18	AR	198/256 (77%)	195 (98%)	3 (2%)	65	82
19	AT	28/124 (23%)	25 (89%)	3 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AU	151/184 (82%)	143 (95%)	8 (5%)	22	52
21	AV	153/158 (97%)	151 (99%)	2 (1%)	69	84
22	AW	244/246 (99%)	234 (96%)	10 (4%)	30	59
23	AX	156/221 (71%)	154 (99%)	2 (1%)	69	84
24	AY	283/337 (84%)	268 (95%)	15 (5%)	22	52
25	Ab	373/451 (83%)	368 (99%)	5 (1%)	69	84
26	Ad	225/250 (90%)	218 (97%)	7 (3%)	40	68
27	Ae	100/172 (58%)	93 (93%)	7 (7%)	15	44
28	Af	111/162 (68%)	103 (93%)	8 (7%)	14	43
29	Ag	238/239 (100%)	231 (97%)	7 (3%)	42	69
30	Aj	237/260 (91%)	230 (97%)	7 (3%)	41	68
31	Al	170/186 (91%)	167 (98%)	3 (2%)	59	79
32	Ao	153/216 (71%)	144 (94%)	9 (6%)	19	49
33	Ap	227/267 (85%)	217 (96%)	10 (4%)	28	58
34	At	116/140 (83%)	114 (98%)	2 (2%)	60	80
35	Av	187/210 (89%)	176 (94%)	11 (6%)	19	49
40	BA	598/727 (82%)	572 (96%)	26 (4%)	29	59
41	BB	271/470 (58%)	240 (89%)	31 (11%)	5	21
42	BC	406/443 (92%)	396 (98%)	10 (2%)	47	72
44	BE	334/386 (86%)	321 (96%)	13 (4%)	32	61
45	BF	299/368 (81%)	289 (97%)	10 (3%)	38	66
46	BG	266/310 (86%)	247 (93%)	19 (7%)	14	44
47	BH	182/297 (61%)	164 (90%)	18 (10%)	8	27
48	BI	268/288 (93%)	255 (95%)	13 (5%)	25	55
49	BJ	136/298 (46%)	128 (94%)	8 (6%)	19	49
50	BK	196/331 (59%)	184 (94%)	12 (6%)	18	48
51	BL	201/262 (77%)	192 (96%)	9 (4%)	27	58
52	BM	209/240 (87%)	197 (94%)	12 (6%)	20	50
53	BN	167/265 (63%)	158 (95%)	9 (5%)	22	52
54	BO	129/225 (57%)	122 (95%)	7 (5%)	22	52
55	BP	162/219 (74%)	155 (96%)	7 (4%)	29	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BQ	182/195 (93%)	175 (96%)	7 (4%)	33	61
57	BR	171/181 (94%)	166 (97%)	5 (3%)	42	69
58	BS	85/164 (52%)	81 (95%)	4 (5%)	26	57
59	BT	147/163 (90%)	140 (95%)	7 (5%)	25	56
60	BU	71/168 (42%)	69 (97%)	2 (3%)	43	70
61	BV	138/163 (85%)	130 (94%)	8 (6%)	20	50
62	BW	163/164 (99%)	158 (97%)	5 (3%)	40	68
63	BX	92/170 (54%)	80 (87%)	12 (13%)	4	16
64	BY	89/151 (59%)	87 (98%)	2 (2%)	52	75
65	BZ	143/160 (89%)	142 (99%)	1 (1%)	84	92
66	Ba	131/144 (91%)	129 (98%)	2 (2%)	65	82
67	Bb	84/135 (62%)	81 (96%)	3 (4%)	35	63
68	Bc	82/134 (61%)	76 (93%)	6 (7%)	14	43
69	Bd	117/120 (98%)	112 (96%)	5 (4%)	29	59
70	Be	89/99 (90%)	85 (96%)	4 (4%)	27	58
71	Bf	45/98 (46%)	44 (98%)	1 (2%)	52	75
72	Bg	65/87 (75%)	60 (92%)	5 (8%)	13	40
73	Bh	79/80 (99%)	74 (94%)	5 (6%)	18	47
All	All	12247/15590 (79%)	11695 (96%)	552 (4%)	31	58

All (552) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	43	PHE
1	A0	116	LEU
1	A0	143	LEU
1	A0	166	ASN
2	A1	28	ARG
2	A1	63	ARG
2	A1	75	VAL
2	A1	97	ARG
2	A1	104	VAL
2	A1	114	LEU
2	A1	133	ASP
2	A1	178	GLN
2	A1	188	ILE

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Mol	Chain	Res	Type
2	A1	192	GLU
2	A1	223	LYS
3	A2	17	VAL
3	A2	22	LEU
3	A2	44	LEU
3	A2	72	GLN
3	A2	89	GLU
3	A2	94	ILE
3	A2	255	ARG
3	A2	270	ASN
3	A2	295	ASN
3	A2	296	VAL
3	A2	338	GLN
3	A2	350	VAL
3	A2	384	LEU
3	A2	470	ASP
4	A3	104	GLN
4	A3	140	ASP
4	A3	151	ARG
4	A3	152	VAL
4	A3	171	ARG
4	A3	181	ASP
5	A4	31	ARG
5	A4	61	ARG
5	A4	128	LYS
5	A4	153	TYR
6	A5	34	GLN
6	A5	49	LEU
6	A5	62	GLU
6	A5	70	CYS
6	A5	76	ARG
7	A6	41	ARG
7	A6	86	LYS
7	A6	87	ILE
7	A6	88	LYS
7	A6	94	LYS
7	A6	99	LYS
7	A6	105	ILE
8	A8	83	ARG
8	A8	96	ARG
8	A8	116	GLN
8	A8	175	ASP

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Mol	Chain	Res	Type
9	A9	60	GLN
9	A9	61	MET
9	A9	63	MET
9	A9	82	ASP
9	A9	99	MET
9	A9	109	LYS
9	A9	110	GLN
10	AE	43	ARG
10	AE	59	CYS
10	AE	73	LEU
10	AE	175	THR
10	AE	190	MET
10	AE	195	GLU
10	AE	215	VAL
10	AE	236	ARG
10	AE	338	ARG
10	AE	345	THR
10	AE	370	ASP
11	AF	26	ASP
11	AF	35	ILE
11	AF	72	ILE
11	AF	105	THR
11	AF	154	ARG
11	AF	165	GLU
11	AF	166	THR
11	AF	182	MET
11	AF	216	VAL
11	AF	217	LYS
11	AF	248	THR
11	AF	257	ARG
11	AF	259	MET
11	AF	280	THR
11	AF	296	ASN
11	AF	368	LEU
11	AF	376	ARG
11	AF	388	GLU
11	AF	394	VAL
12	AI	20	ILE
12	AI	32	VAL
12	AI	48	ARG
12	AI	100	LEU
12	AI	126	LYS

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Mol	Chain	Res	Type
12	AI	158	THR
12	AI	181	THR
12	AI	183	ARG
13	AJ	14	ARG
13	AJ	27	ARG
13	AJ	46	LYS
13	AJ	98	THR
14	AK	16	THR
14	AK	19	VAL
14	AK	24	ASN
14	AK	90	THR
14	AK	172	LEU
14	AK	174	GLU
14	AK	207	GLU
14	AK	208	GLN
14	AK	209	GLN
14	AK	216	ARG
14	AK	218	ARG
14	AK	219	ARG
14	AK	230	GLN
14	AK	231	ARG
14	AK	314	ARG
14	AK	321	ARG
14	AK	326	GLU
15	AN	31	ASP
15	AN	43	ARG
15	AN	54	LEU
15	AN	143	VAL
15	AN	148	THR
16	AP	25	MET
16	AP	34	LEU
16	AP	45	ARG
16	AP	46	ASN
16	AP	73	ARG
16	AP	111	ASN
16	AP	133	ARG
16	AP	163	ARG
16	AP	209	ARG
16	AP	225	ARG
16	AP	283	ARG
16	AP	315	ARG
16	AP	322	LYS

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Mol	Chain	Res	Type
16	AP	373	ARG
16	AP	374	LEU
17	AQ	26	ARG
17	AQ	30	ARG
17	AQ	33	ASP
17	AQ	44	ILE
18	AR	121	ASP
18	AR	186	PHE
18	AR	196	GLU
19	AT	21	PHE
19	AT	24	LEU
19	AT	35	MET
20	AU	15	LEU
20	AU	50	ARG
20	AU	82	ASN
20	AU	136	LEU
20	AU	173	ARG
20	AU	189	ASN
20	AU	194	LEU
20	AU	195	ILE
21	AV	147	ARG
21	AV	203	GLN
22	AW	14	LEU
22	AW	33	ARG
22	AW	55	THR
22	AW	75	GLN
22	AW	76	LEU
22	AW	82	TRP
22	AW	84	ARG
22	AW	112	LEU
22	AW	198	VAL
22	AW	273	ILE
23	AX	62	HIS
23	AX	63	LYS
24	AY	1	MET
24	AY	6	ARG
24	AY	36	ARG
24	AY	58	LEU
24	AY	68	ARG
24	AY	96	ARG
24	AY	190	MET
24	AY	202	GLU

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Mol	Chain	Res	Type
24	AY	205	ARG
24	AY	224	GLU
24	AY	225	VAL
24	AY	256	LEU
24	AY	278	ARG
24	AY	287	GLN
24	AY	299	MET
25	Ab	74	ASP
25	Ab	105	ASN
25	Ab	355	VAL
25	Ab	385	ILE
25	Ab	455	ARG
26	Ad	67	MET
26	Ad	80	LYS
26	Ad	100	ILE
26	Ad	153	GLU
26	Ad	173	SER
26	Ad	192	GLU
26	Ad	243	ARG
27	Ae	75	ARG
27	Ae	80	LEU
27	Ae	87	VAL
27	Ae	98	VAL
27	Ae	148	ILE
27	Ae	153	PHE
27	Ae	154	ARG
28	Af	60	GLN
28	Af	65	LEU
28	Af	72	ASP
28	Af	125	THR
28	Af	127	MET
28	Af	135	ILE
28	Af	162	ARG
28	Af	169	ARG
29	Ag	33	LEU
29	Ag	91	ASN
29	Ag	117	LEU
29	Ag	134	ARG
29	Ag	168	CYS
29	Ag	175	ARG
29	Ag	224	VAL
30	Aj	53	ARG

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Mol	Chain	Res	Type
30	Aj	77	GLN
30	Aj	78	ARG
30	Aj	168	ARG
30	Aj	179	ARG
30	Aj	205	ARG
30	Aj	210	ASP
31	Al	15	THR
31	Al	23	ARG
31	Al	191	VAL
32	Ao	25	ASN
32	Ao	54	GLN
32	Ao	57	MET
32	Ao	158	ARG
32	Ao	163	ARG
32	Ao	226	ARG
32	Ao	243	LYS
32	Ao	244	PHE
32	Ao	246	VAL
33	Ap	52	ARG
33	Ap	56	ASN
33	Ap	62	LYS
33	Ap	74	ARG
33	Ap	123	LYS
33	Ap	234	VAL
33	Ap	278	ASN
33	Ap	280	LEU
33	Ap	284	ASP
33	Ap	285	TYR
34	At	44	LEU
34	At	143	THR
35	Av	47	ARG
35	Av	99	ARG
35	Av	146	THR
35	Av	167	ARG
35	Av	198	LYS
35	Av	207	ARG
35	Av	210	LEU
35	Av	213	ARG
35	Av	227	LYS
35	Av	233	THR
35	Av	237	LYS
40	BA	129	PHE

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Mol	Chain	Res	Type
40	BA	133	THR
40	BA	151	ASP
40	BA	190	THR
40	BA	254	ARG
40	BA	266	LEU
40	BA	326	LEU
40	BA	328	VAL
40	BA	336	THR
40	BA	340	LEU
40	BA	344	GLU
40	BA	396	ARG
40	BA	401	THR
40	BA	412	LEU
40	BA	419	THR
40	BA	495	ARG
40	BA	526	ARG
40	BA	567	THR
40	BA	569	LEU
40	BA	589	MET
40	BA	593	THR
40	BA	699	ASN
40	BA	714	ASN
40	BA	767	ARG
40	BA	799	ASP
40	BA	809	ASP
41	BB	66	GLU
41	BB	75	MET
41	BB	94	THR
41	BB	100	GLU
41	BB	105	LEU
41	BB	132	GLU
41	BB	136	TRP
41	BB	138	CYS
41	BB	152	ARG
41	BB	169	SER
41	BB	174	ASP
41	BB	180	GLU
41	BB	188	LEU
41	BB	206	ASP
41	BB	213	LEU
41	BB	215	ARG
41	BB	230	THR

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Mol	Chain	Res	Type
41	BB	234	ILE
41	BB	240	HIS
41	BB	244	LYS
41	BB	251	ILE
41	BB	256	ARG
41	BB	259	GLU
41	BB	344	CYS
41	BB	356	ASN
41	BB	357	THR
41	BB	360	ASP
41	BB	379	ARG
41	BB	390	LEU
41	BB	395	GLU
41	BB	413	LEU
42	BC	116	ARG
42	BC	230	MET
42	BC	268	LEU
42	BC	362	VAL
42	BC	413	LYS
42	BC	427	LEU
42	BC	490	LEU
42	BC	494	LEU
42	BC	501	CYS
42	BC	522	LEU
44	BE	28	LEU
44	BE	29	ASN
44	BE	32	LEU
44	BE	61	MET
44	BE	88	ARG
44	BE	128	ILE
44	BE	144	VAL
44	BE	190	ARG
44	BE	335	LYS
44	BE	354	GLU
44	BE	358	ASN
44	BE	359	LYS
44	BE	442	THR
45	BF	50	LEU
45	BF	128	LYS
45	BF	131	LEU
45	BF	181	THR
45	BF	183	ARG

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Mol	Chain	Res	Type
45	BF	237	LEU
45	BF	345	LEU
45	BF	360	THR
45	BF	398	ARG
45	BF	420	ARG
46	BG	50	ARG
46	BG	56	ARG
46	BG	65	MET
46	BG	74	ARG
46	BG	102	GLN
46	BG	106	ASP
46	BG	162	SER
46	BG	164	GLN
46	BG	165	GLU
46	BG	176	LEU
46	BG	177	ASP
46	BG	178	THR
46	BG	180	LEU
46	BG	181	VAL
46	BG	183	ARG
46	BG	189	MET
46	BG	295	ARG
46	BG	339	GLU
46	BG	350	LEU
47	BH	74	ARG
47	BH	113	LEU
47	BH	119	VAL
47	BH	135	ARG
47	BH	146	GLU
47	BH	149	ARG
47	BH	156	LEU
47	BH	168	THR
47	BH	172	MET
47	BH	174	LEU
47	BH	178	GLU
47	BH	192	LYS
47	BH	236	ARG
47	BH	253	GLN
47	BH	254	TRP
47	BH	255	PHE
47	BH	257	ASP
47	BH	258	THR

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Mol	Chain	Res	Type
48	BI	60	GLN
48	BI	63	LEU
48	BI	71	LYS
48	BI	84	LEU
48	BI	139	ARG
48	BI	140	PHE
48	BI	144	HIS
48	BI	245	ASN
48	BI	254	ARG
48	BI	276	ILE
48	BI	299	ARG
48	BI	319	ARG
48	BI	338	CYS
49	BJ	223	THR
49	BJ	234	THR
49	BJ	250	LEU
49	BJ	261	ARG
49	BJ	270	ARG
49	BJ	288	LYS
49	BJ	292	ARG
49	BJ	307	ARG
50	BK	98	THR
50	BK	140	LEU
50	BK	150	ASP
50	BK	193	VAL
50	BK	194	ARG
50	BK	224	MET
50	BK	285	GLN
50	BK	300	TRP
50	BK	302	VAL
50	BK	328	LEU
50	BK	340	ARG
50	BK	379	LEU
51	BL	53	ARG
51	BL	103	ASN
51	BL	122	LYS
51	BL	123	LEU
51	BL	125	GLU
51	BL	141	ASN
51	BL	180	LEU
51	BL	256	ARG
51	BL	291	LEU

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Mol	Chain	Res	Type
52	BM	74	ARG
52	BM	113	ASN
52	BM	141	THR
52	BM	148	LYS
52	BM	160	ARG
52	BM	163	LEU
52	BM	178	GLU
52	BM	184	MET
52	BM	223	THR
52	BM	236	ARG
52	BM	237	THR
52	BM	241	MET
53	BN	22	ARG
53	BN	36	GLU
53	BN	60	ARG
53	BN	71	GLN
53	BN	177	ARG
53	BN	180	GLU
53	BN	182	GLU
53	BN	199	ASP
53	BN	219	ARG
54	BO	135	LEU
54	BO	139	LEU
54	BO	142	GLU
54	BO	144	GLN
54	BO	169	MET
54	BO	193	ARG
54	BO	219	ARG
55	BP	36	ARG
55	BP	39	LEU
55	BP	121	ARG
55	BP	152	ASN
55	BP	176	THR
55	BP	205	TYR
55	BP	214	ASN
56	BQ	101	ASP
56	BQ	115	ASP
56	BQ	116	GLU
56	BQ	119	GLU
56	BQ	121	LYS
56	BQ	215	LEU
56	BQ	227	LEU

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Mol	Chain	Res	Type
57	BR	19	TYR
57	BR	41	LEU
57	BR	48	ARG
57	BR	160	GLN
57	BR	175	GLU
58	BS	26	ARG
58	BS	29	ASN
58	BS	30	GLU
58	BS	32	ARG
59	BT	14	LYS
59	BT	17	LYS
59	BT	33	ASN
59	BT	72	LEU
59	BT	105	VAL
59	BT	152	ASN
59	BT	174	ILE
60	BU	116	ARG
60	BU	117	ILE
61	BV	43	ARG
61	BV	52	PHE
61	BV	54	GLN
61	BV	59	ARG
61	BV	60	MET
61	BV	148	MET
61	BV	154	ARG
61	BV	161	LYS
62	BW	11	ARG
62	BW	50	ARG
62	BW	75	ARG
62	BW	91	SER
62	BW	175	THR
63	BX	64	ASN
63	BX	67	VAL
63	BX	68	ASP
63	BX	71	MET
63	BX	72	VAL
63	BX	120	ASN
63	BX	149	VAL
63	BX	155	ARG
63	BX	165	ARG
63	BX	170	LEU
63	BX	171	THR

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Mol	Chain	Res	Type
63	BX	173	HIS
64	BY	79(C)	LYS
64	BY	150	GLN
65	BZ	76	ARG
66	Ba	25	GLN
66	Ba	37	ARG
67	Bb	47	ARG
67	Bb	53	ARG
67	Bb	120	ARG
68	Bc	21	LEU
68	Bc	29	ARG
68	Bc	32	ARG
68	Bc	37	ARG
68	Bc	54	ASN
68	Bc	82	GLU
69	Bd	52	ARG
69	Bd	54	MET
69	Bd	57	LEU
69	Bd	58	LEU
69	Bd	102	LEU
70	Be	49	ARG
70	Be	54	LEU
70	Be	63	CYS
70	Be	71	SER
71	Bf	79	GLU
72	Bg	27	ASN
72	Bg	35	LEU
72	Bg	50	ASN
72	Bg	100	ARG
72	Bg	104	THR
73	Bh	6	CYS
73	Bh	53	MET
73	Bh	56	LYS
73	Bh	71	ARG
73	Bh	88	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (237) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	108	GLN
1	A0	166	ASN
2	A1	16	ASN

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Mol	Chain	Res	Type
2	A1	62	GLN
2	A1	138	ASN
3	A2	59	ASN
3	A2	72	GLN
3	A2	167	HIS
3	A2	194	GLN
3	A2	270	ASN
3	A2	314	HIS
3	A2	389	HIS
4	A3	82	ASN
4	A3	104	GLN
4	A3	144	GLN
5	A4	56	GLN
7	A6	77	GLN
8	A8	68	GLN
10	AE	191	ASN
10	AE	214	HIS
10	AE	354	HIS
11	AF	64	HIS
11	AF	83	HIS
11	AF	192	ASN
11	AF	193	HIS
11	AF	223	ASN
11	AF	265	HIS
11	AF	296	ASN
11	AF	331	ASN
11	AF	346	HIS
11	AF	377	ASN
12	AI	18	HIS
12	AI	76	HIS
12	AI	96	ASN
12	AI	120	ASN
13	AJ	81	ASN
14	AK	24	ASN
14	AK	144	HIS
14	AK	230	GLN
14	AK	246	ASN
15	AN	19	HIS
15	AN	21	HIS
15	AN	30	ASN
15	AN	68	GLN
15	AN	82	HIS

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Mol	Chain	Res	Type
15	AN	141	HIS
15	AN	164	HIS
15	AN	166	HIS
16	AP	81	HIS
16	AP	84	GLN
16	AP	89	GLN
16	AP	111	ASN
16	AP	199	HIS
16	AP	259	HIS
16	AP	310	HIS
16	AP	346	HIS
16	AP	348	ASN
16	AP	349	GLN
16	AP	362	ASN
17	AQ	47	GLN
17	AQ	164	HIS
18	AR	65	HIS
18	AR	223	HIS
18	AR	229	HIS
18	AR	242	HIS
20	AU	46	GLN
20	AU	73	HIS
21	AV	75	ASN
21	AV	87	HIS
21	AV	100	GLN
21	AV	206	ASN
22	AW	12	HIS
22	AW	40	HIS
22	AW	172	HIS
22	AW	183	GLN
23	AX	62	HIS
23	AX	126	HIS
24	AY	64	HIS
24	AY	89	GLN
24	AY	168	HIS
24	AY	177	HIS
25	Ab	105	ASN
25	Ab	122	HIS
25	Ab	205	HIS
25	Ab	351	GLN
25	Ab	419	GLN
25	Ab	471	ASN

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Mol	Chain	Res	Type
26	Ad	151	GLN
26	Ad	188	GLN
26	Ad	284	HIS
27	Ae	48	ASN
28	Af	86	ASN
28	Af	101	HIS
28	Af	104	HIS
28	Af	156	HIS
28	Af	164	HIS
28	Af	168	GLN
29	Ag	27	GLN
29	Ag	84	ASN
29	Ag	91	ASN
29	Ag	101	HIS
29	Ag	170	GLN
29	Ag	204	HIS
29	Ag	244	HIS
30	Aj	22	GLN
30	Aj	37	GLN
30	Aj	90	HIS
30	Aj	225	GLN
32	Ao	25	ASN
32	Ao	54	GLN
32	Ao	113	GLN
33	Ap	37	ASN
33	Ap	55	HIS
33	Ap	79	GLN
33	Ap	83	HIS
33	Ap	197	GLN
33	Ap	278	ASN
34	At	20	HIS
34	At	147	HIS
34	At	148	GLN
35	Av	34	GLN
35	Av	118	ASN
40	BA	301	HIS
40	BA	380	ASN
40	BA	484	HIS
40	BA	490	ASN
40	BA	502	HIS
40	BA	531	GLN
40	BA	539	ASN

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Mol	Chain	Res	Type
40	BA	693	HIS
40	BA	699	ASN
40	BA	714	ASN
40	BA	734	HIS
40	BA	781	HIS
41	BB	82	HIS
41	BB	162	GLN
41	BB	170	GLN
41	BB	218	HIS
41	BB	240	HIS
41	BB	242	GLN
41	BB	356	ASN
41	BB	359	HIS
41	BB	420	ASN
42	BC	62	GLN
42	BC	71	GLN
42	BC	86	GLN
42	BC	108	GLN
42	BC	115	GLN
42	BC	131	GLN
42	BC	165	HIS
42	BC	207	GLN
42	BC	282	HIS
42	BC	289	ASN
42	BC	292	ASN
42	BC	340	HIS
44	BE	23	GLN
44	BE	25	HIS
44	BE	29	ASN
44	BE	78	HIS
44	BE	125	GLN
44	BE	270	HIS
44	BE	350	ASN
44	BE	361	GLN
45	BF	250	HIS
45	BF	298	ASN
45	BF	332	HIS
45	BF	387	ASN
46	BG	35	GLN
46	BG	115	HIS
46	BG	287	HIS
46	BG	305	HIS

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Mol	Chain	Res	Type
46	BG	340	GLN
47	BH	99	GLN
47	BH	102	ASN
47	BH	122	HIS
47	BH	134	GLN
47	BH	239	ASN
47	BH	246	GLN
48	BI	45	HIS
48	BI	60	GLN
48	BI	106	HIS
48	BI	144	HIS
48	BI	148	ASN
48	BI	223	GLN
48	BI	263	HIS
49	BJ	333	ASN
50	BK	108	GLN
50	BK	200	ASN
50	BK	212	GLN
50	BK	227	GLN
50	BK	285	GLN
51	BL	83	HIS
51	BL	99	HIS
51	BL	103	ASN
51	BL	141	ASN
51	BL	226	HIS
52	BM	88	GLN
52	BM	89	HIS
52	BM	113	ASN
53	BN	28	ASN
54	BO	101	GLN
54	BO	131	HIS
55	BP	152	ASN
55	BP	213	HIS
55	BP	214	ASN
56	BQ	147	ASN
57	BR	16	GLN
57	BR	96	GLN
57	BR	164	HIS
59	BT	46	GLN
59	BT	51	HIS
60	BU	156	GLN
61	BV	31	GLN

Continued on next page...

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Mol	Chain	Res	Type
61	BV	74	ASN
62	BW	46	HIS
62	BW	61	ASN
62	BW	65	ASN
62	BW	100	GLN
62	BW	149	ASN
64	BY	79(B)	HIS
64	BY	79(H)	HIS
64	BY	80	GLN
64	BY	150	GLN
65	BZ	96	GLN
65	BZ	155	GLN
67	Bb	128	GLN
68	Bc	66	HIS
68	Bc	97	GLN
69	Bd	49	ASN
69	Bd	67	HIS
69	Bd	97	GLN
69	Bd	123	ASN
70	Be	72	HIS
71	Bf	92	HIS
71	Bf	104	ASN
72	Bg	27	ASN
73	Bh	37	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	AA	581/1178 (49%)	289 (49%)	19 (3%)

All (289) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
39	AA	2	U
39	AA	4	U
39	AA	5	U
39	AA	10	A
39	AA	11	U
39	AA	12	U
39	AA	13	A
39	AA	16	A

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Mol	Chain	Res	Type
39	AA	17	A
39	AA	18	G
39	AA	20	A
39	AA	21	U
39	AA	28	A
39	AA	29	U
39	AA	32	U
39	AA	34	G
39	AA	38	U
39	AA	40	U
39	AA	41	U
39	AA	42	A
39	AA	43	U
39	AA	44	A
39	AA	46	U
39	AA	47	U
39	AA	50	A
39	AA	53	A
39	AA	54	A
39	AA	57	A
39	AA	58	U
39	AA	59	U
39	AA	60	U
39	AA	64	U
39	AA	65	U
39	AA	68	G
39	AA	69	U
39	AA	70	G
39	AA	71	U
39	AA	72	A
39	AA	73	G
39	AA	74	U
39	AA	75	A
39	AA	77	A
39	AA	79	U
39	AA	80	U
39	AA	81	A
39	AA	82	U
39	AA	83	U
39	AA	84	A
39	AA	85	U
39	AA	86	U

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Mol	Chain	Res	Type
39	AA	87	U
39	AA	88	G
39	AA	89	U
39	AA	93	A
39	AA	98	U
39	AA	101	A
39	AA	103	U
39	AA	104	A
39	AA	105	G
39	AA	106	G
39	AA	111	U
39	AA	112	U
39	AA	113	A
39	AA	114	U
39	AA	115	A
39	AA	119	A
39	AA	120	A
39	AA	124	U
39	AA	125	U
39	AA	126	A
39	AA	130	U
39	AA	131	U
39	AA	133	U
39	AA	134	U
39	AA	135	G
39	AA	136	U
39	AA	137	U
39	AA	146	A
39	AA	147	G
39	AA	149	U
39	AA	150	A
39	AA	152	A
39	AA	154	A
39	AA	158	A
39	AA	159	U
39	AA	162	A
39	AA	164	U
39	AA	168	A
39	AA	170	A
39	AA	171	U
39	AA	172	U
39	AA	174	A

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Mol	Chain	Res	Type
39	AA	176	A
39	AA	177	U
39	AA	178	A
39	AA	179	A
39	AA	180	U
39	AA	183	U
39	AA	186	A
39	AA	187	A
39	AA	189	A
39	AA	282	A
39	AA	283	A
39	AA	284	U
39	AA	285	A
39	AA	288	G
39	AA	289	U
39	AA	290	A
39	AA	296	A
39	AA	297	U
39	AA	299	U
39	AA	301	A
39	AA	327	U
39	AA	328	U
39	AA	331	C
39	AA	336	U
39	AA	344	A
39	AA	370	U
39	AA	371	A
39	AA	375	A
39	AA	378	A
39	AA	379	U
39	AA	380	G
39	AA	381	U
39	AA	383	A
39	AA	384	U
39	AA	385	A
39	AA	387	A
39	AA	388	U
39	AA	393	A
39	AA	394	U
39	AA	404	U
39	AA	411	A
39	AA	418	G

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Mol	Chain	Res	Type
39	AA	419	U
39	AA	421	C
39	AA	423	A
39	AA	425	U
39	AA	426	A
39	AA	427	U
39	AA	428	A
39	AA	438	U
39	AA	440	U
39	AA	441	A
39	AA	443	A
39	AA	446	A
39	AA	447	U
39	AA	448	A
39	AA	455	U
39	AA	456	U
39	AA	457	A
39	AA	458	U
39	AA	460	U
39	AA	461	U
39	AA	462	U
39	AA	463	U
39	AA	468	A
39	AA	469	G
39	AA	470	G
39	AA	472	A
39	AA	473	A
39	AA	474	A
39	AA	475	U
39	AA	476	G
39	AA	477	A
39	AA	479	A
39	AA	481	G
39	AA	483	A
39	AA	484	U
39	AA	485	A
39	AA	486	A
39	AA	487	A
39	AA	488	U
39	AA	489	G
39	AA	490	G
39	AA	491	A

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Mol	Chain	Res	Type
39	AA	492	U
39	AA	493	A
39	AA	494	U
39	AA	495	A
39	AA	496	A
39	AA	498	U
39	AA	500	A
39	AA	503	A
39	AA	504	U
39	AA	507	A
39	AA	509	U
39	AA	513	U
39	AA	514	G
39	AA	515	U
39	AA	516	U
39	AA	518	A
39	AA	519	A
39	AA	520	U
39	AA	524	A
39	AA	525	A
39	AA	526	G
39	AA	527	U
39	AA	529	U
39	AA	530	U
39	AA	531	U
39	AA	532	U
39	AA	533	A
39	AA	535	U
39	AA	536	A
39	AA	537	U
39	AA	538	U
39	AA	540	U
39	AA	544	G
39	AA	545	U
39	AA	546	A
39	AA	548	A
39	AA	549	G
39	AA	551	A
39	AA	554	A
39	AA	555	U
39	AA	556	U
39	AA	557	A

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Mol	Chain	Res	Type
39	AA	558	U
39	AA	559	A
39	AA	560	G
39	AA	562	G
39	AA	563	U
39	AA	564	A
39	AA	565	U
39	AA	566	A
39	AA	567	G
39	AA	568	U
39	AA	570	U
39	AA	571	U
39	AA	572	U
39	AA	573	U
39	AA	574	A
39	AA	575	A
39	AA	795	A
39	AA	801	A
39	AA	802	G
39	AA	803	U
39	AA	815	U
39	AA	818	A
39	AA	819	A
39	AA	825	A
39	AA	826	A
39	AA	827	U
39	AA	828	A
39	AA	830	A
39	AA	836	A
39	AA	837	A
39	AA	838	A
39	AA	844	A
39	AA	845	A
39	AA	883	U
39	AA	884	A
39	AA	885	U
39	AA	886	G
39	AA	887	A
39	AA	892	U
39	AA	893	A
39	AA	948	A
39	AA	949	U

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Mol	Chain	Res	Type
39	AA	950	U
39	AA	951	C
39	AA	952	U
39	AA	953	U
39	AA	954	U
39	AA	955	G
39	AA	1100	U
39	AA	1106	U
39	AA	1107	U
39	AA	1110	A
39	AA	1111	A
39	AA	1112	U
39	AA	1113	U
39	AA	1157	A
39	AA	1158	G
39	AA	1159	A
39	AA	1160	A
39	AA	1163	A
39	AA	1164	A
39	AA	1165	G
39	AA	1166	A
39	AA	1168	U
39	AA	1169	A
39	AA	1170	U
39	AA	1171	A
39	AA	1172	A
39	AA	1173	U
39	AA	1174	U
39	AA	1175	U

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	AA	40	U
39	AA	69	U
39	AA	86	U
39	AA	125	U
39	AA	171	U
39	AA	335	G
39	AA	379	U
39	AA	384	U
39	AA	387	A

Continued on next page...

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Mol	Chain	Res	Type
39	AA	392	A
39	AA	418	G
39	AA	422	A
39	AA	425	U
39	AA	440	U
39	AA	485	A
39	AA	528	A
39	AA	534	U
39	AA	951	C
39	AA	1164	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 13 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
88	NAD	Av	301	-	42,48,48	1.98	9 (21%)	50,73,73	1.82	10 (20%)

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
88	NAD	Av	301	-	-	3/26/62/62	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	Av	301	NAD	C3N-C7N	-7.74	1.38	1.50
88	Av	301	NAD	C2A-N3A	4.51	1.39	1.32
88	Av	301	NAD	C2N-N1N	3.87	1.39	1.35
88	Av	301	NAD	C2A-N1A	3.03	1.39	1.33
88	Av	301	NAD	C5A-C4A	-2.84	1.33	1.40
88	Av	301	NAD	C6A-C5A	-2.80	1.32	1.43
88	Av	301	NAD	O4B-C1B	2.61	1.44	1.41
88	Av	301	NAD	C2D-C1D	-2.50	1.50	1.53
88	Av	301	NAD	C2B-C1B	-2.38	1.50	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	Av	301	NAD	N3A-C2A-N1A	-6.69	118.23	128.68
88	Av	301	NAD	O4D-C1D-C2D	-4.68	100.08	106.93
88	Av	301	NAD	PN-O3-PA	-4.30	118.06	132.83
88	Av	301	NAD	C3D-C2D-C1D	-3.90	95.10	100.98
88	Av	301	NAD	C2B-C3B-C4B	-3.19	96.45	102.64
88	Av	301	NAD	C5A-C6A-N6A	-2.83	116.05	120.35
88	Av	301	NAD	C3B-C2B-C1B	-2.18	97.69	100.98
88	Av	301	NAD	C3N-C7N-N7N	-2.12	115.21	117.75
88	Av	301	NAD	O4B-C1B-C2B	-2.11	103.84	106.93
88	Av	301	NAD	C2D-C3D-C4D	-2.04	98.67	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	Av	301	NAD	O4D-C4D-C5D-O5D
88	Av	301	NAD	C3D-C4D-C5D-O5D
88	Av	301	NAD	O4B-C4B-C5B-O5B

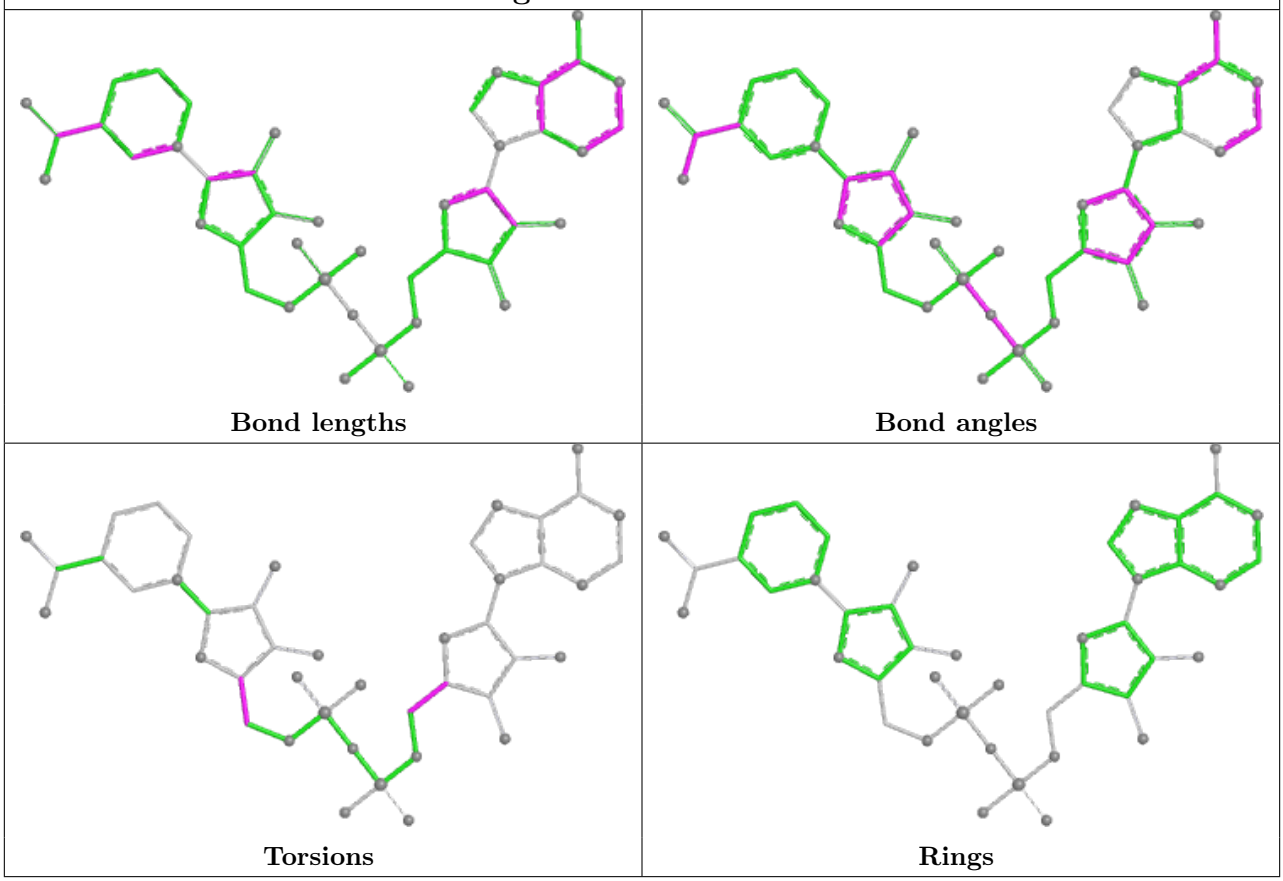
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

Ligand NAD Av 301



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:

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Mol	Chain	Number of breaks
77	UD	3
39	AA	1
14	AK	1
8	A8	1
21	AV	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UD	90:UNK	C	136:UNK	N	14.30
1	UD	158:UNK	C	159:UNK	N	11.31
1	UD	68:UNK	C	69:UNK	N	9.93
1	AA	448:A	O3'	454:U	P	9.07
1	AK	250:LEU	C	251:THR	N	5.73
1	A8	40:PRO	C	41:LYS	N	5.37
1	AV	56:ALA	C	57:ASN	N	5.05

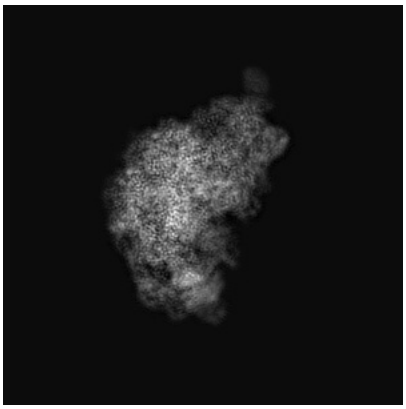
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0231. These allow visual inspection of the internal detail of the map and identification of artifacts.

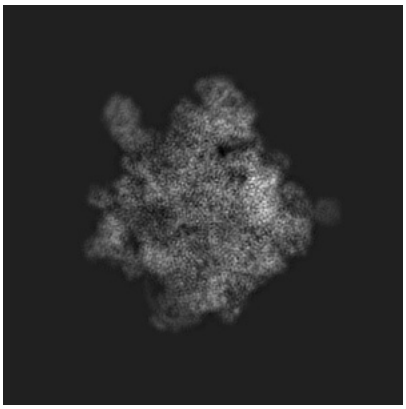
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

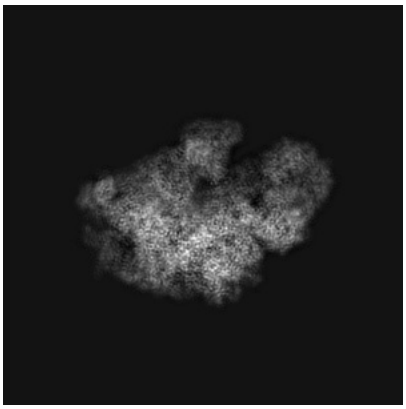
6.1.1 Primary map



X

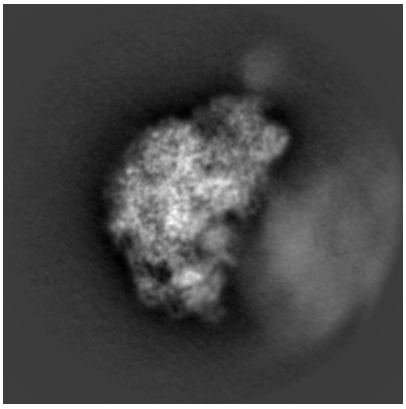


Y

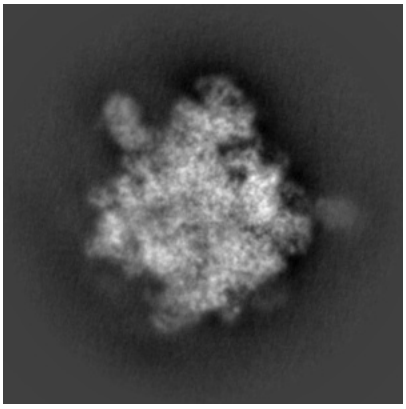


Z

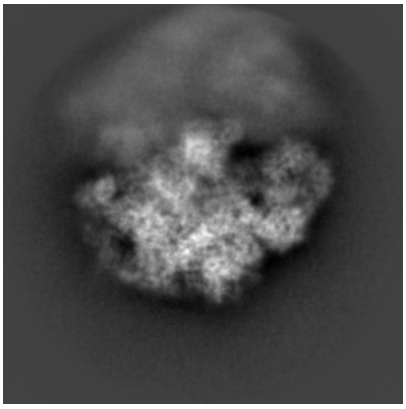
6.1.2 Raw map



X



Y

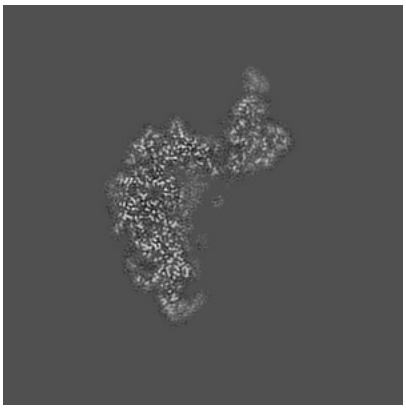


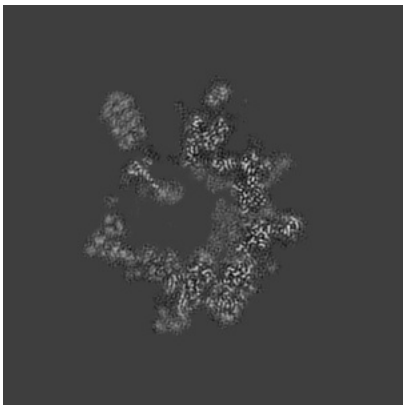
Z

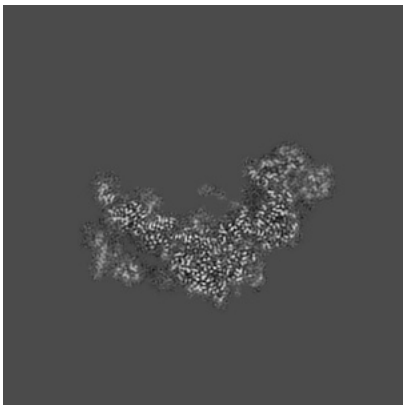
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

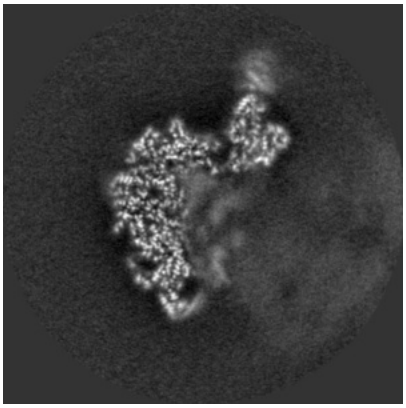
6.2.1 Primary map

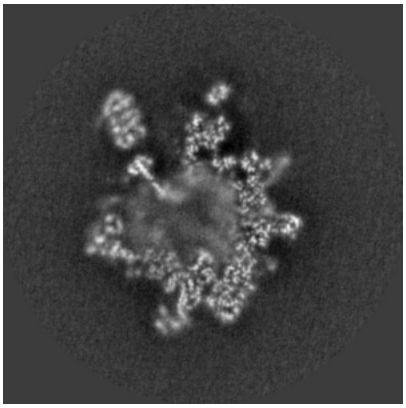

X Index: 160

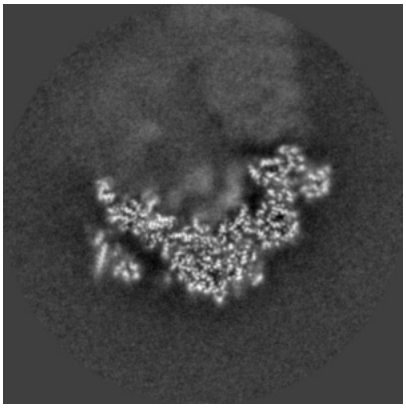

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

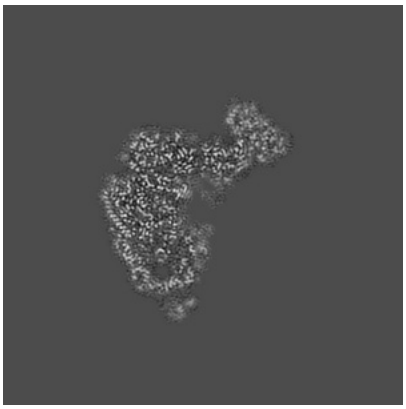

Y Index: 160


Z Index: 160

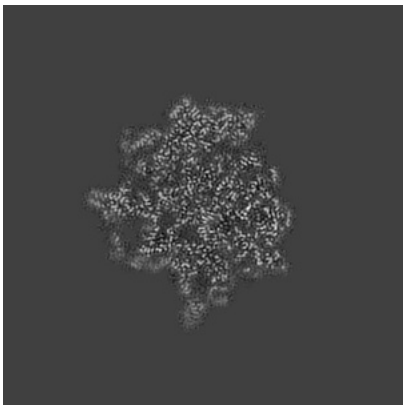
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

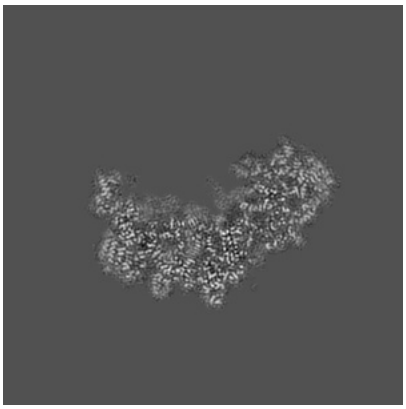
6.3.1 Primary map



X Index: 171

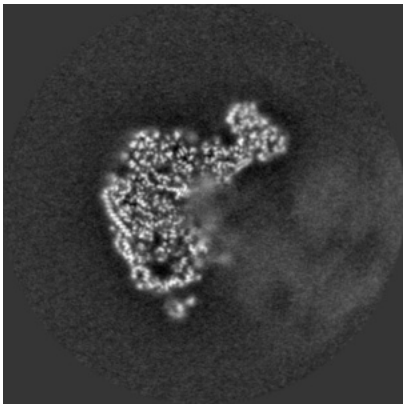


Y Index: 134

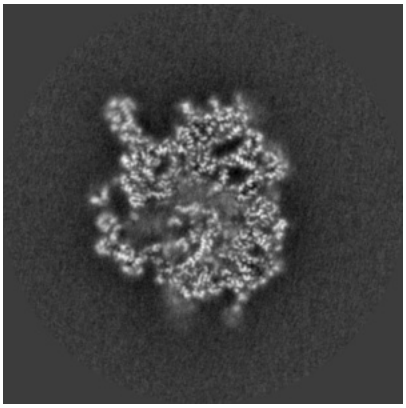


Z Index: 169

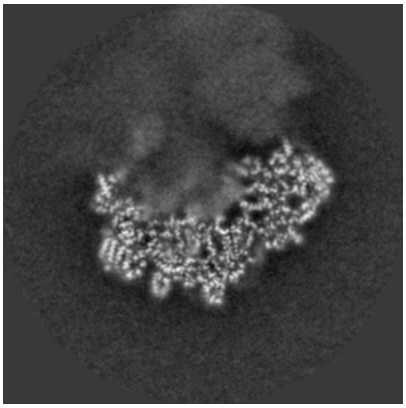
6.3.2 Raw map



X Index: 171



Y Index: 147

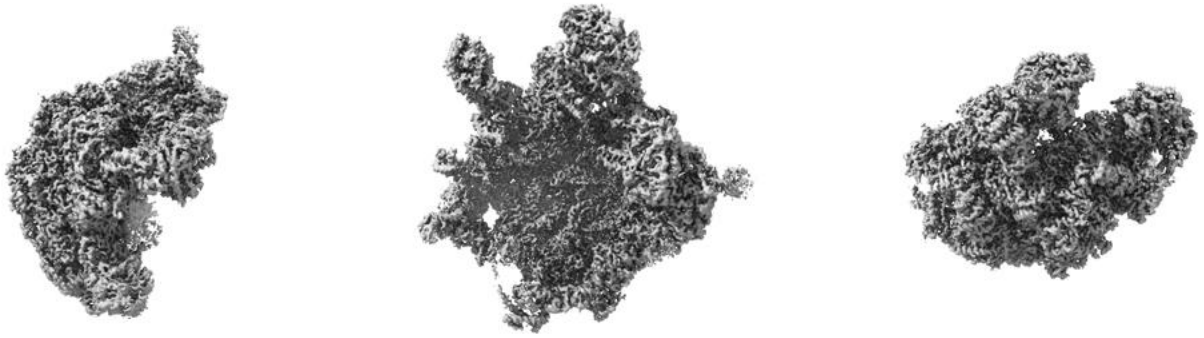


Z Index: 169

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

6.4 Orthogonal surface views (i)

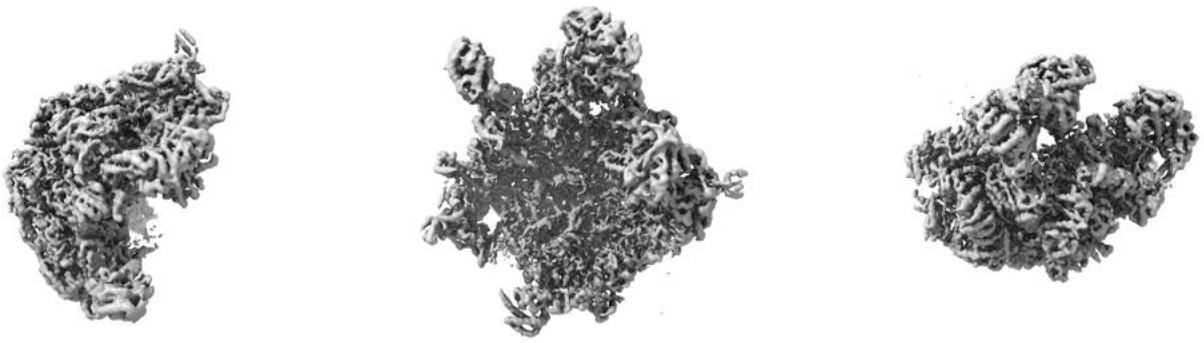
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

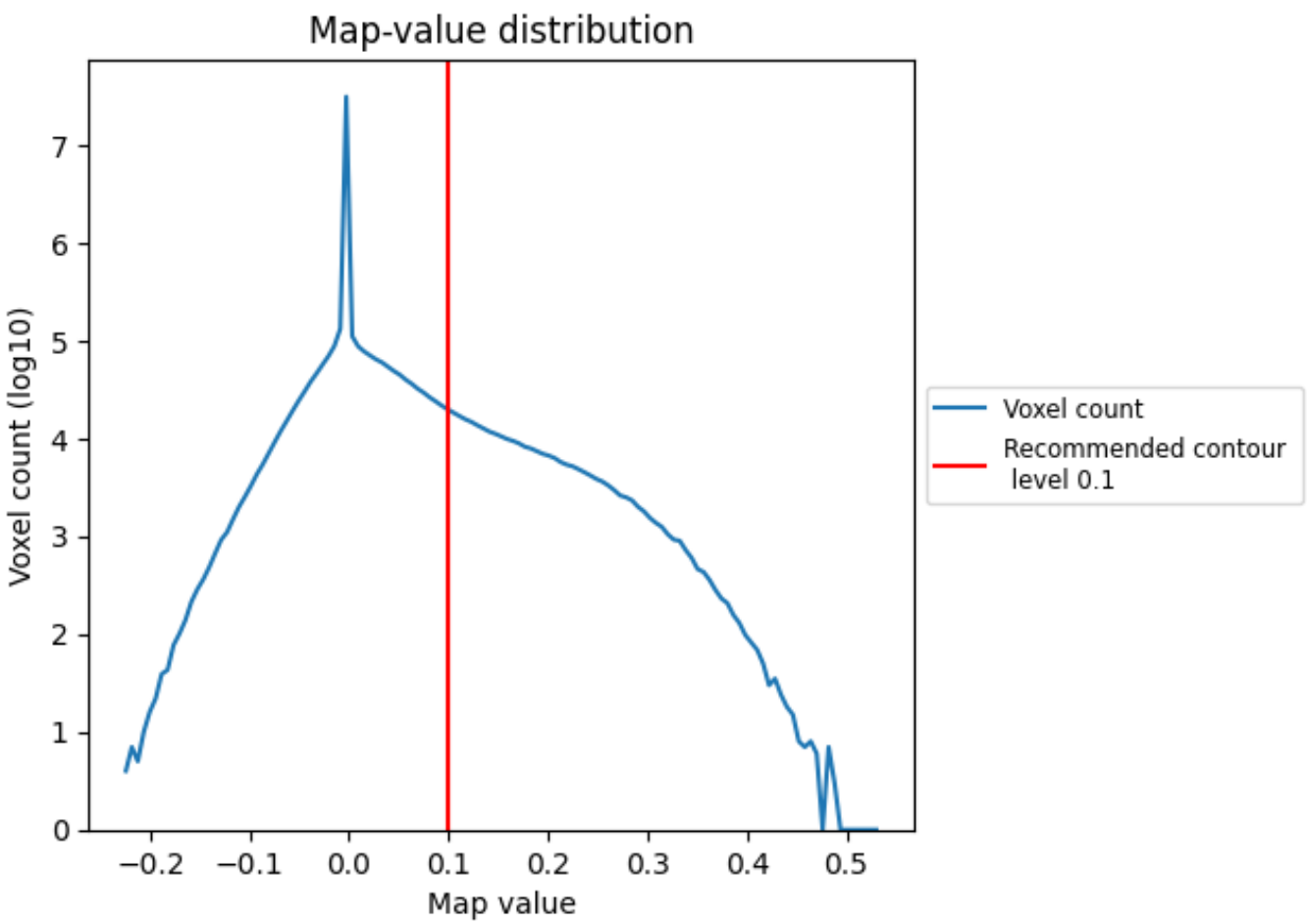
6.5 Mask visualisation (i)

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

7 Map analysis (i)

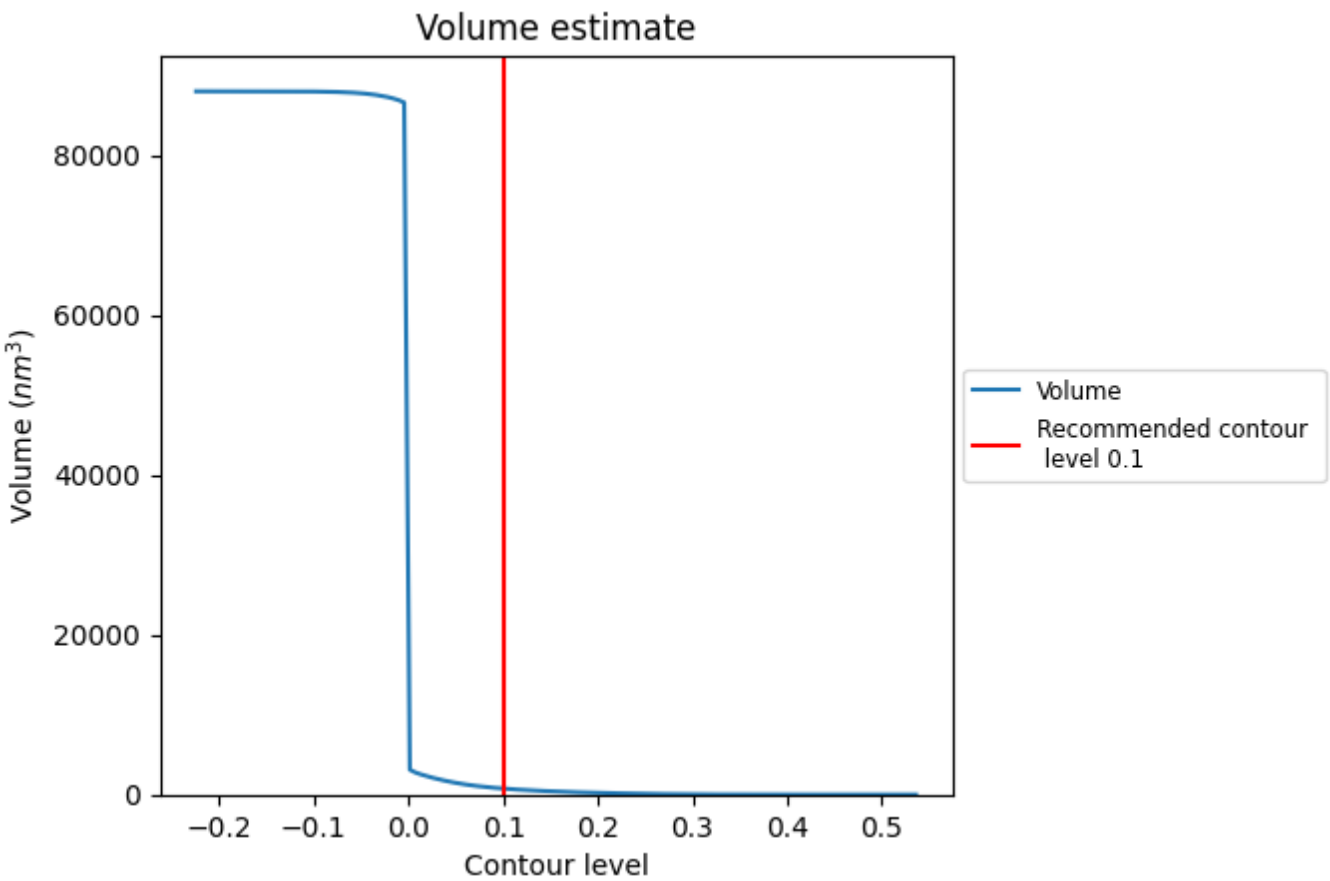
This section contains the results of statistical analysis of the map.

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.

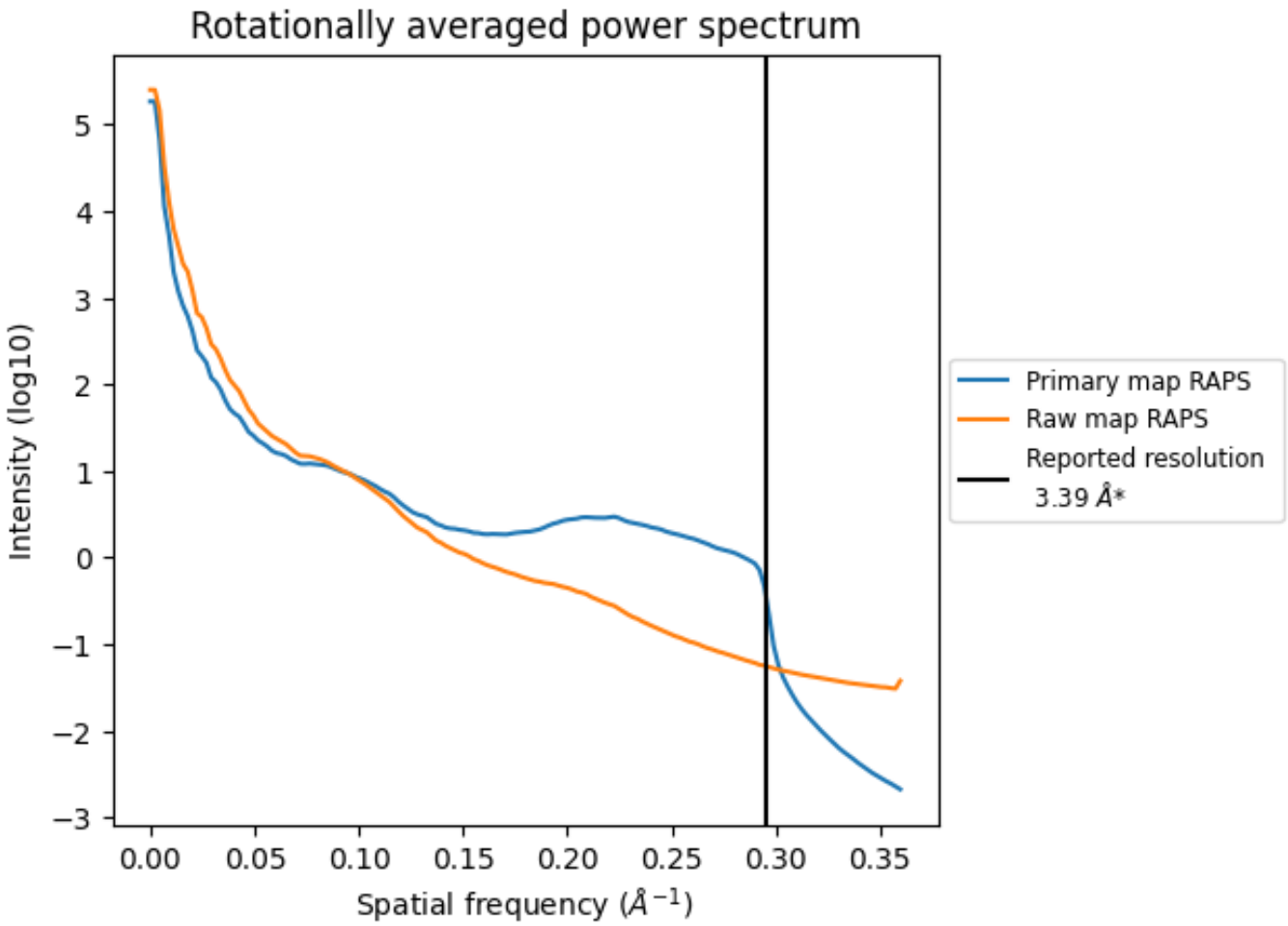
7.2 Volume estimate (i)



The volume at the recommended contour level is 751 nm^3; this corresponds to an approximate mass of 678 kDa.

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

7.3 Rotationally averaged power spectrum (i)

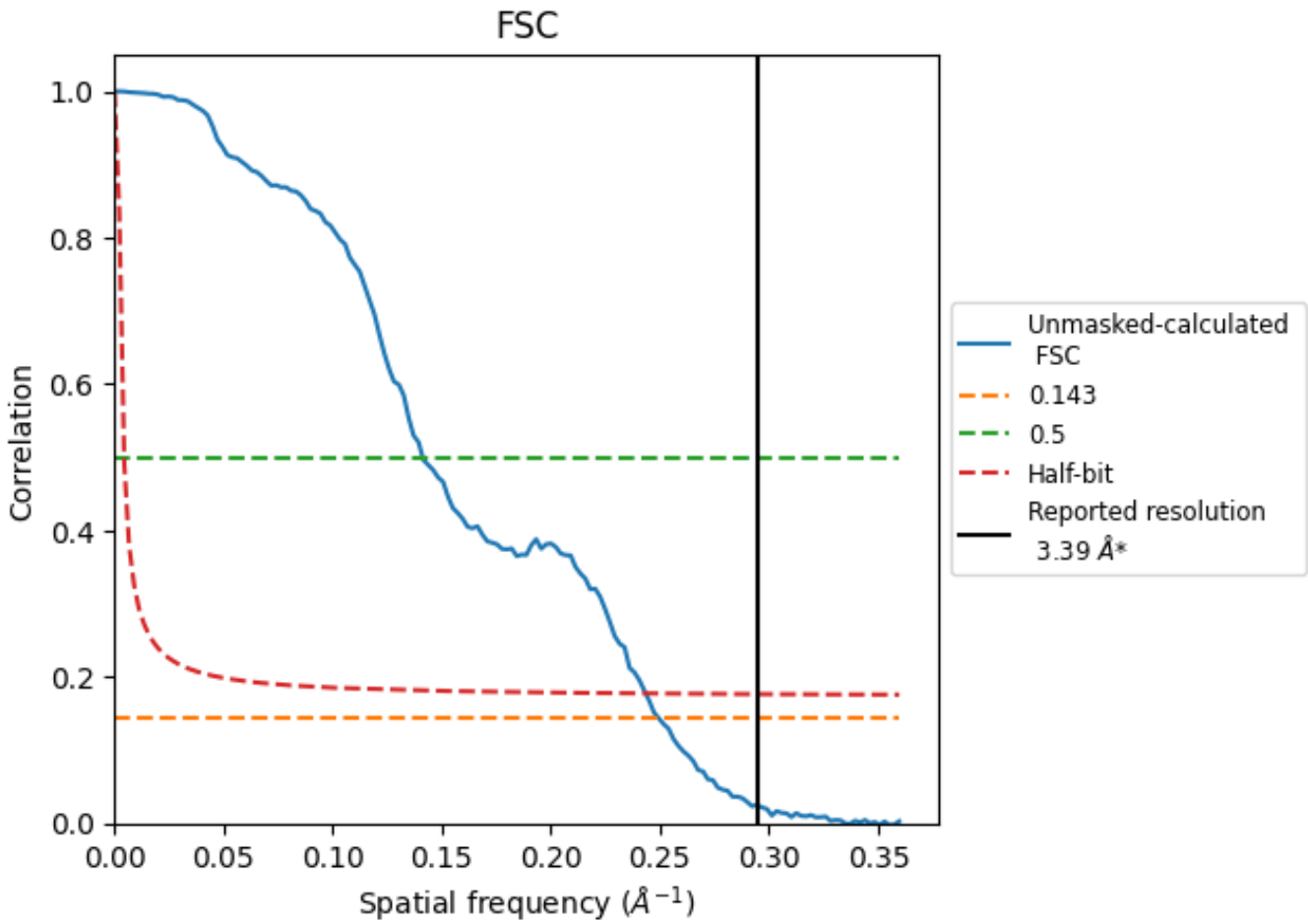


*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

8.2 Resolution estimates (i)

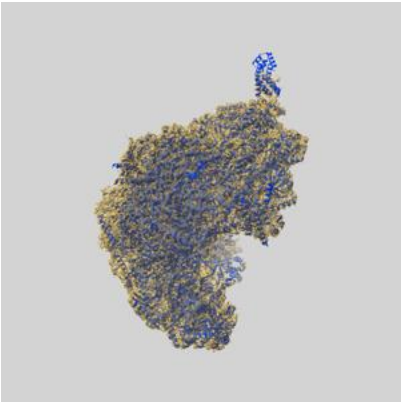
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.08	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.39 by more than 10 %

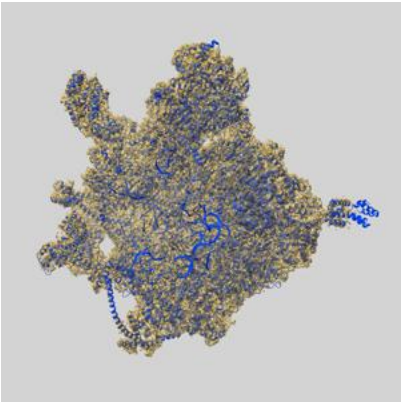
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0231 and PDB model 6HIX. Per-residue inclusion information can be found in section 3 on page 23.

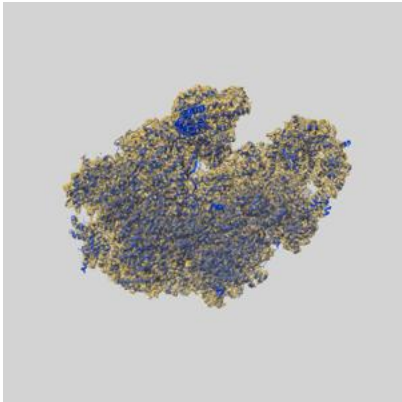
9.1 Map-model overlay (i)



X



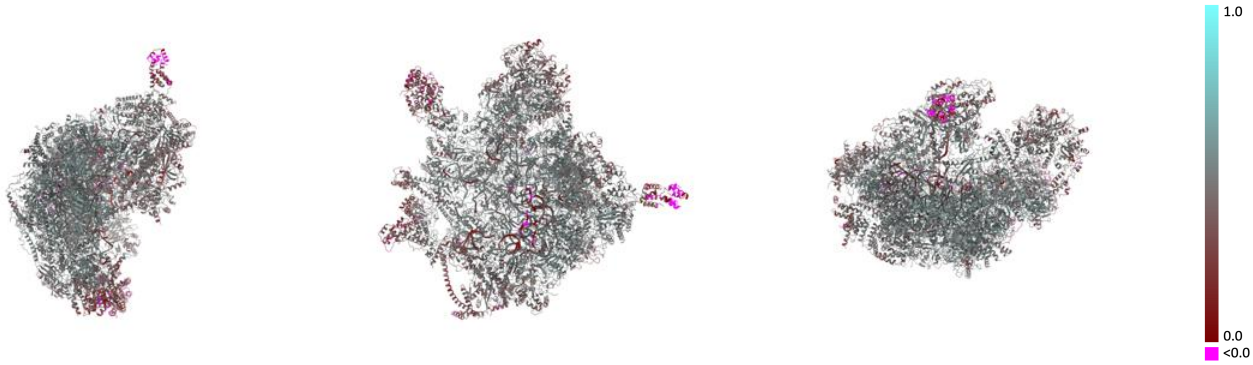
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

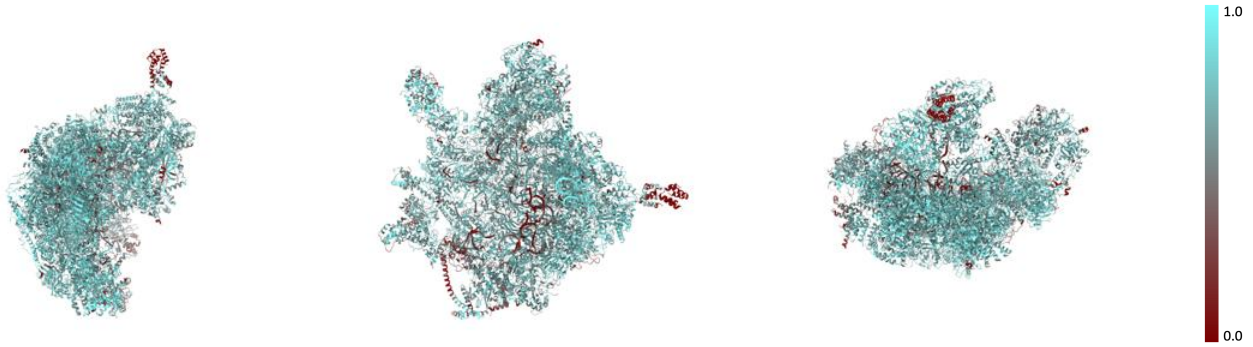
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

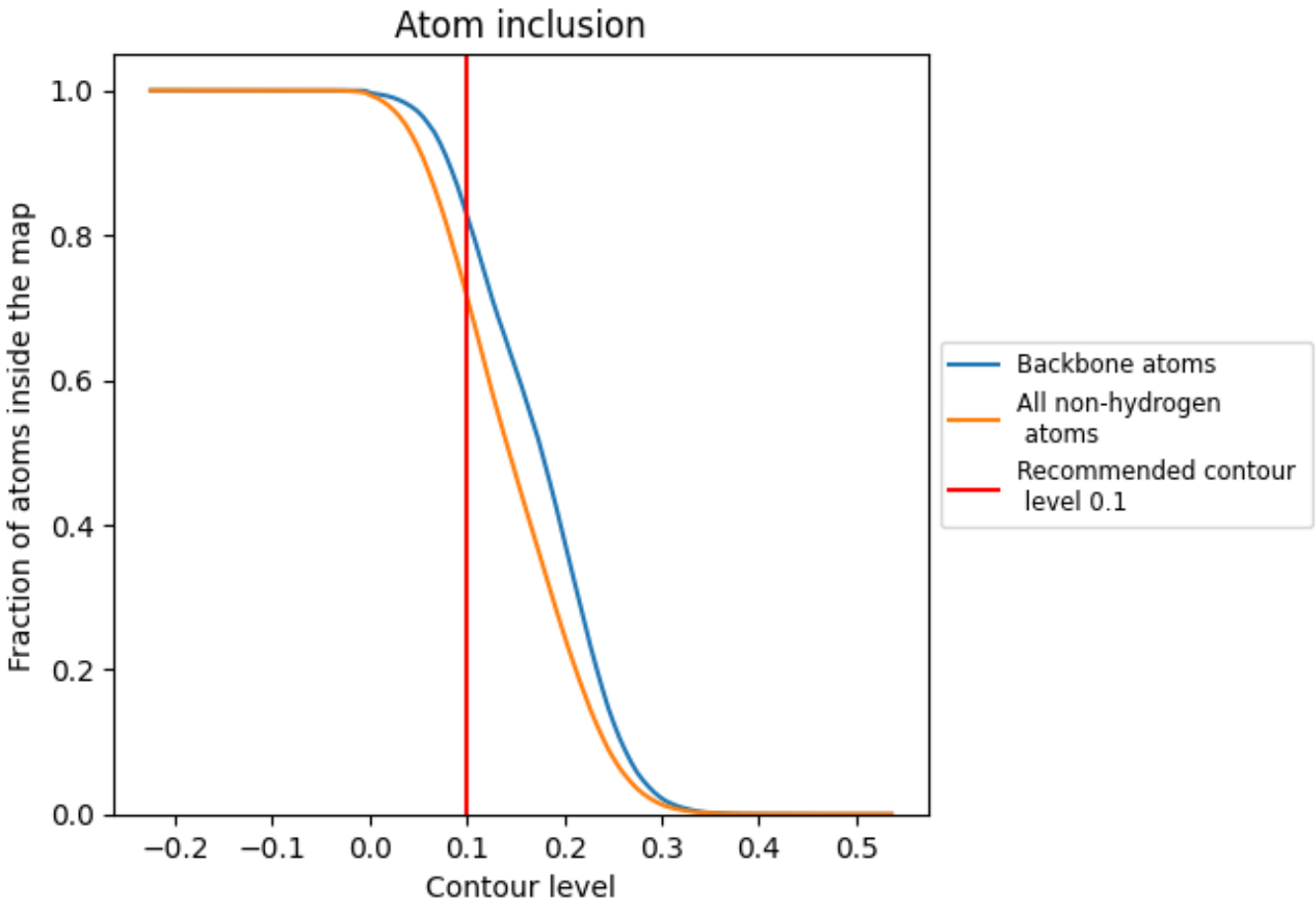
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7159	0.4690
A0	0.7174	0.5000
A1	0.7087	0.4740
A2	0.7984	0.5020
A3	0.7968	0.5290
A4	0.6252	0.4470
A5	0.7532	0.5120
A6	0.6129	0.4720
A8	0.6891	0.4970
A9	0.6539	0.4950
AA	0.6662	0.4290
AB	0.4571	0.3200
AC	0.5143	0.2850
AD	0.0000	-0.0810
AE	0.7383	0.5000
AF	0.7961	0.5270
AG	0.0148	0.0120
AI	0.7687	0.5000
AJ	0.6720	0.4230
AK	0.7180	0.4390
AN	0.7258	0.5130
AP	0.7804	0.5170
AQ	0.6805	0.4990
AR	0.7584	0.4910
AT	0.6777	0.4690
AU	0.7586	0.5150
AV	0.7696	0.5100
AW	0.7477	0.5180
AX	0.7411	0.4970
AY	0.7080	0.4620
Ab	0.7542	0.4880
Ad	0.6952	0.4460
Ae	0.7780	0.4990
Af	0.7371	0.4950
Ag	0.7727	0.4930

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Chain	Atom inclusion	Q-score
Aj	0.6740	0.3980
Al	0.7511	0.5160
Ao	0.7590	0.5150
Ap	0.7418	0.5020
At	0.6938	0.4710
Av	0.7351	0.4970
BA	0.7644	0.4990
BB	0.6439	0.3940
BC	0.7875	0.5060
BD	0.6966	0.2880
BE	0.7347	0.4730
BF	0.7845	0.5120
BG	0.6847	0.3960
BH	0.7378	0.4660
BI	0.7883	0.4930
BJ	0.6494	0.4060
BK	0.4881	0.3780
BL	0.7405	0.4820
BM	0.7813	0.5030
BN	0.6154	0.3960
BO	0.6571	0.4360
BP	0.6846	0.4790
BQ	0.7923	0.5100
BR	0.7832	0.5130
BS	0.6837	0.4540
BT	0.8111	0.5130
BU	0.7348	0.4630
BV	0.6958	0.4420
BW	0.8317	0.5190
BX	0.3563	0.4030
BY	0.6848	0.4450
BZ	0.7243	0.4600
Ba	0.8010	0.5200
Bb	0.7373	0.4550
Bc	0.7086	0.4810
Bd	0.6992	0.4680
Be	0.7189	0.5000
Bf	0.6850	0.4930
Bg	0.7195	0.4870
Bh	0.4986	0.4120
UA	0.6014	0.3140
UB	0.6667	0.4210

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Chain	Atom inclusion	Q-score
UC	0.3889	0.3870
UD	0.4030	0.3690
UE	0.6742	0.4730
UF	0.7500	0.4920
UG	0.5972	0.4630
UH	0.7500	0.5140
UI	0.4118	0.4170
UK	0.7667	0.4570
UL	0.6333	0.4470
UM	0.1944	0.3000
UN	0.1806	0.3030
UU	0.4242	0.3880
UV	0.6667	0.4970
UW	0.2143	0.2140
UX	0.6667	0.4540