



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 04:03 AM UTC

PDB ID : 7PUB / pdb_00007pub
EMDB ID : EMD-13661
Title : Late assembly intermediate of the Trypanosoma brucei mitoribosomal small subunit
Authors : Lenarcic, T.; Leibundgut, M.; Saurer, M.; Ramrath, D.J.F.; Fluegel, T.; Boehringer, D.; Ban, N.
Deposited on : 2021-09-29
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

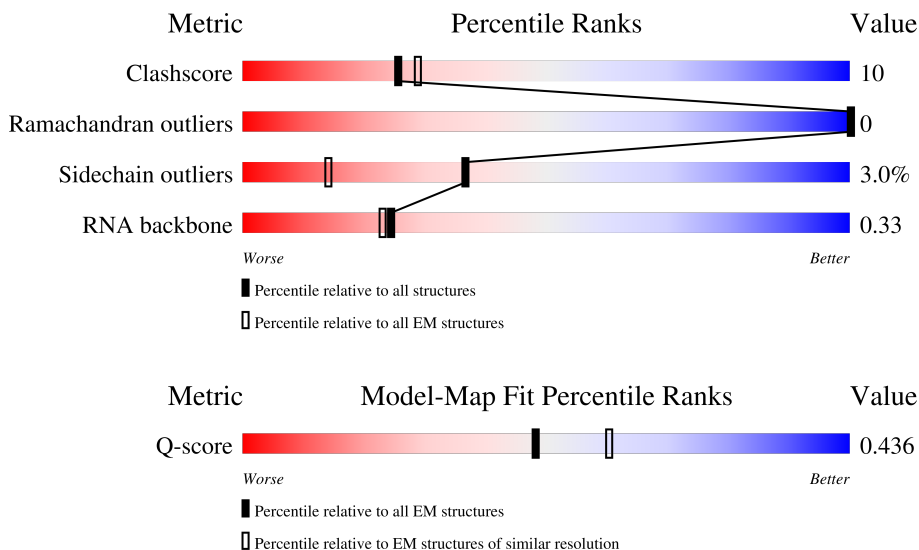
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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














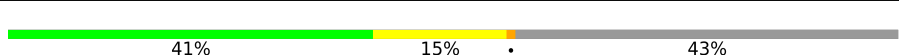
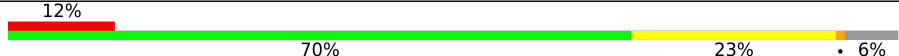
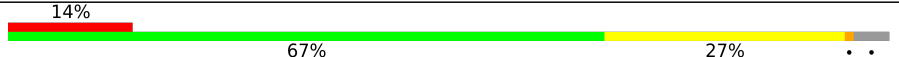
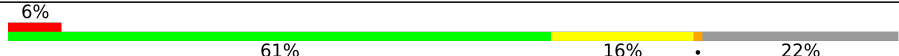
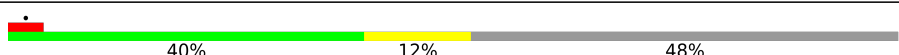
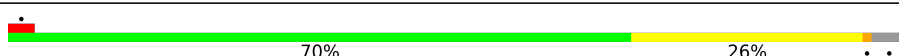
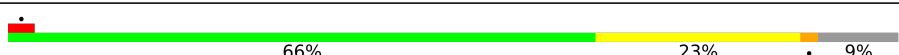
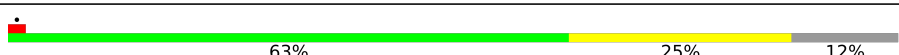
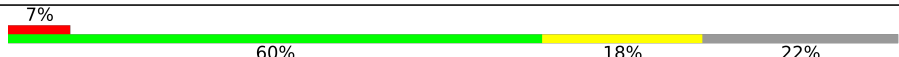




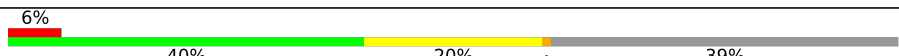
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CA	621	
2	CC	74	
3	CE	435	

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Mol	Chain	Length	Quality of chain
4	CF	160	
5	CH	282	
6	CI	443	
7	CJ	817	
8	CK	326	
9	CL	87	
10	CN	166	
11	CO	429	
12	CP	188	
13	CQ	307	
14	CR	320	
15	CS	244	
16	CU	193	
17	Ca	602	
18	Cb	325	
19	Cd	440	
20	Cg	498	
21	Ci	181	
22	Cj	257	
23	Ck	874	
24	Cm	215	
25	Cn	250	
26	Cp	187	
27	Cq	263	
28	Cr	439	





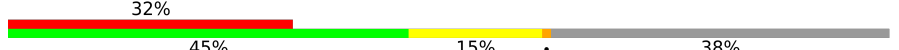

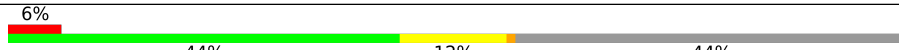

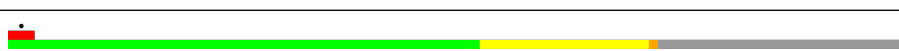

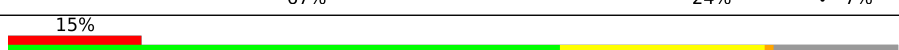
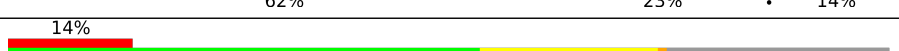

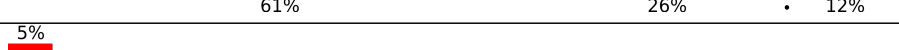
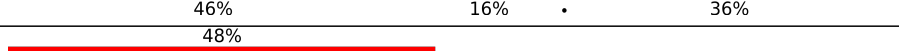
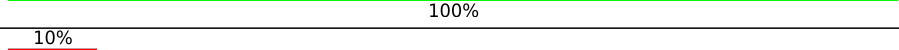
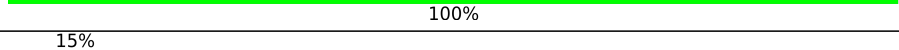
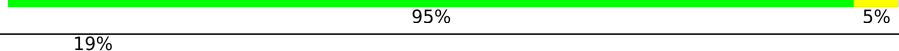
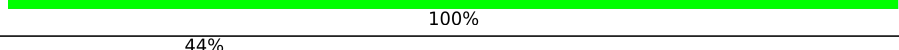
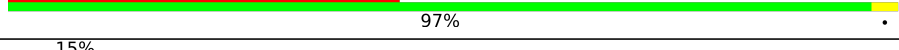
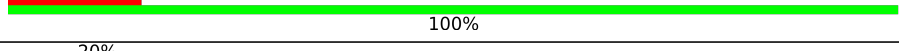
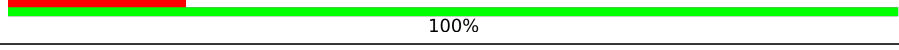
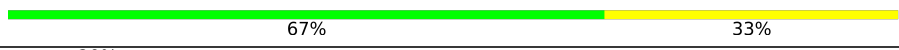
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Mol	Chain	Length	Quality of chain
29	Cv	1211	6% 64% 21% 14%
30	DA	1788	9% 65% 22% 13%
31	DB	1181	6% 66% 27% 6%
32	DC	1165	6% 65% 28% 7%
33	DD	812	6% 70% 27% 2%
34	DE	747	6% 57% 21% 21%
35	DF	666	6% 65% 23% 12%
36	DG	631	6% 62% 24% 13%
37	DH	581	6% 67% 28% 2%
38	DI	407	5% 68% 27% 2%
39	DJ	396	6% 67% 22% 10%
40	DK	324	5% 60% 19% 19%
41	DL	307	14% 72% 22% 5%
42	DM	294	6% 74% 25% 2%
43	DN	293	6% 55% 30% 14%
44	DO	282	6% 56% 22% 22%
45	DP	274	6% 47% 28% 24%
46	DQ	268	7% 63% 31% 5%
47	DR	270	6% 64% 26% 7%
48	DS	261	6% 69% 24% 7%
49	DT	247	6% 61% 34% 2%
50	DU	228	10% 69% 24% 7%
51	DV	183	6% 63% 23% 13%
52	DW	179	6% 66% 23% 10%
53	DX	169	6% 59% 22% 18%

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Mol	Chain	Length	Quality of chain
54	DY	163	
55	DZ	94	
56	Da	64	
57	F3	966	
58	F6	676	
59	F7	679	
60	F9	608	
61	FO	334	
62	Ff	848	
63	Fg	550	
64	Fh	318	
65	Fi	629	
66	IA	787	
67	IB	803	
68	U6	21	
68	UJ	21	
69	U7	40	
70	UE	53	
71	UF	39	
72	UG	13	
73	UI	10	
74	UK	3	
75	UL	20	

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 212864 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 RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	CA	621	12330	5513	1927	4269	621	0	0

- Molecule 2 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CC	74	646	451	96	98	1	0	0

- Molecule 3 is a protein called Ribosomal_S5_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CE	426	3459	2188	642	613	16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	341	ARG	LYS	variant	UNP Q38AX6

- Molecule 4 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CF	149	1240	791	217	226	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S8, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CH	273	2228	1387	432	398	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CH	74	ASN	SER	variant	UNP Q388R7

- Molecule 6 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CI	427	3410	2148	615	630	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	370	ALA	VAL	variant	UNP Q57W62

- Molecule 7 is a protein called LysM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CJ	803	6535	4133	1152	1221	29	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	311	LEU	TYR	variant	UNP Q57Z45
CJ	484	HIS	ARG	variant	UNP Q57Z45
CJ	488	SER	ASN	variant	UNP Q57Z45
CJ	629	ARG	LYS	variant	UNP Q57Z45

- Molecule 8 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CK	298	2447	1520	465	445	17	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	variant	UNP Q389T7
CK	138	UNK	ILE	conflict	UNP Q389T7

- Molecule 9 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CL	87	733	503	113	107	10	0	0

- Molecule 10 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CN	157	1322	843	251	220	8	0	0

- Molecule 11 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	CO	308	2552	1615	476	448	13	0	0

- Molecule 12 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	CP	180	1489	956	274	250	9	0	0

- Molecule 13 is a protein called 30S Ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	CQ	226	1866	1186	355	317	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CQ	138	ALA	VAL	variant	UNP Q38DP8

- Molecule 14 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	CR	267	2210	1398	405	402	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CR	8	ILE	VAL	variant	UNP Q38AS2

- Molecule 15 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	CS	139	1149	743	205	195	6	0	0

- Molecule 16 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	CU	181	1522	957	303	250	12	0	0

- Molecule 17 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Ca	575	4911	3146	875	867	23	0	0

- Molecule 18 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Cb	252	2056	1300	368	380	8	0	0

- Molecule 19 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Cd	230	1961	1242	358	350	11	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cd	299	UNK	GLY	conflict	UNP Q38DK6
Cd	364	UNK	GLY	conflict	UNP Q38DK6

- Molecule 20 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Cg	480	3895	2494	682	699	20	0	0

- Molecule 21 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Ci	164	1343	845	246	243	9	0	0

- Molecule 22 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Cj	227	1799	1142	311	342	4	0	0

- Molecule 23 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Ck	682	5442	3411	990	1016	25	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	variant	UNP Q387C7
Ck	144	PHE	LEU	variant	UNP Q387C7
Ck	253	TYR	PHE	variant	UNP Q387C7
Ck	339	GLU	VAL	variant	UNP Q387C7
Ck	815	GLY	ARG	variant	UNP Q387C7
Ck	871	GLY	GLU	variant	UNP Q387C7

- Molecule 24 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Cm	145	1184	735	230	210	9	0	0

- Molecule 25 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Cn	62	528	345	105	75	3	0	0

- Molecule 26 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Cp	173	1466	928	265	268	5	0	0

- Molecule 27 is a protein called Superoxide dismutase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Cq	252	2005	1285	342	369	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cq	48	THR	ALA	variant	UNP Q586A1
Cq	167	MET	VAL	variant	UNP Q586A1

- Molecule 28 is a protein called Sod_Fe_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Cr	267	2083	1317	382	369	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cr	351	LYS	GLU	variant	UNP Q585I1

- Molecule 29 is a protein called ECH_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Cv	1040	8404	5291	1508	1568	37	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cv	1179	GLU	GLY	variant	UNP Q383R4

- Molecule 30 is a protein called mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	DA	1552	12448	7861	2220	2329	38	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	1181	THR	ILE	variant	UNP Q57UJ2
DA	1333	ALA	VAL	variant	UNP Q57UJ2
DA	1700	ARG	HIS	variant	UNP Q57UJ2
DA	1761	LYS	ARG	variant	UNP Q57UJ2

- Molecule 31 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	DB	1111	9148	5691	1717	1711	29	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DB	23	VAL	ALA	variant	UNP Q586P5
DB	359	ILE	THR	variant	UNP Q586P5
DB	384	GLN	HIS	variant	UNP Q586P5
DB	402	THR	ILE	variant	UNP Q586P5
DB	423	THR	ALA	variant	UNP Q586P5
DB	586	ARG	HIS	variant	UNP Q586P5
DB	593	ARG	LYS	variant	UNP Q586P5
DB	647	SER	GLY	variant	UNP Q586P5

- Molecule 32 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	DC	1089	8709	5498	1538	1642	31	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DC	53	ALA	THR	variant	UNP Q57YB5
DC	365	LYS	GLU	variant	UNP Q57YB5
DC	385	THR	ALA	variant	UNP Q57YB5
DC	405	ILE	VAL	variant	UNP Q57YB5
DC	641	SER	PRO	variant	UNP Q57YB5
DC	651	LYS	GLU	variant	UNP Q57YB5
DC	731	GLU	ASP	variant	UNP Q57YB5
DC	814	GLN	HIS	variant	UNP Q57YB5
DC	1097	ALA	VAL	variant	UNP Q57YB5
DC	1113	THR	ILE	variant	UNP Q57YB5

- Molecule 33 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	DD	790	6513	4121	1181	1170	41	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DD	371	PRO	SER	variant	UNP Q385L8
DD	599	ALA	VAL	variant	UNP Q385L8

- Molecule 34 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	DE	588	4798	3052	868	859	19	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DE	378	UNK	LYS	variant	UNP Q386Q7
DE	384	UNK	THR	variant	UNP Q386Q7

- Molecule 35 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	DF	589	4738	2974	895	844	25	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DF	18	THR	ALA	variant	UNP Q38ET1
DF	258	ASP	ASN	variant	UNP Q38ET1
DF	372	ASN	ASP	variant	UNP Q38ET1
DF	406	ASN	SER	variant	UNP Q38ET1
DF	510	ASP	GLY	variant	UNP Q38ET1
DF	577	ALA	VAL	variant	UNP Q38ET1
DF	636	UNK	GLY	conflict	UNP Q38ET1
DF	638	LYS	ARG	variant	UNP Q38ET1

- Molecule 36 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	DG	552	4482	2820	818	813	31	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DG	428	ASN	SER	variant	UNP Q57ZP8
DG	429	GLY	SER	variant	UNP Q57ZP8

- Molecule 37 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	DH	559	4541	2849	843	828	21	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DH	191	HIS	GLN	variant	UNP Q580V1
DH	194	PRO	ARG	variant	UNP Q580V1
DH	488	GLY	SER	variant	UNP Q580V1

- Molecule 38 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	DI	390	3182	2020	554	594	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	92	GLU	GLY	variant	UNP Q587C2
DI	116	ASP	GLU	variant	UNP Q587C2

- Molecule 39 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	DJ	357	2914	1858	512	530	14	0	0

- Molecule 40 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	DK	263	2083	1312	374	392	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DK	61	SER	PRO	variant	UNP Q38BP1
DK	257	GLY	SER	variant	UNP Q38BP1

- Molecule 41 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	DL	291	2360	1495	441	412	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DL	274	THR	ALA	variant	UNP Q38BS2

- Molecule 42 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	DM	294	2430	1533	459	426	12	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DM	69	PHE	TYR	variant	UNP Q57XL2
DM	97	ASN	SER	variant	UNP Q57XL2
DM	138	SER	PRO	variant	UNP Q57XL2
DM	173	ALA	THR	variant	UNP Q57XL2
DM	206	ALA	THR	variant	UNP Q57XL2

- Molecule 43 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	DN	253	2062	1313	374	365	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DN	51	GLY	SER	variant	UNP Q38D60

- Molecule 44 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	DO	221	1796	1123	325	338	10	0	0

- Molecule 45 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	DP	207	1760	1132	312	307	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DP	3	HIS	ARG	variant	UNP Q38F25

- Molecule 46 is a protein called AKAP7_NLS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	DQ	255	2055	1290	388	368	9	0	0

- Molecule 47 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	DR	250	2019	1301	368	340	10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DR	65	GLY	SER	variant	UNP Q57UA2
DR	94	GLY	GLU	variant	UNP Q57UA2
DR	128	PRO	SER	variant	UNP Q57UA2
DR	229	ARG	GLN	variant	UNP Q57UA2

- Molecule 48 is a protein called mS66.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	DS	243	1950	1216	364	356	14	0	0

- Molecule 49 is a protein called Rhodanese domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	DT	239	2058	1321	364	362	11	0	0

- Molecule 50 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	DU	213	1754	1103	310	335	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DU	119	ILE	LEU	variant	UNP Q582T9
DU	152	ILE	VAL	variant	UNP Q582T9

- Molecule 51 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	DV	160	1346	855	252	235	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	variant	UNP Q57UZ6

- Molecule 52 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	DW	161	1359	866	260	228	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DW	74	THR	MET	variant	UNP Q383N9

- Molecule 53 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	DX	139	1174	747	223	197	7	0	0

- Molecule 54 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	DY	154	1295	829	247	214	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DY	34	HIS	ASP	variant	UNP Q57YD4

- Molecule 55 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	DZ	82	697	457	113	123	4	0	0

- Molecule 56 is a protein called mS74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Da	34	305	193	67	43	2	0	0

- Molecule 57 is a protein called mt-SAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	F3	252	2003	1259	354	378	12	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	44	THR	ALA	variant	UNP Q38E61
F3	190	VAL	ILE	variant	UNP Q38E61
F3	303	ALA	SER	variant	UNP Q38E61
F3	418	ASP	ASN	variant	UNP Q38E61

- Molecule 58 is a protein called mt-SAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	F6	416	3358	2124	580	636	18	0	0

- Molecule 59 is a protein called mt-SAF7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	F7	576	4584	2922	792	837	33	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F7	36	ILE	THR	variant	UNP Q57UW6
F7	470	GLU	LYS	variant	UNP Q57UW6
F7	474	VAL	ALA	variant	UNP Q57UW6

- Molecule 60 is a protein called mt-SAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	F9	342	2815	1736	530	539	10	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F9	117	ALA	SER	variant	UNP Q57YC0
F9	145	TYR	HIS	variant	UNP Q57YC0
F9	316	LYS	GLU	variant	UNP Q57YC0
F9	412	GLY	VAL	variant	UNP Q57YC0
F9	449	VAL	ALA	variant	UNP Q57YC0
F9	537	GLY	SER	variant	UNP Q57YC0

- Molecule 61 is a protein called mt-SAF22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	FO	267	2236	1407	432	385	12	0	0

- Molecule 62 is a protein called DNA photolyase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	Ff	614	4941	3135	885	898	23	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ff	109	ALA	VAL	variant	UNP Q382U6
Ff	127	UNK	TYR	conflict	UNP Q382U6
Ff	138	GLN	ARG	variant	UNP Q382U6
Ff	200	CYS	SER	variant	UNP Q382U6
Ff	319	ALA	THR	variant	UNP Q382U6
Ff	334	ASN	THR	variant	UNP Q382U6
Ff	350	ILE	THR	variant	UNP Q382U6
Ff	362	ALA	VAL	variant	UNP Q382U6
Ff	844	THR	SER	variant	UNP Q382U6

- Molecule 63 is a protein called Acyl transferase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	Fg	513	3994	2512	698	754	30	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fg	90	LYS	ARG	variant	UNP Q38DK4
Fg	152	VAL	LEU	variant	UNP Q38DK4
Fg	159	ILE	VAL	variant	UNP Q38DK4
Fg	363	MET	ARG	variant	UNP Q38DK4
Fg	399	UNK	GLU	conflict	UNP Q38DK4
Fg	525	LYS	ARG	variant	UNP Q38DK4

- Molecule 64 is a protein called mt-SAF37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Fh	274	2230	1384	420	411	15	0	0

- Molecule 65 is a protein called mt-SAF38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Fi	469	3734	2363	683	665	23	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fi	35	THR	SER	variant	UNP Q57ZP1
Fi	69	GLY	SER	variant	UNP Q57ZP1
Fi	185	PRO	HIS	variant	UNP Q57ZP1

- Molecule 66 is a protein called Translation initiation factor IF-2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	IA	693	5414	3397	972	1018	27	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
IA	373	LYS	GLU	variant	UNP Q57WE3
IA	451	ILE	VAL	variant	UNP Q57WE3
IA	584	ASN	SER	variant	UNP Q57WE3
IA	679	ASP	VAL	variant	UNP Q57WE3

- Molecule 67 is a protein called mt-SAF39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	IB	511	4103	2561	764	760	18	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
IB	136	LYS	GLU	variant	UNP Q387Q6
IB	226	ASP	ASN	variant	UNP Q387Q6
IB	237	CYS	SER	variant	UNP Q387Q6
IB	259	THR	ARG	variant	UNP Q387Q6
IB	268	GLU	LYS	variant	UNP Q387Q6
IB	275	CYS	TYR	variant	UNP Q387Q6
IB	312	THR	SER	variant	UNP Q387Q6
IB	459	ASP	ALA	variant	UNP Q387Q6
IB	572	HIS	ARG	variant	UNP Q387Q6

- Molecule 68 is a protein called Unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
68	U6	21	105	63	21	21	0	0
68	UJ	21	105	63	21	21	0	0

- Molecule 69 is a protein called Unk7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
69	U7	40	200	120	40	40	0	0

- Molecule 70 is a protein called UnkE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
70	UE	53	265	159	53	53	0	0

- Molecule 71 is a protein called UnkF.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
71	UF	39	195	117	39	39	0	0

- Molecule 72 is a protein called UnkG.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
72	UG	13	65	39	13	13	0	0

- Molecule 73 is a protein called UnkI.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
73	UI	10	50	30	10	10	0	0

- Molecule 74 is a protein called UnkK.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
74	UK	3	15	9	3	3	0	0

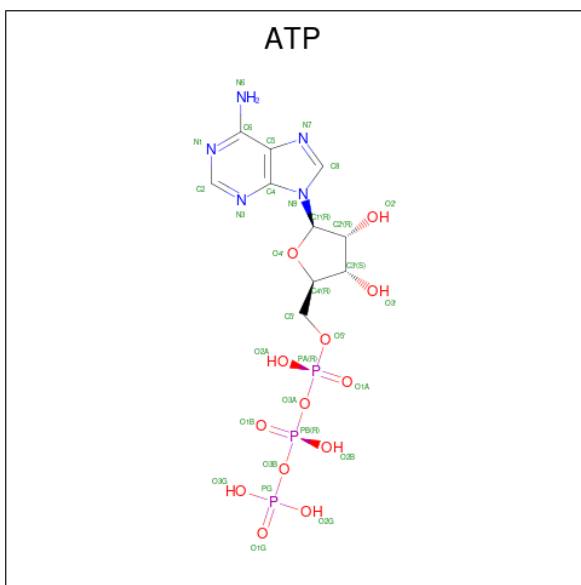
- Molecule 75 is a protein called UnkL.

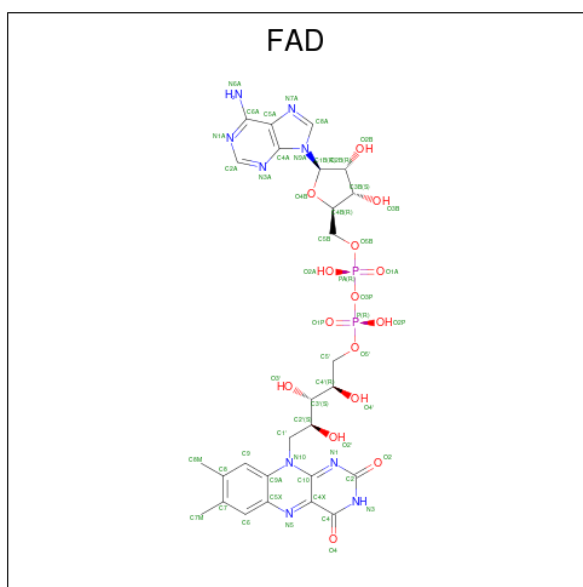
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
75	UL	20	100	60	20	20	0	0

- Molecule 76 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
76	CA	3	3	3	0
76	CQ	1	1	1	0
76	Cg	1	1	1	0
76	IA	1	1	1	0

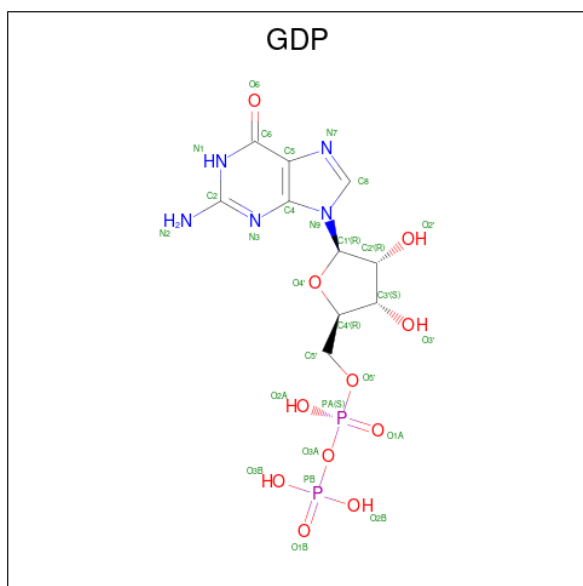
- Molecule 77 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).





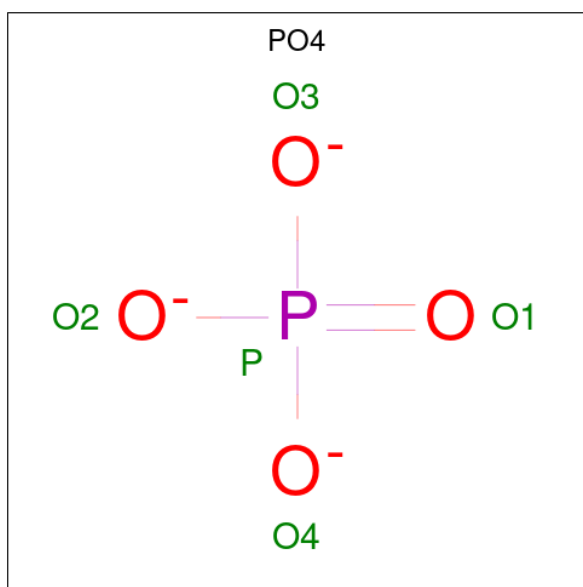
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
80	Ff	1	53	27	9	15	2	0

- Molecule 81 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
81	IA	1	28	10	5	11	2	0

- Molecule 82 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
82	IA	1	Total	O	P	0
			5	4	1	

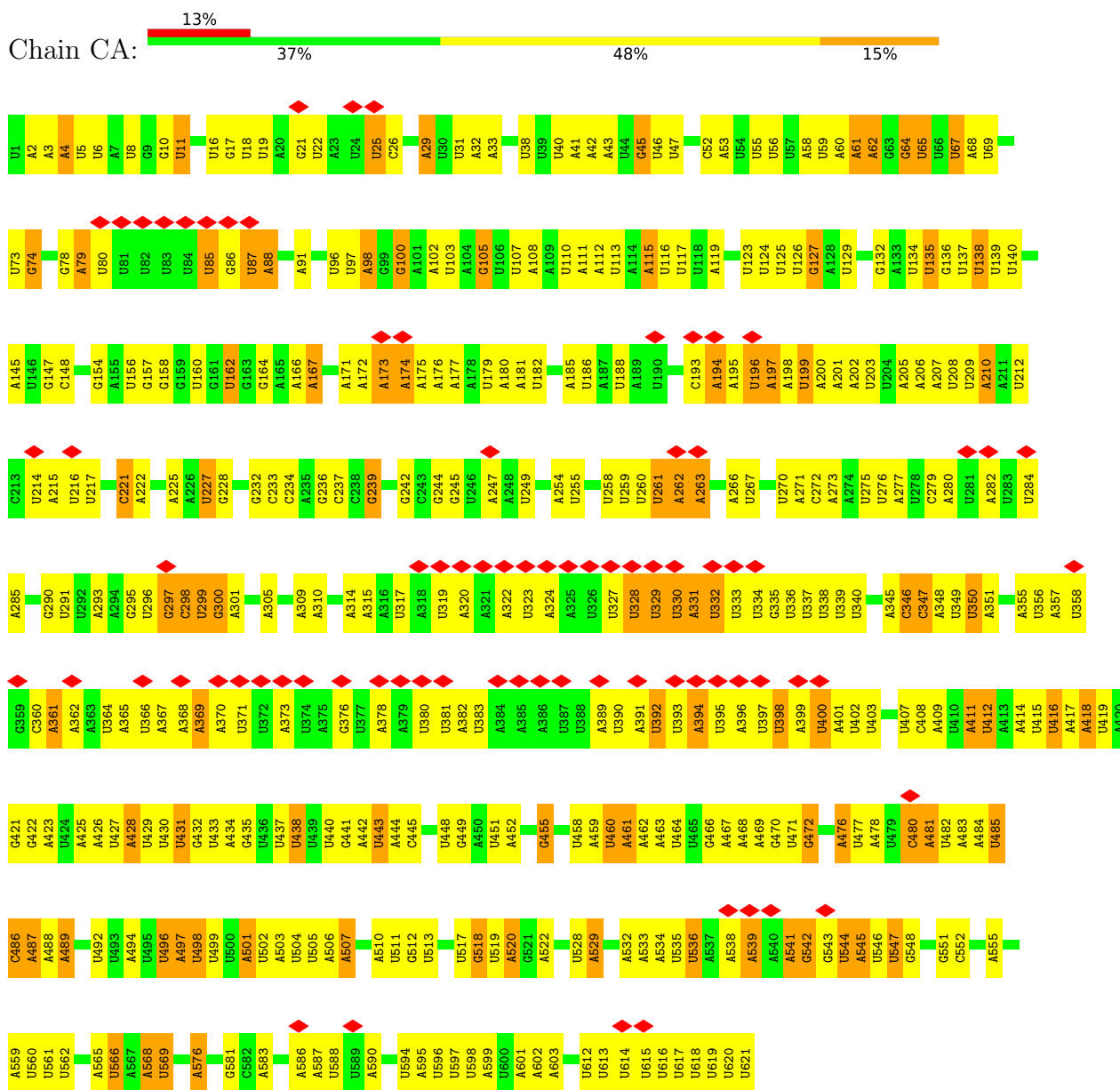
- Molecule 83 is water.

Mol	Chain	Residues	Atoms		AltConf
83	Cg	3	Total	O	0
			3	3	
83	IA	2	Total	O	0
			2	2	

3 Residue-property plots

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.

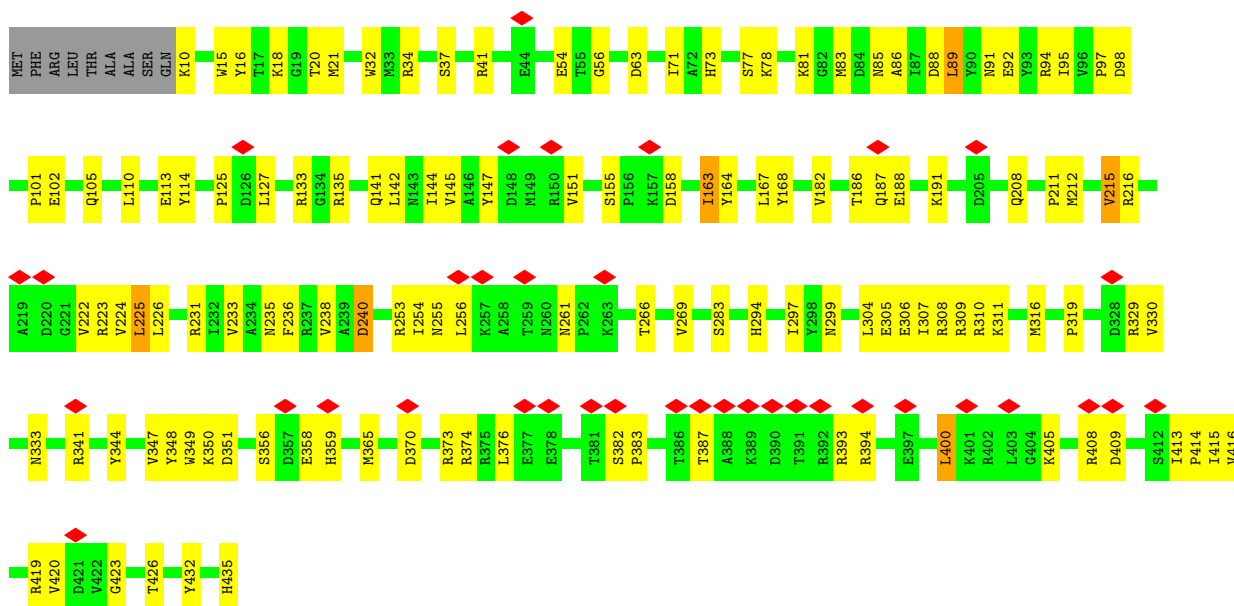
- Molecule 1: 9S rRNA



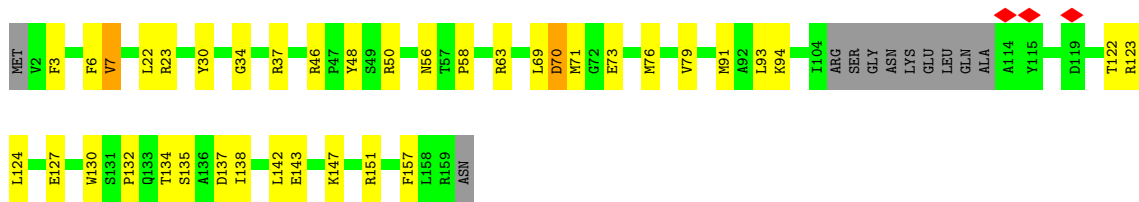
- Molecule 2: uS3m



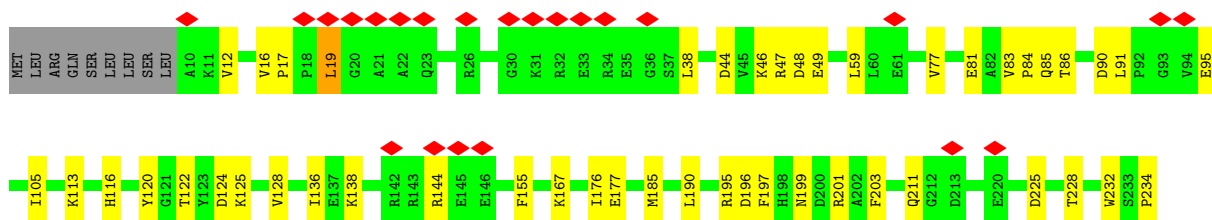
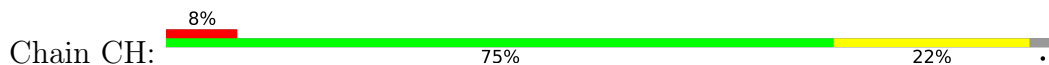
• Molecule 3: Ribosomal_S5_C domain-containing protein

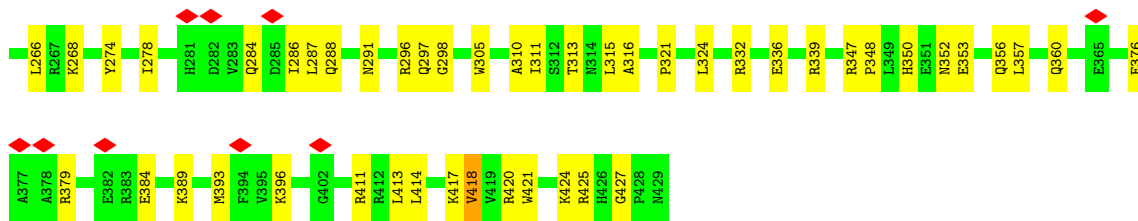


• Molecule 4: bS6m

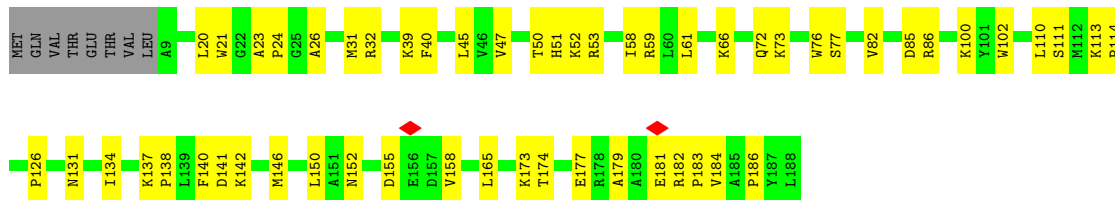


• Molecule 5: 30S ribosomal protein S8, putative

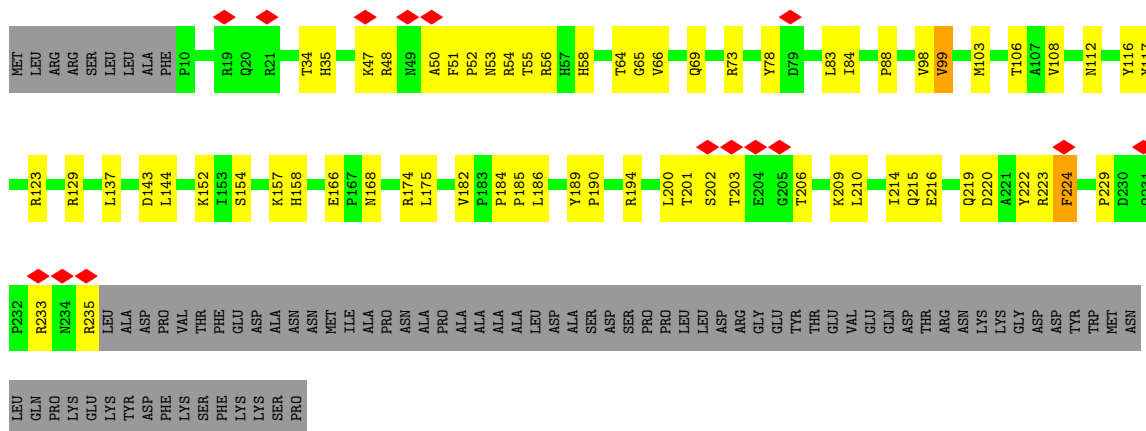




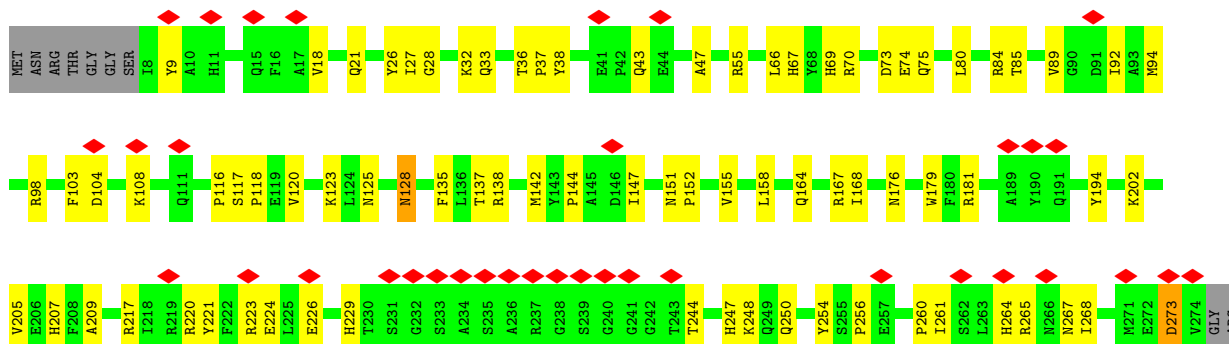
• Molecule 12: bS16m



• Molecule 13: 30S Ribosomal protein S17, putative



• Molecule 14: bS18m



SER VAL
LYS PHE
ASN ARG
PRO HIS
THR THR
VAL VAL
PRO THR
GLY THR
MET MET
SER SER
THR THR
LYS LYS
MET MET
VAL VAL
LYS LYS
LYS LYS
PHE PHE
HIS HIS
ASN ASN
LEU LEU
LEU LEU
TYR TYR
SER SER
SER SER
THR THR
SER SER
VAL VAL
LYS LYS
VAL VAL
PHE PHE
ARG ARG
MET MET
GLY GLY
PHE PHE
SER SER
ASN ASN
PRO PRO
THR THR
LEU LEU
GLY GLY
ILE ILE
LYS LYS
VAL VAL

• Molecule 15: uS19m



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

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

Q152 F156
F156 F156
E159 E159
M160 M160
Y161 Y161
I162 I162
W166 W166
K169 K169
F170 F170
F171 F171
K174 K174
R175 R175
Q176 Q176
V177 V177
H182 H182
R190 R190
I197 I197
S204 S204
R205 R205
V206 V206
G209 G209
N213 N213
K217 K217
M220 M220
D221 D221
L222 L222
I223 I223
D224 D224
L228 L228
T229 T229
Q232 Q232
R233 R233
L234 L234
R238 R238
P243 P243
LYS LYS

• Molecule 16: bS21m



MET LEU
HIS THR
THR THR
ARG ARG
LEU LEU
TRP TRP
GLY GLY
Y12 Y12
M13 M13
M14 M14
Y15 Y15
H16 H16
R17 R17
K18 K18
A19 A19
K27 K27
H32 H32
S36 S36
Y39 Y39
P43 P43
W44 W44
V45 V45
V48 V48
N51 N51
E54 E54
T55 T55
L56 L56
V57 V57
D58 D58
R59 R59
R60 R60
M62 M62
V65 V65
F76 F76
Y79 Y79
Q80 Q80
E81 E81
K82 K82
E92 E92
M112 M112
T116 T116

M117 K118
E121 D122
R126 L126
M128 T128
Q132 V135
H143 T146
D147 M148
V149 A150
R151 E152
R153 A157
R158 R159
R160 Q161
V162 R163
L165 P166
M167 V168
M169 Y175
Q180 I181
H182 M183
D184 R185
Y188 R189
M190 R191
V192 ASN

• Molecule 17: mS22



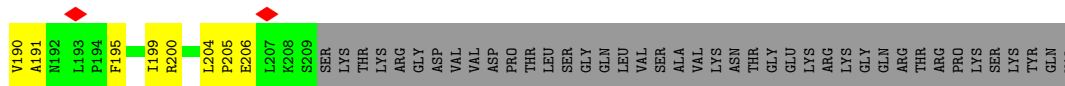
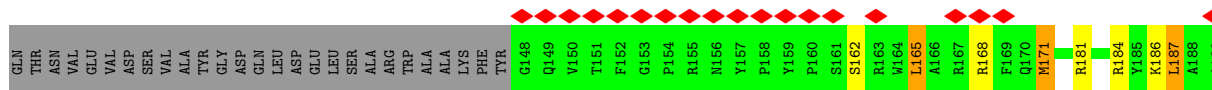
MET LEU
ARG ARG
ARG ARG
ALA ALA
TYR TYR
ILE ILE
GLN GLN
ARG ARG
ARG ARG
TYR TYR
PRO PRO
PHE PHE
ASN ASN
LYS LYS
ARG ARG
GLY GLY
PRO PRO
ARG ARG
GLU GLU
H21 H21
W24 W24
K25 K25
H26 H26
H27 H27
V28 V28
L29 L29
T30 T30
E31 E31
P32 P32
P33 P33
LYS LYS
PRO PRO
LEU LEU
GLN GLN
TRP TRP
ARG ARG
D40 D40
P41 P41
K42 K42
W44 W44
T45 T45
R46 R46
D47 D47
L48 L48
S49 S49
V50 V50
M51 M51
K52 K52
S53 S53
F54 F54
D55 D55
A56 A56
R65 R65
P66 P66
R67 R67

D70 M71
D72 E73
A74 L75
F78 M79
D80 M81
P82 L85
K86 R89
Y90 D91
M106 S109
L110 L111
L112 K116
M120 A121
I124 Y127
R132 A135
S136 G137
K138 D139
T141 D145
D146 M150
E154 R155
M165 A166
G167 L179
M180

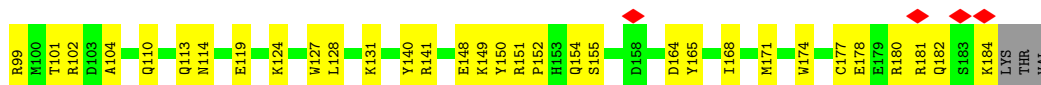
E181 K184
D187 R193
E196 H197
R200 R201
I202 L205
D213 W216
L217 E218
A219 L220
T221 Q222
N223 S224
P225 H226
L227 N227
K228 E229
Q230 Q230
L231 Q232
R233 K234
I235 A236
F237 Q238
T239 S240
L241 Q242
T243 P244
E245 F246
F247 D248
M249 R252
L253 E256
D260

L267 G268
P269 E270
L271 F272
A273 L274
W275 D276
K277 A278
P283 P284
E285 R286
L297 V298
L302 V303
M304 H305
H306 F307
K308 Y311
D312 A313
C314 V315
E316 F317
D318 S320
F326 A327
L328 E329
W330 V334
R335 A336
R337 K338
H339 G340
L341 F342
Y343 G344
K345 M346

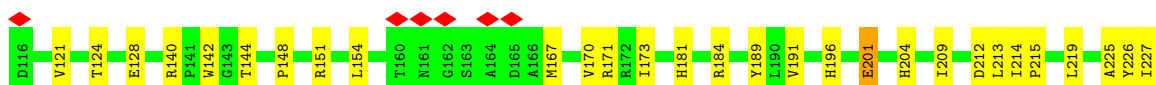
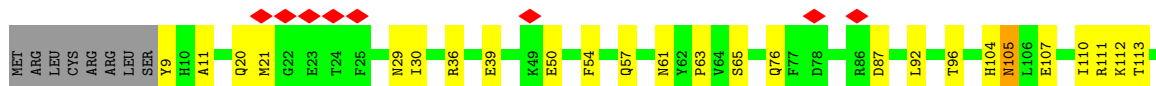
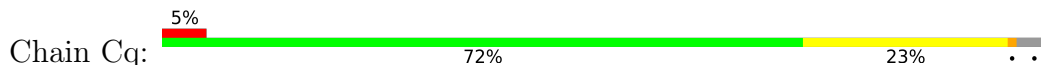
R347 T354
F355 D358
L361 F362
R363 D364
L365 V366
N367 R368
R384 D391
D398 G412
R413 T414
C415 Q419
Q420 Y421
H430 H431
R432 Q433
K437 W442
M443 F444
V449 M450
H453 L459
E460 R474
L480 E487
M488 R489
A490 W491
Y492



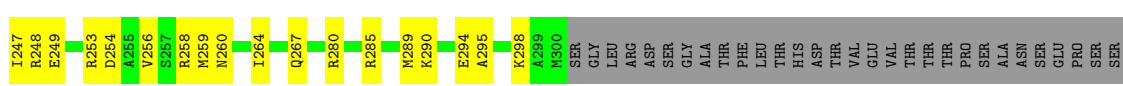
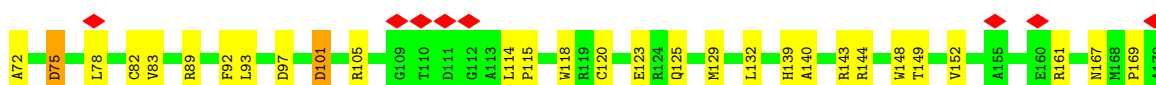
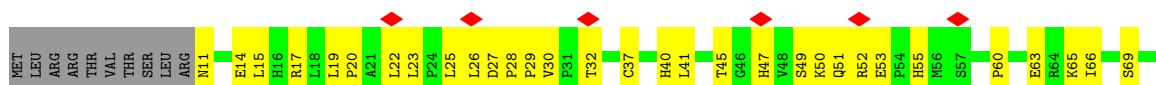
• Molecule 26: Protein FYV4, mitochondrial



• Molecule 27: Superoxide dismutase, putative

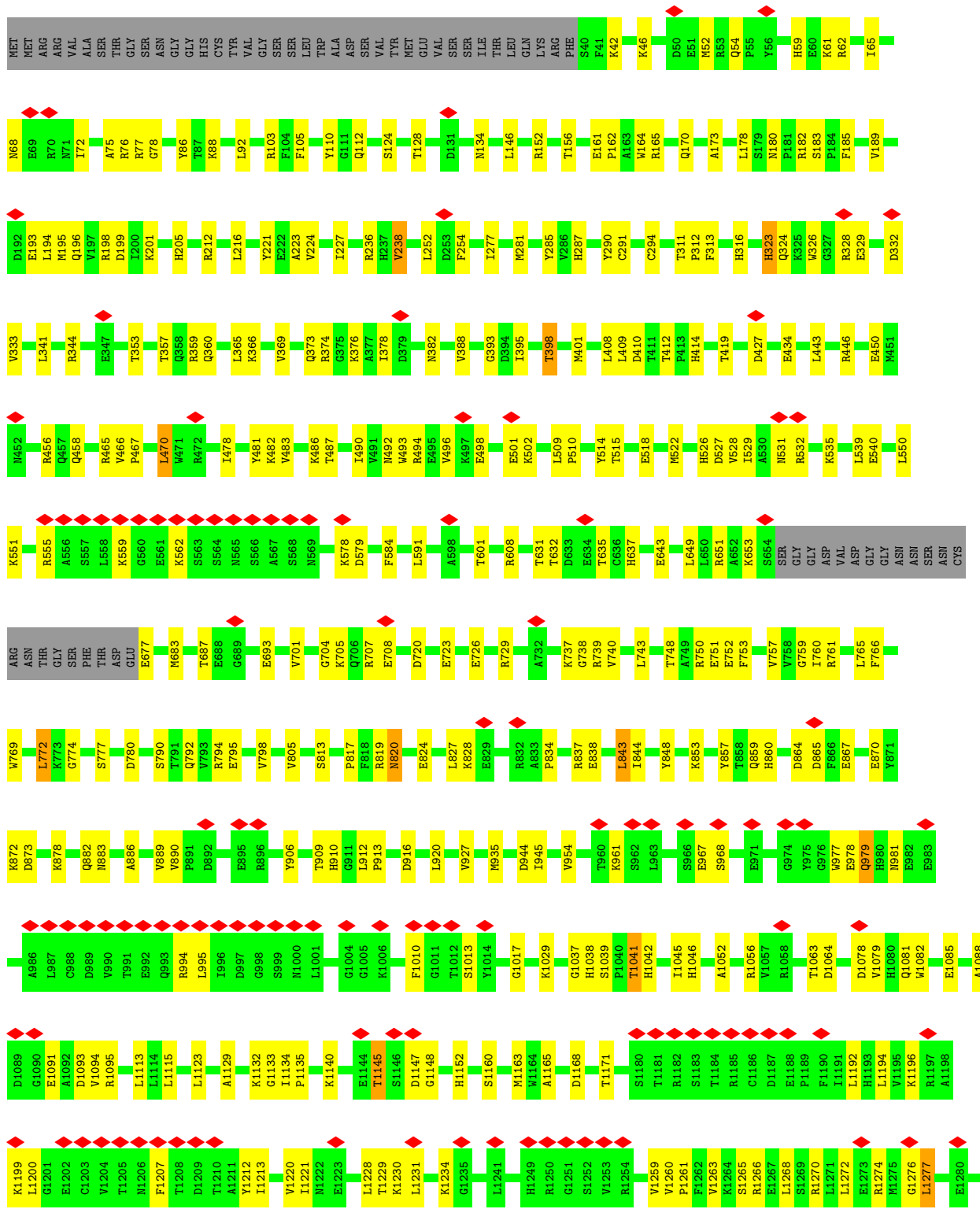


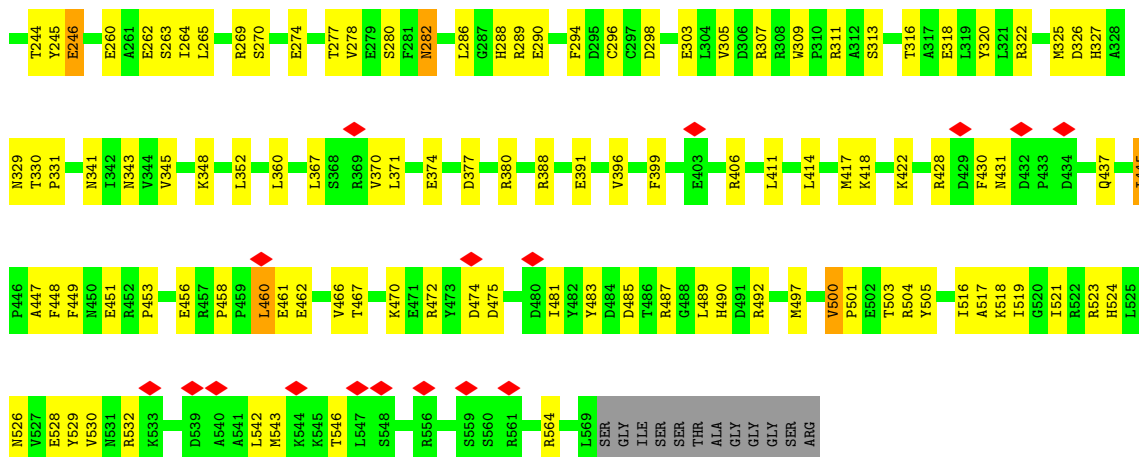
• Molecule 28: Sod_Fe_C domain-containing protein



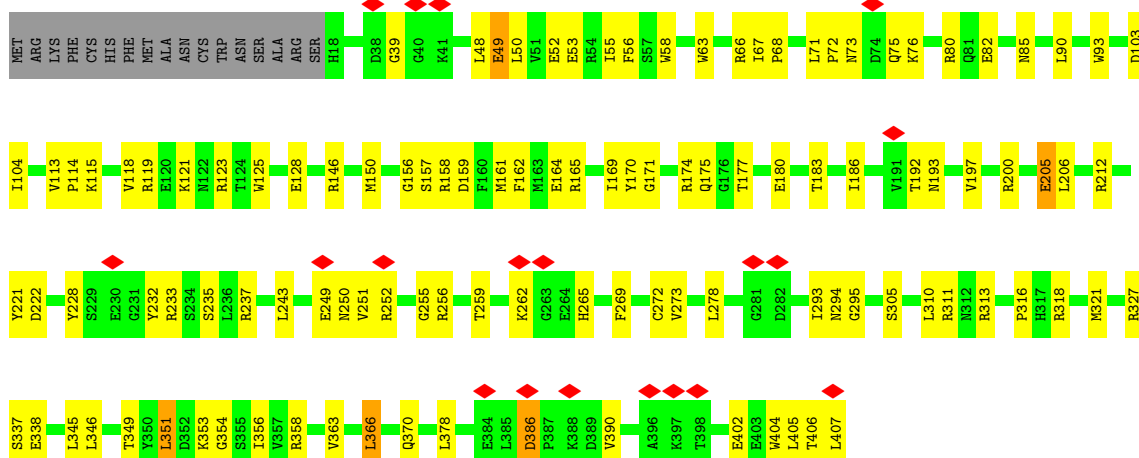
ASP
GLU
MET
ASP
ARG
ALA
VAL
LYS
ASN
ALA
ALA
GLU
ASP
SER
SER
TYR
TRP
ALA
ALA
GLY
GLY
ASP
ASP
VAL
VAL
VAL
VAL
THR
THR
ASP
ASP
ALA
ASN
VAL
VAL
PRO
THR
VAL
MET
GLU
ASP
GLY
ASP
ASP
SER
SER
SER

• Molecule 30: mS48

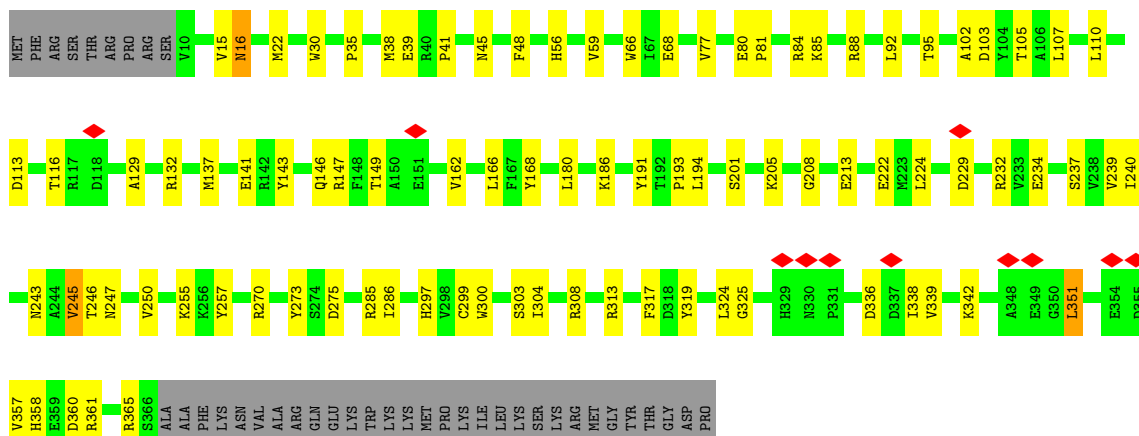




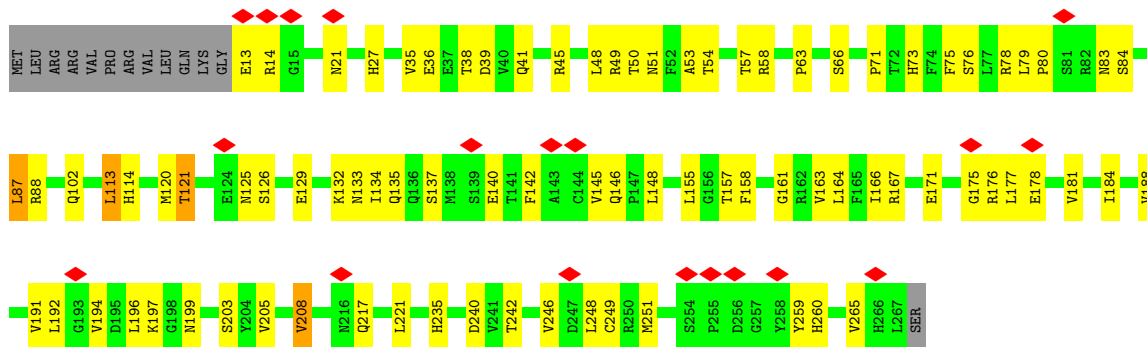
• Molecule 38: mS56



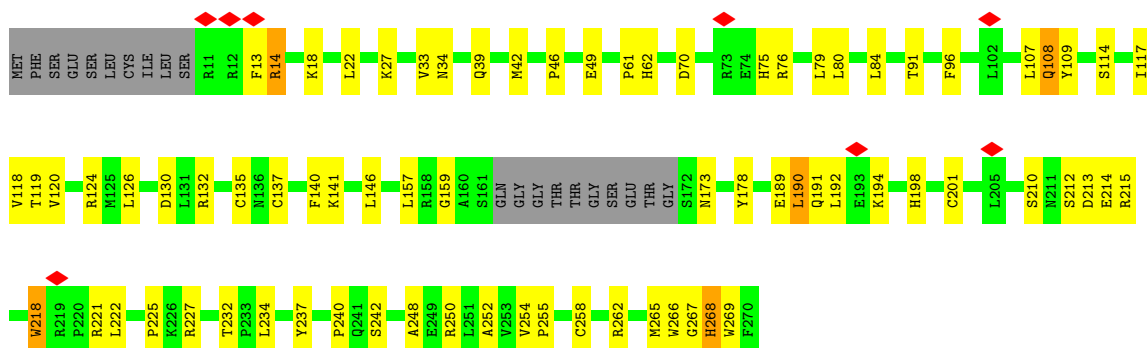
• Molecule 39: mS57



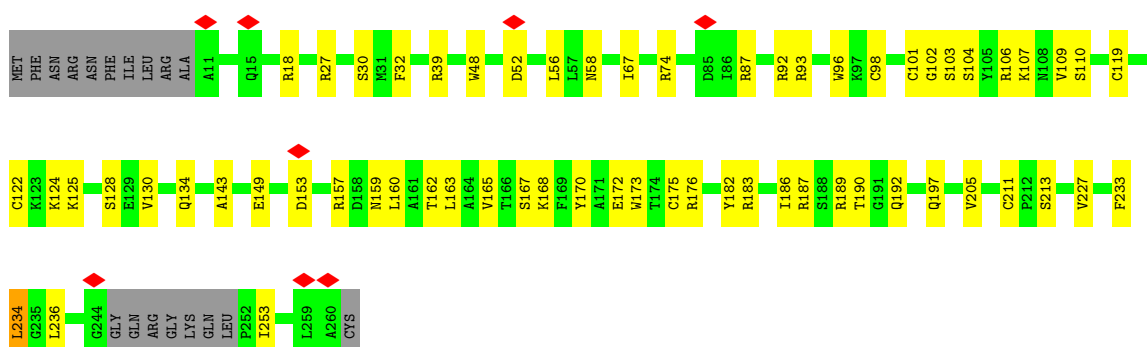
• Molecule 40: mS58



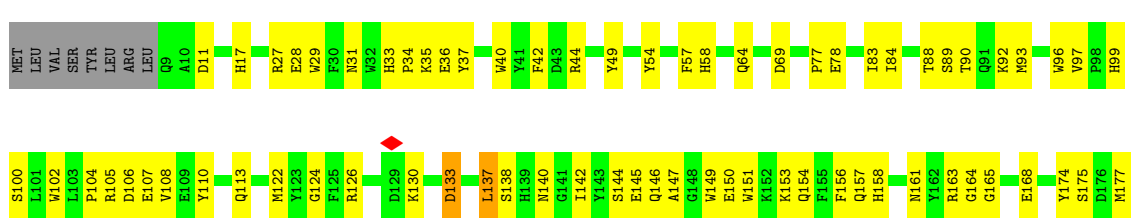
• Molecule 47: mS65



• Molecule 48: mS66

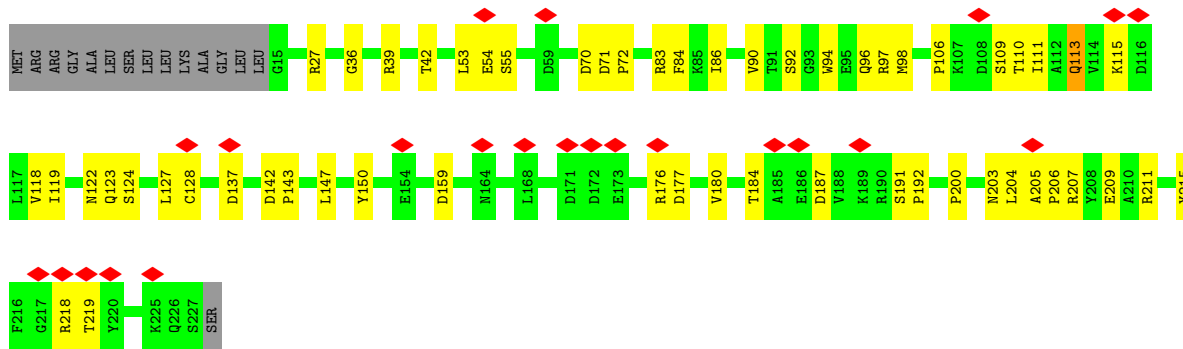


• Molecule 49: Rhodanese domain-containing protein

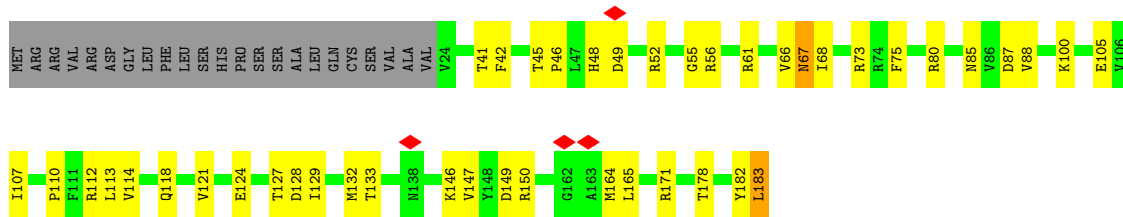




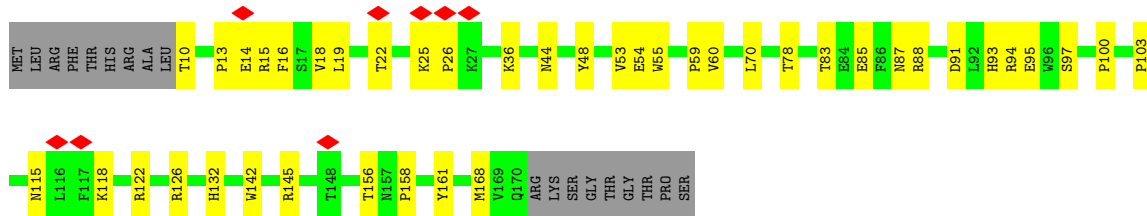
• Molecule 50: Ubiquitin-like domain-containing protein



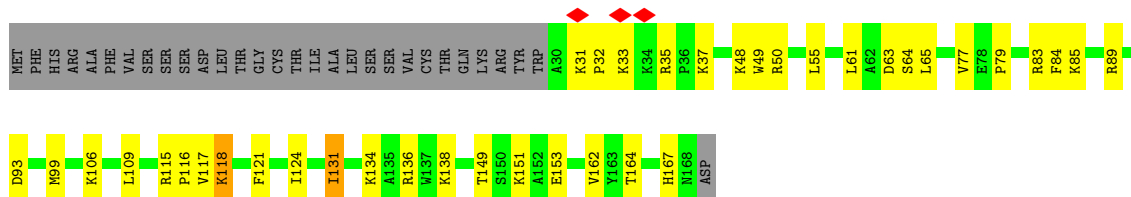
• Molecule 51: mS69



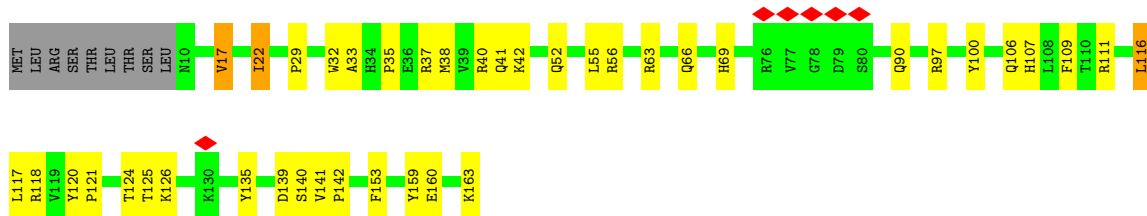
• Molecule 52: mS70



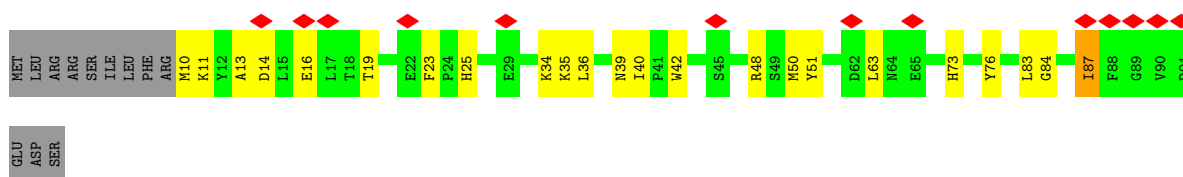
• Molecule 53: mS71



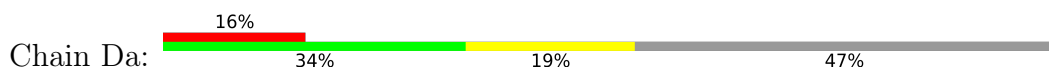
• Molecule 54: mS72



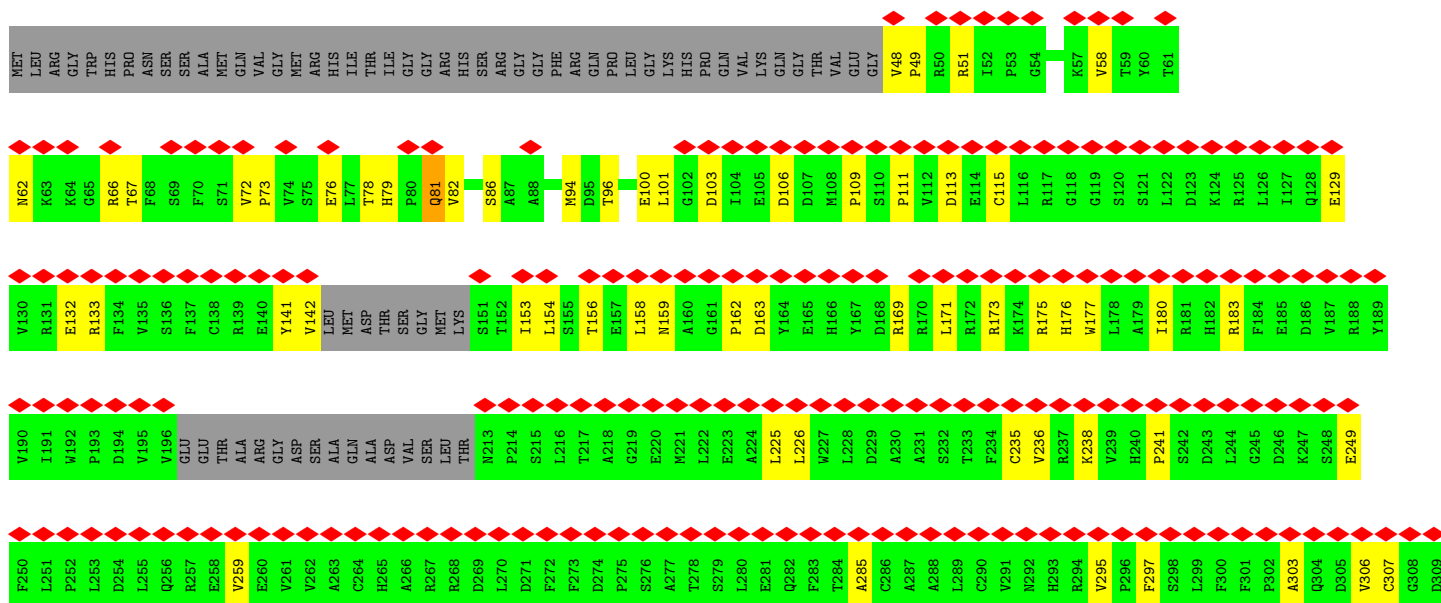
• Molecule 55: mS73

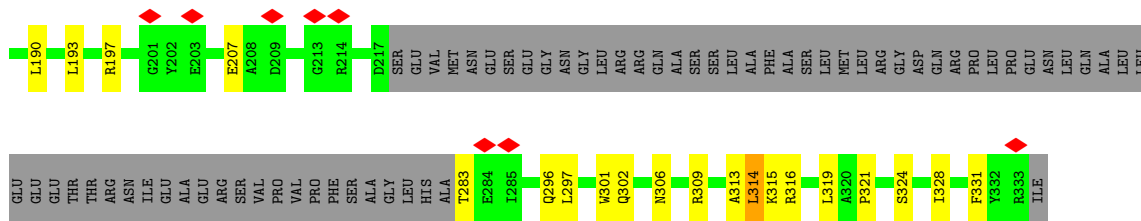


• Molecule 56: mS74

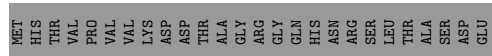
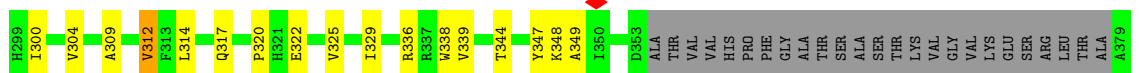
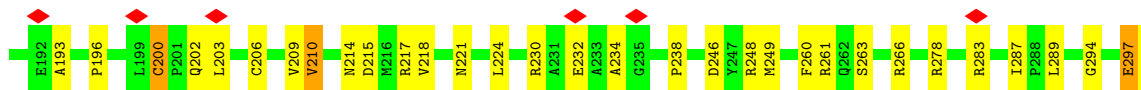
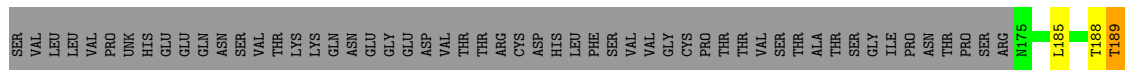
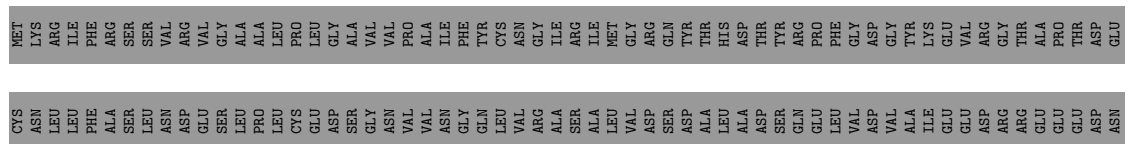


• Molecule 57: mt-SAF3

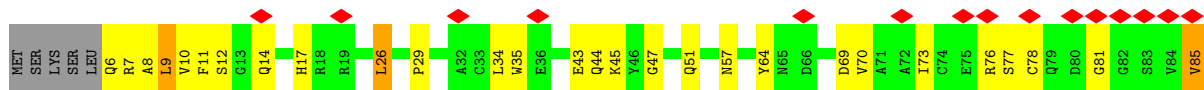


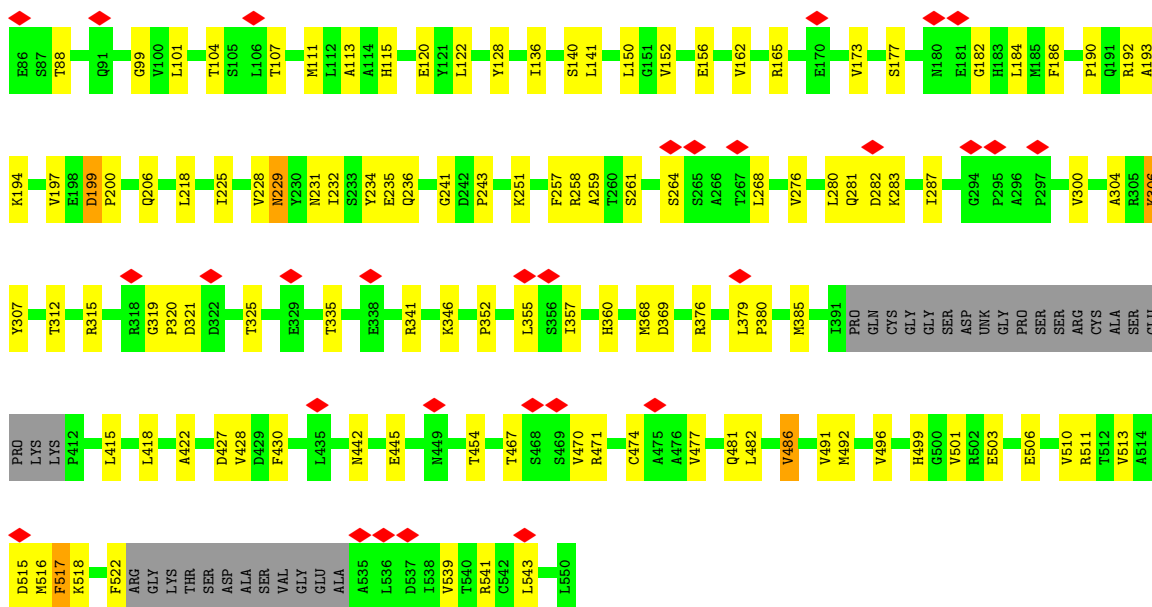


• Molecule 62: DNA photolyase, putative

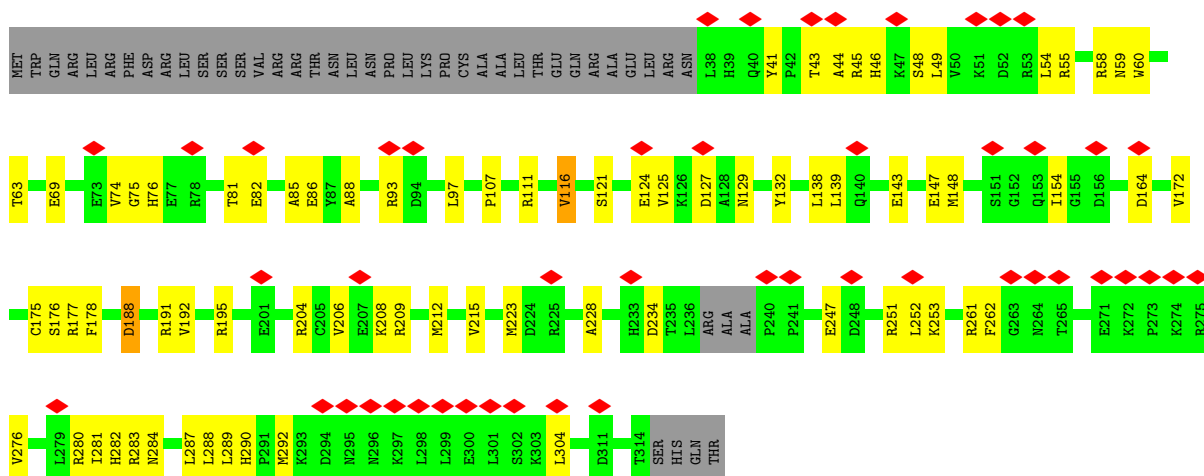


• Molecule 63: Acyl transferase-like protein

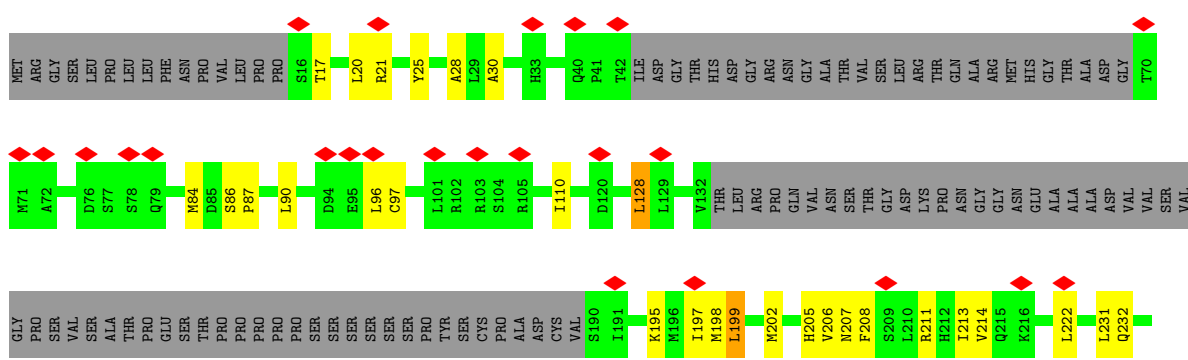


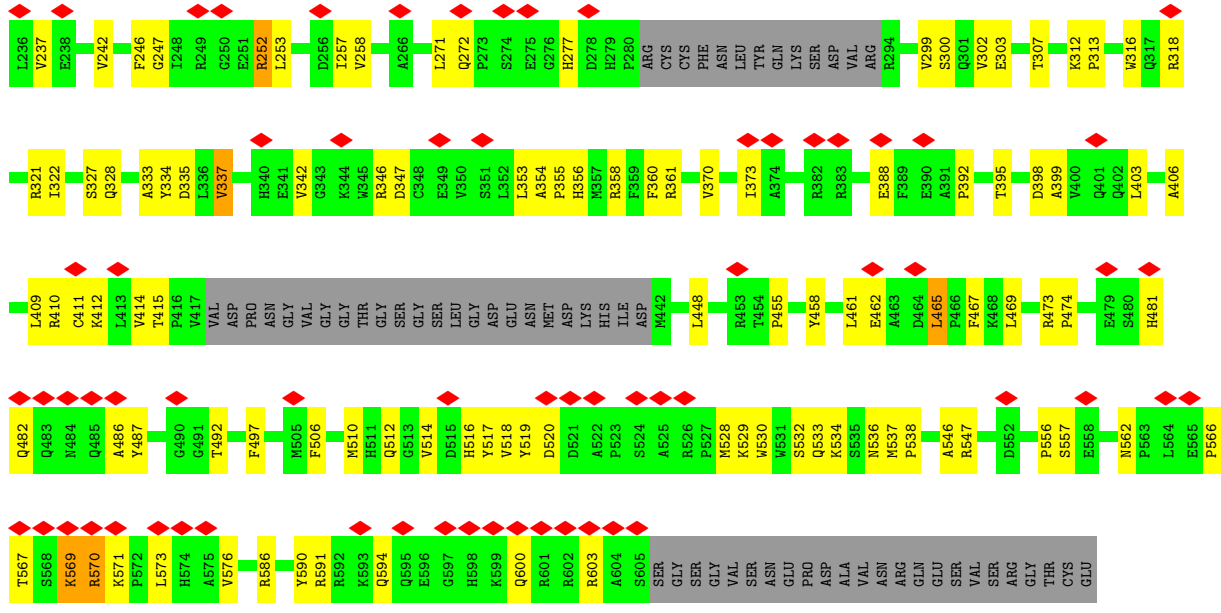


• Molecule 64: mt-SAF37

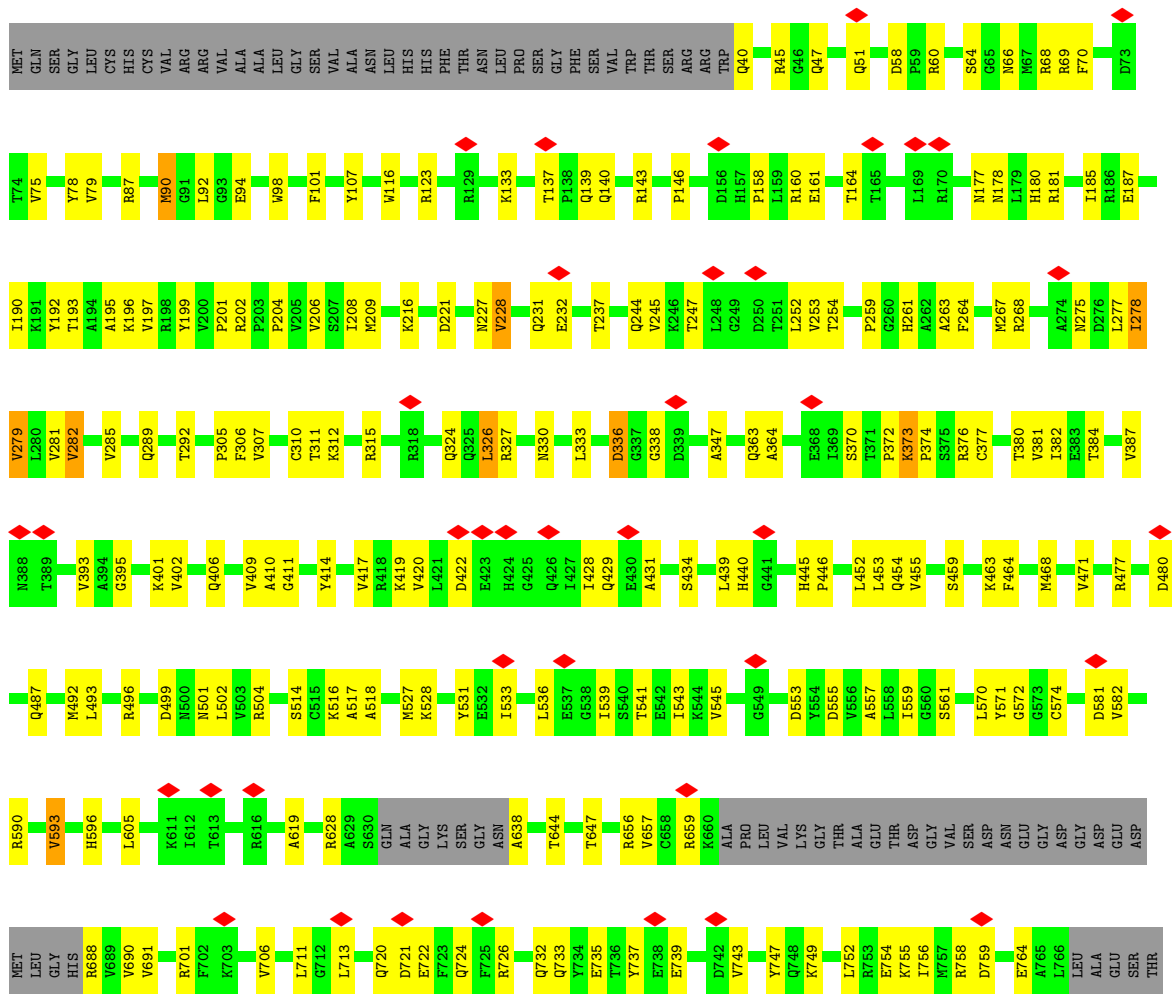


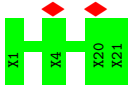
• Molecule 65: mt-SAF38



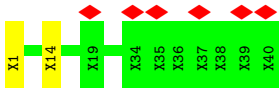


• Molecule 66: Translation initiation factor IF-2, putative

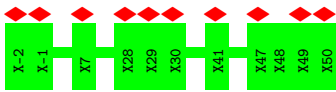




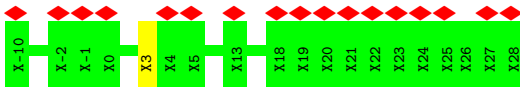
- Molecule 69: Unk7



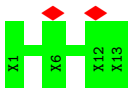
- Molecule 70: UnkE



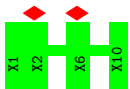
- Molecule 71: UnkF



- Molecule 72: UnkG



- Molecule 73: UnkI

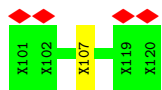


- Molecule 74: UnkK



- Molecule 75: UnkL





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.222	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	500.4, 500.4, 500.4	wwPDB
Map dimensions	360, 360, 360	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: FAD, PO4, ZN, MG, ATP, UTP, GDP

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	CA	0.09	0/13759	0.18	0/21382
2	CC	0.11	0/666	0.29	0/900
3	CE	0.11	0/3547	0.25	0/4798
4	CF	0.10	0/1266	0.24	0/1708
5	CH	0.10	0/2276	0.24	0/3071
6	CI	0.10	0/3479	0.25	0/4693
7	CJ	0.10	0/6725	0.25	0/9152
8	CK	0.09	0/2502	0.24	0/3357
9	CL	0.11	0/759	0.27	0/1026
10	CN	0.11	0/1361	0.25	0/1840
11	CO	0.10	0/2614	0.24	0/3520
12	CP	0.10	0/1533	0.26	0/2074
13	CQ	0.10	0/1919	0.23	0/2595
14	CR	0.10	0/2276	0.24	0/3087
15	CS	0.10	0/1183	0.24	0/1593
16	CU	0.09	0/1560	0.23	0/2094
17	Ca	0.10	0/5066	0.23	0/6852
18	Cb	0.10	0/2105	0.24	0/2842
19	Cd	0.10	0/2016	0.21	0/2715
20	Cg	0.08	0/4016	0.21	0/5455
21	Ci	0.10	0/1383	0.23	0/1871
22	Cj	0.09	0/1849	0.23	0/2521
23	Ck	0.09	0/5540	0.23	0/7490
24	Cm	0.09	0/1215	0.25	0/1630
25	Cn	0.08	0/543	0.22	0/725
26	Cp	0.09	0/1511	0.23	0/2049
27	Cq	0.09	0/2066	0.23	0/2815
28	Cr	0.11	0/2131	0.26	0/2895
29	Cv	0.09	0/8625	0.24	0/11690
30	DA	0.09	0/12744	0.23	0/17248
31	DB	0.10	0/9369	0.24	0/12692
32	DC	0.11	0/8913	0.27	0/12092

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	DD	0.09	0/6699	0.24	0/9072
34	DE	0.10	0/4920	0.26	0/6666
35	DF	0.10	0/4847	0.26	0/6569
36	DG	0.11	0/4578	0.26	0/6202
37	DH	0.11	0/4645	0.28	0/6295
38	DI	0.10	0/3248	0.25	0/4401
39	DJ	0.10	0/2999	0.24	0/4071
40	DK	0.10	0/2123	0.24	0/2865
41	DL	0.10	0/2420	0.24	0/3262
42	DM	0.10	0/2488	0.24	0/3362
43	DN	0.09	0/2118	0.25	0/2874
44	DO	0.11	0/1832	0.27	0/2471
45	DP	0.10	0/1813	0.25	0/2457
46	DQ	0.09	0/2105	0.24	0/2855
47	DR	0.09	0/2084	0.27	0/2841
48	DS	0.08	0/1997	0.22	0/2694
49	DT	0.10	0/2133	0.25	0/2889
50	DU	0.09	0/1799	0.25	0/2438
51	DV	0.11	0/1382	0.28	0/1871
52	DW	0.10	0/1407	0.25	0/1916
53	DX	0.11	0/1207	0.27	0/1620
54	DY	0.11	0/1337	0.27	0/1814
55	DZ	0.10	0/725	0.25	0/984
56	Da	0.08	0/317	0.22	0/422
57	F3	0.08	0/2049	0.22	0/2782
58	F6	0.09	0/3434	0.24	0/4661
59	F7	0.09	0/4684	0.26	0/6341
60	F9	0.10	0/2863	0.25	0/3835
61	FO	0.10	0/2292	0.25	0/3096
62	Ff	0.10	0/5082	0.24	0/6918
63	Fg	0.10	0/4074	0.26	0/5522
64	Fh	0.10	0/2278	0.26	0/3073
65	Fi	0.10	0/3833	0.28	0/5202
66	IA	0.12	0/5512	0.27	0/7462
67	IB	0.10	0/4193	0.26	0/5672
All	All	0.10	0/218034	0.24	0/297947

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	12330	0	6168	233	0
2	CC	646	0	682	23	0
3	CE	3459	0	3440	97	0
4	CF	1240	0	1232	28	0
5	CH	2228	0	2204	48	0
6	CI	3410	0	3384	85	0
7	CJ	6535	0	6274	148	0
8	CK	2447	0	2379	83	0
9	CL	733	0	738	22	0
10	CN	1322	0	1304	55	0
11	CO	2552	0	2554	61	0
12	CP	1489	0	1510	49	0
13	CQ	1866	0	1869	63	0
14	CR	2210	0	2122	74	0
15	CS	1149	0	1154	33	0
16	CU	1522	0	1527	39	0
17	Ca	4911	0	4735	142	0
18	Cb	2056	0	2031	48	0
19	Cd	1961	0	1892	53	0
20	Cg	3895	0	3777	88	0
21	Ci	1343	0	1301	53	0
22	Cj	1799	0	1751	56	0
23	Ck	5442	0	5455	119	0
24	Cm	1184	0	1141	32	0
25	Cn	528	0	563	14	0
26	Cp	1466	0	1426	44	0
27	Cq	2005	0	1916	49	0
28	Cr	2083	0	2107	61	0
29	Cv	8404	0	8091	191	0
30	DA	12448	0	12128	266	0
31	DB	9148	0	8834	240	0
32	DC	8709	0	8502	235	0
33	DD	6513	0	6300	169	0
34	DE	4798	0	4756	119	0
35	DF	4738	0	4717	114	0
36	DG	4482	0	4404	99	0
37	DH	4541	0	4491	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	DI	3182	0	3153	72	0
39	DJ	2914	0	2820	65	0
40	DK	2083	0	2071	61	0
41	DL	2360	0	2352	61	0
42	DM	2430	0	2427	56	0
43	DN	2062	0	2047	63	0
44	DO	1796	0	1746	55	0
45	DP	1760	0	1723	56	0
46	DQ	2055	0	2036	57	0
47	DR	2019	0	2024	61	0
48	DS	1950	0	1904	46	0
49	DT	2058	0	1928	68	0
50	DU	1754	0	1687	38	0
51	DV	1346	0	1335	36	0
52	DW	1359	0	1342	32	0
53	DX	1174	0	1175	32	0
54	DY	1295	0	1290	37	0
55	DZ	697	0	644	23	0
56	Da	305	0	286	11	0
57	F3	2003	0	1945	43	0
58	F6	3358	0	3280	77	0
59	F7	4584	0	4547	115	0
60	F9	2815	0	2745	63	0
61	FO	2236	0	2210	72	0
62	Ff	4941	0	4789	104	0
63	Fg	3994	0	3953	95	0
64	Fh	2230	0	2186	67	0
65	Fi	3734	0	3703	93	0
66	IA	5414	0	5443	144	0
67	IB	4103	0	4045	101	0
68	U6	105	0	23	0	0
68	UJ	105	0	23	0	0
69	U7	200	0	43	3	0
70	UE	265	0	56	0	0
71	UF	195	0	44	1	0
72	UG	65	0	15	0	0
73	UI	50	0	12	0	0
74	UK	15	0	6	1	0
75	UL	100	0	22	1	0
76	CA	3	0	0	0	0
76	CQ	1	0	0	0	0
76	Cg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	IA	1	0	0	0	0
77	Cg	31	0	12	0	0
78	Cr	1	0	0	0	0
78	DA	1	0	0	0	0
78	DS	2	0	0	0	0
79	DJ	29	0	11	3	0
80	Ff	53	0	31	0	0
81	IA	28	0	12	1	0
82	IA	5	0	0	1	0
83	Cg	3	0	0	0	0
83	IA	2	0	0	0	0
All	All	212864	0	202005	4246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4246 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DE:33:ILE:N	34:DE:547:THR:HG1	1.66	0.93
7:CJ:716:ARG:HE	21:CI:77:ARG:HE	1.20	0.85
57:F3:103:ASP:HB2	61:FO:65:ARG:HH22	1.42	0.85
11:CO:263:LEU:O	11:CO:274:TYR:OH	1.96	0.83
36:DG:292:GLU:O	36:DG:296:ASP:HB2	1.79	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	CC	72/74 (97%)	66 (92%)	6 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CE	424/435 (98%)	406 (96%)	18 (4%)	0	100	100
4	CF	145/160 (91%)	139 (96%)	6 (4%)	0	100	100
5	CH	271/282 (96%)	263 (97%)	8 (3%)	0	100	100
6	CI	423/443 (96%)	411 (97%)	12 (3%)	0	100	100
7	CJ	799/817 (98%)	771 (96%)	28 (4%)	0	100	100
8	CK	294/326 (90%)	284 (97%)	10 (3%)	0	100	100
9	CL	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
10	CN	155/166 (93%)	149 (96%)	6 (4%)	0	100	100
11	CO	306/429 (71%)	292 (95%)	14 (5%)	0	100	100
12	CP	178/188 (95%)	171 (96%)	7 (4%)	0	100	100
13	CQ	224/307 (73%)	219 (98%)	5 (2%)	0	100	100
14	CR	265/320 (83%)	258 (97%)	7 (3%)	0	100	100
15	CS	137/244 (56%)	132 (96%)	5 (4%)	0	100	100
16	CU	179/193 (93%)	175 (98%)	4 (2%)	0	100	100
17	Ca	571/602 (95%)	549 (96%)	22 (4%)	0	100	100
18	Cb	248/325 (76%)	236 (95%)	12 (5%)	0	100	100
19	Cd	228/440 (52%)	223 (98%)	5 (2%)	0	100	100
20	Cg	478/498 (96%)	473 (99%)	5 (1%)	0	100	100
21	Ci	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
22	Cj	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
23	Ck	676/874 (77%)	666 (98%)	10 (2%)	0	100	100
24	Cm	143/215 (66%)	138 (96%)	5 (4%)	0	100	100
25	Cn	60/250 (24%)	59 (98%)	1 (2%)	0	100	100
26	Cp	171/187 (91%)	167 (98%)	4 (2%)	0	100	100
27	Cq	250/263 (95%)	241 (96%)	9 (4%)	0	100	100
28	Cr	263/439 (60%)	258 (98%)	5 (2%)	0	100	100
29	Cv	1032/1211 (85%)	994 (96%)	38 (4%)	0	100	100
30	DA	1546/1788 (86%)	1513 (98%)	33 (2%)	0	100	100
31	DB	1109/1181 (94%)	1076 (97%)	33 (3%)	0	100	100
32	DC	1081/1165 (93%)	1023 (95%)	58 (5%)	0	100	100
33	DD	786/812 (97%)	758 (96%)	28 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DE	576/747 (77%)	549 (95%)	27 (5%)	0	100	100
35	DF	585/666 (88%)	559 (96%)	26 (4%)	0	100	100
36	DG	542/631 (86%)	529 (98%)	13 (2%)	0	100	100
37	DH	555/581 (96%)	530 (96%)	25 (4%)	0	100	100
38	DI	388/407 (95%)	372 (96%)	16 (4%)	0	100	100
39	DJ	355/396 (90%)	351 (99%)	4 (1%)	0	100	100
40	DK	257/324 (79%)	249 (97%)	8 (3%)	0	100	100
41	DL	287/307 (94%)	283 (99%)	4 (1%)	0	100	100
42	DM	292/294 (99%)	277 (95%)	15 (5%)	0	100	100
43	DN	249/293 (85%)	243 (98%)	6 (2%)	0	100	100
44	DO	219/282 (78%)	207 (94%)	12 (6%)	0	100	100
45	DP	205/274 (75%)	198 (97%)	7 (3%)	0	100	100
46	DQ	253/268 (94%)	249 (98%)	4 (2%)	0	100	100
47	DR	246/270 (91%)	240 (98%)	6 (2%)	0	100	100
48	DS	239/261 (92%)	238 (100%)	1 (0%)	0	100	100
49	DT	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
50	DU	211/228 (92%)	204 (97%)	7 (3%)	0	100	100
51	DV	158/183 (86%)	144 (91%)	14 (9%)	0	100	100
52	DW	159/179 (89%)	152 (96%)	7 (4%)	0	100	100
53	DX	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
54	DY	152/163 (93%)	145 (95%)	7 (5%)	0	100	100
55	DZ	80/94 (85%)	78 (98%)	2 (2%)	0	100	100
56	Da	32/64 (50%)	31 (97%)	1 (3%)	0	100	100
57	F3	246/966 (26%)	243 (99%)	3 (1%)	0	100	100
58	F6	410/676 (61%)	402 (98%)	8 (2%)	0	100	100
59	F7	566/679 (83%)	544 (96%)	22 (4%)	0	100	100
60	F9	338/608 (56%)	329 (97%)	9 (3%)	0	100	100
61	FO	263/334 (79%)	255 (97%)	8 (3%)	0	100	100
62	Ff	610/848 (72%)	593 (97%)	17 (3%)	0	100	100
63	Fg	507/550 (92%)	487 (96%)	20 (4%)	0	100	100
64	Fh	270/318 (85%)	259 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	Fi	459/629 (73%)	438 (95%)	21 (5%)	0	100	100
66	IA	687/787 (87%)	668 (97%)	19 (3%)	0	100	100
67	IB	507/803 (63%)	491 (97%)	16 (3%)	0	100	100
All	All	24263/29685 (82%)	23456 (97%)	807 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CC	73/73 (100%)	68 (93%)	5 (7%)	14	42
3	CE	365/372 (98%)	353 (97%)	12 (3%)	33	55
4	CF	135/144 (94%)	132 (98%)	3 (2%)	45	63
5	CH	237/246 (96%)	235 (99%)	2 (1%)	73	76
6	CI	360/371 (97%)	352 (98%)	8 (2%)	45	63
7	CJ	710/723 (98%)	686 (97%)	24 (3%)	32	55
8	CK	259/283 (92%)	254 (98%)	5 (2%)	50	65
9	CL	79/79 (100%)	76 (96%)	3 (4%)	29	53
10	CN	142/150 (95%)	136 (96%)	6 (4%)	26	51
11	CO	270/377 (72%)	262 (97%)	8 (3%)	36	57
12	CP	160/168 (95%)	157 (98%)	3 (2%)	50	65
13	CQ	201/270 (74%)	193 (96%)	8 (4%)	28	52
14	CR	233/279 (84%)	224 (96%)	9 (4%)	28	53
15	CS	123/220 (56%)	119 (97%)	4 (3%)	33	55
16	CU	159/169 (94%)	157 (99%)	2 (1%)	61	71
17	Ca	518/543 (95%)	508 (98%)	10 (2%)	50	65
18	Cb	219/277 (79%)	213 (97%)	6 (3%)	39	59
19	Cd	207/381 (54%)	205 (99%)	2 (1%)	68	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Cg	424/437 (97%)	416 (98%)	8 (2%)	50	65
21	Ci	144/160 (90%)	139 (96%)	5 (4%)	32	54
22	Cj	194/219 (89%)	192 (99%)	2 (1%)	68	74
23	Ck	589/746 (79%)	578 (98%)	11 (2%)	50	65
24	Cm	124/184 (67%)	122 (98%)	2 (2%)	55	68
25	Cn	54/210 (26%)	51 (94%)	3 (6%)	19	46
26	Cp	161/175 (92%)	156 (97%)	5 (3%)	35	57
27	Cq	210/221 (95%)	204 (97%)	6 (3%)	37	57
28	Cr	223/369 (60%)	215 (96%)	8 (4%)	31	54
29	Cv	894/1033 (86%)	869 (97%)	25 (3%)	38	58
30	DA	1319/1514 (87%)	1273 (96%)	46 (4%)	32	54
31	DB	976/1030 (95%)	953 (98%)	23 (2%)	43	61
32	DC	923/985 (94%)	889 (96%)	34 (4%)	30	54
33	DD	693/711 (98%)	671 (97%)	22 (3%)	34	56
34	DE	514/642 (80%)	501 (98%)	13 (2%)	42	61
35	DF	499/560 (89%)	481 (96%)	18 (4%)	31	54
36	DG	481/543 (89%)	464 (96%)	17 (4%)	32	54
37	DH	489/504 (97%)	470 (96%)	19 (4%)	28	53
38	DI	350/365 (96%)	341 (97%)	9 (3%)	40	60
39	DJ	313/347 (90%)	302 (96%)	11 (4%)	32	54
40	DK	218/261 (84%)	208 (95%)	10 (5%)	24	49
41	DL	249/263 (95%)	243 (98%)	6 (2%)	43	61
42	DM	252/252 (100%)	248 (98%)	4 (2%)	55	68
43	DN	225/256 (88%)	216 (96%)	9 (4%)	28	52
44	DO	185/229 (81%)	182 (98%)	3 (2%)	55	68
45	DP	187/239 (78%)	184 (98%)	3 (2%)	55	68
46	DQ	227/239 (95%)	219 (96%)	8 (4%)	32	54
47	DR	219/235 (93%)	210 (96%)	9 (4%)	27	52
48	DS	213/228 (93%)	208 (98%)	5 (2%)	44	62
49	DT	220/228 (96%)	212 (96%)	8 (4%)	31	54
50	DU	190/201 (94%)	185 (97%)	5 (3%)	40	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	DV	145/165 (88%)	137 (94%)	8 (6%)	19	46
52	DW	148/163 (91%)	145 (98%)	3 (2%)	48	64
53	DX	122/149 (82%)	118 (97%)	4 (3%)	33	55
54	DY	137/146 (94%)	134 (98%)	3 (2%)	45	63
55	DZ	72/84 (86%)	69 (96%)	3 (4%)	26	51
56	Da	30/59 (51%)	30 (100%)	0	100	100
57	F3	223/809 (28%)	217 (97%)	6 (3%)	39	59
58	F6	368/590 (62%)	350 (95%)	18 (5%)	22	48
59	F7	493/577 (85%)	474 (96%)	19 (4%)	28	53
60	F9	288/504 (57%)	284 (99%)	4 (1%)	59	70
61	FO	234/290 (81%)	226 (97%)	8 (3%)	32	55
62	Ff	519/715 (73%)	499 (96%)	20 (4%)	28	53
63	Fg	441/469 (94%)	426 (97%)	15 (3%)	32	55
64	Fh	242/281 (86%)	237 (98%)	5 (2%)	47	64
65	Fi	404/536 (75%)	389 (96%)	15 (4%)	30	54
66	IA	586/661 (89%)	560 (96%)	26 (4%)	25	50
67	IB	435/675 (64%)	420 (97%)	15 (3%)	32	55
All	All	21296/25584 (83%)	20647 (97%)	649 (3%)	37	57

5 of 649 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	DS	253	ILE
63	Fg	9	LEU
50	DU	147	LEU
48	DS	234	LEU
58	F6	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 426 such sidechains are listed below:

Mol	Chain	Res	Type
33	DD	176	HIS
39	DJ	146	GLN
65	Fi	218	HIS
33	DD	585	ASN

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Mol	Chain	Res	Type
36	DG	12	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	620/621 (99%)	252 (40%)	2 (0%)

5 of 252 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	CA	2	A
1	CA	3	A
1	CA	4	A
1	CA	6	U
1	CA	11	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	299	U
1	CA	512	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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$
82	PO4	IA	1001	76	4,4,4	0.96	0	6,6,6	0.47	0
81	GDP	IA	1000	76	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
79	UTP	DJ	401	-	29,30,30	0.57	0	43,47,47	0.70	0
80	FAD	Ff	901	-	58,58,58	0.32	0	85,89,89	0.27	0
77	ATP	Cg	1000	76	32,33,33	0.34	0	48,52,52	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	GDP	IA	1000	76	-	2/16/32/32	0/3/3/3
80	FAD	Ff	901	-	-	11/34/50/50	0/6/6/6
77	ATP	Cg	1000	76	-	3/22/38/38	0/3/3/3
79	UTP	DJ	401	-	-	4/22/38/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	IA	1000	GDP	C5-C4	3.12	1.47	1.38
81	IA	1000	GDP	C6-N1	-2.42	1.34	1.38
81	IA	1000	GDP	C5-N7	-2.08	1.34	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	IA	1000	GDP	C5-C4-N3	-6.03	118.79	128.39
81	IA	1000	GDP	C2-N3-C4	4.98	120.88	112.30
81	IA	1000	GDP	N9-C4-N3	4.52	134.99	125.95
81	IA	1000	GDP	C6-C5-N7	3.20	136.11	130.29
81	IA	1000	GDP	C4-C5-N7	-2.46	106.77	110.67

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
79	DJ	401	UTP	O4'-C1'-N1-C2

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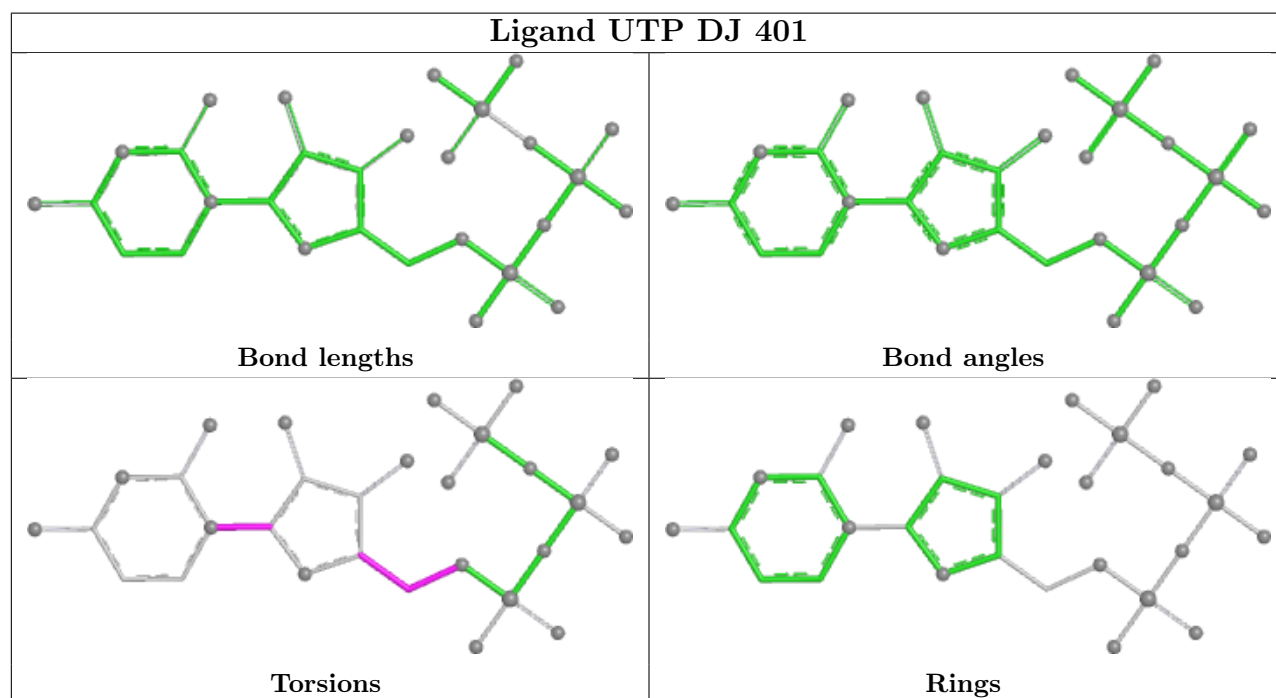
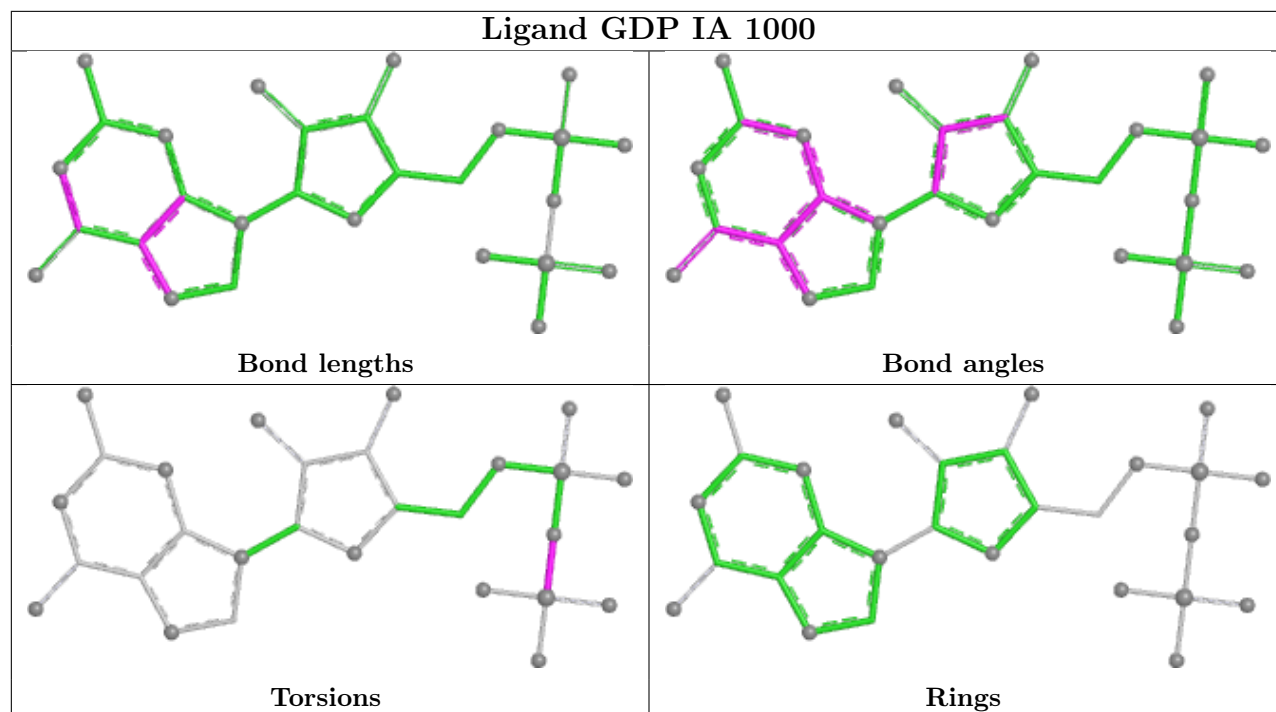
Mol	Chain	Res	Type	Atoms
80	Ff	901	FAD	C5B-O5B-PA-O3P
80	Ff	901	FAD	N10-C1'-C2'-O2'
80	Ff	901	FAD	N10-C1'-C2'-C3'
80	Ff	901	FAD	C2'-C3'-C4'-O4'

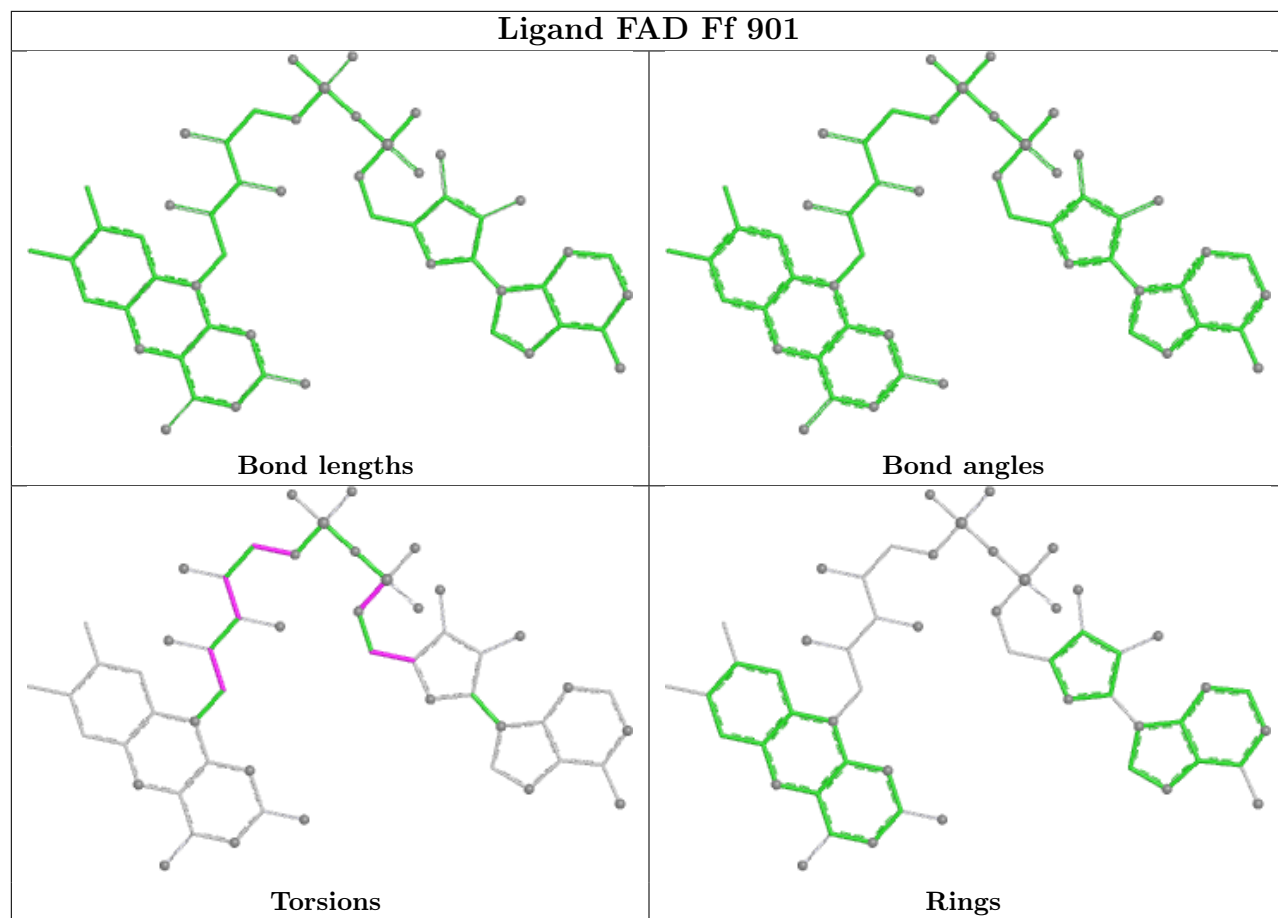
There are no ring outliers.

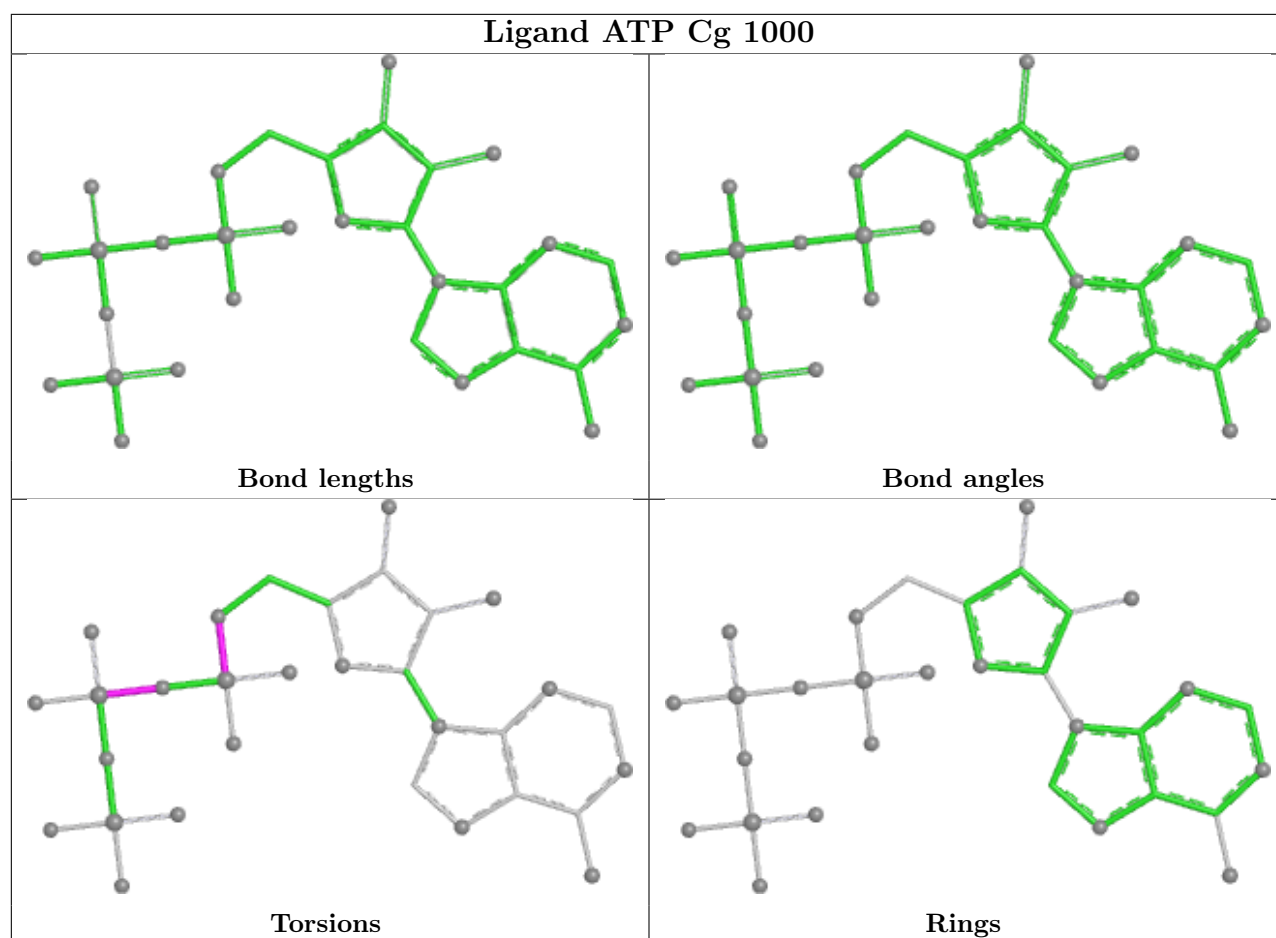
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	IA	1001	PO4	1	0
81	IA	1000	GDP	1	0
79	DJ	401	UTP	3	0

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







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

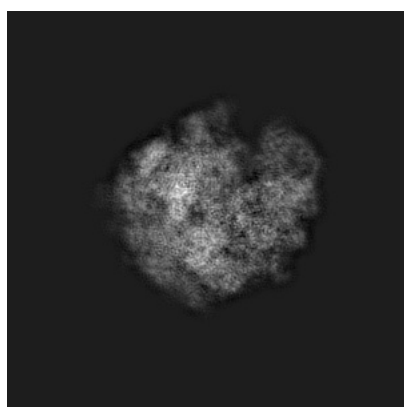
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13661. These allow visual inspection of the internal detail of the map and identification of artifacts.

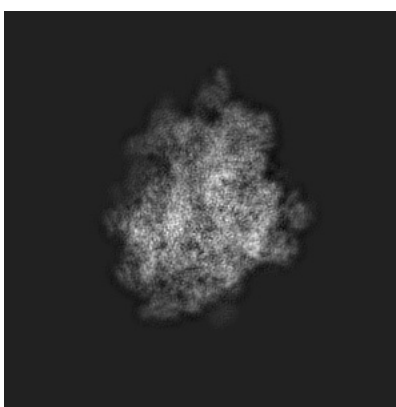
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

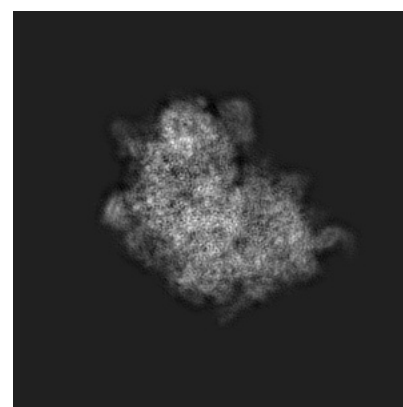
6.1.1 Primary map



X



Y

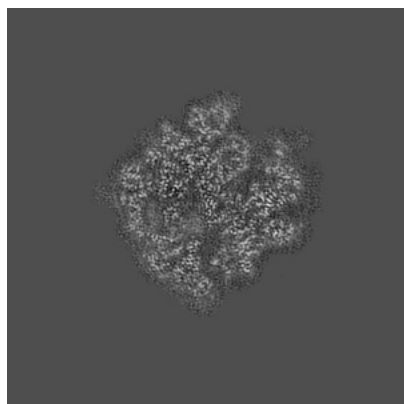


Z

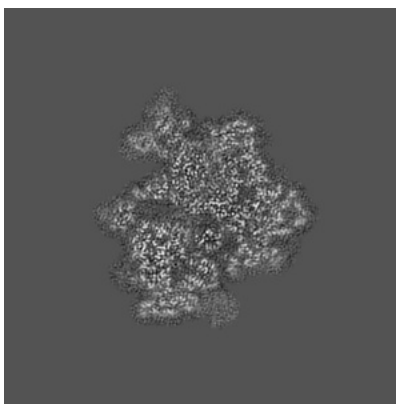
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

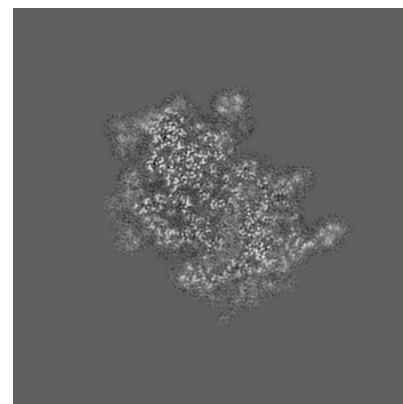
6.2.1 Primary map



X Index: 180



Y Index: 180

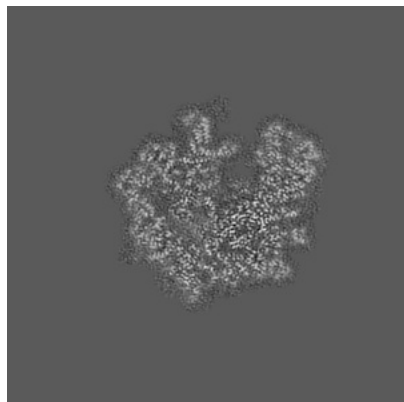


Z Index: 180

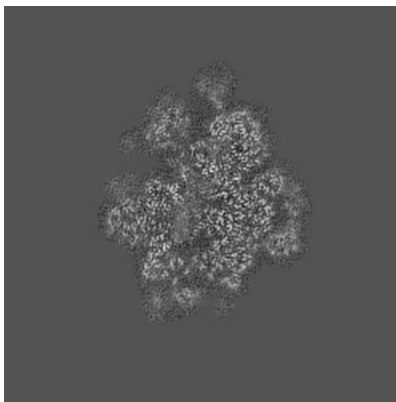
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

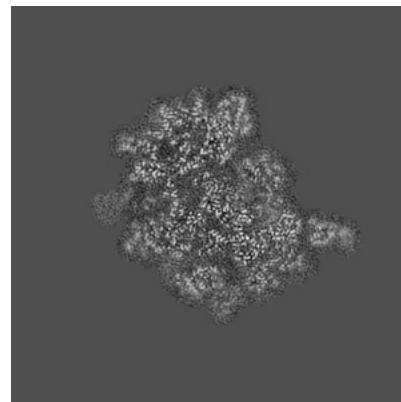
6.3.1 Primary map



X Index: 158



Y Index: 165

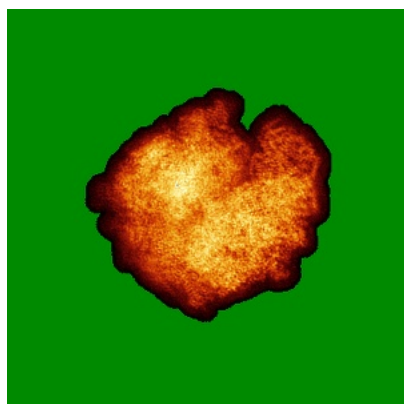


Z Index: 192

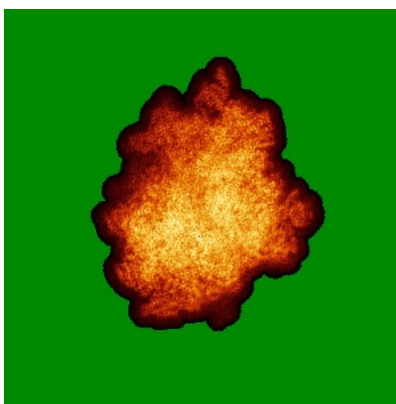
The images above show the largest variance slices of the map in three orthogonal directions.

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

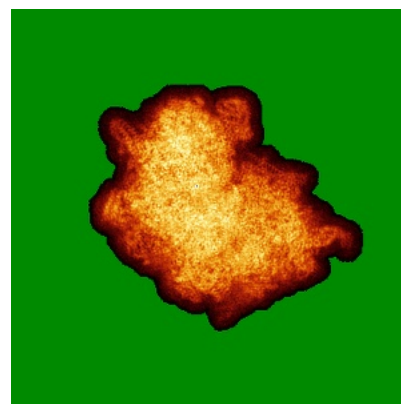
6.4.1 Primary map



X



Y

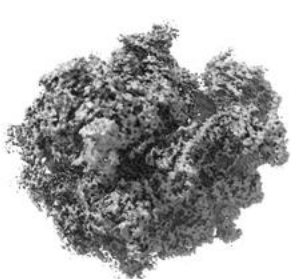


Z

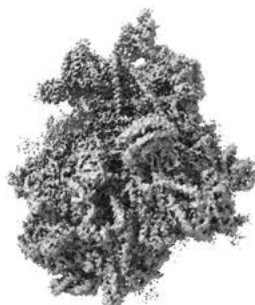
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

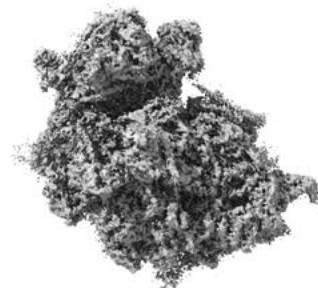
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

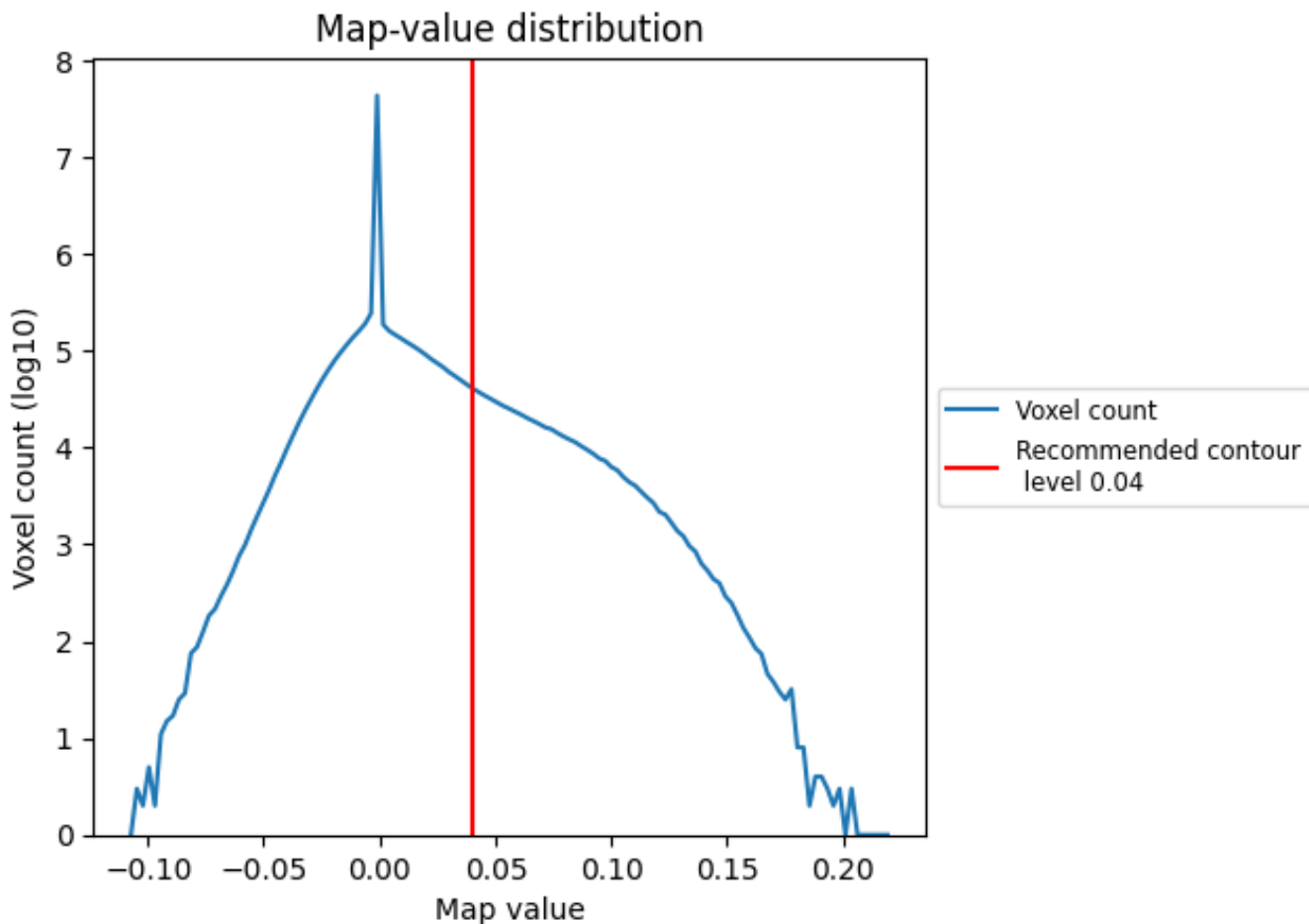
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

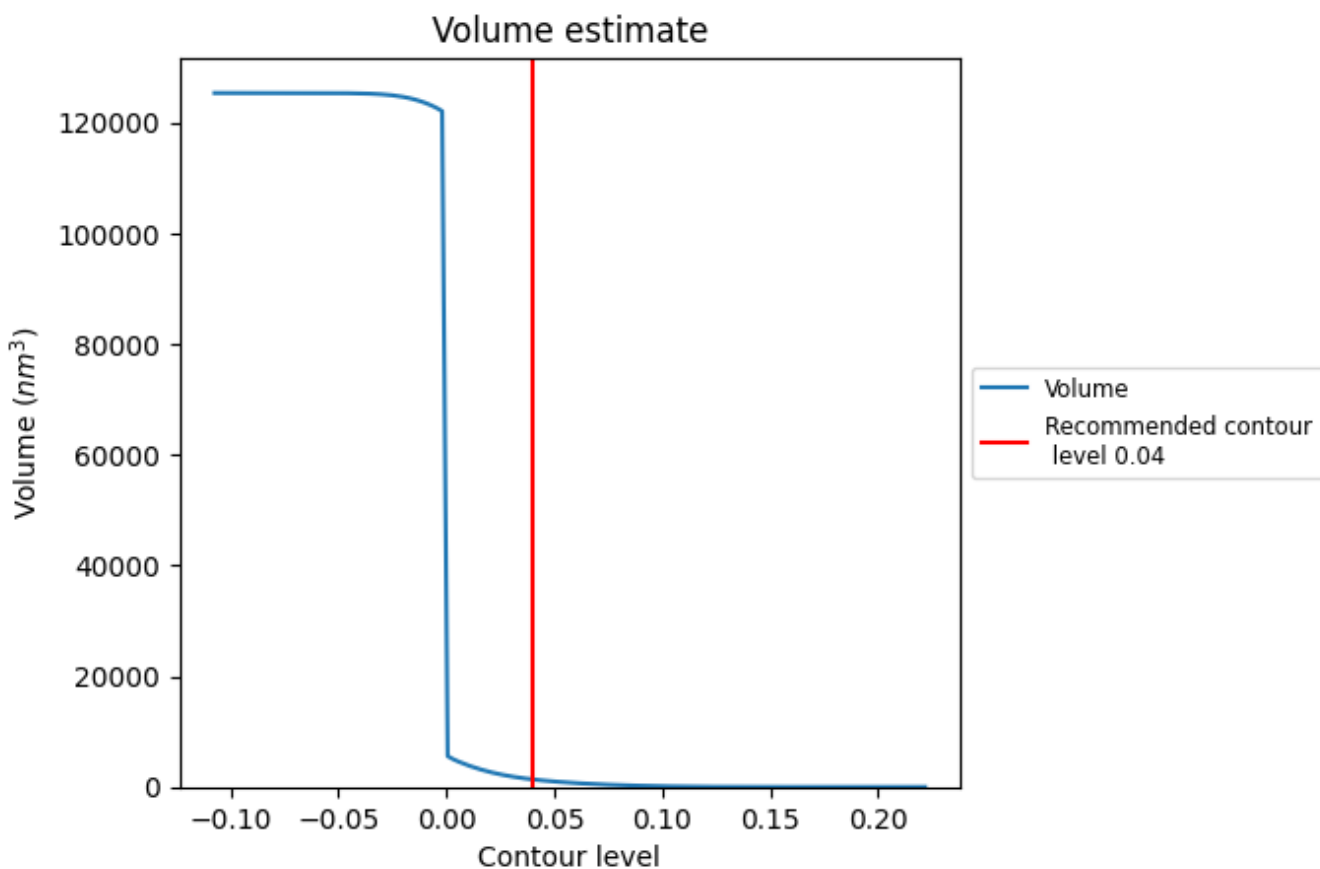
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

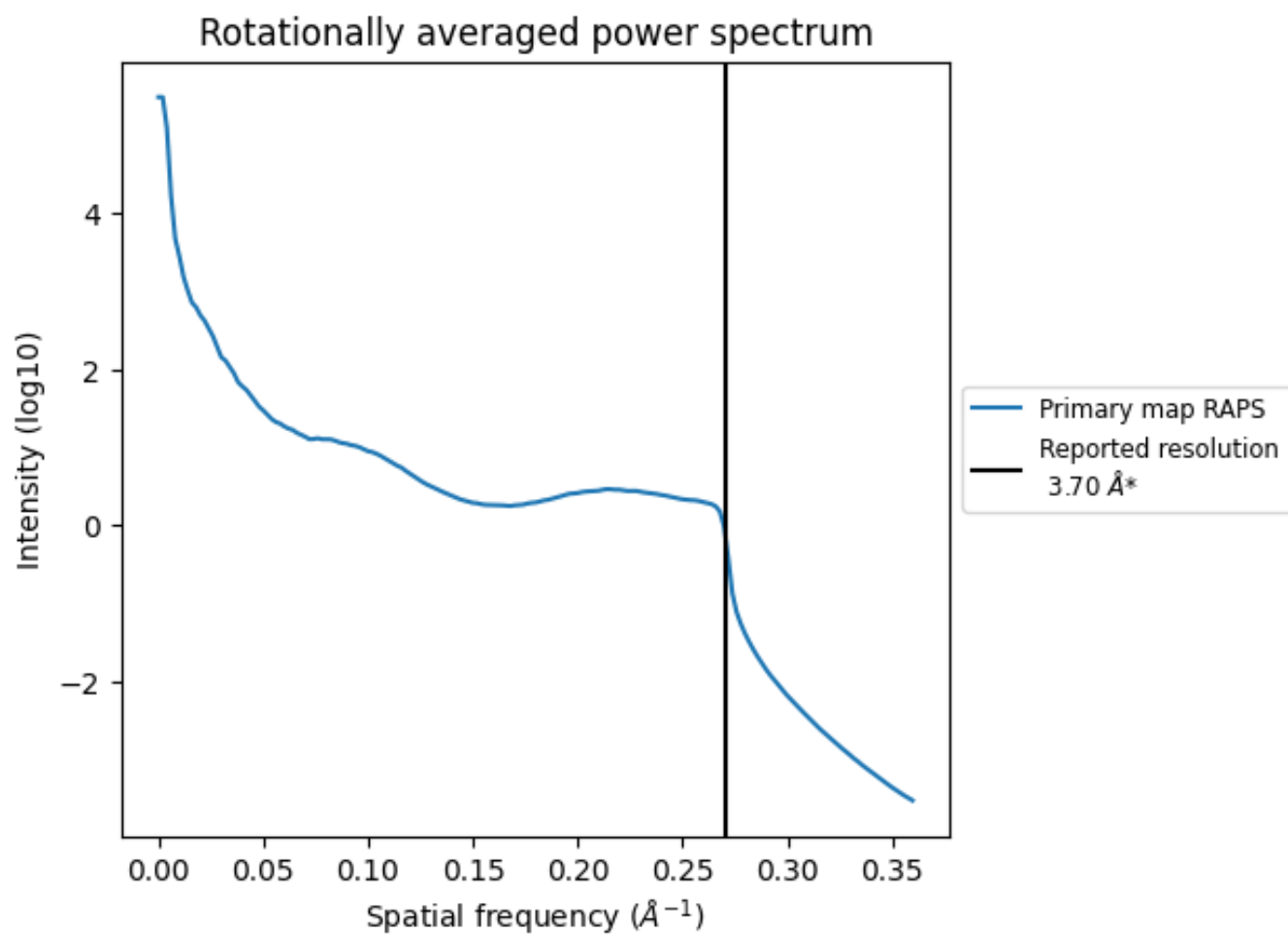
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1367 nm³; this corresponds to an approximate mass of 1235 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 0.270\AA^{-1}

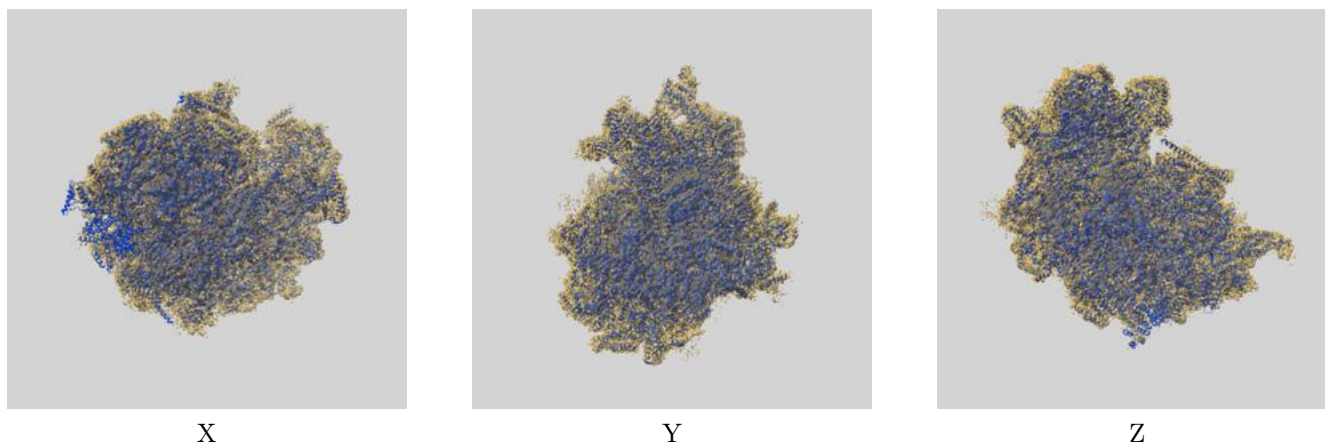
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

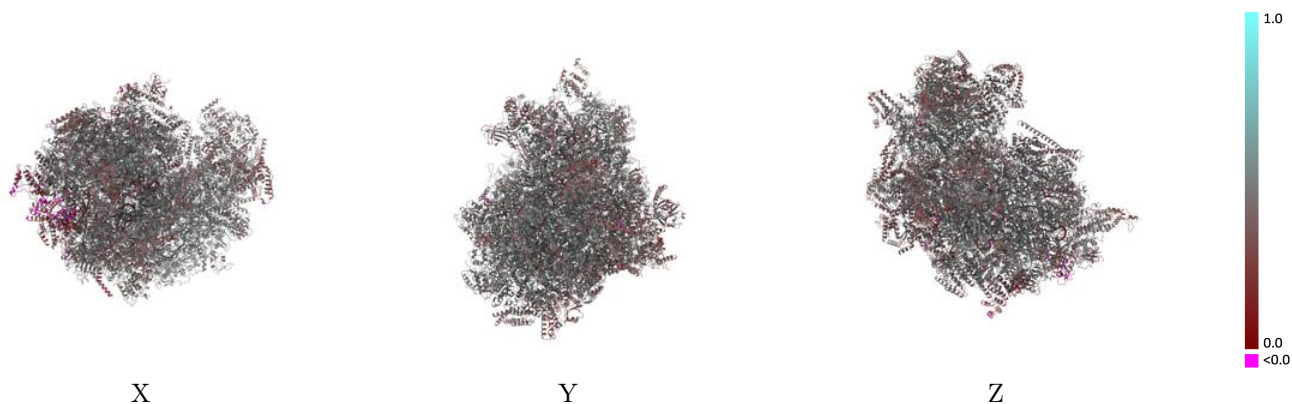
This section contains information regarding the fit between EMDB map EMD-13661 and PDB model 7PUB. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



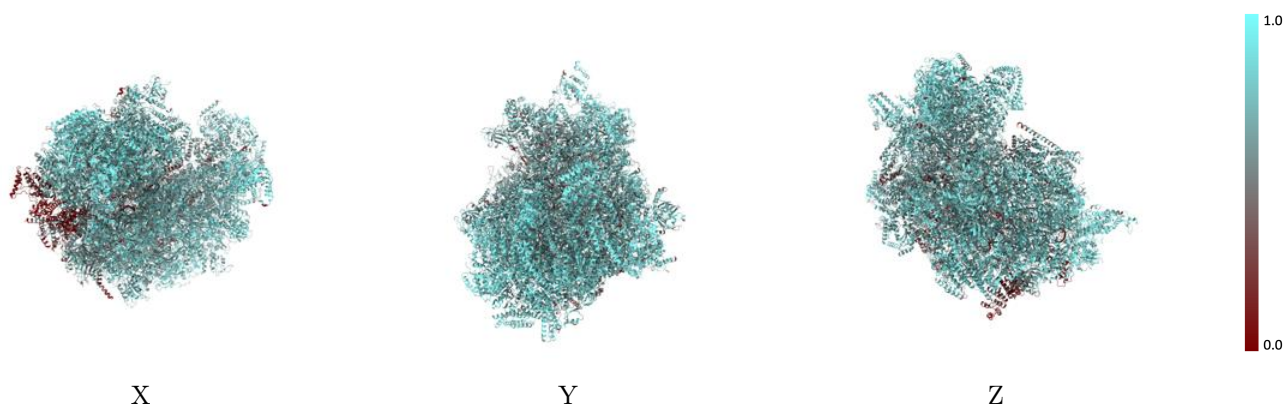
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



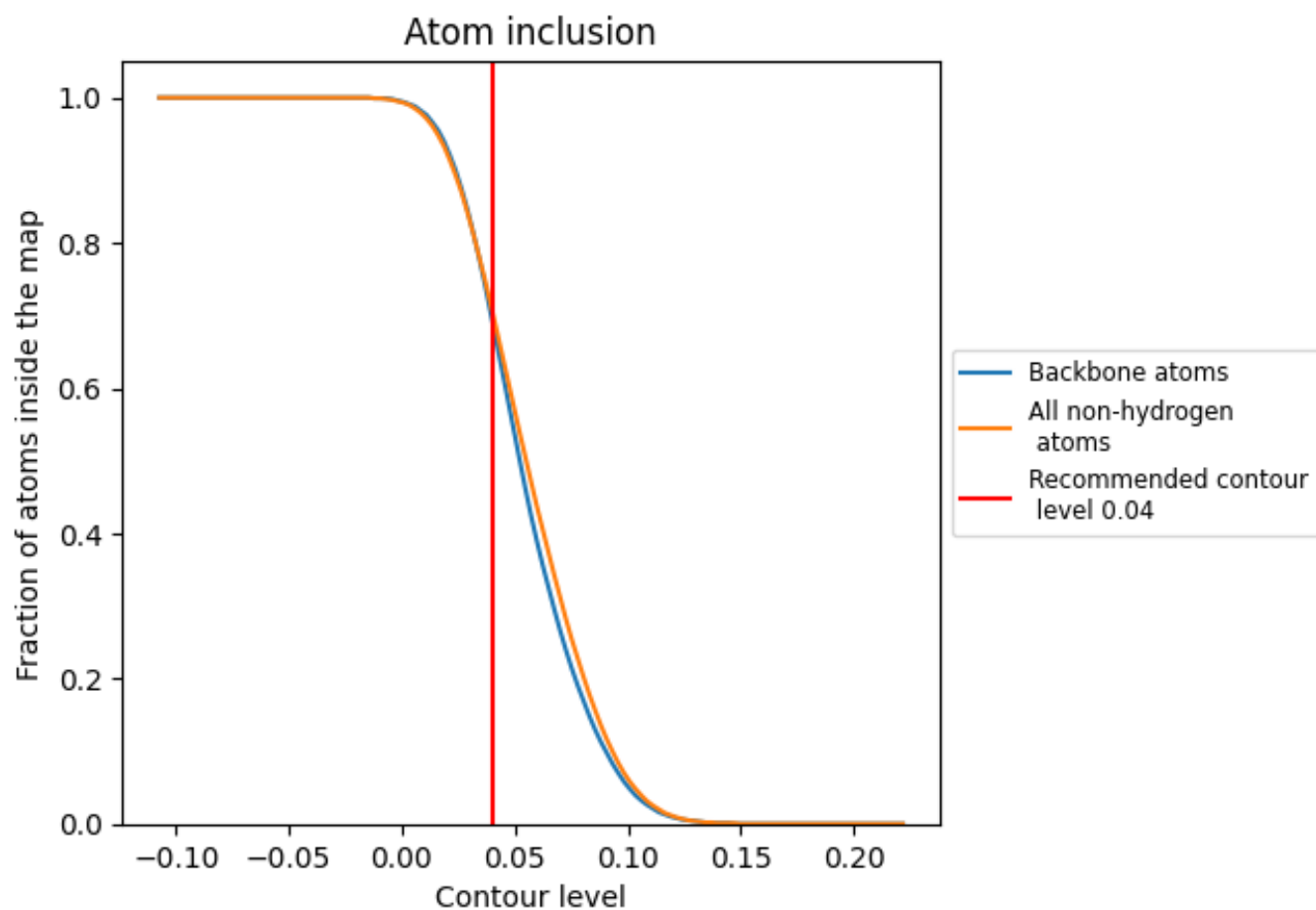
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.4360
CA	 0.7550	 0.4250
CC	 0.6620	 0.4760
CE	 0.6950	 0.4700
CF	 0.7820	 0.4500
CH	 0.6990	 0.4650
CI	 0.7100	 0.4570
CJ	 0.7850	 0.4760
CK	 0.7150	 0.4410
CL	 0.6770	 0.4740
CN	 0.8160	 0.4970
CO	 0.7250	 0.4420
CP	 0.7870	 0.4760
CQ	 0.7380	 0.4790
CR	 0.6760	 0.4530
CS	 0.8250	 0.4850
CU	 0.6630	 0.4440
Ca	 0.6580	 0.4460
Cb	 0.6930	 0.4330
Cd	 0.7700	 0.4470
Cg	 0.8260	 0.4660
Ci	 0.8320	 0.4950
Cj	 0.8230	 0.4410
Ck	 0.7570	 0.4360
Cm	 0.5120	 0.3880
Cn	 0.5280	 0.4310
Cp	 0.7630	 0.4340
Cq	 0.7560	 0.4430
Cr	 0.7010	 0.3850
Cv	 0.7420	 0.4560
DA	 0.7100	 0.4140
DB	 0.7730	 0.4580
DC	 0.7830	 0.4050
DD	 0.7840	 0.4530
DE	 0.7670	 0.4120



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Chain	Atom inclusion	Q-score
DF	0.8280	0.4630
DG	0.7700	0.4150
DH	0.7720	0.4640
DI	0.7820	0.4510
DJ	0.7980	0.4640
DK	0.7690	0.4550
DL	0.6340	0.4630
DM	0.7670	0.4590
DN	0.7340	0.4620
DO	0.7600	0.4290
DP	0.8270	0.4090
DQ	0.6800	0.4240
DR	0.8150	0.4230
DS	0.7940	0.4500
DT	0.8160	0.4840
DU	0.6730	0.4450
DV	0.7860	0.4790
DW	0.7890	0.4610
DX	0.8370	0.4650
DY	0.7970	0.4690
DZ	0.6410	0.4590
Da	0.6150	0.4420
F3	0.1220	0.1800
F6	0.4070	0.3160
F7	0.3270	0.3290
F9	0.6640	0.4400
FO	0.7170	0.4510
Ff	0.7490	0.4530
Fg	0.6900	0.4100
Fh	0.6030	0.4360
Fi	0.5830	0.4190
IA	0.6890	0.4450
IB	0.6770	0.4480
U6	0.4480	0.3440
U7	0.6850	0.4160
UE	0.6340	0.4640
UF	0.5080	0.4100
UG	0.6150	0.4680
UI	0.7000	0.3140
UJ	0.7240	0.3360
UK	0.9330	0.4980
UL	0.6500	0.4290