wwPDB EM Validation Summary Report

Nov 27, 2022 – 02:33 PM EST

PDB ID	:	6X89
EMDB ID	:	EMD-22090
Title	:	Vigna radiata mitochondrial complex I*
Authors	:	Letts, J.A.; Maldonado, M.; Padavannil, A.; Zhou, L.; Guo, F.
Deposited on	:	2020-06-01
Resolution	:	3.90 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:

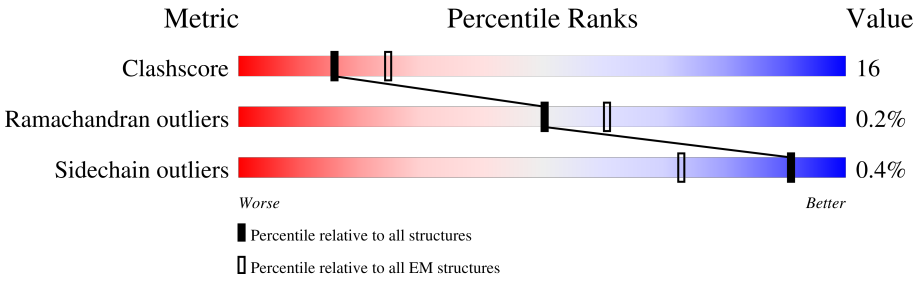
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.90 Å.

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



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

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	A	18	11% 100%
2	A2	98	12% 62% 32% 6%
3	A5	169	11% 48% 27% 25%
4	A6	132	8% 89%
5	A7	127	26% 65% 19% 14%
6	A9	396	36% 49% 33% 17%
7	AL	156	31% 58% 28% 13%
8	S1	746	8% 60% 32% 8%

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Mol	Chain	Length	Quality of chain
9	S2	394	6% 62% 35%
10	S3	190	8% 62% 33%
11	S4	146	58% 12% 31%
12	S6	103	6% 50% 20% 30%
13	S7	213	7% 52% 21% 26%
14	S8	222	7% 59% 21% 18%
15	V1	491	12% 56% 32% 12%
16	V2	251	13% 53% 32% 14%
17	1M	325	16% 60% 38%
18	2M	488	17% 61% 38%
19	3M	118	12% 51% 23% 26%
20	4L	100	7% 52% 34% 14%
21	6M	205	9% 54% 21% 25%
22	A1	65	12% 71% 25% 5%
23	A3	63	13% 59% 11% 30%
24	A8	106	7% 69% 29%
25	AM	143	20% 73% 25%
26	B	25	8% 100%
27	C	43	40% 79% 21%
28	C2	81	15% 83% 6% 11%
29	P2	115	25% 74%
30	S5	399	11% 6% 83%
31	X1	101	66% 32%
32	G1	270	51% 34% 14%
33	G2	273	5% 47% 40% 14%

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Mol	Chain	Length	Quality of chain
34	L2	256	5% 51% 30% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	SF4	S1	802	-	-	X	-
37	SF4	S7	301	-	-	X	-
37	SF4	S8	302	-	-	X	-
37	SF4	V1	500	-	-	X	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 45017 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 Unknown Peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	18	90	54	18	18	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A2	92	718	456	126	133	3	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A5	126	1009	642	166	197	4	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	A6	15	129	88	18	23	0	0

- Molecule 5 is a protein called NDUA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A7	109	868	549	150	166	3	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A9	328	Total	C	N	O	S	0	0
			2548	1641	435	461	11		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AL	135	Total	C	N	O	S	0	0
			1128	718	203	206	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S1	688	Total	C	N	O	S	0	0
			5268	3304	931	1000	33		

- Molecule 9 is a protein called NDUS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S2	382	Total	C	N	O	S	0	0
			3044	1926	539	556	23		

- Molecule 10 is a protein called NDUS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S3	184	Total	C	N	O	S	0	0
			1559	1004	269	280	6		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S4	101	Total	C	N	O	S	0	0
			811	521	147	142	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S6	72	Total	C	N	O	S	0	0
			563	355	97	105	6		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S7	158	Total	C	N	O	S	0	0
			1254	804	221	215	14		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S8	181	Total	C	N	O	S	0	0
			1484	930	251	292	11		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V1	433	Total	C	N	O	S	0	0
			3343	2108	594	617	24		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V2	216	Total	C	N	O	S	0	0
			1676	1063	286	316	11		

- Molecule 17 is a protein called NU1M.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1M	318	Total	C	N	O	S	0	0
			2463	1657	378	413	15		

- Molecule 18 is a protein called NU2M.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2M	488	Total	C	N	O	S	0	0
			3795	2537	578	651	29		

- Molecule 19 is a protein called NU3M.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3M	87	Total	C	N	O	S	0	0
			710	490	100	116	4		

- Molecule 20 is a protein called NU4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4L	86	Total	C	N	O	S	0	0
			670	447	104	112	7		

- Molecule 21 is a protein called NU6M.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6M	153	Total	C	N	O	S	0	0
			1142	773	172	189	8		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A1	62	Total	C	N	O	S	0	0
			490	309	93	83	5		

- Molecule 23 is a protein called uncharacterized protein LOC106754061.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A3	44	Total	C	N	O	S	0	0
			332	221	52	56	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A8	105	Total	C	N	O	S	0	0
			823	508	145	159	11		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AM	142	Total	C	N	O	S	0	0
			1134	731	202	197	4		

- Molecule 26 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	B	25	Total 125	C 75	N 25	O 25	0	0

- Molecule 27 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C	43	Total 215	C 129	N 43	O 43	0	0

- Molecule 28 is a protein called NDUC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C2	72	Total 571	C 364	N 102	O 101	S 4	0	0

- Molecule 29 is a protein called Protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	P2	30	Total 214	C 140	N 39	O 35	0	0

- Molecule 30 is a protein called serine/arginine-rich-splicing factor SR34 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S5	66	Total 560	C 345	N 108	O 100	S 7	0	0

- Molecule 31 is a protein called NDUX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X1	99	Total 750	C 479	N 126	O 140	S 5	0	0

- Molecule 32 is a protein called gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G1	231	Total 1769	C 1122	N 311	O 330	S 6	0	0

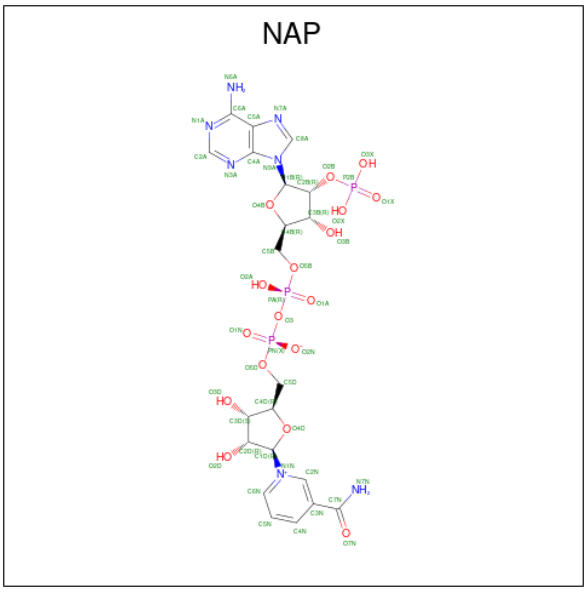
- Molecule 33 is a protein called gamma carbonic anhydrase 1, mitochondrial-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	G2	236	Total	C	N	O	S	0	0
			1799	1131	324	339	5		

- Molecule 34 is a protein called gamma carbonic anhydrase-like 2, mitochondrial.

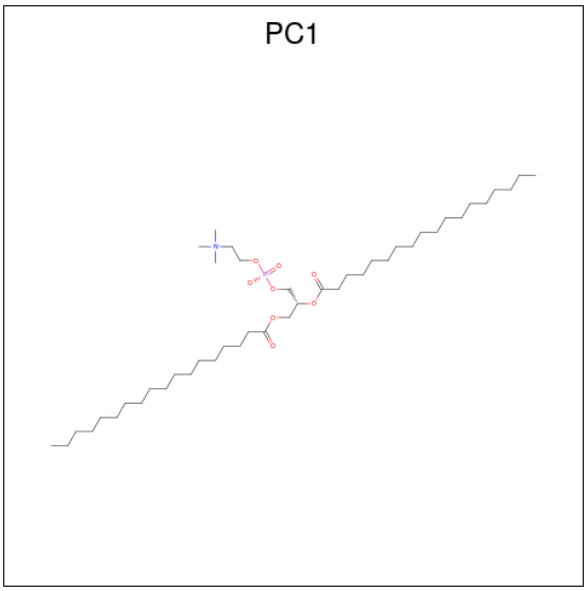
Mol	Chain	Residues	Atoms					AltConf	Trace
34	L2	207	Total	C	N	O	S	0	0
			1611	1033	276	297	5		

- Molecule 35 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



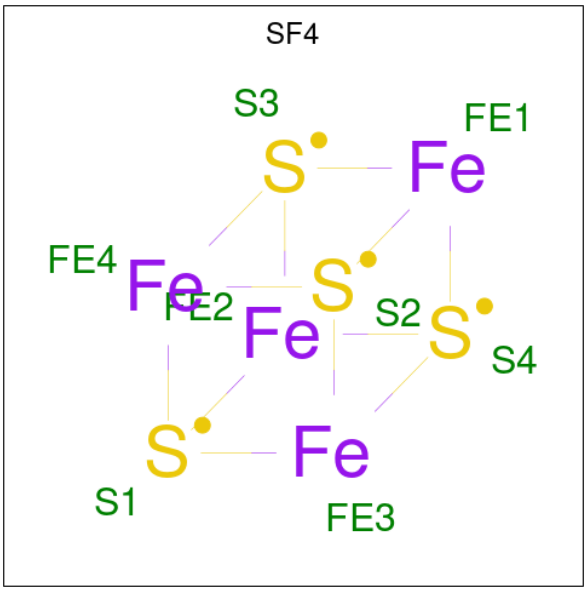
Mol	Chain	Residues	Atoms					AltConf
35	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 36 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



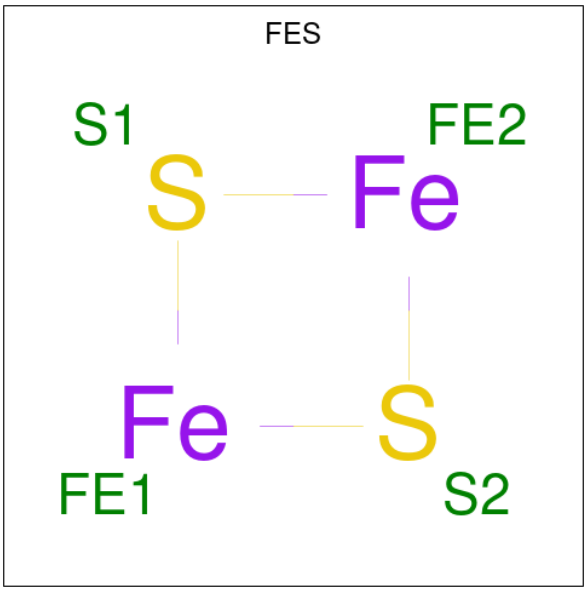
Mol	Chain	Residues	Atoms					AltConf
36	AL	1	Total	C	N	O	P	0
			29	19	1	8	1	
36	S2	1	Total	C	N	O	P	0
			45	35	1	8	1	
36	A1	1	Total	C	N	O	P	0
			37	27	1	8	1	
36	C2	1	Total	C	N	O	P	0
			37	27	1	8	1	
36	G1	1	Total	C	N	O	P	0
			67	47	2	16	2	
36	G1	1	Total	C	N	O	P	0
			67	47	2	16	2	

- Molecule 37 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
37	S1	1	Total	Fe	S	0
			16	8	8	
37	S1	1	Total	Fe	S	0
			16	8	8	
37	S7	1	Total	Fe	S	0
			8	4	4	
37	S8	1	Total	Fe	S	0
			16	8	8	
37	S8	1	Total	Fe	S	0
			16	8	8	
37	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 38 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

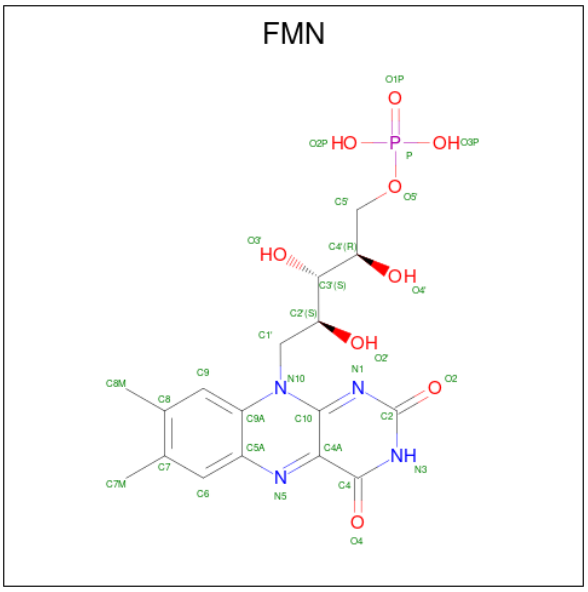


Mol	Chain	Residues	Atoms	AltConf
38	S1	1	Total Fe S 4 2 2	0
38	V2	1	Total Fe S 4 2 2	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
39	S6	1	Total Zn 1 1	0
39	G1	1	Total Zn 1 1	0

- Molecule 40 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



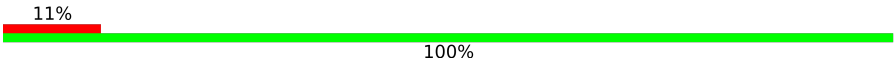
Mol	Chain	Residues	Atoms					AltConf
40	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

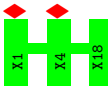
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Unknown Peptide

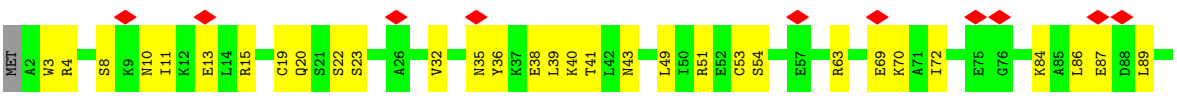
Chain A:

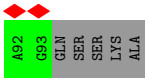




• Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

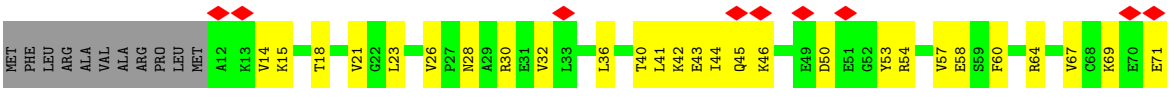
Chain A2:

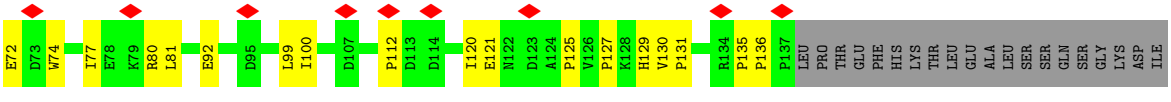




• Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial

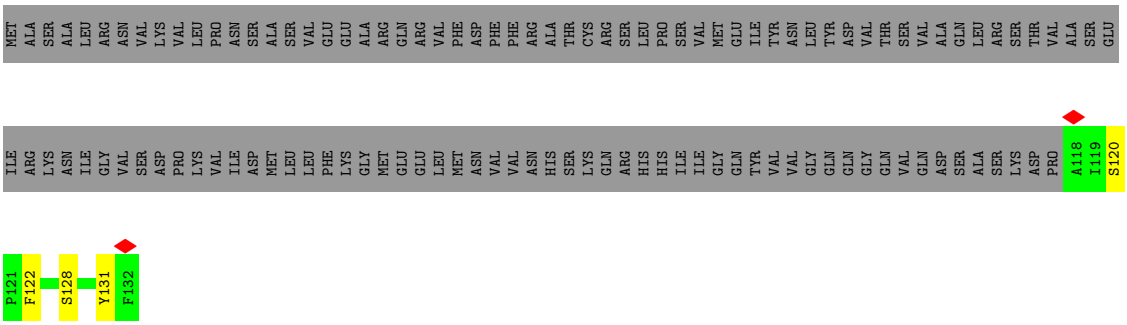
Chain A5:





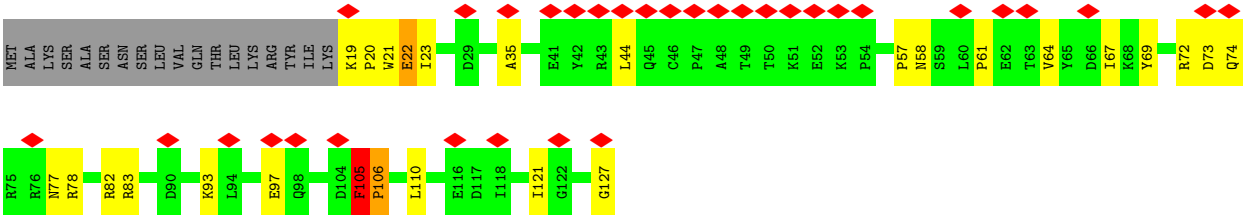
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:



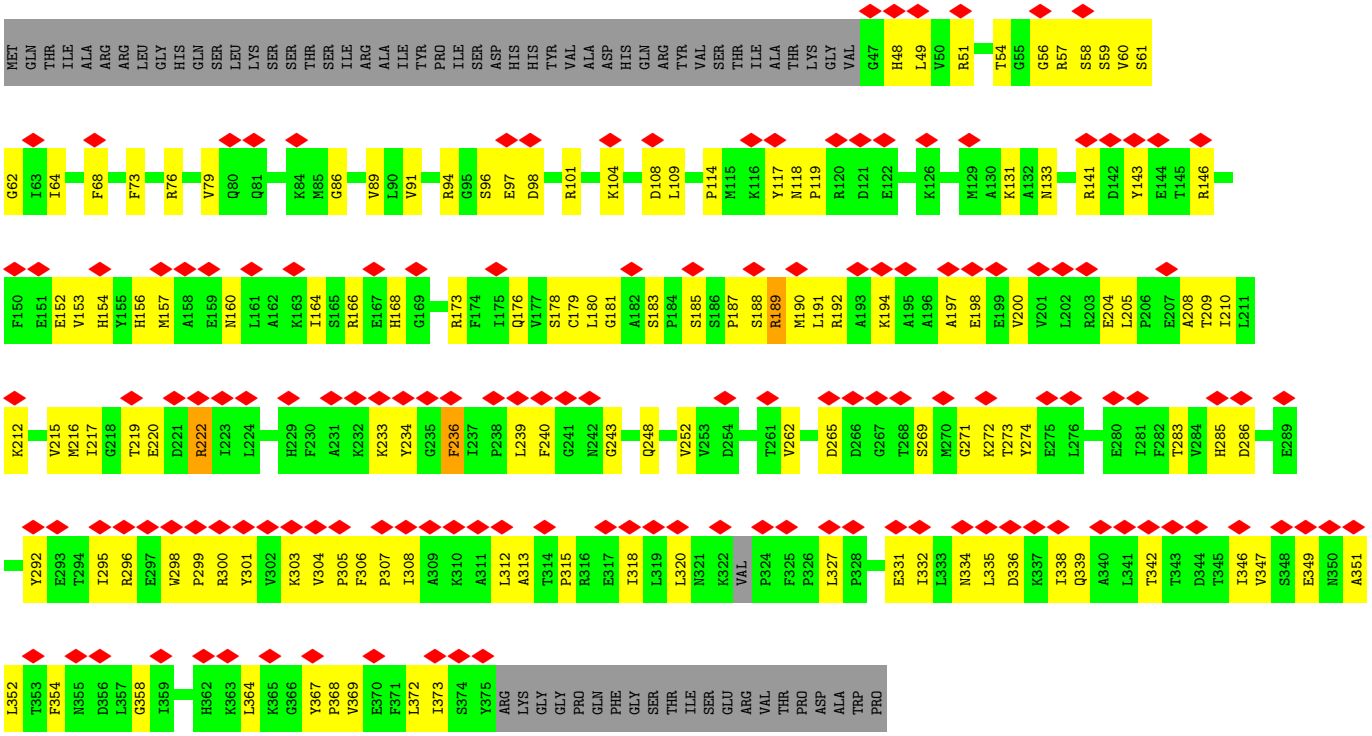
• Molecule 5: NDUA7

Chain A7:



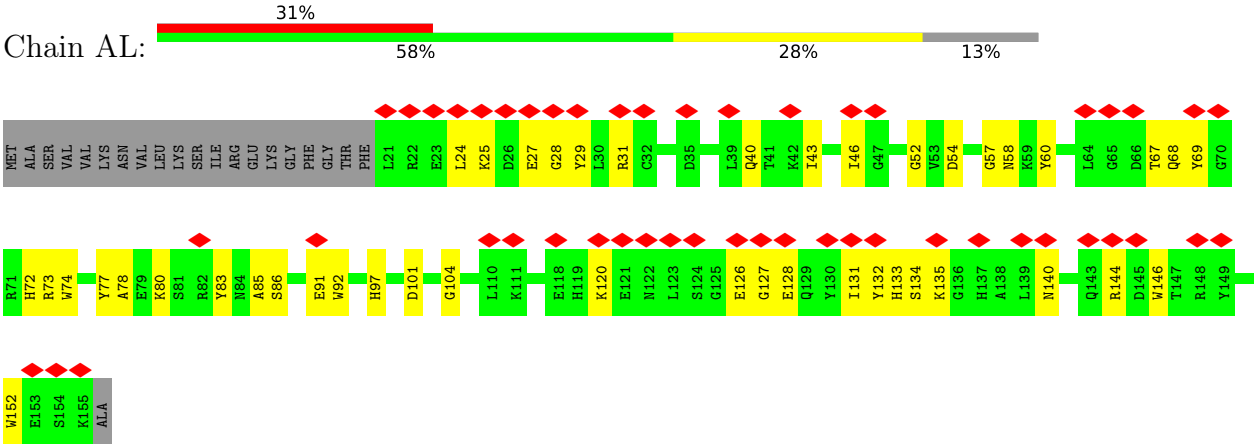
• Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial isoform X1

Chain A9:



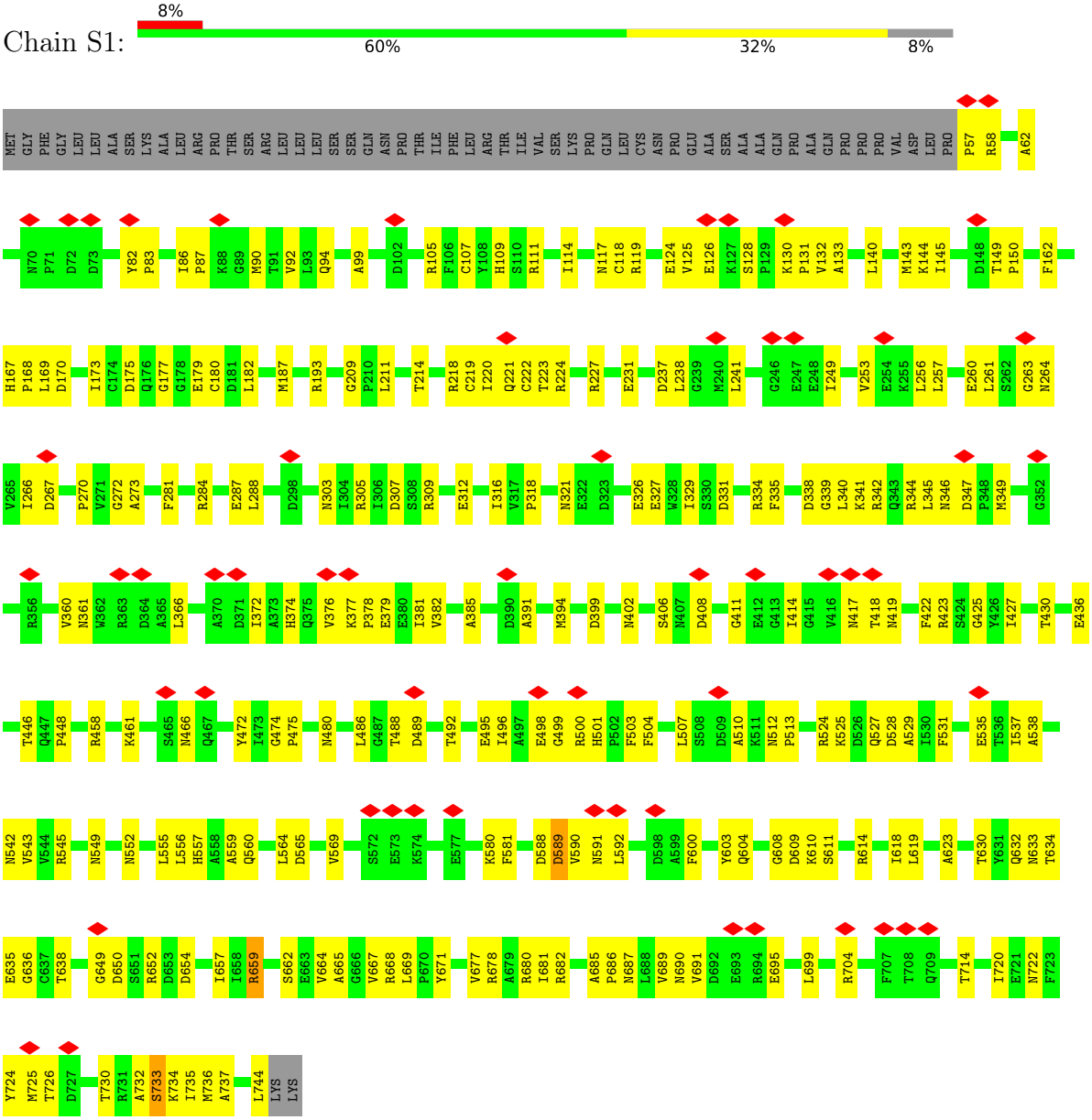
• Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:



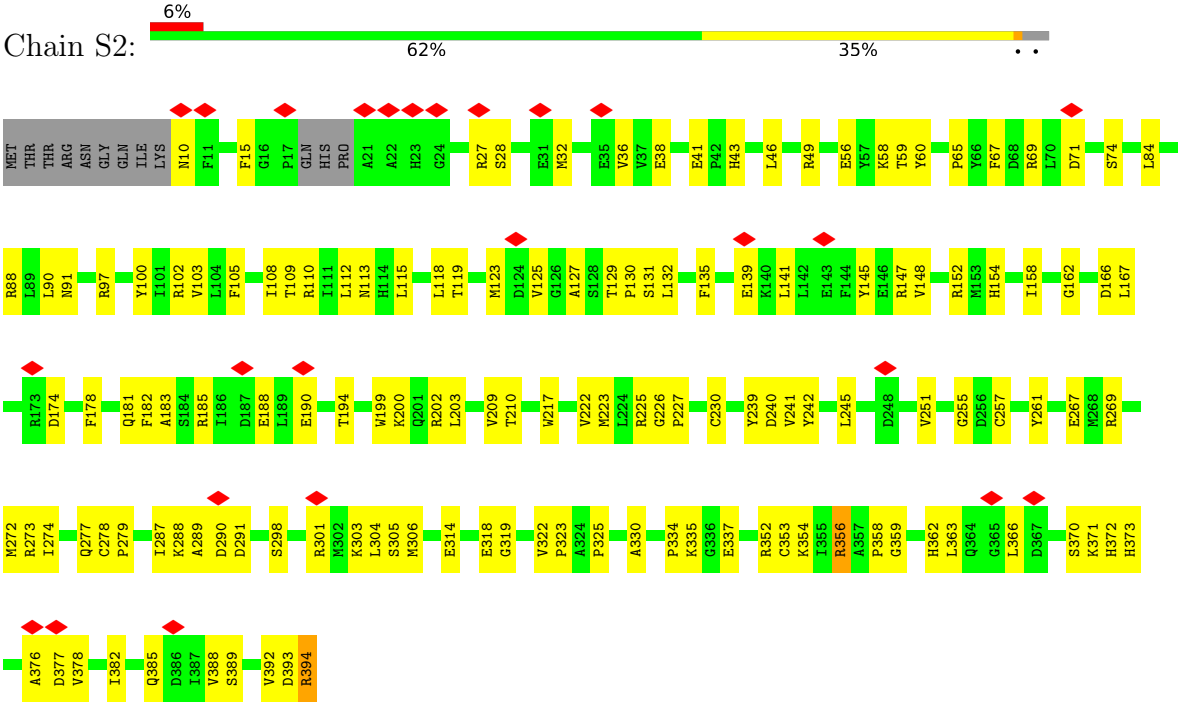
• Molecule 8: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial

Chain S1:



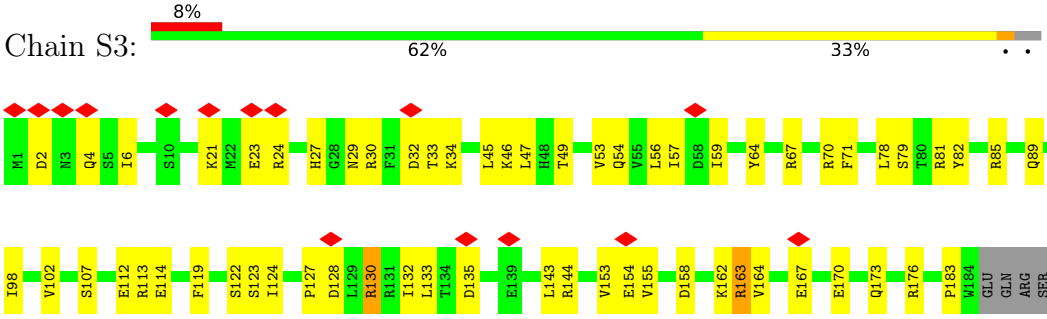
• Molecule 9: NDUS2

Chain S2:



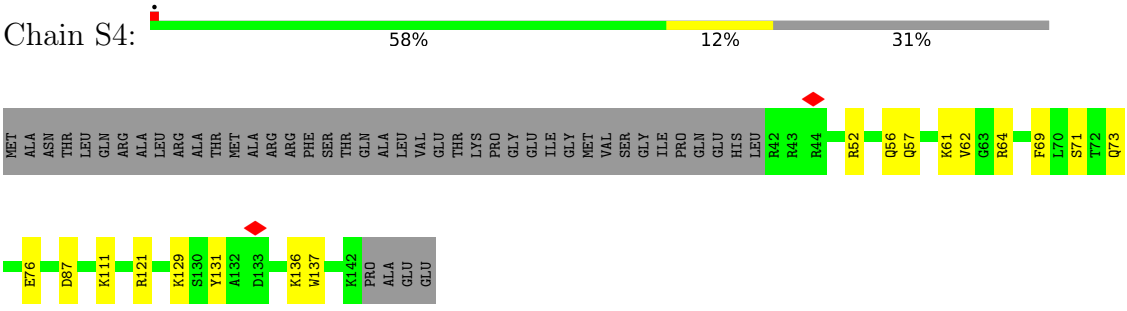
• Molecule 10: NDUS3

Chain S3:



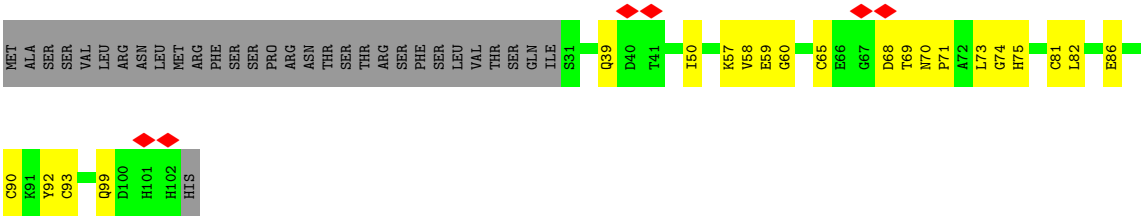
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:



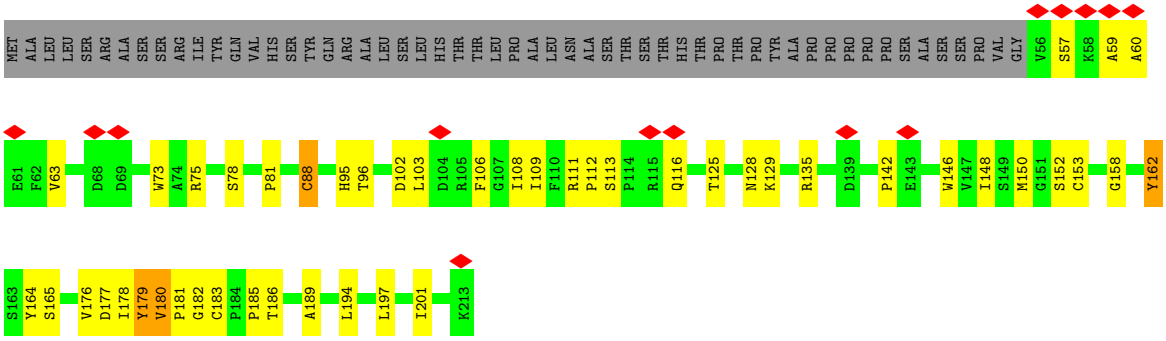
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:



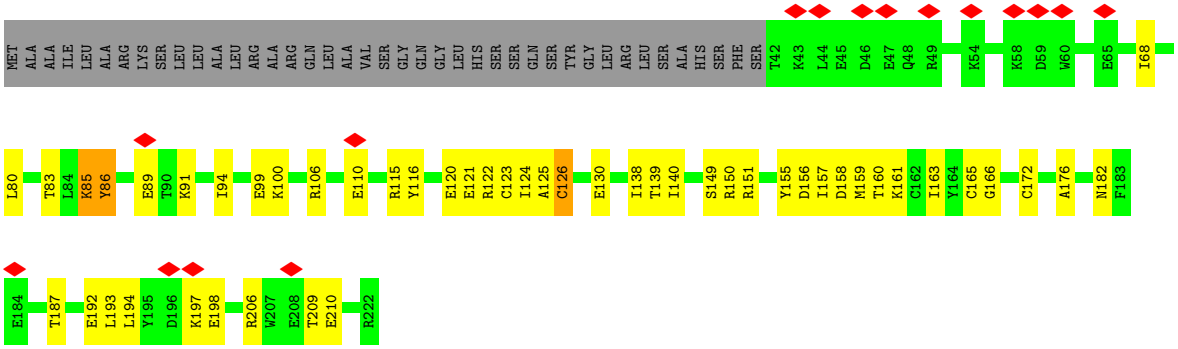
• Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:



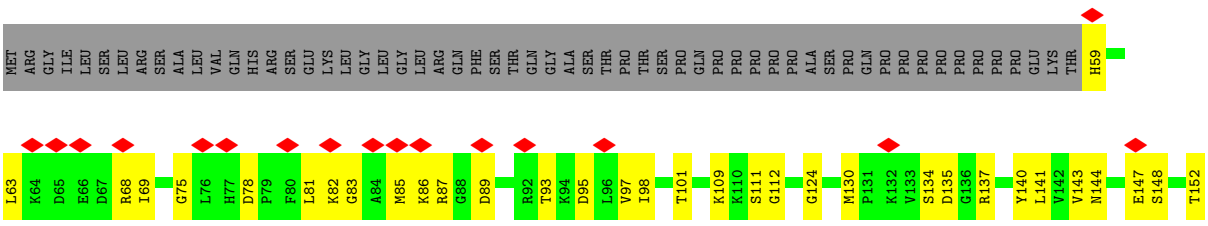
• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

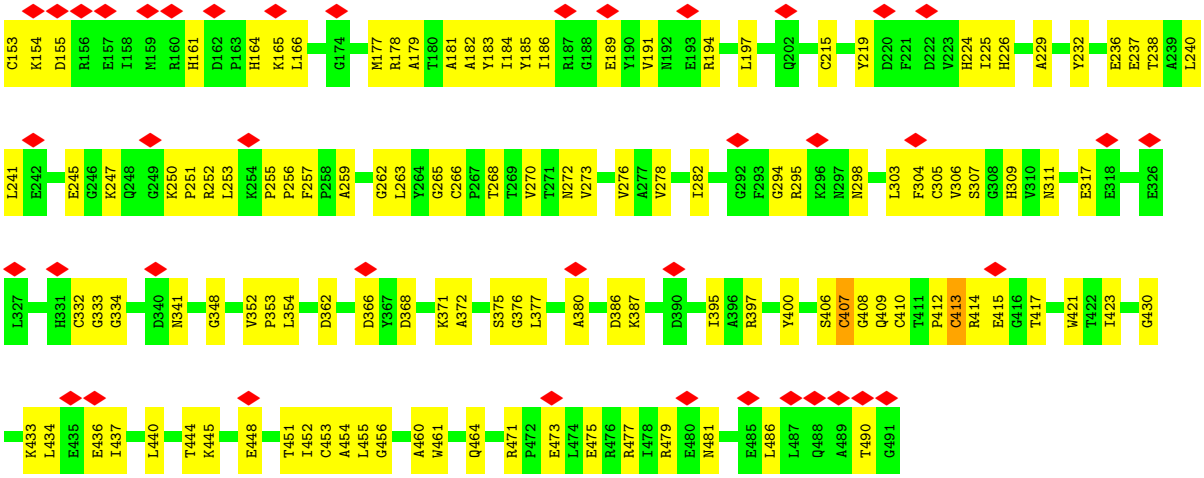
Chain S8:



• Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

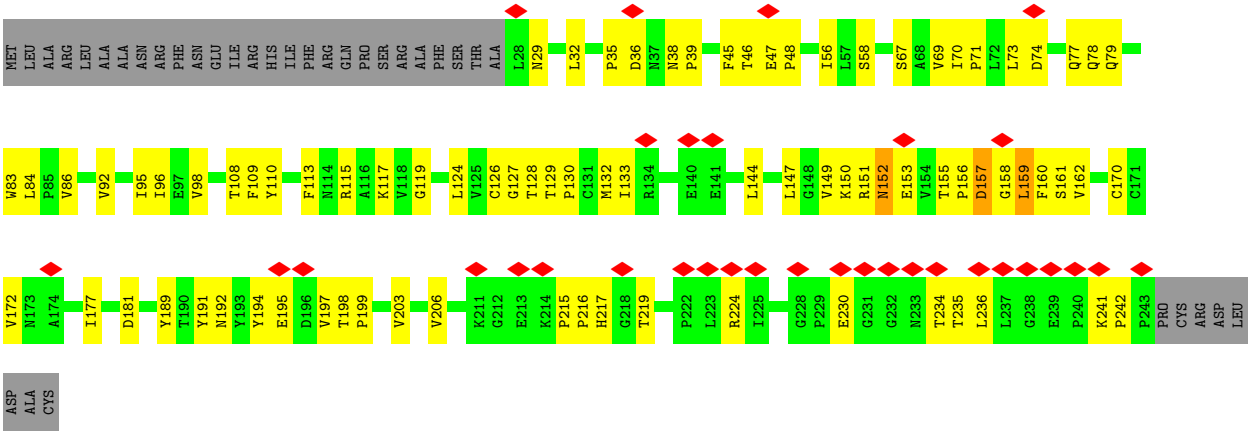
Chain V1:





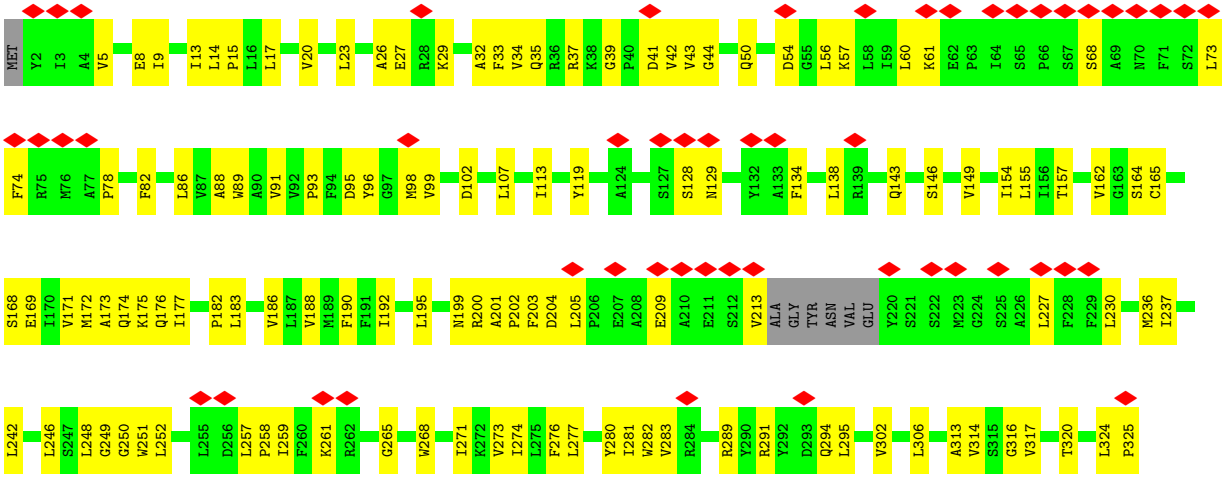
• Molecule 16: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:



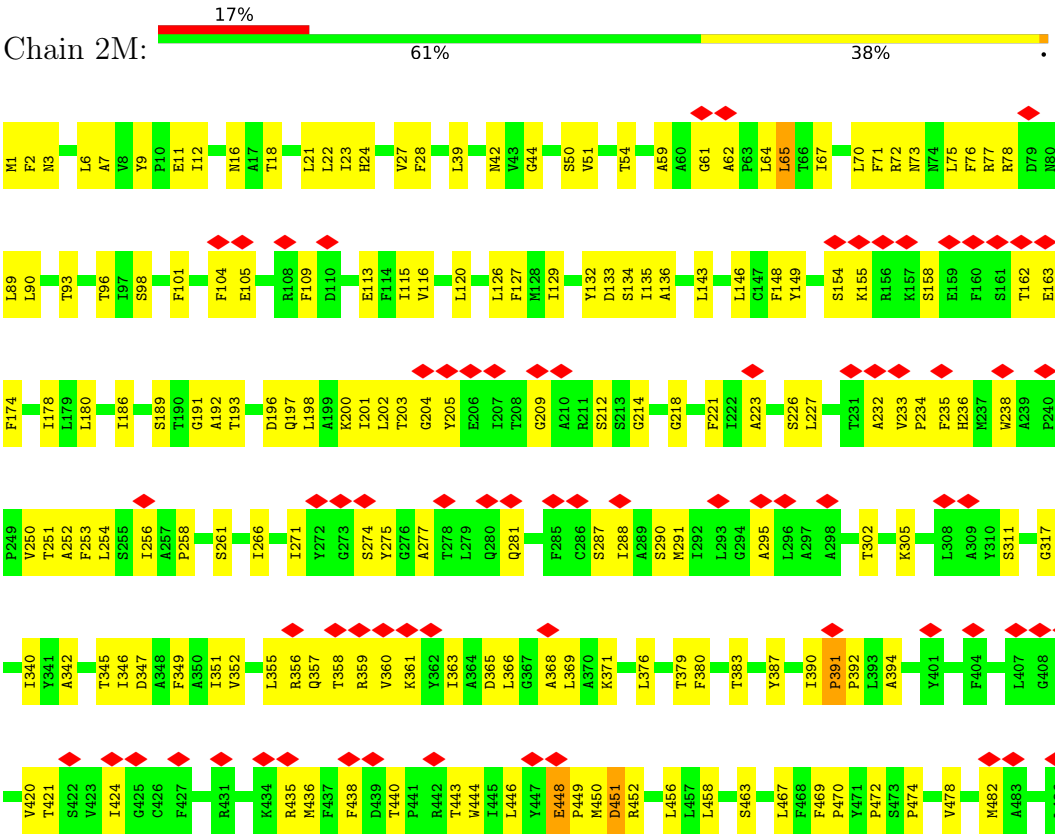
• Molecule 17: NU1M

Chain 1M:



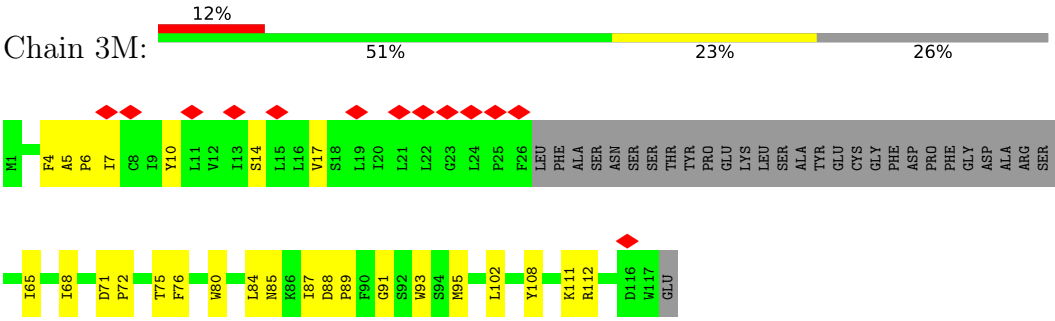
• Molecule 18: NU2M

Chain 2M:



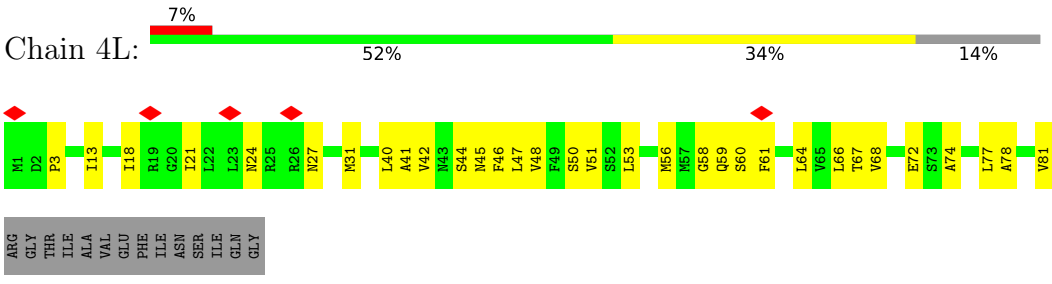
• Molecule 19: NU3M

Chain 3M:



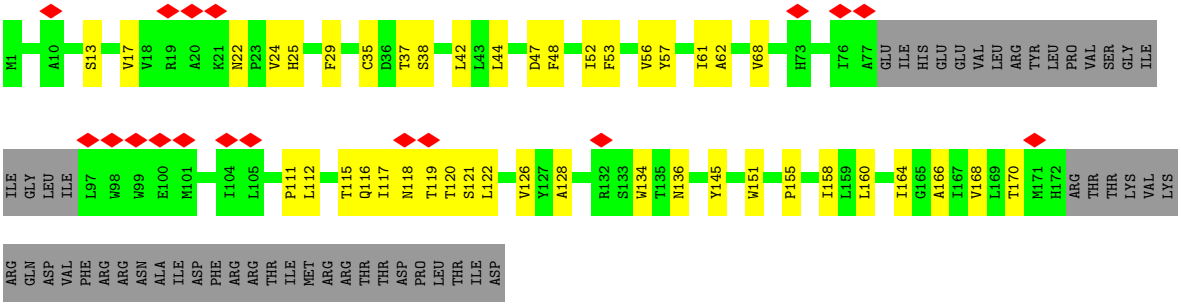
• Molecule 20: NU4L

Chain 4L:

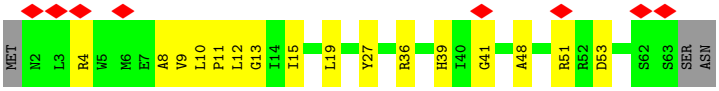


• Molecule 21: NU6M

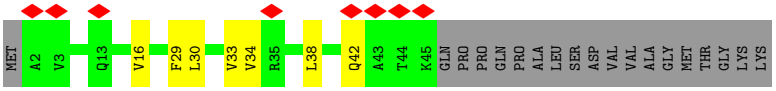
Chain 6M:



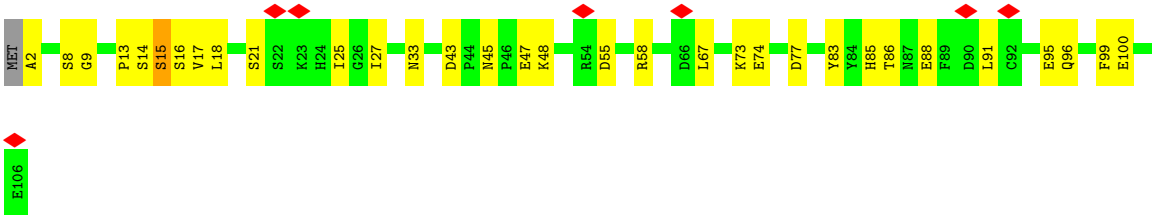
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



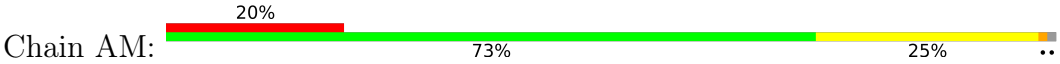
• Molecule 23: uncharacterized protein LOC106754061

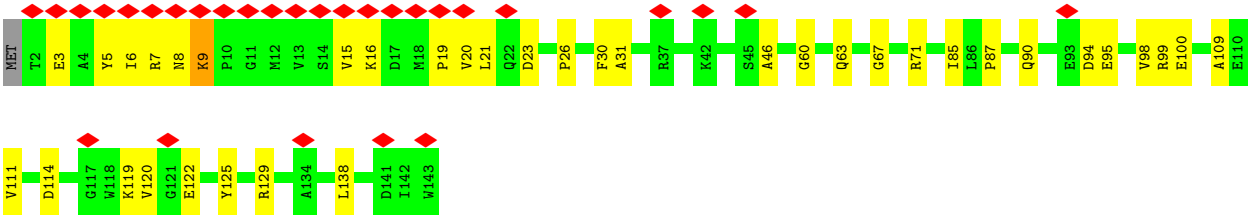


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



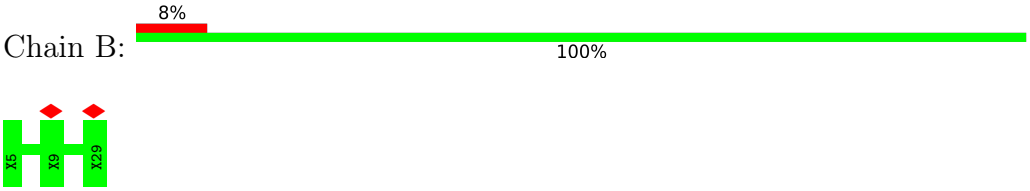
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A





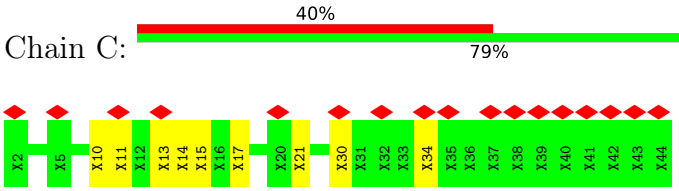
• Molecule 26: Unknown Peptide

Chain B:



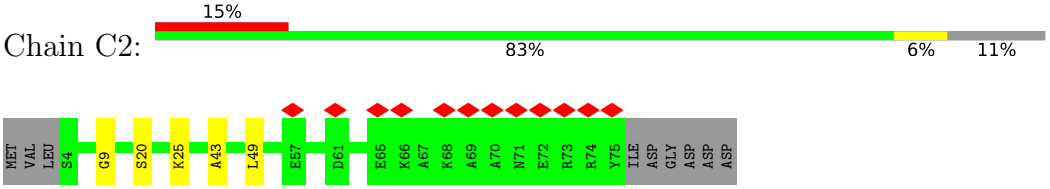
• Molecule 27: Unknown Peptide

Chain C:



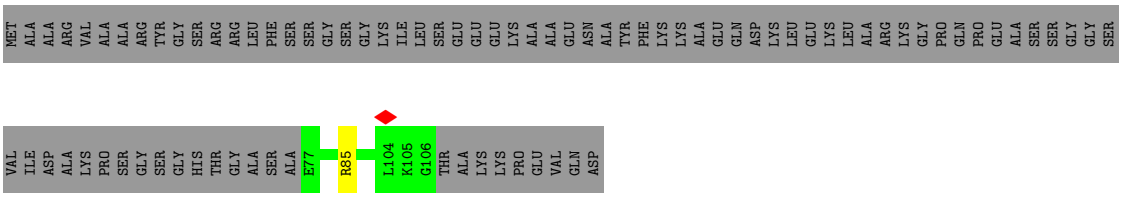
• Molecule 28: NDUC2

Chain C2:



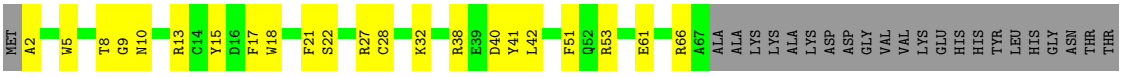
• Molecule 29: Protein At2g27730, mitochondrial

Chain P2:



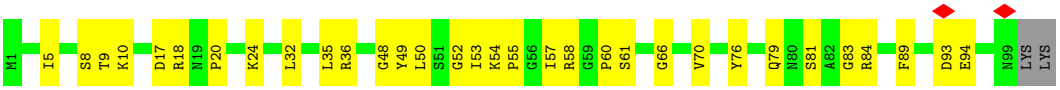
• Molecule 30: serine/arginine-rich-splicing factor SR34 isoform X2

Chain S5:



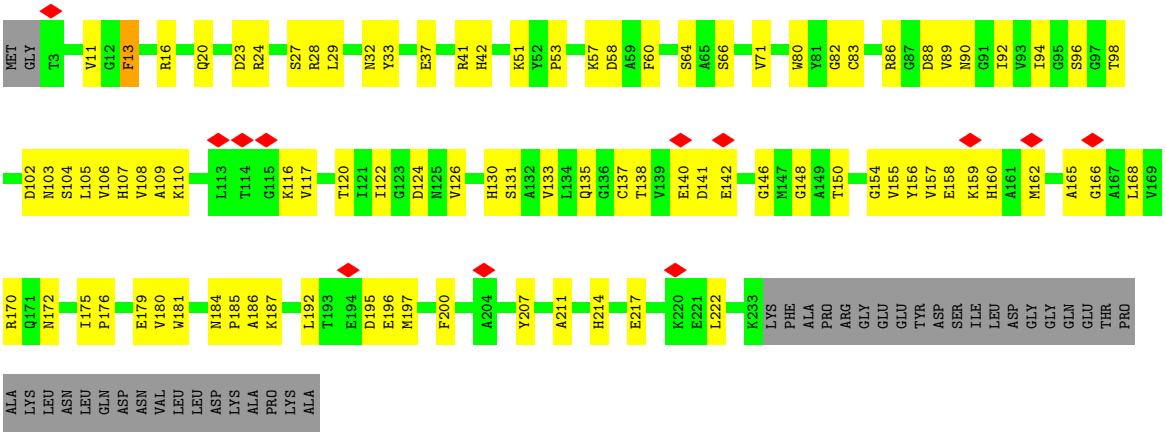
• Molecule 31: NDUX1

Chain X1:



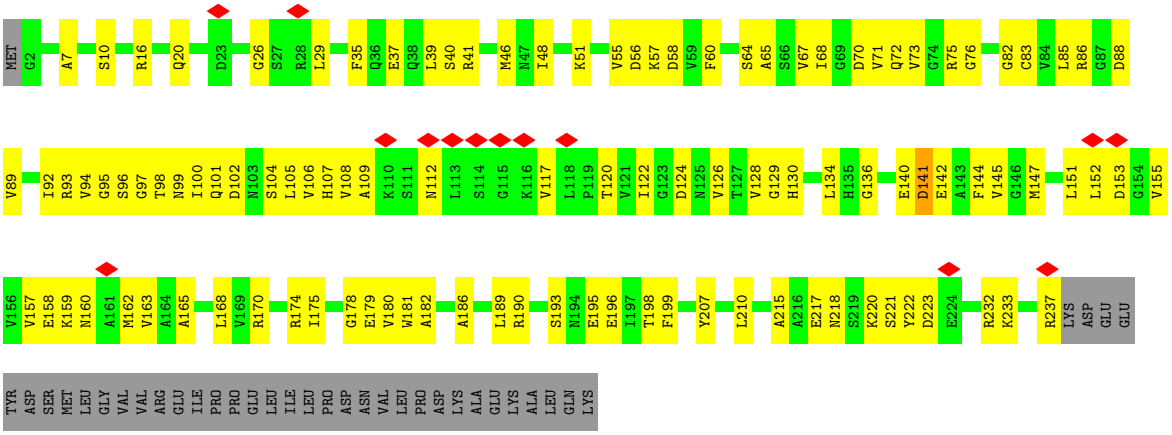
• Molecule 32: gamma carbonic anhydrase 1, mitochondrial

Chain G1:



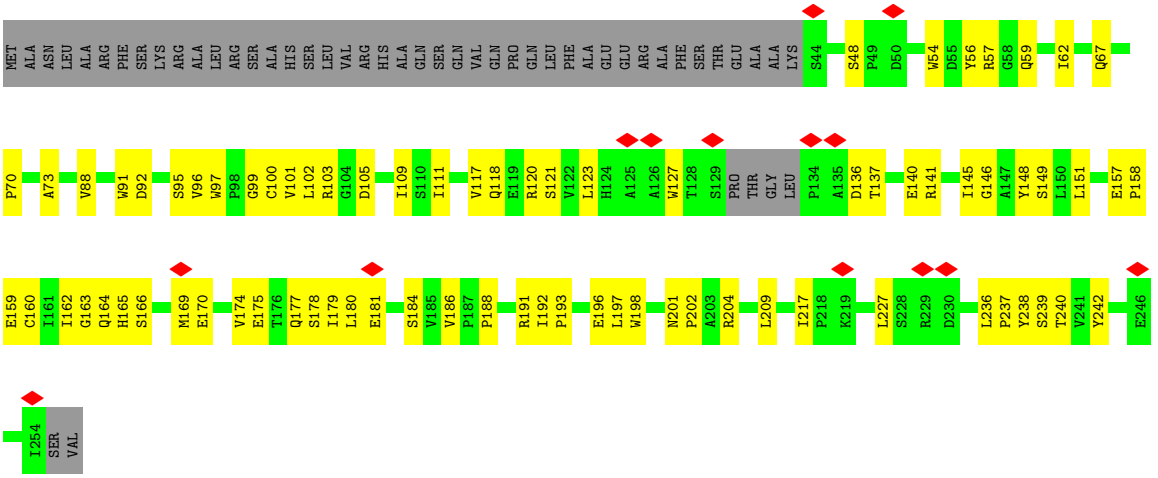
• Molecule 33: gamma carbonic anhydrase 1, mitochondrial-like

Chain G2:



• Molecule 34: gamma carbonic anhydrase-like 2, mitochondrial

Chain L2:


MET ALA ASN LEU ALA ARG PHE SER LYS ARG ALA LEU ARG SER ALA HIS SER LEU VAL ARG HIS ALA GLN SER GLN VAL GLN PRO GLN LEU PHE ALA GLU GLU ARG ALA PHE SER THR GLU ALA ALA LYS S44 S48 P49 D50 W54 D55 Y56 R57 G58 Q59 I62 Q67
P70 A73 V88 W91 D92 S95 V96 W97 P98 G99 C100 V101 L102 R103 G104 D105 I109 S110 I111 V117 Q118 E119 R120 S121 V122 L123 H124 A125 A126 W127 T128 S129 PRO THR GLY LEU P134 A135 D136 T137 E140 R141 I145 G146 A147 Y148 S149 L150 L151 E157 P158
E159 C160 I161 I162 G163 Q164 H165 S166 M169 E170 V174 E175 T176 Q177 S178 I179 L180 E181 S184 V185 V186 P187 P188 R191 I192 P193 E196 L197 W198 N201 P202 A203 R204 L209 I217 P218 K219 L227 S228 R229 D230 L236 P237 Y238 S239 T240 V241 Y242 E246
I254 SER VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34407	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	86.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.246	Depositor
Minimum map value	-24.127	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.082	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	426.5984, 426.5984, 426.5984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	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: FES, SF4, PC1, ZN, NAP, FMN

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	#$\|Z\|>5$
2	A2	0.32	0/728	0.49	0/976
3	A5	0.34	0/1032	0.47	0/1401
4	A6	0.37	0/134	0.39	0/179
5	A7	0.34	0/890	0.52	0/1210
6	A9	0.31	0/2605	0.50	0/3532
7	AL	0.35	0/1163	0.52	0/1573
8	S1	0.37	0/5364	0.52	1/7274 (0.0%)
9	S2	0.42	0/3114	0.52	0/4213
10	S3	0.39	0/1605	0.50	0/2174
11	S4	0.39	0/837	0.45	0/1131
12	S6	0.34	0/578	0.56	0/786
13	S7	0.44	0/1289	0.49	0/1747
14	S8	0.43	0/1512	0.49	0/2036
15	V1	0.35	0/3416	0.48	0/4612
16	V2	0.35	0/1720	0.48	0/2344
17	1M	0.42	0/2532	0.51	0/3450
18	2M	0.38	0/3895	0.50	0/5287
19	3M	0.41	0/733	0.47	0/999
20	4L	0.39	0/679	0.53	0/916
21	6M	0.40	0/1166	0.50	0/1596
22	A1	0.32	0/501	0.40	0/674
23	A3	0.33	0/338	0.41	0/458
24	A8	0.33	0/836	0.46	0/1118
25	AM	0.37	0/1169	0.49	0/1585
28	C2	0.35	0/582	0.42	0/784
29	P2	0.34	0/218	0.40	0/296
30	S5	0.40	0/572	0.43	0/760
31	X1	0.42	0/768	0.48	0/1043
32	G1	0.39	0/1806	0.54	0/2449
33	G2	0.38	0/1829	0.52	0/2475
34	L2	0.42	0/1650	0.55	0/2250
All	All	0.38	0/45261	0.50	1/61328 (0.0%)

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
5	A7	0	1
6	A9	0	1
8	S1	0	2
10	S3	0	1
13	S7	0	1
16	V2	0	3
18	2M	0	3
25	AM	0	2
33	G2	0	1
All	All	0	15

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S1	57	PRO	N-CA-CB	5.96	110.45	103.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A7	105	PHE	Peptide
6	A9	236	PHE	Peptide
8	S1	589	ASP	Peptide
8	S1	733	SER	Peptide
10	S3	94	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	90	0	22	0	0
2	A2	718	0	749	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A5	1009	0	998	40	0
4	A6	129	0	118	4	0
5	A7	868	0	860	29	0
6	A9	2548	0	2612	99	0
7	AL	1128	0	1074	47	0
8	S1	5268	0	5271	211	0
9	S2	3044	0	2998	111	0
10	S3	1559	0	1516	57	0
11	S4	811	0	792	17	0
12	S6	563	0	548	18	0
13	S7	1254	0	1251	42	0
14	S8	1484	0	1435	52	0
15	V1	3343	0	3323	129	0
16	V2	1676	0	1647	58	0
17	1M	2463	0	2560	98	0
18	2M	3795	0	3893	153	0
19	3M	710	0	730	25	0
20	4L	670	0	726	32	0
21	6M	1142	0	1168	40	0
22	A1	490	0	490	18	0
23	A3	332	0	356	7	0
24	A8	823	0	809	24	0
25	AM	1134	0	1124	38	0
26	B	125	0	28	0	0
27	C	215	0	47	5	0
28	C2	571	0	579	4	0
29	P2	214	0	205	1	0
30	S5	560	0	530	24	0
31	X1	750	0	743	25	0
32	G1	1769	0	1747	88	0
33	G2	1799	0	1801	90	0
34	L2	1611	0	1620	65	0
35	A9	48	0	25	7	0
36	A1	37	0	48	1	0
36	AL	29	0	32	2	0
36	C2	37	0	48	6	0
36	G1	67	0	82	5	0
36	S2	45	0	64	1	0
37	S1	16	0	0	6	0
37	S7	8	0	0	2	0
37	S8	16	0	0	2	0
37	V1	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	S1	4	0	0	0	0
38	V2	4	0	0	0	0
39	G1	1	0	0	0	0
39	S6	1	0	0	0	0
40	V1	31	0	19	3	0
All	All	45017	0	44688	1452	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 16.

The worst 5 of 1452 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)
18:2M:256:ILE:HD13	18:2M:346:ILE:HG22	1.55	0.88
34:L2:109:ILE:HG22	34:L2:137:THR:HB	1.58	0.85
24:A8:45:ASN:HD22	24:A8:48:LYS:HG2	1.45	0.81
32:G1:86:ARG:NH1	32:G1:88:ASP:OD2	2.14	0.81
32:G1:158:GLU:HG2	32:G1:159:LYS:HG2	1.63	0.81

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	A2	90/98 (92%)	75 (83%)	15 (17%)	0	100 100
3	A5	124/169 (73%)	105 (85%)	18 (14%)	1 (1%)	19 57
4	A6	13/132 (10%)	7 (54%)	6 (46%)	0	100 100
5	A7	107/127 (84%)	86 (80%)	18 (17%)	3 (3%)	5 34
6	A9	324/396 (82%)	257 (79%)	66 (20%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AL	133/156 (85%)	104 (78%)	29 (22%)	0	100	100
8	S1	686/746 (92%)	582 (85%)	103 (15%)	1 (0%)	51	84
9	S2	378/394 (96%)	325 (86%)	53 (14%)	0	100	100
10	S3	182/190 (96%)	143 (79%)	38 (21%)	1 (0%)	29	67
11	S4	99/146 (68%)	91 (92%)	8 (8%)	0	100	100
12	S6	70/103 (68%)	45 (64%)	25 (36%)	0	100	100
13	S7	156/213 (73%)	130 (83%)	25 (16%)	1 (1%)	25	63
14	S8	179/222 (81%)	152 (85%)	27 (15%)	0	100	100
15	V1	431/491 (88%)	367 (85%)	64 (15%)	0	100	100
16	V2	214/251 (85%)	172 (80%)	39 (18%)	3 (1%)	11	46
17	1M	314/325 (97%)	279 (89%)	35 (11%)	0	100	100
18	2M	486/488 (100%)	431 (89%)	54 (11%)	1 (0%)	47	79
19	3M	83/118 (70%)	77 (93%)	6 (7%)	0	100	100
20	4L	84/100 (84%)	79 (94%)	5 (6%)	0	100	100
21	6M	149/205 (73%)	138 (93%)	11 (7%)	0	100	100
22	A1	60/65 (92%)	54 (90%)	6 (10%)	0	100	100
23	A3	42/63 (67%)	41 (98%)	1 (2%)	0	100	100
24	A8	103/106 (97%)	88 (85%)	14 (14%)	1 (1%)	15	52
25	AM	140/143 (98%)	109 (78%)	31 (22%)	0	100	100
28	C2	70/81 (86%)	68 (97%)	2 (3%)	0	100	100
29	P2	28/115 (24%)	26 (93%)	2 (7%)	0	100	100
30	S5	64/399 (16%)	55 (86%)	9 (14%)	0	100	100
31	X1	97/101 (96%)	88 (91%)	9 (9%)	0	100	100
32	G1	229/270 (85%)	186 (81%)	43 (19%)	0	100	100
33	G2	234/273 (86%)	197 (84%)	37 (16%)	0	100	100
34	L2	203/256 (79%)	168 (83%)	35 (17%)	0	100	100
All	All	5572/6942 (80%)	4725 (85%)	834 (15%)	13 (0%)	50	79

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A7	22	GLU
24	A8	15	SER

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Mol	Chain	Res	Type
6	A9	189	ARG
16	V2	39	PRO
16	V2	158	GLY

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	A2	76/81 (94%)	76 (100%)	0	100	100
3	A5	112/149 (75%)	112 (100%)	0	100	100
4	A6	14/118 (12%)	14 (100%)	0	100	100
5	A7	95/111 (86%)	95 (100%)	0	100	100
6	A9	276/334 (83%)	275 (100%)	1 (0%)	91	94
7	AL	117/134 (87%)	117 (100%)	0	100	100
8	S1	571/622 (92%)	570 (100%)	1 (0%)	93	96
9	S2	328/339 (97%)	324 (99%)	4 (1%)	71	83
10	S3	173/179 (97%)	171 (99%)	2 (1%)	71	83
11	S4	82/119 (69%)	82 (100%)	0	100	100
12	S6	64/94 (68%)	64 (100%)	0	100	100
13	S7	133/180 (74%)	131 (98%)	2 (2%)	65	80
14	S8	162/193 (84%)	159 (98%)	3 (2%)	57	75
15	V1	349/400 (87%)	347 (99%)	2 (1%)	86	91
16	V2	186/216 (86%)	186 (100%)	0	100	100
17	1M	266/271 (98%)	265 (100%)	1 (0%)	91	94
18	2M	407/408 (100%)	406 (100%)	1 (0%)	93	96
19	3M	79/105 (75%)	79 (100%)	0	100	100
20	4L	75/86 (87%)	75 (100%)	0	100	100
21	6M	119/186 (64%)	119 (100%)	0	100	100
22	A1	49/52 (94%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	A3	36/51 (71%)	36 (100%)	0	100	100
24	A8	95/96 (99%)	95 (100%)	0	100	100
25	AM	115/116 (99%)	115 (100%)	0	100	100
28	C2	58/66 (88%)	58 (100%)	0	100	100
29	P2	17/85 (20%)	17 (100%)	0	100	100
30	S5	59/349 (17%)	58 (98%)	1 (2%)	60	78
31	X1	82/84 (98%)	82 (100%)	0	100	100
32	G1	185/216 (86%)	184 (100%)	1 (0%)	88	93
33	G2	192/226 (85%)	191 (100%)	1 (0%)	88	93
34	L2	177/217 (82%)	176 (99%)	1 (1%)	86	91
All	All	4749/5883 (81%)	4728 (100%)	21 (0%)	91	94

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	V1	413	CYS
30	S5	66	ARG
34	L2	165	HIS
32	G1	13	PHE
18	2M	65	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
24	A8	45	ASN
34	L2	164	GLN
25	AM	90	GLN
31	X1	79	GLN
9	S2	121	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
40	FMN	V1	501	-	33,33,33	0.31	0	48,50,50	0.35	0
38	FES	S1	803	8	0,4,4	-	-	-		
35	NAP	A9	401	-	45,52,52	1.41	5 (11%)	56,80,80	1.38	6 (10%)
37	SF4	S8	301	14	0,12,12	-	-	-		
38	FES	V2	300	16	0,4,4	-	-	-		
36	PC1	G1	701	-	26,26,53	0.43	0	32,34,61	0.39	0
37	SF4	S7	301	-	0,12,12	-	-	-		
36	PC1	G1	702	-	39,39,53	0.34	0	45,47,61	0.36	0
36	PC1	S2	401	-	44,44,53	0.32	0	50,52,61	0.30	0
37	SF4	S1	801	8	0,12,12	-	-	-		
36	PC1	A1	101	-	36,36,53	0.34	0	42,44,61	0.32	0
36	PC1	C2	101	-	36,36,53	0.36	0	42,44,61	0.38	0
37	SF4	S1	802	8	0,12,12	-	-	-		
37	SF4	S8	302	14	0,12,12	-	-	-		
36	PC1	AL	401	-	28,28,53	0.39	0	34,36,61	0.43	0
37	SF4	V1	500	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	FMN	V1	501	-	-	6/18/18/18	0/3/3/3
38	FES	S1	803	8	-	-	0/1/1/1
35	NAP	A9	401	-	-	20/31/67/67	0/5/5/5
37	SF4	S8	301	14	-	-	0/6/5/5
38	FES	V2	300	16	-	-	0/1/1/1
36	PC1	G1	701	-	-	6/30/30/57	-
37	SF4	S7	301	-	-	-	0/6/5/5
36	PC1	G1	702	-	-	12/43/43/57	-
36	PC1	S2	401	-	-	12/48/48/57	-
37	SF4	S1	801	8	-	-	0/6/5/5
36	PC1	A1	101	-	-	10/40/40/57	-
36	PC1	C2	101	-	-	11/40/40/57	-
37	SF4	S1	802	8	-	-	0/6/5/5
37	SF4	S8	302	14	-	-	0/6/5/5
36	PC1	AL	401	-	-	7/32/32/57	-
37	SF4	V1	500	-	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A9	401	NAP	C4N-C3N	5.54	1.48	1.39
35	A9	401	NAP	C5N-C4N	4.61	1.48	1.38
35	A9	401	NAP	C6N-C5N	-2.85	1.32	1.38
35	A9	401	NAP	C2N-C3N	-2.53	1.35	1.39
35	A9	401	NAP	C2N-N1N	2.19	1.37	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A9	401	NAP	C5N-C4N-C3N	-7.16	111.87	120.34
35	A9	401	NAP	C6N-N1N-C2N	-3.49	118.80	121.97
35	A9	401	NAP	C3N-C2N-N1N	2.80	123.16	120.43
35	A9	401	NAP	C6N-C5N-C4N	2.39	122.91	119.44
35	A9	401	NAP	C5A-C6A-N6A	2.26	123.78	120.35

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A9	401	NAP	C5B-O5B-PA-O1A
35	A9	401	NAP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
35	A9	401	NAP	C2B-O2B-P2B-O1X
35	A9	401	NAP	C2B-O2B-P2B-O3X
35	A9	401	NAP	O4D-C1D-N1N-C2N

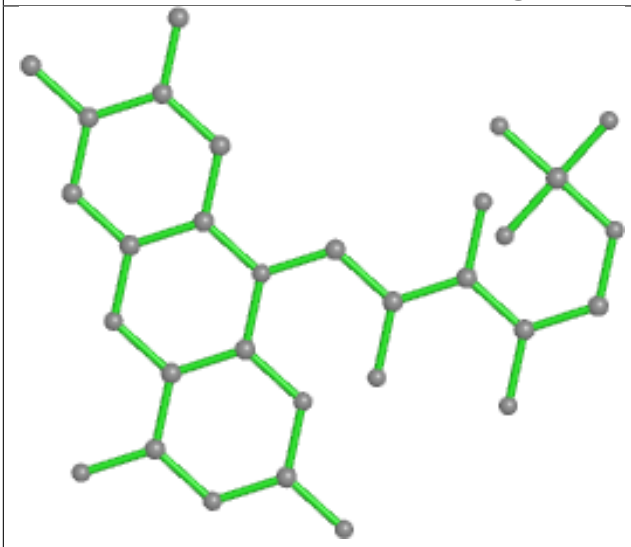
There are no ring outliers.

13 monomers are involved in 38 short contacts:

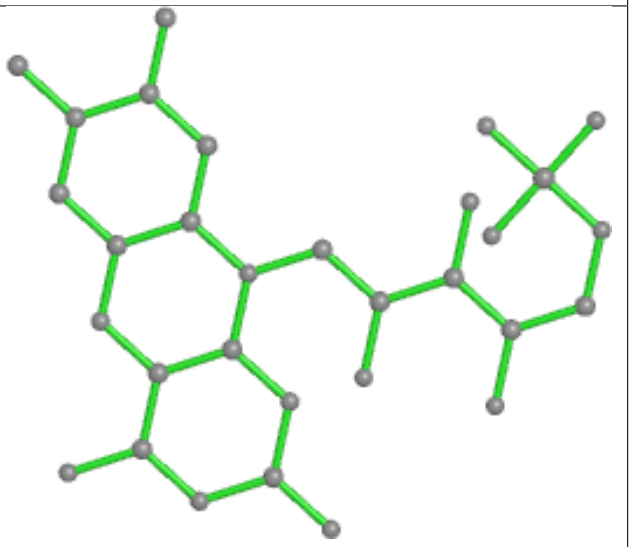
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	V1	501	FMN	3	0
35	A9	401	NAP	7	0
36	G1	701	PC1	3	0
37	S7	301	SF4	2	0
36	G1	702	PC1	5	0
36	S2	401	PC1	1	0
37	S1	801	SF4	1	0
36	A1	101	PC1	1	0
36	C2	101	PC1	6	0
37	S1	802	SF4	5	0
37	S8	302	SF4	2	0
36	AL	401	PC1	2	0
37	V1	500	SF4	3	0

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 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.

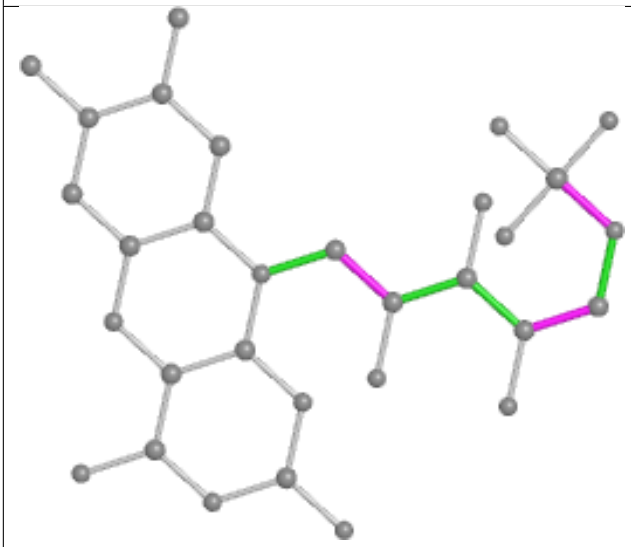
Ligand FMN V1 501



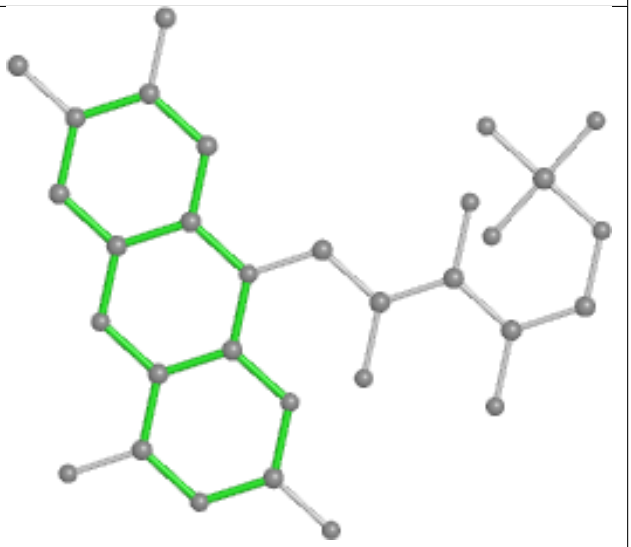
Bond lengths



Bond angles

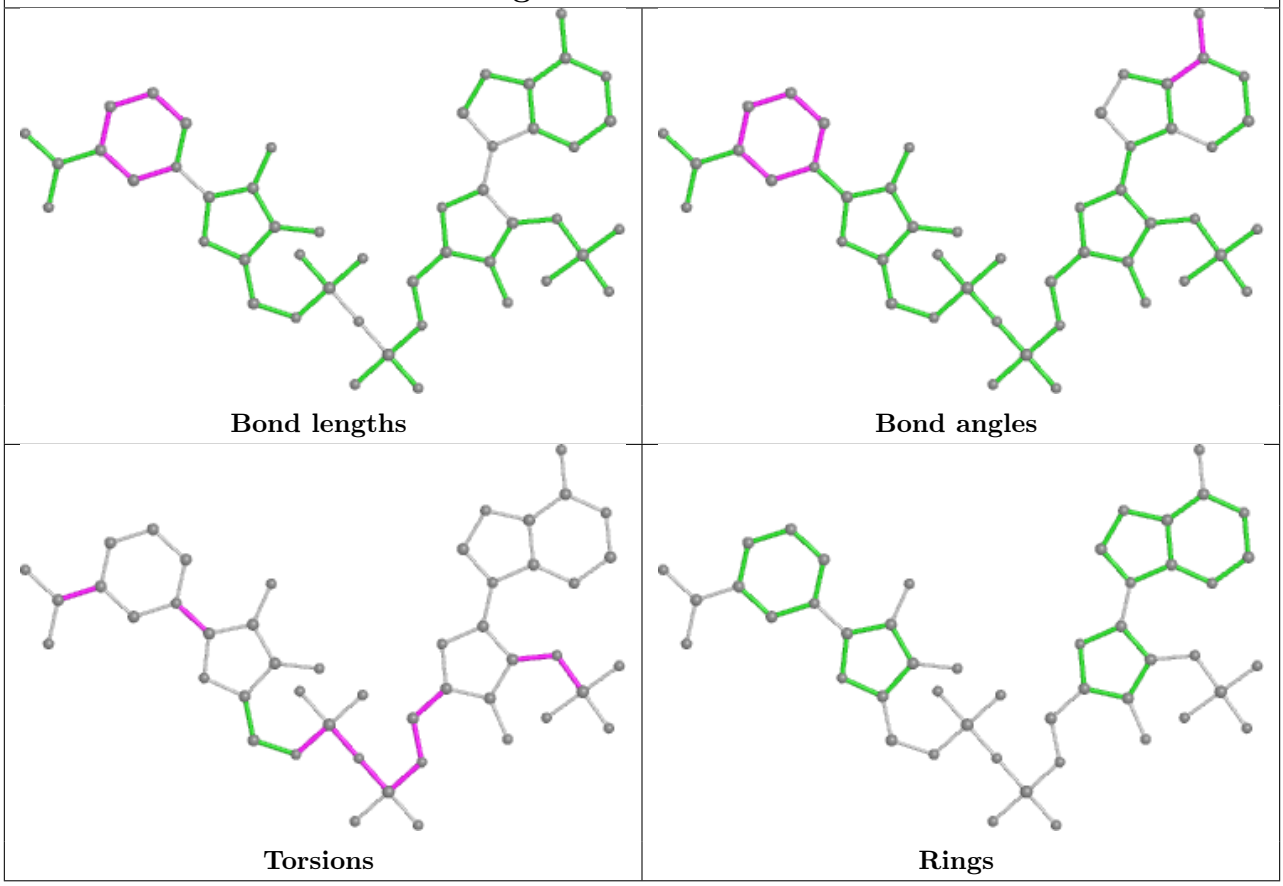


Torsions

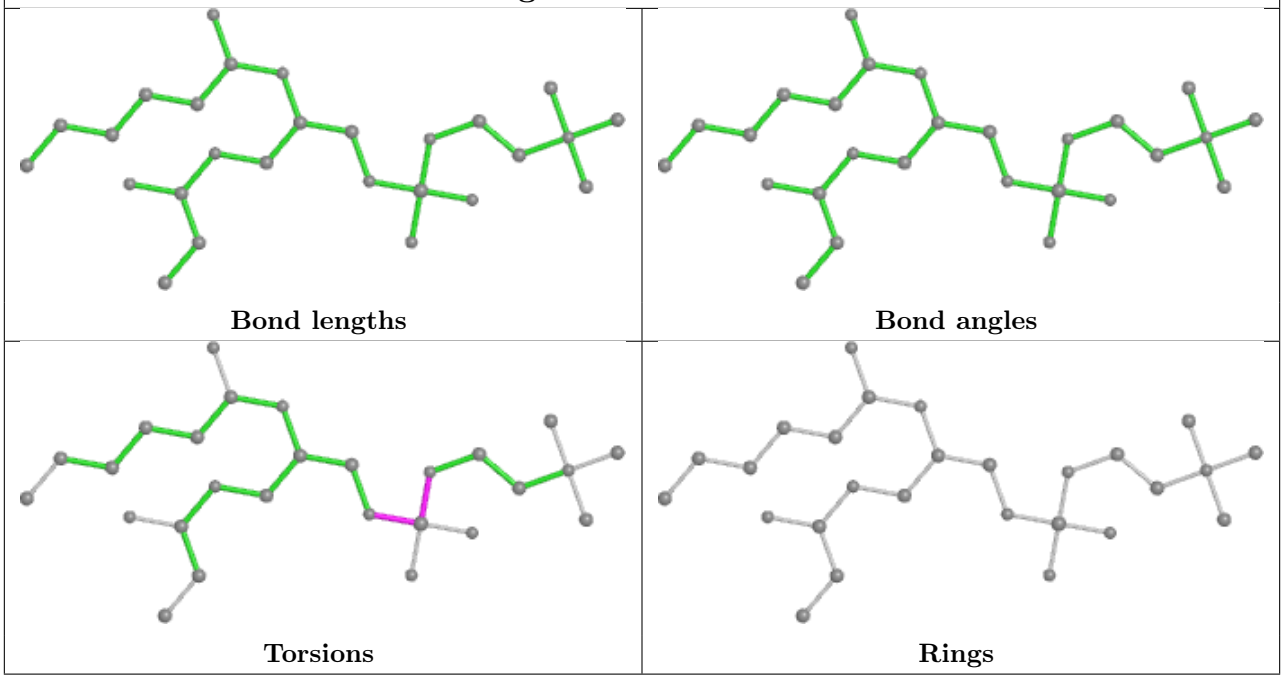


Rings

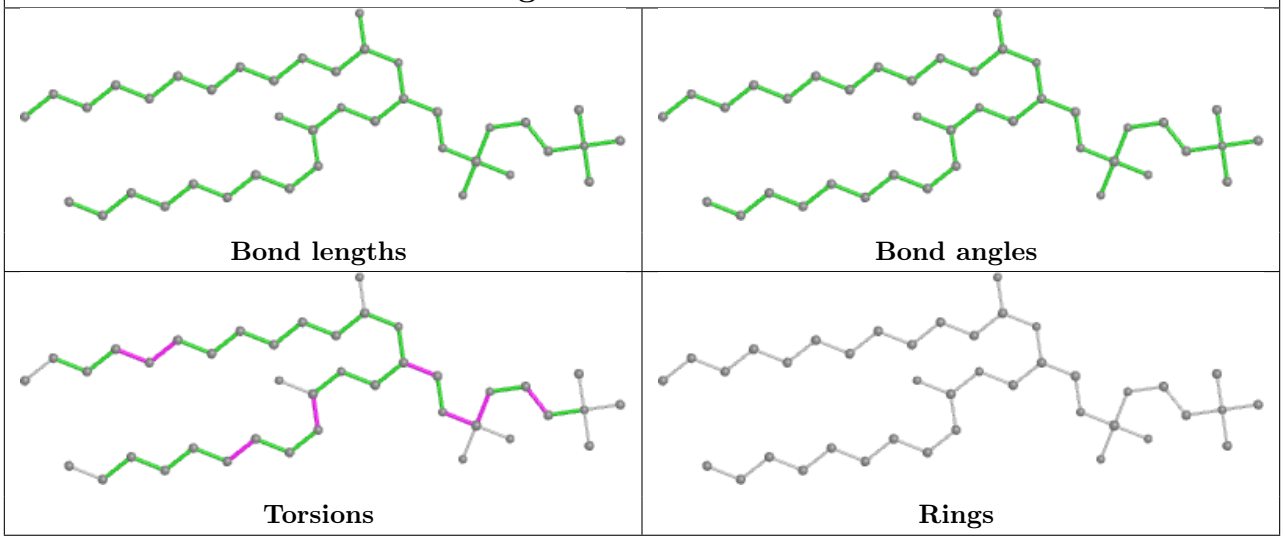
Ligand NAP A9 401



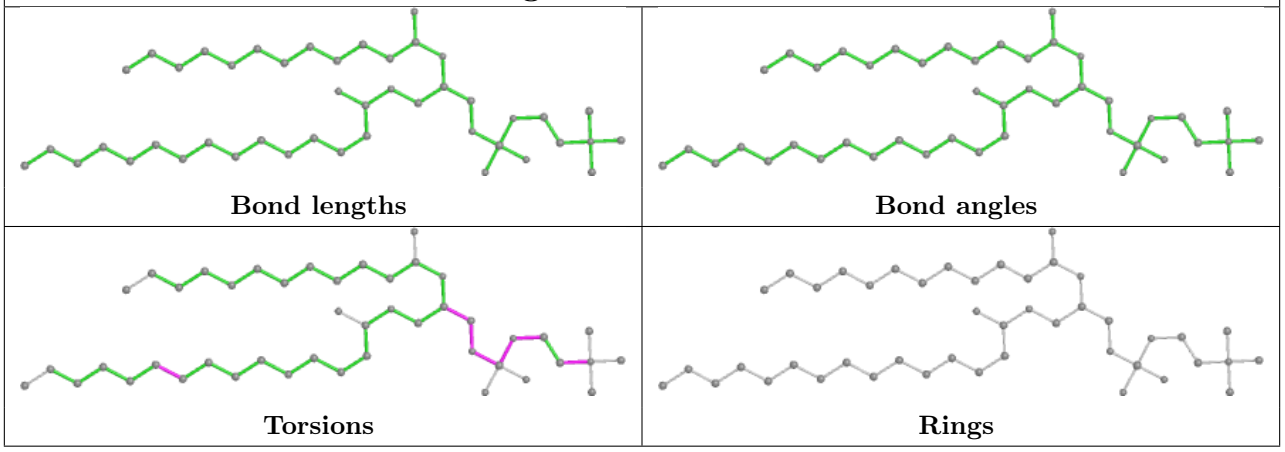
Ligand PC1 G1 701



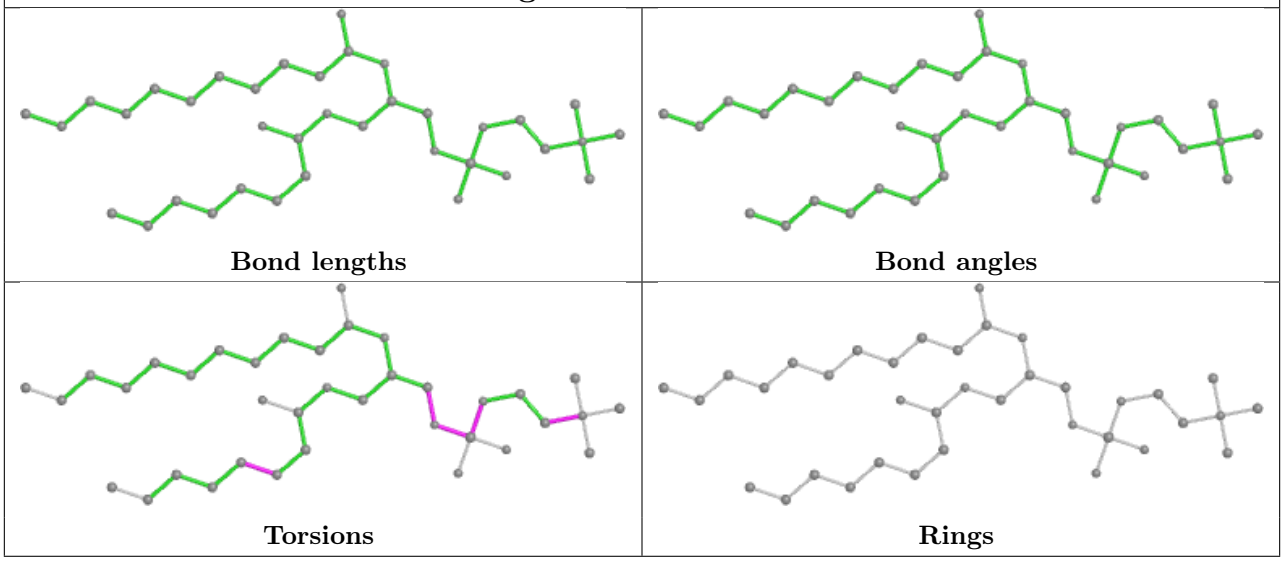
Ligand PC1 G1 702



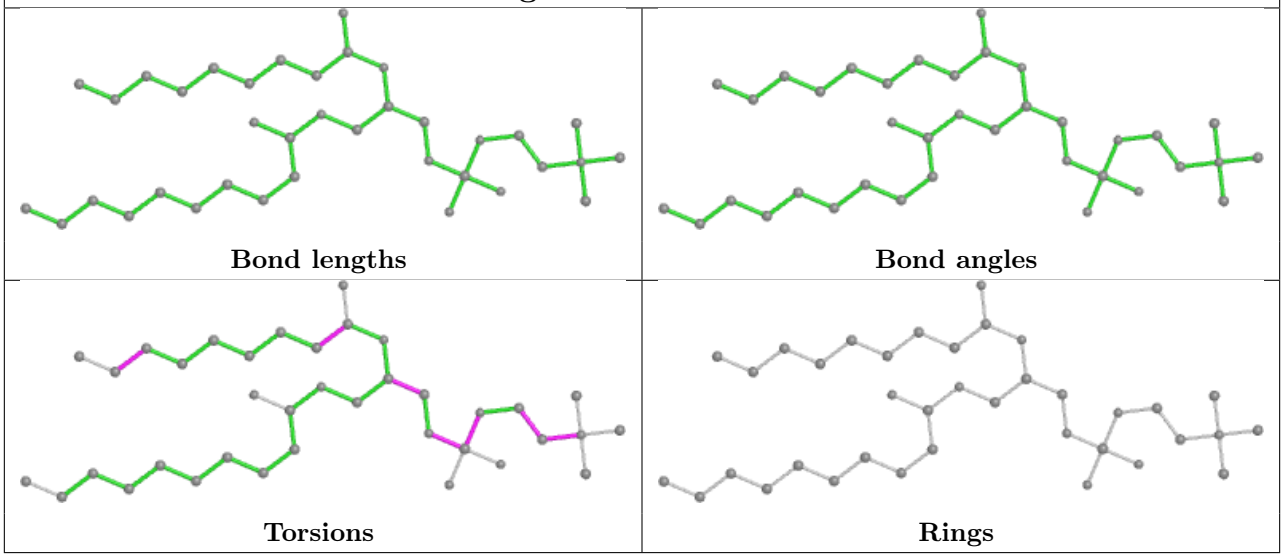
Ligand PC1 S2 401



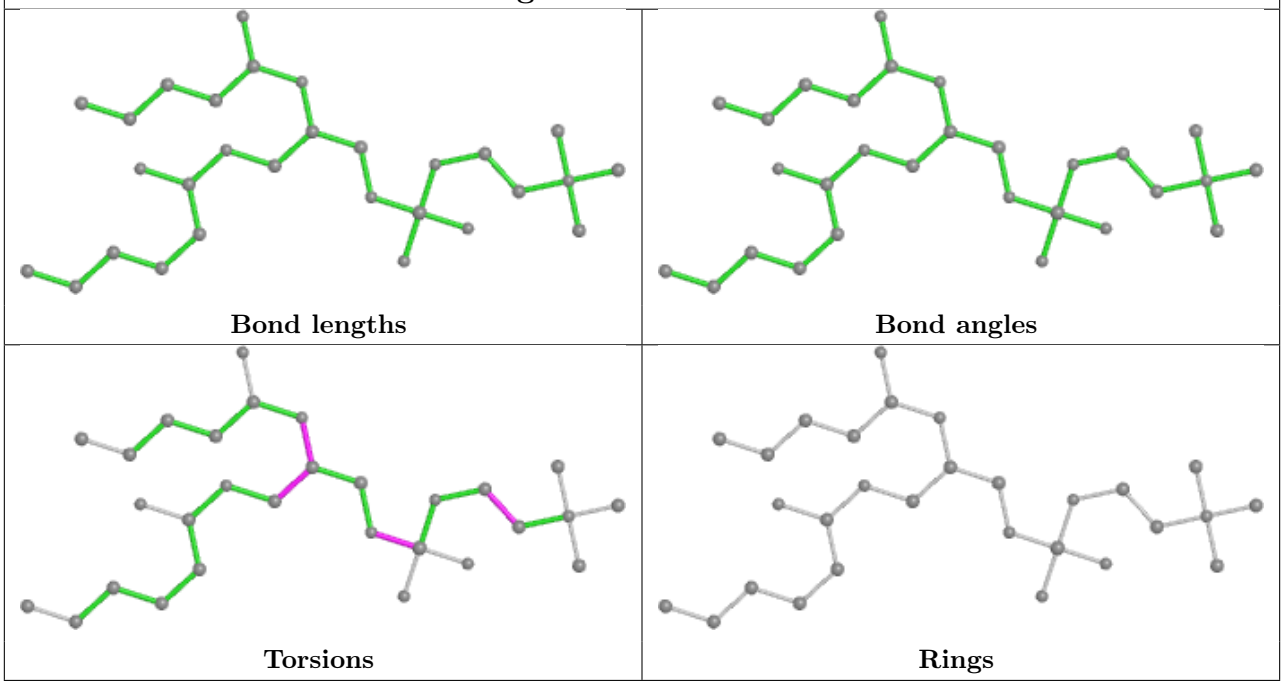
Ligand PC1 A1 101



Ligand PC1 C2 101



Ligand PC1 AL 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	20:UNK	C	21:UNK	N	3.16

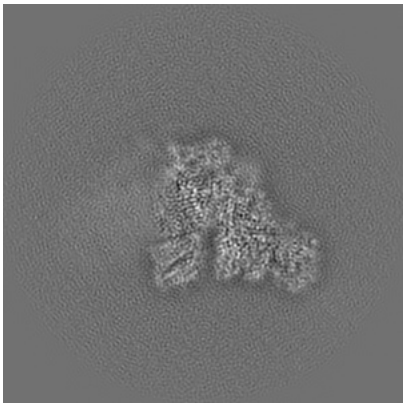
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22090. These allow visual inspection of the internal detail of the map and identification of artifacts.

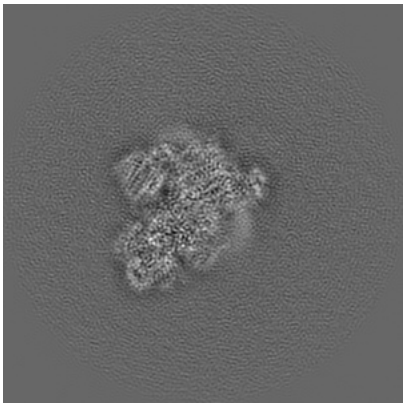
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

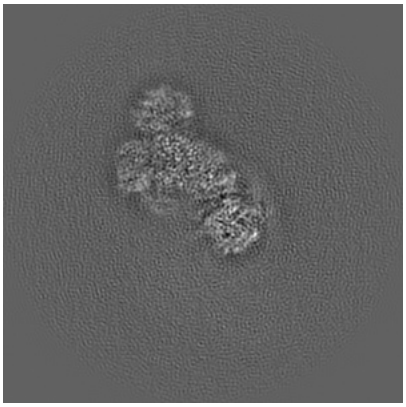
6.1.1 Primary map



X



Y

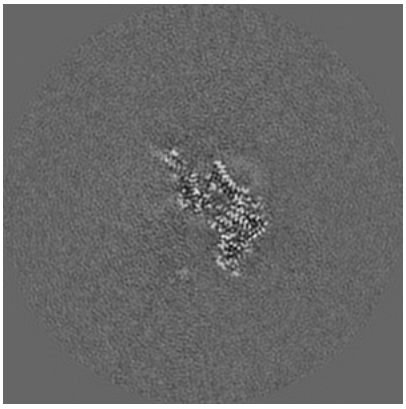


Z

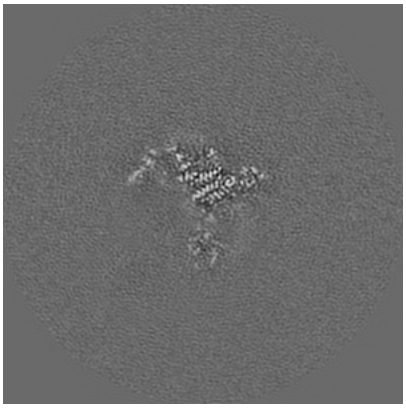
The images above show the map projected in three orthogonal directions.

6.2 Central slices

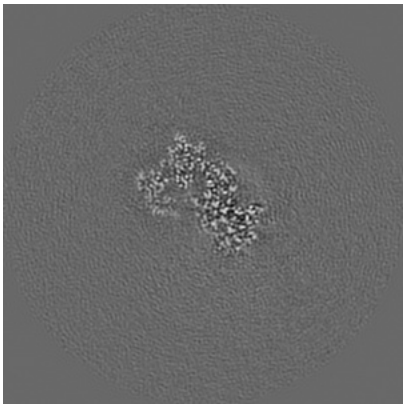
6.2.1 Primary map



X Index: 256



Y Index: 256

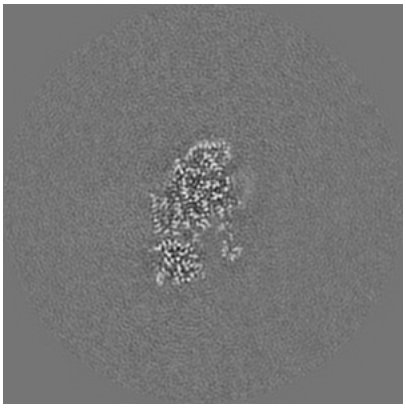


Z Index: 256

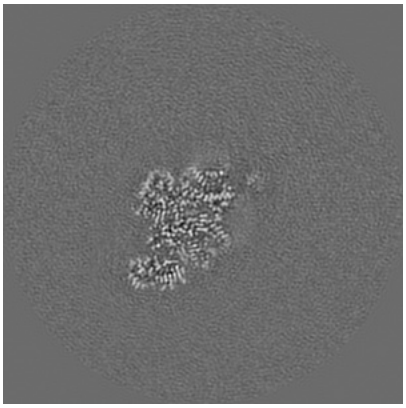
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

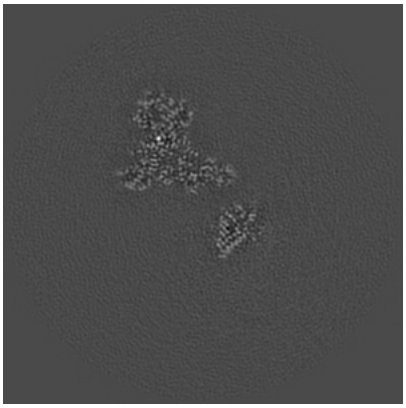
6.3.1 Primary map



X Index: 288



Y Index: 291

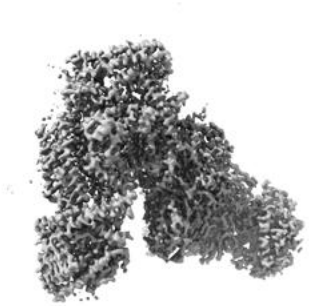


Z Index: 199

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

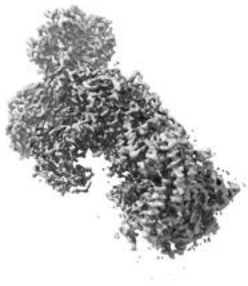
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

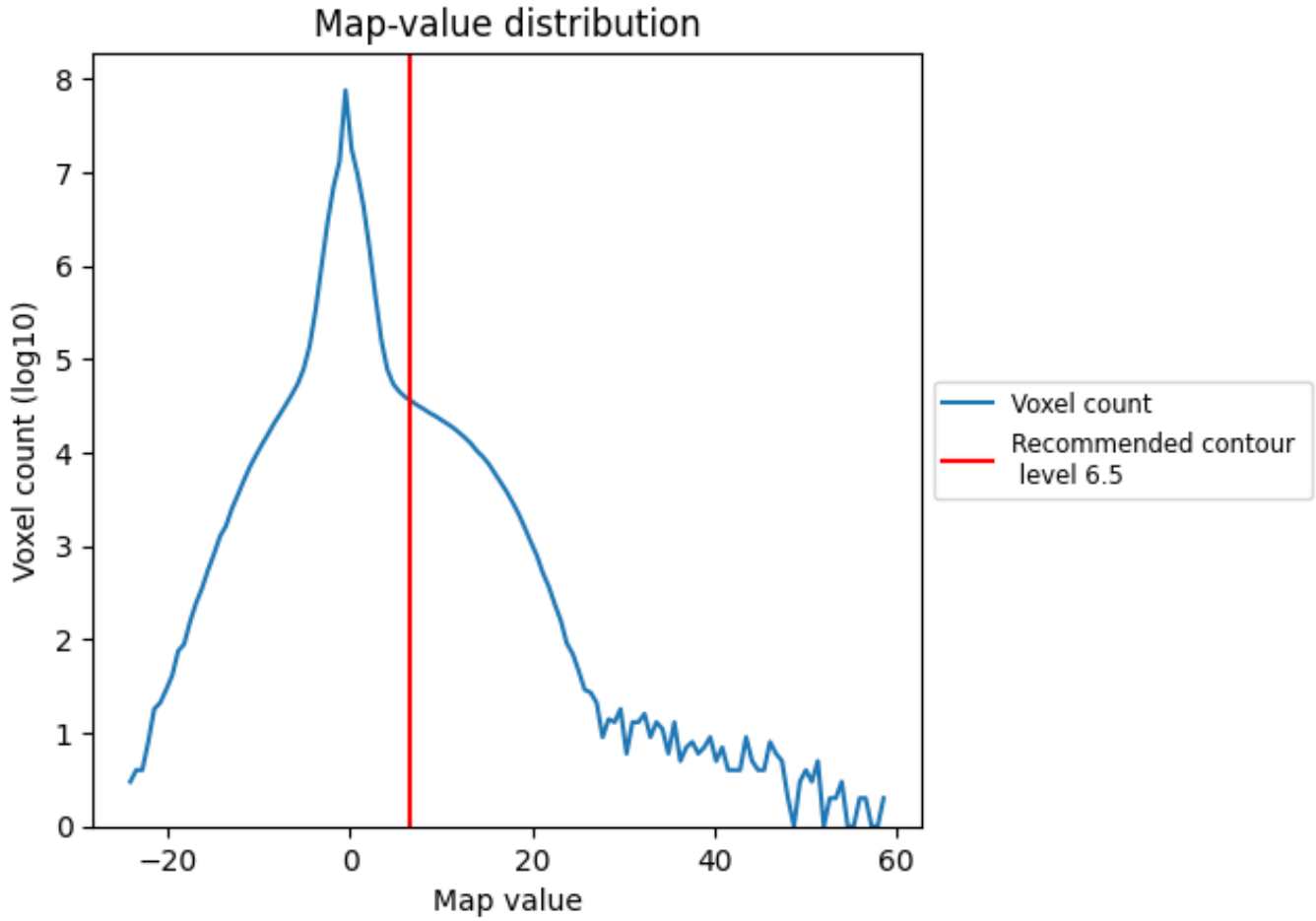
6.5 Mask visualisation (i)

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

7 Map analysis

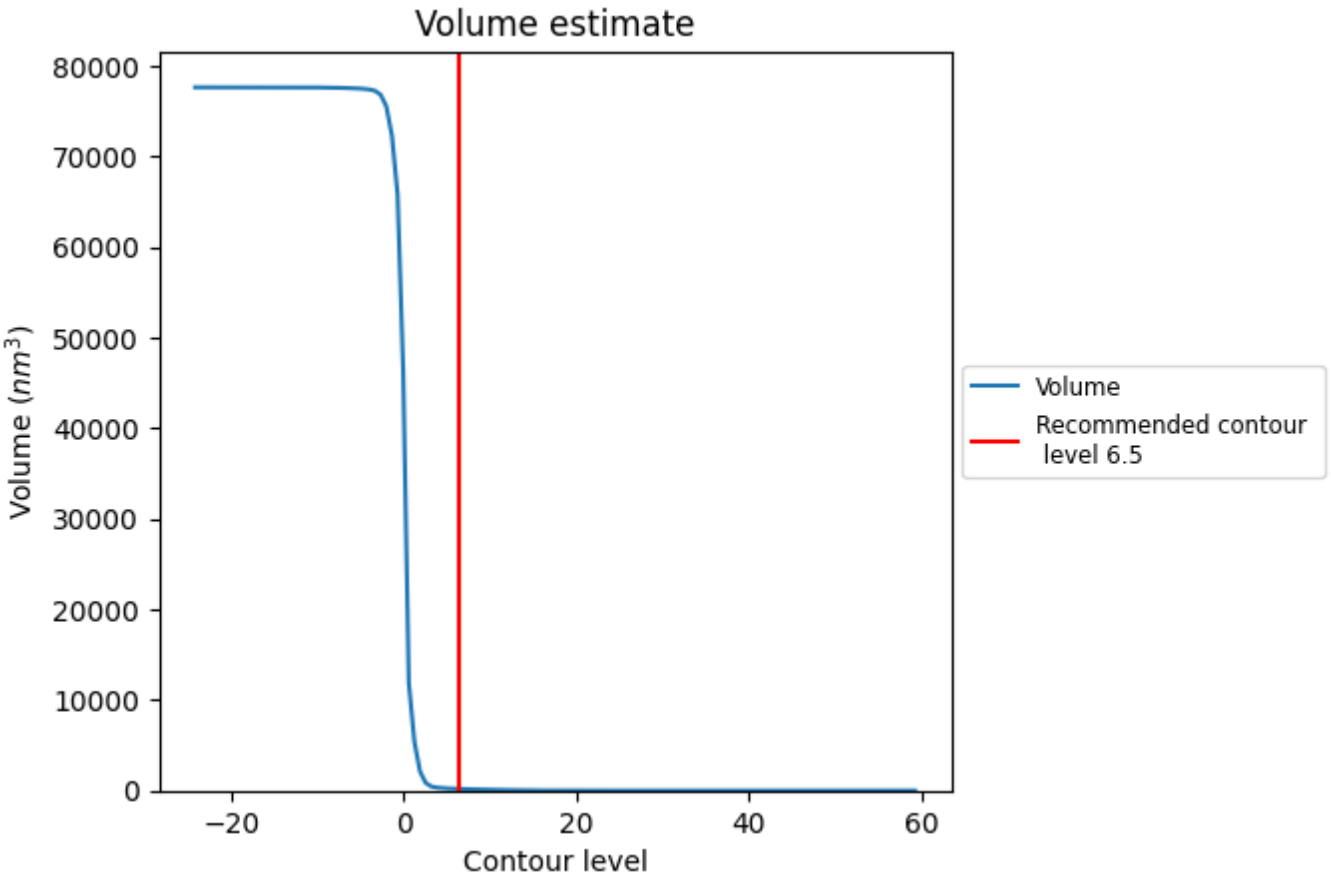
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

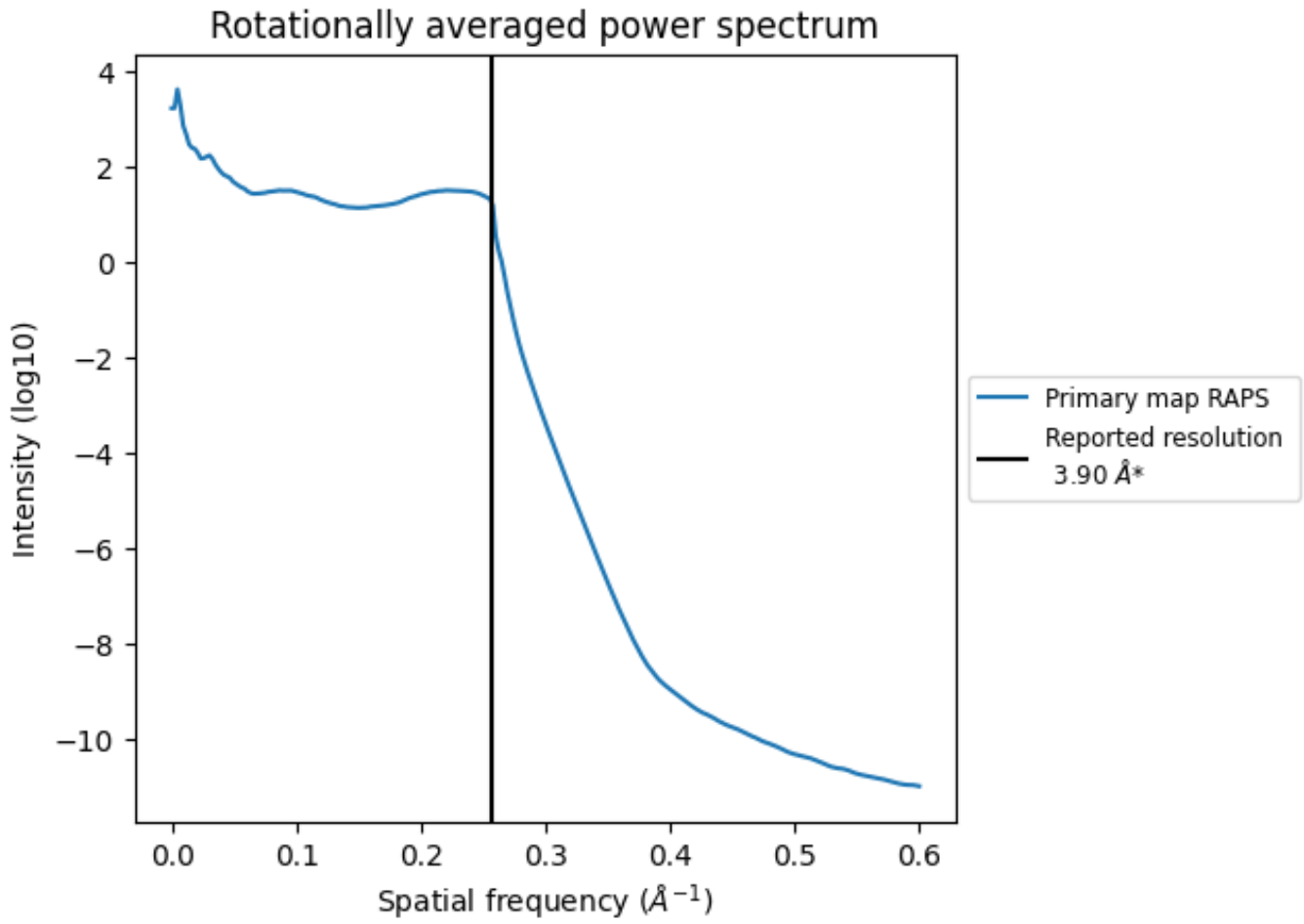
7.2 Volume estimate (i)



The volume at the recommended contour level is 183 nm^3; this corresponds to an approximate mass of 166 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 0.256 Å^{-1}

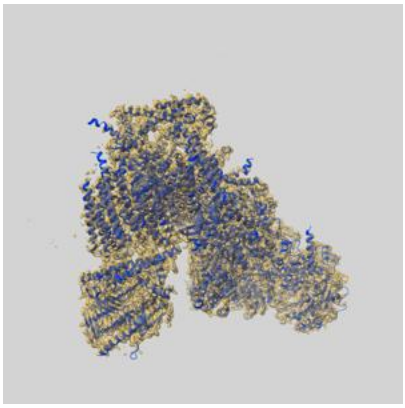
8 Fourier-Shell correlation (i)

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

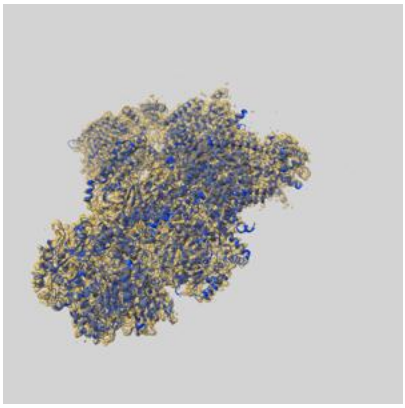
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22090 and PDB model 6X89. Per-residue inclusion information can be found in section 3 on page 15.

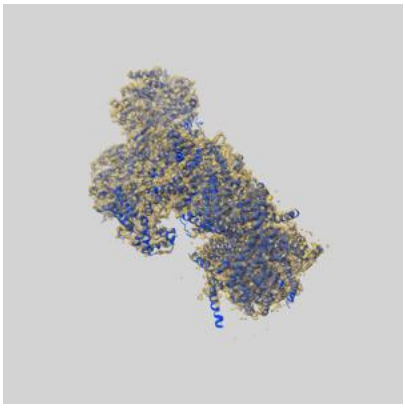
9.1 Map-model overlay



X



Y



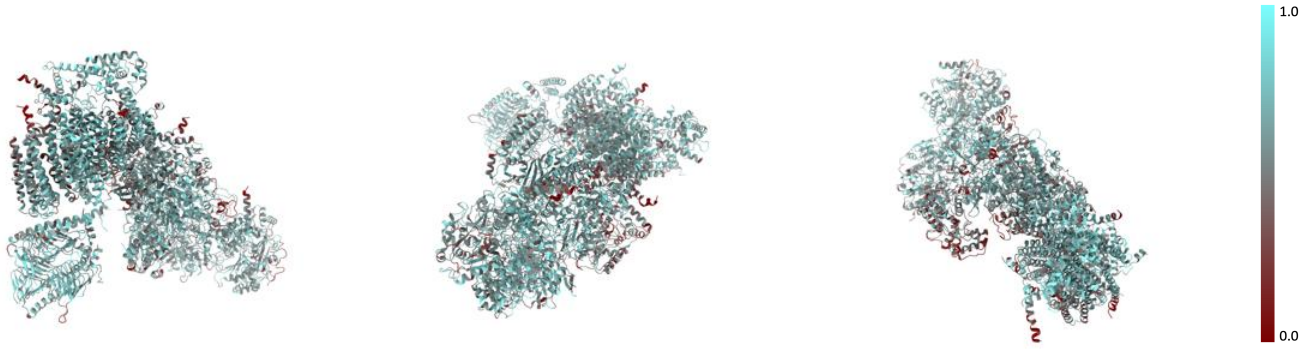
Z

The images above show the 3D surface view of the map at the recommended contour level 6.5 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)

This section was not generated.

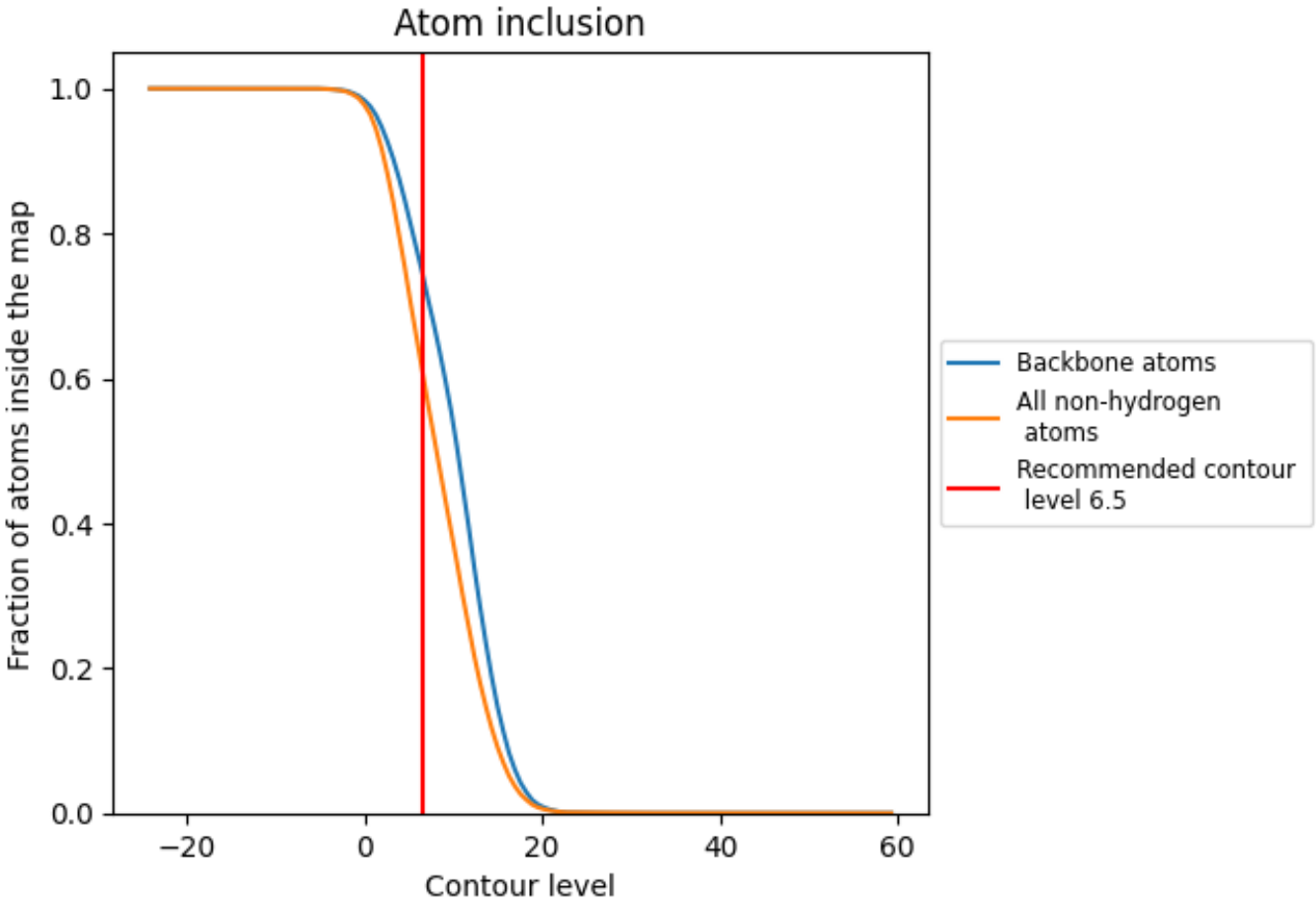
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.5).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 61% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.6116
1M	0.5894
2M	0.5865
3M	0.6037
4L	0.6248
6M	0.6398
A	0.7111
A1	0.5612
A2	0.5952
A3	0.5137
A5	0.5776
A6	0.6457
A7	0.4876
A8	0.6613
A9	0.4297
AL	0.4858
AM	0.5933
B	0.6960
C	0.4791
C2	0.5882
G1	0.6608
G2	0.6572
L2	0.6868
P2	0.6699
S1	0.6452
S2	0.6629
S3	0.6581
S4	0.6848
S5	0.7058
S6	0.6607
S7	0.6408
S8	0.6420
V1	0.5993
V2	0.5972
X1	0.7143