



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 01:09 PM EDT

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](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

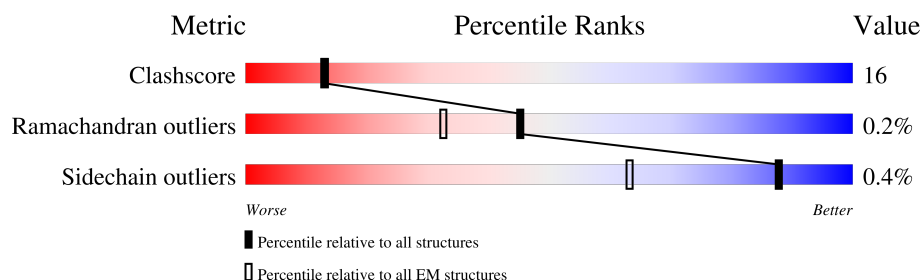
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	A	18	
2	A2	98	
3	A5	169	
4	A6	132	
5	A7	127	
6	A9	396	
7	AL	156	
8	S1	746	


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Mol	Chain	Length	Quality of chain
9	S2	394	
10	S3	190	
11	S4	146	
12	S6	103	
13	S7	213	
14	S8	222	
15	V1	491	
16	V2	251	
17	1M	325	
18	2M	488	
19	3M	118	
20	4L	100	
21	6M	205	
22	A1	65	
23	A3	63	
24	A8	106	
25	AM	143	
26	B	25	
27	C	43	
28	C2	81	
29	P2	115	
30	S5	399	
31	X1	101	
32	G1	270	
33	G2	273	

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Mol	Chain	Length	Quality of chain
34	L2	256	

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
1	A	18	Total	C	N	O	0	0
			90	54	18	18		

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

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

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

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

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

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

- Molecule 5 is a protein called NDUA7.

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

- 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	C	N	O	0	0
			125	75	25	25		

- Molecule 27 is a protein called Unknown Peptide.

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

- Molecule 28 is a protein called NDUC2.

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

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

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

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

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

- Molecule 31 is a protein called NDUX1.

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

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

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

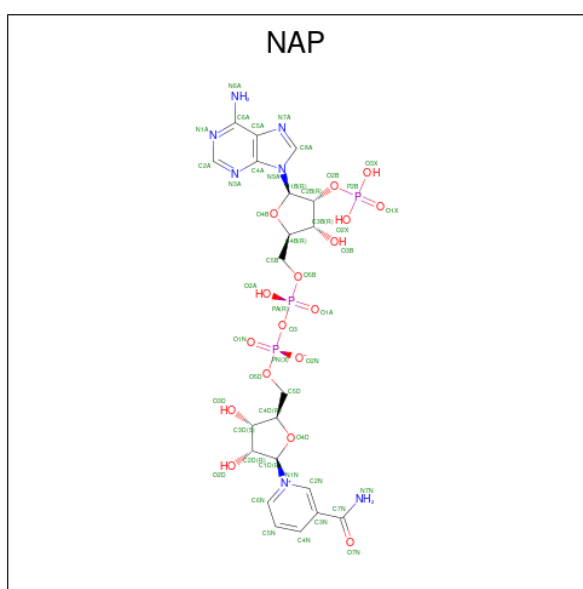
- Molecule 33 is a protein called gamma carbonic anhydrase 1, mitochondrial-like.

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.

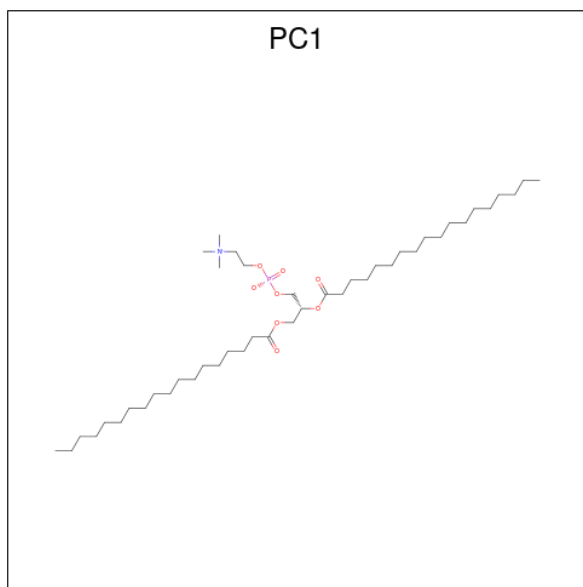
Mol	Chain	Residues	Atoms					AltConf	Trace
34	L2	207	Total	C	N	O	S	0	0
			1611	1033	276	297	5		

- 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
			27	17	1	8	1	
36	G1	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 37 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 38 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

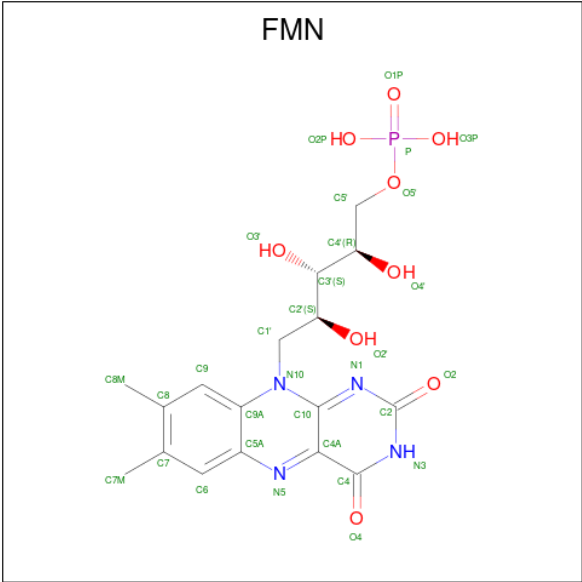


Mol	Chain	Residues	Atoms			AltConf
38	S1	1	Total	Fe	S	0
			4	2	2	
38	V2	1	Total	Fe	S	0
			4	2	2	

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

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

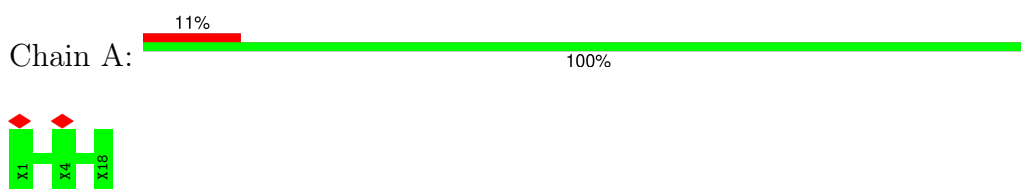
- Molecule 40 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



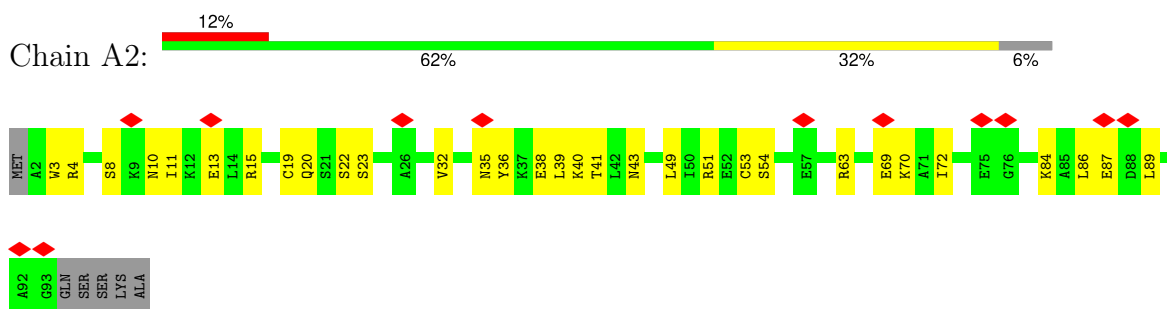
### 3 Residue-property plots [i](#)

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.

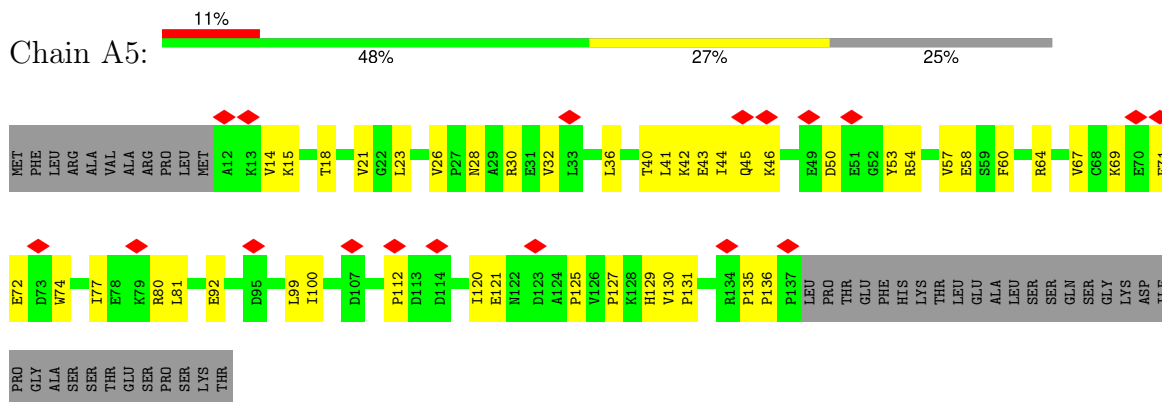
- Molecule 1: Unknown Peptide



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

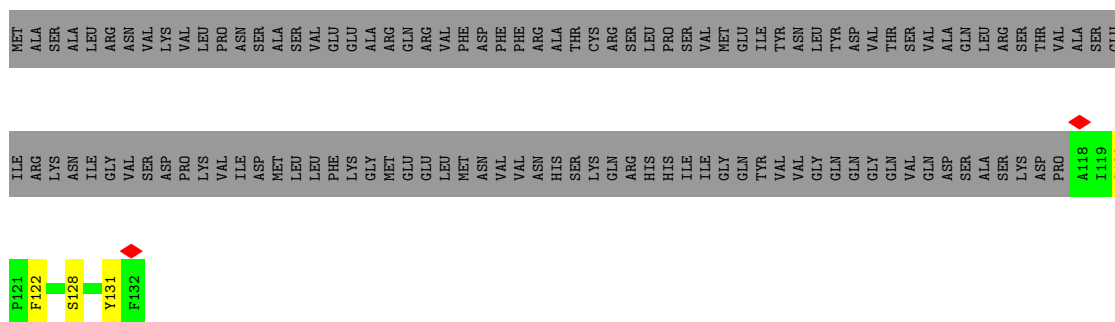


- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial

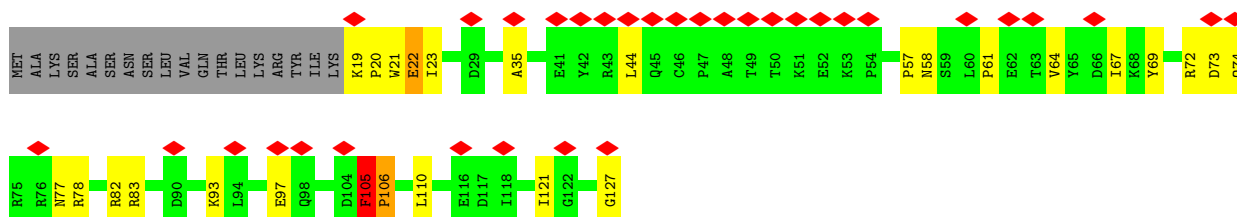


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

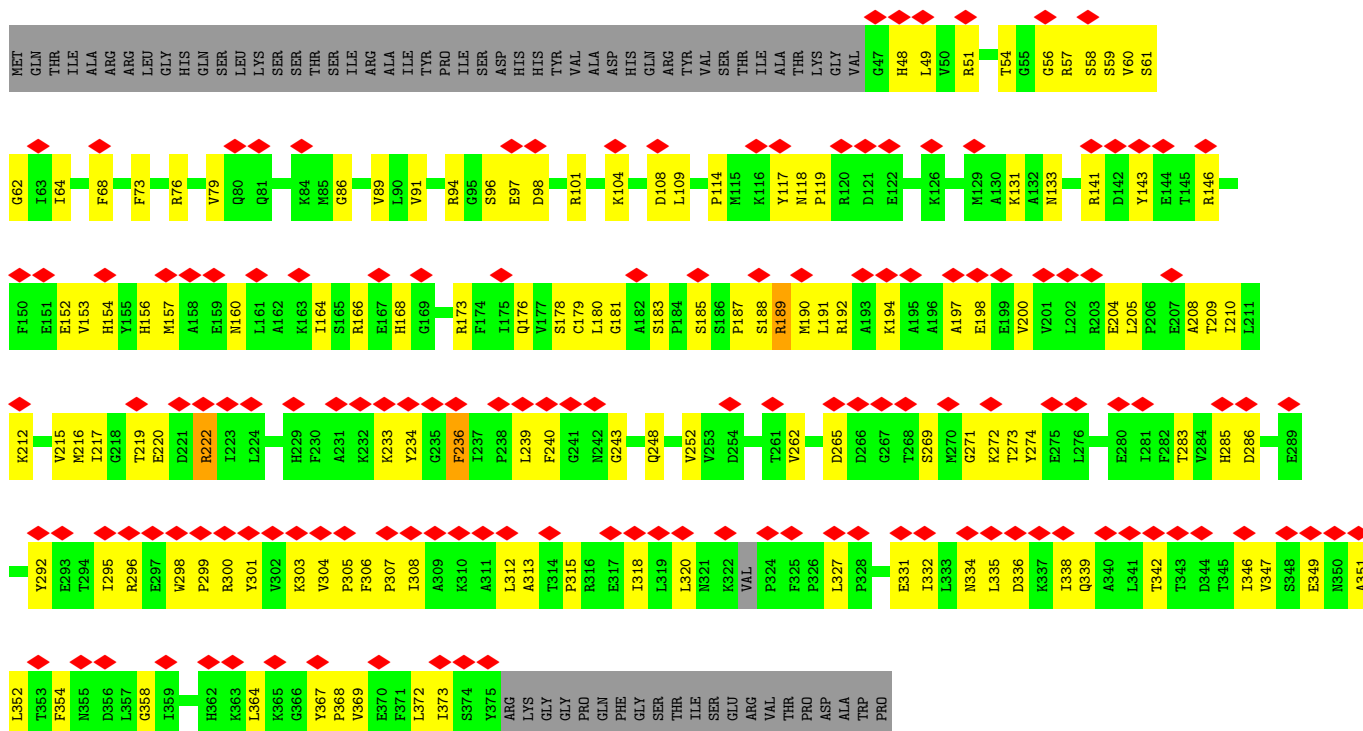




- Molecule 5: NDUA7

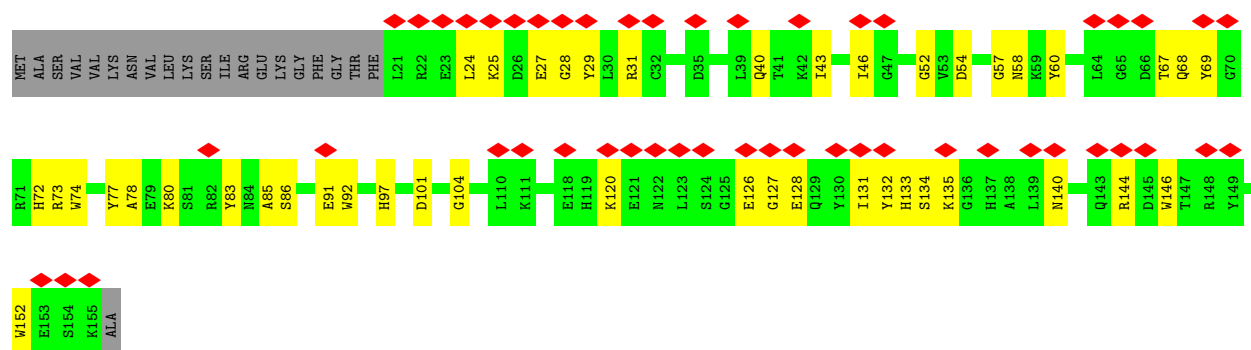


- Molecule 6: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial isoform X1

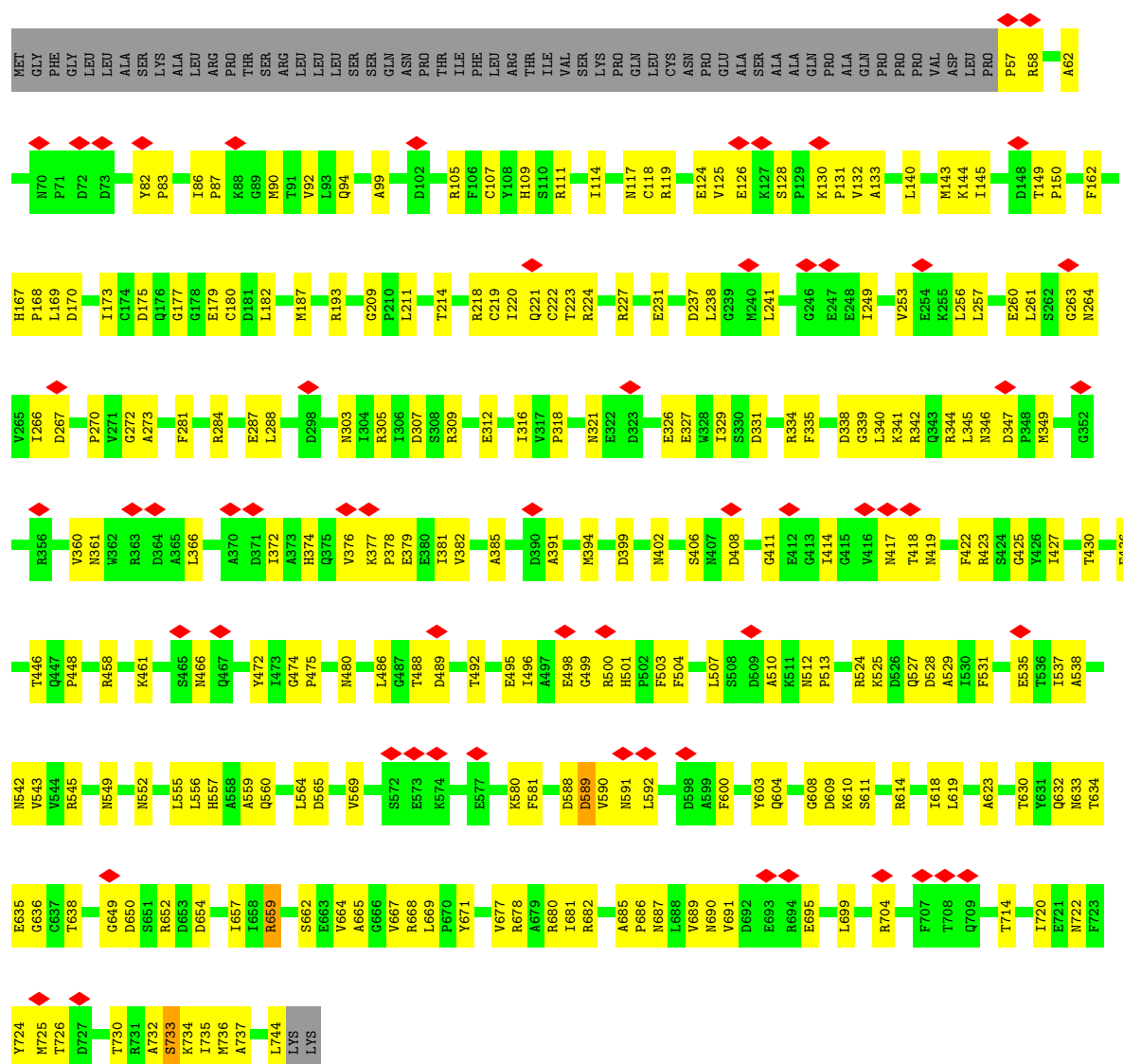


- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



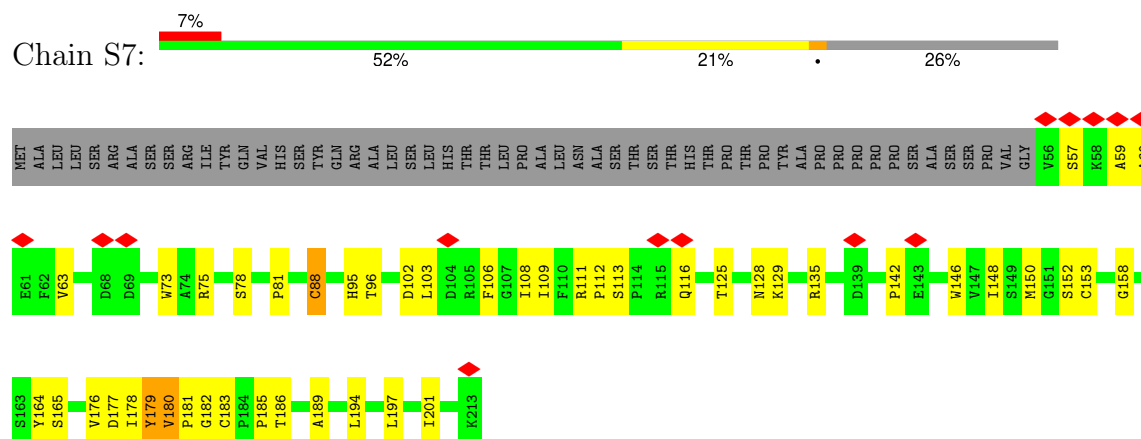


• Molecule 8: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial

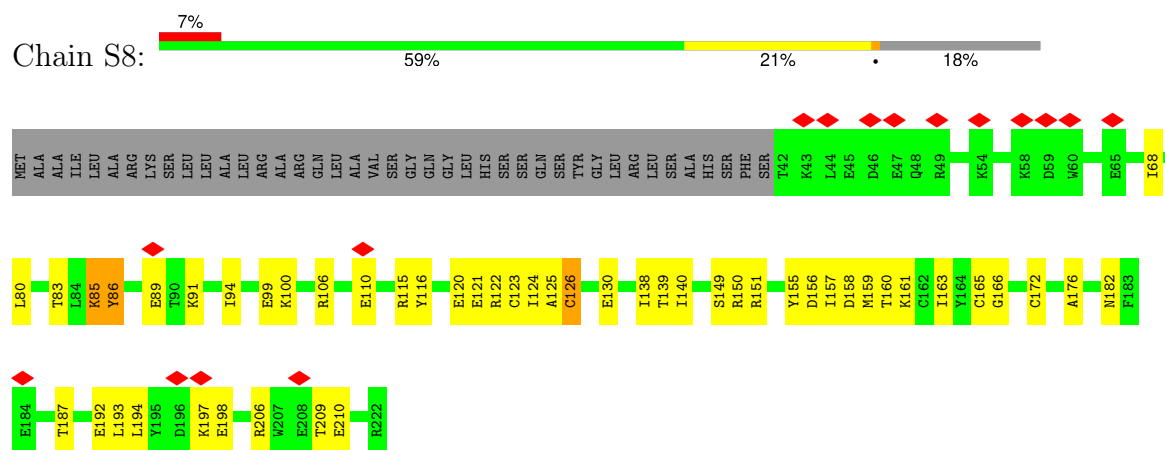




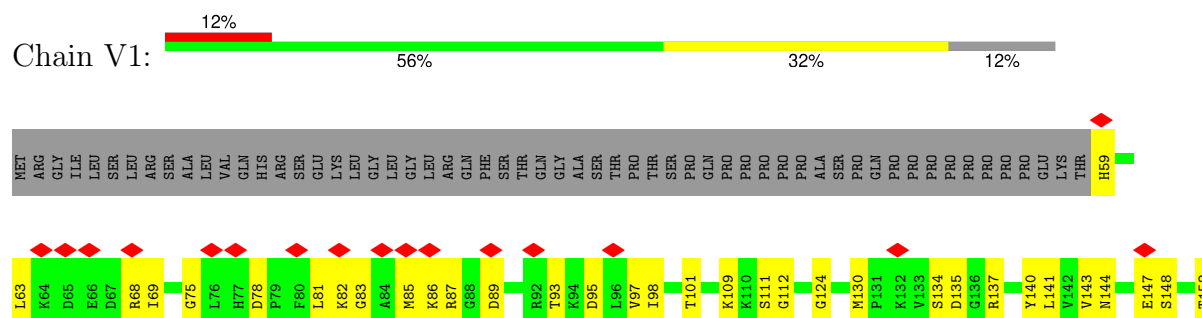
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

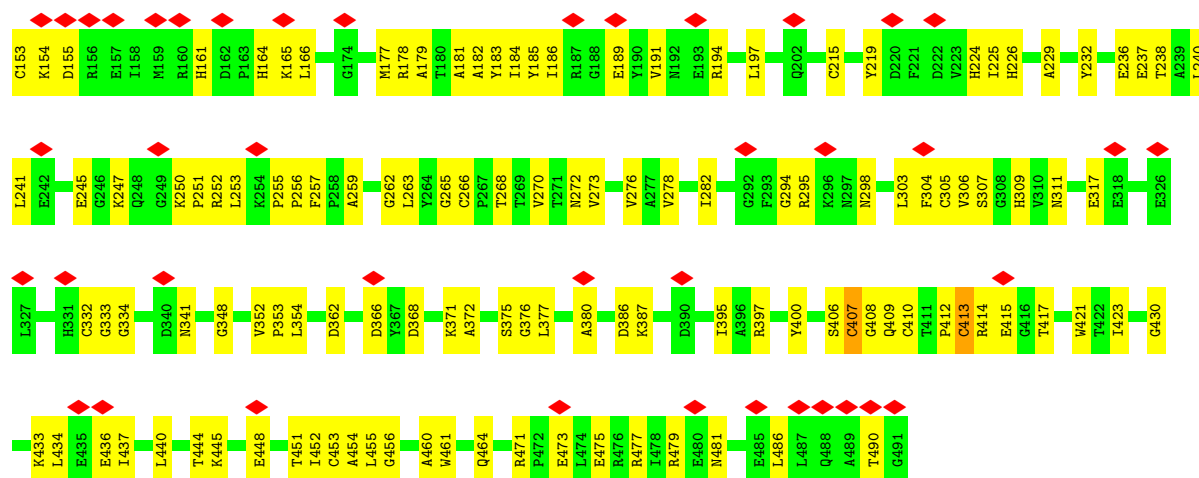


- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

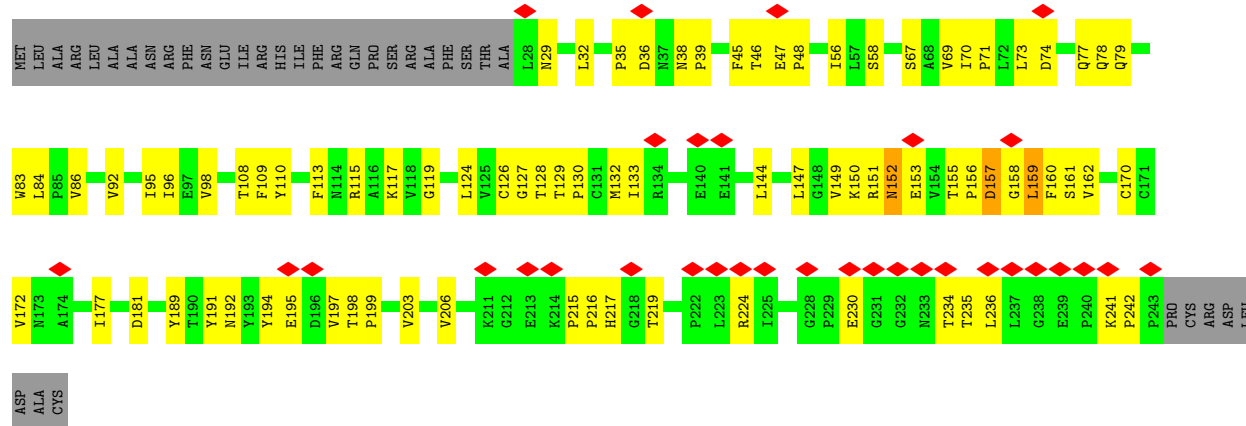


- Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

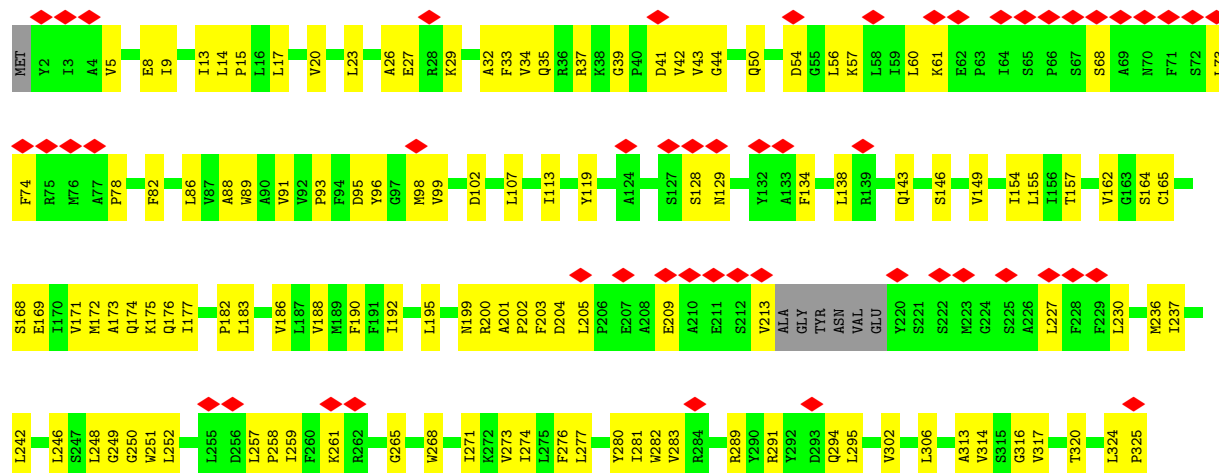




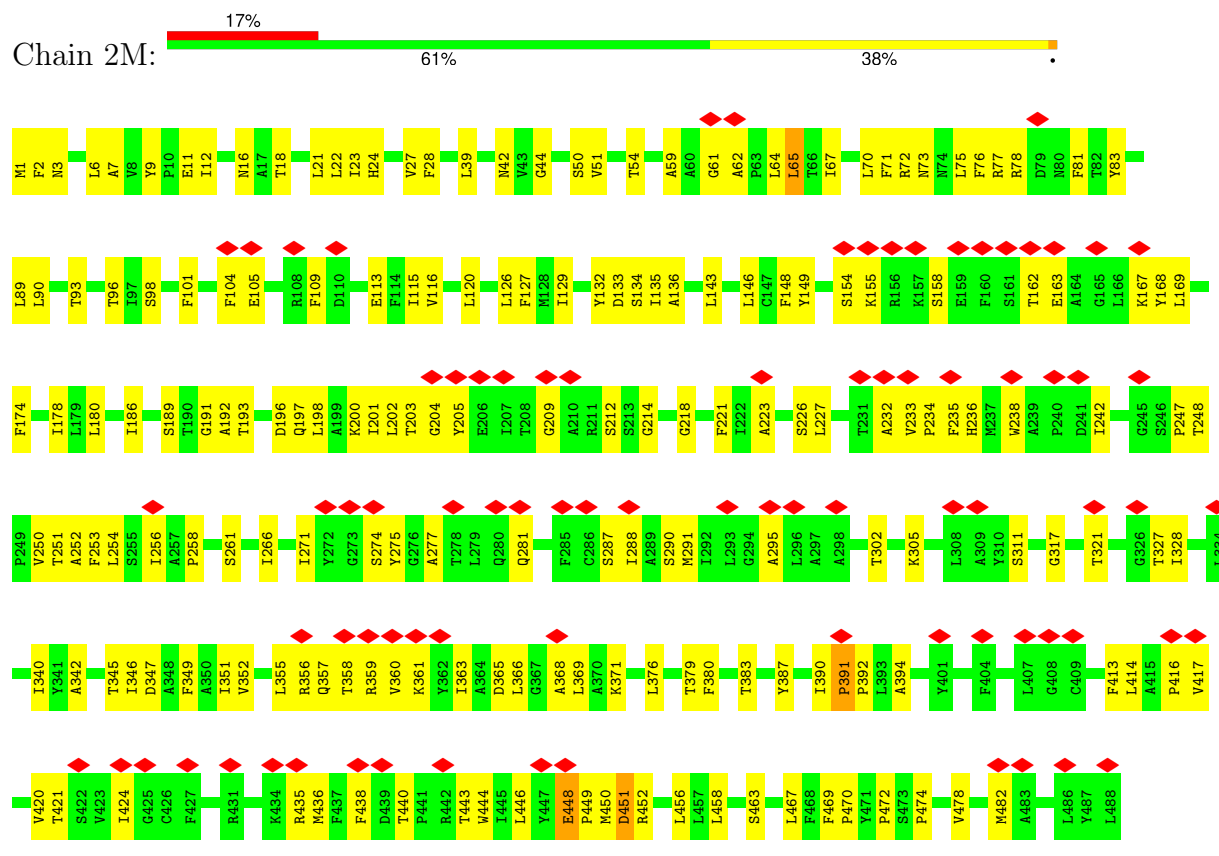
• Molecule 16: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



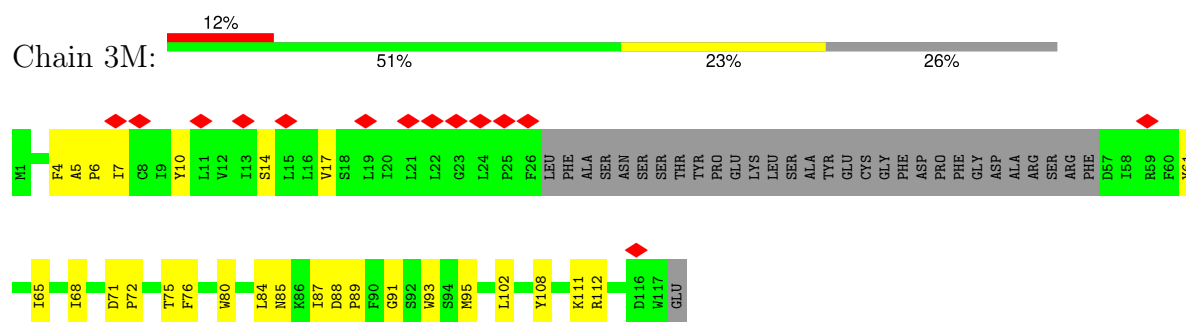
• Molecule 17: NU1M



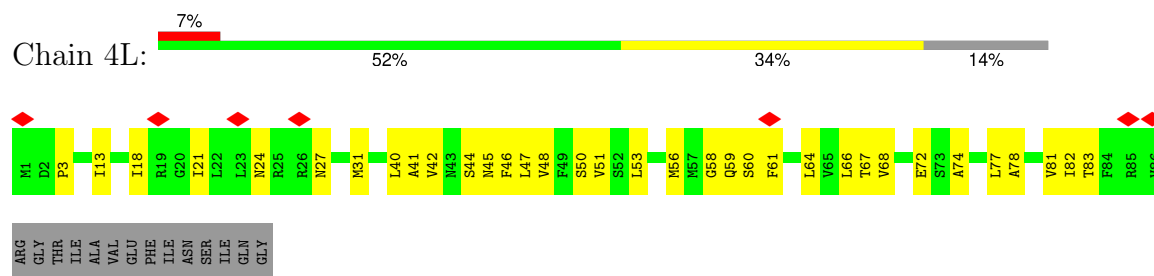
- Molecule 18: NU2M



- Molecule 19: NU3M

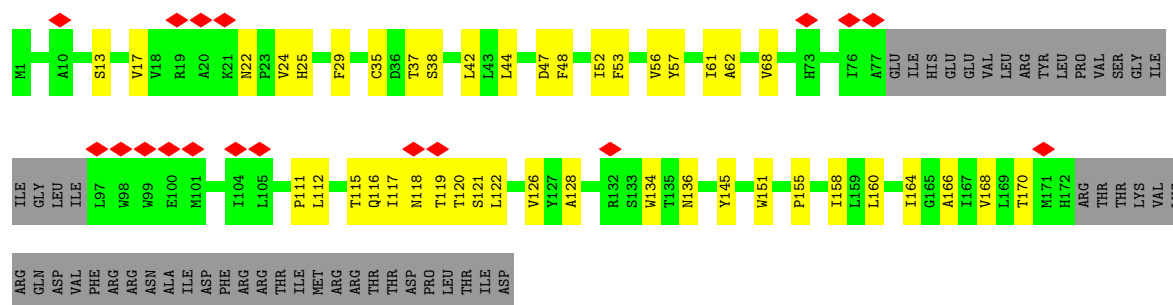


- Molecule 20: NU4L



- Molecule 21: NU6M





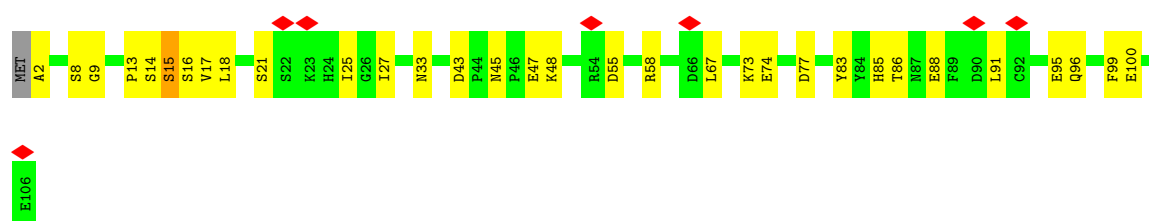
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



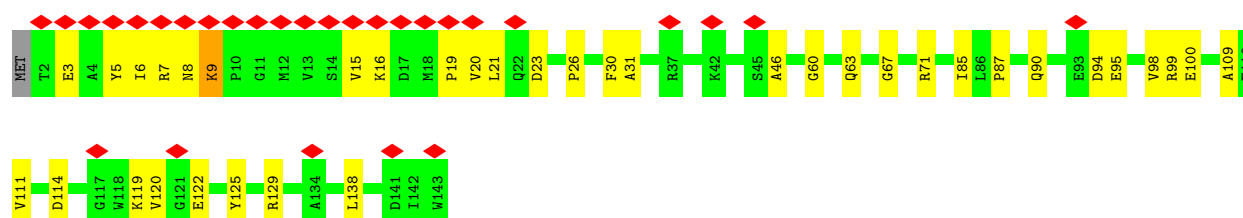
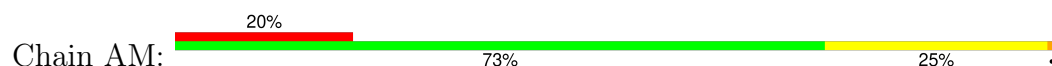
- Molecule 23: uncharacterized protein LOC106754061



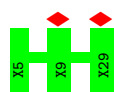
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B

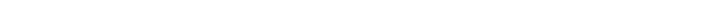


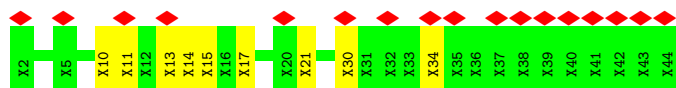
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A




- Molecule 26: Unknown Peptide



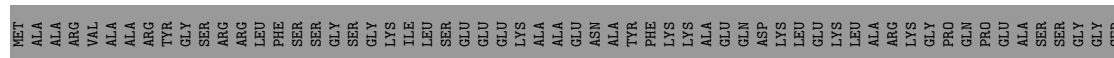
- Chain C:  40% 79% 21%



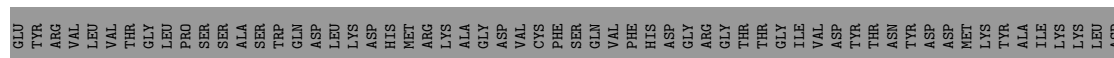
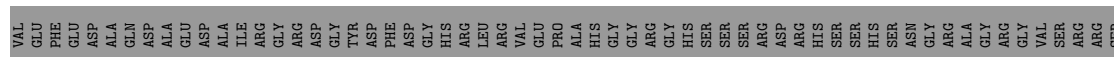
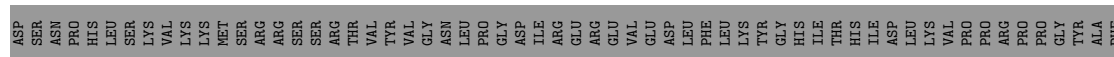
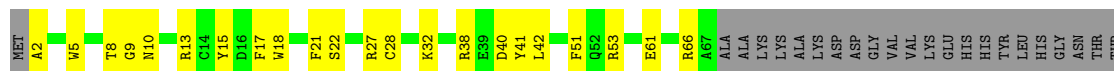
- Chain C2: 



- Chain P2:  25% 74%



- Chain S5:  11% 6% 83%



SER  
ARG  
SER  
ARG  
SER  
LYS  
SER  
LEU  
SER  
ARG

• Molecule 31: NDUX1

Chain X1:  66% 32%

H1 I5 S8 T9 K10 D17 R18 R19 P20 K24 L32 L35 R36 G48 Y49 L50 L51 G52 I53 K54 P55 G56 I57 R58 G59 P60 S61 G66 V70 Y76 Q79 R80 S81 A82 G83 R84 F89 D93 E94 R99 LYS LYS

• Molecule 32: gamma carbonic anhydrase 1, mitochondrial

Chain G1:  51% 34% 14%

MET GLY T3 V11 G12 F13 R16 Q20 D23 R24 S27 R28 L29 N32 Y33 E37 R41 H42 K51 K51 V52 P53 K57 D58 A59 F60 S64 A65 S66 V71 W80 W81 G82 C83 R86 G87 D88 V89 N90 G91 I92 V93 I94 G95 S96 G97 T98

D102 M103 S104 L105 V106 H107 V108 K110 K111 L113 T114 G115 K116 V117 T120 I121 I122 G123 D124 M125 V126 H130 S131 A132 V133 L134 G135 G136 C137 T138 V139 E140 D141 E142 G146 H147 G148 H149 T150 G154 V155 V156 V157 E158 K159 H160 I161 M162 A165 S166 G166 G167 L168 V169

R170 G171 M172 I175 P176 E179 V180 W181 M184 P185 A186 K187 T193 E194 D195 E196 M197 F200 A204 Y207 A211 H214 E217 K220 F221 L222 R233 LYS PHE ALA PRO ARG GLU GLU TYR ASP SER ILE LEU ASP GLY GLN GLN GLU THR PRO

ALA LYS LEU LEU GLN ASP ASN VAL LEU ASP LYS ALA PRO LYS ALA

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

Chain G2:  5% 47% 40% 14%

MET G2 A7 S10 R16 Q20 D23 G26 S27 R28 L29 F35 Q36 E37 Q38 L39 S40 R41 M46 M47 I48 K51 V55 D56 K57 D58 V59 F60 S64 A65 S66 V67 I68 G69 D70 V71 V72 V73 G74 R75 G76 G82 C83 V84 L85 R86 G87 D88

V89 I92 R93 V94 G95 S96 G97 N98 N99 I100 Q101 H103 S104 L105 V106 H107 V108 K109 A110 S111 N112 L113 S114 G115 K116 V117 L118 P119 T120 V121 I122 G123 D124 H125 V126 V127 V128 G129 H130 L134 H135 G136 E140 D141 A142 A143 F144 V145 G146 M147 L151 L152 D153 G154 V155

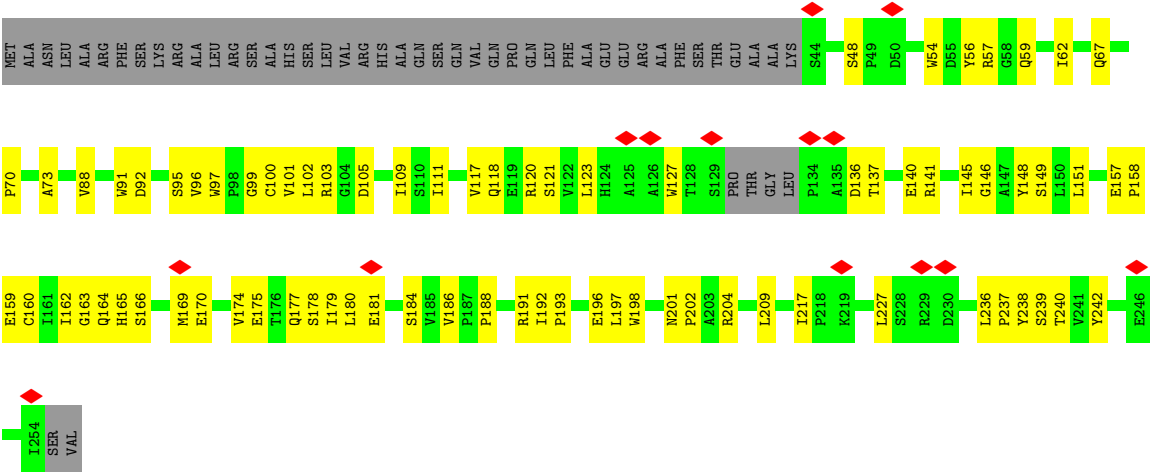
V156 V157 K159 N160 A161 V163 A164 A165 L168 V169 R170 R174 I175 G178 E179 V180 V181 A182 A186 L189 R190 S193 R194 E195 E196 T198 F199 Y207 L210 A215 A216 E217 N218 S219 K220 S221 Y222 D223 E224 R232 K233 R237 LYS ASP GLU GLU

TYR ASP SER MET LEU VAL VAL ARG GLU ILE PRO PRO GLU LEU ILE LEU PRO ASP ASN VAL V181 LEU PRO ASP LYS ALA GLU LYS LEU GLN LYS

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

Chain L2:  5% 51% 30% 19%





## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NAP, ZN, PC1, FMN, FES

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(°)	Ideal(°)
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%)	16	51
4	A6	13/132 (10%)	7 (54%)	6 (46%)	0	100	100
5	A7	107/127 (84%)	86 (80%)	18 (17%)	3 (3%)	4	28
6	A9	324/396 (82%)	257 (79%)	66 (20%)	1 (0%)	37	70

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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%)	48	80
9	S2	378/394 (96%)	325 (86%)	53 (14%)	0	100	100
10	S3	182/190 (96%)	143 (79%)	38 (21%)	1 (0%)	25	60
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%)	22	57
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%)	9	39
17	1M	314/325 (97%)	279 (89%)	35 (11%)	0	100	100
18	2M	486/488 (100%)	431 (89%)	54 (11%)	1 (0%)	44	75
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%)	13	46
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%)	45	75

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%)	89	91
7	AL	117/134 (87%)	117 (100%)	0	100	100
8	S1	571/622 (92%)	570 (100%)	1 (0%)	92	94
9	S2	328/339 (97%)	324 (99%)	4 (1%)	67	78
10	S3	173/179 (97%)	171 (99%)	2 (1%)	67	78
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%)	60	74
14	S8	162/193 (84%)	159 (98%)	3 (2%)	52	70
15	V1	349/400 (87%)	347 (99%)	2 (1%)	84	88
16	V2	186/216 (86%)	186 (100%)	0	100	100
17	1M	266/271 (98%)	265 (100%)	1 (0%)	89	91
18	2M	407/408 (100%)	406 (100%)	1 (0%)	92	94
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%)	56	72
31	X1	82/84 (98%)	82 (100%)	0	100	100
32	G1	185/216 (86%)	184 (100%)	1 (0%)	86	90
33	G2	192/226 (85%)	191 (100%)	1 (0%)	86	90
34	L2	177/217 (82%)	176 (99%)	1 (1%)	84	88
All	All	4749/5883 (81%)	4728 (100%)	21 (0%)	88	91

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 ⓘ

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 oligosaccharides 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	$\# Z  > 2$
38	FES	V2	300	16	0,4,4	-	-	-		
36	PC1	AL	401	-	28,28,53	0.39	0	34,36,61	0.45	0
36	PC1	S2	401	-	44,44,53	0.31	0	50,52,61	0.32	0
36	PC1	A1	101	-	36,36,53	0.34	0	42,44,61	0.34	0
36	PC1	G1	701	-	26,26,53	0.43	0	32,34,61	0.41	0
37	SF4	S1	802	8	0,12,12	-	-	-		
37	SF4	S8	301	14	0,12,12	-	-	-		
37	SF4	S8	302	14	0,12,12	-	-	-		
37	SF4	S7	301	-	0,12,12	-	-	-		
37	SF4	S1	801	8	0,12,12	-	-	-		
36	PC1	G1	702	-	39,39,53	0.34	0	45,47,61	0.38	0
35	NAP	A9	401	-	46,52,52	1.55	5 (10%)	61,80,80	1.45	5 (8%)
38	FES	S1	803	8	0,4,4	-	-	-		
40	FMN	V1	501	-	33,33,33	0.32	0	48,50,50	0.32	0
36	PC1	C2	101	-	36,36,53	0.37	0	42,44,61	0.41	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
38	FES	V2	300	16	-	-	0/1/1/1
36	PC1	AL	401	-	-	7/32/32/57	-
36	PC1	S2	401	-	-	11/48/48/57	-
36	PC1	A1	101	-	-	10/40/40/57	-
36	PC1	G1	701	-	-	6/30/30/57	-
37	SF4	S1	802	8	-	-	0/6/5/5
37	SF4	S8	301	14	-	-	0/6/5/5
37	SF4	S8	302	14	-	-	0/6/5/5
37	SF4	S7	301	-	-	-	0/6/5/5
37	SF4	S1	801	8	-	-	0/6/5/5
36	PC1	G1	702	-	-	11/43/43/57	-
35	NAP	A9	401	-	-	19/31/67/67	0/5/5/5
40	FMN	V1	501	-	-	6/18/18/18	0/3/3/3
38	FES	S1	803	8	-	-	0/1/1/1
36	PC1	C2	101	-	-	9/40/40/57	-
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	6.19	1.48	1.39
35	A9	401	NAP	C5N-C4N	5.69	1.48	1.38
35	A9	401	NAP	C6N-C5N	-3.04	1.32	1.38
35	A9	401	NAP	C2N-C3N	-2.47	1.35	1.39
35	A9	401	NAP	C2N-N1N	2.41	1.37	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A9	401	NAP	C5N-C4N-C3N	-8.64	111.87	120.36
35	A9	401	NAP	C6N-N1N-C2N	-3.62	118.80	121.88
35	A9	401	NAP	C6N-C5N-C4N	2.40	122.91	119.45
35	A9	401	NAP	C5A-C6A-N6A	2.28	123.78	120.31
35	A9	401	NAP	C2N-C3N-C4N	2.10	120.70	118.26

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

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

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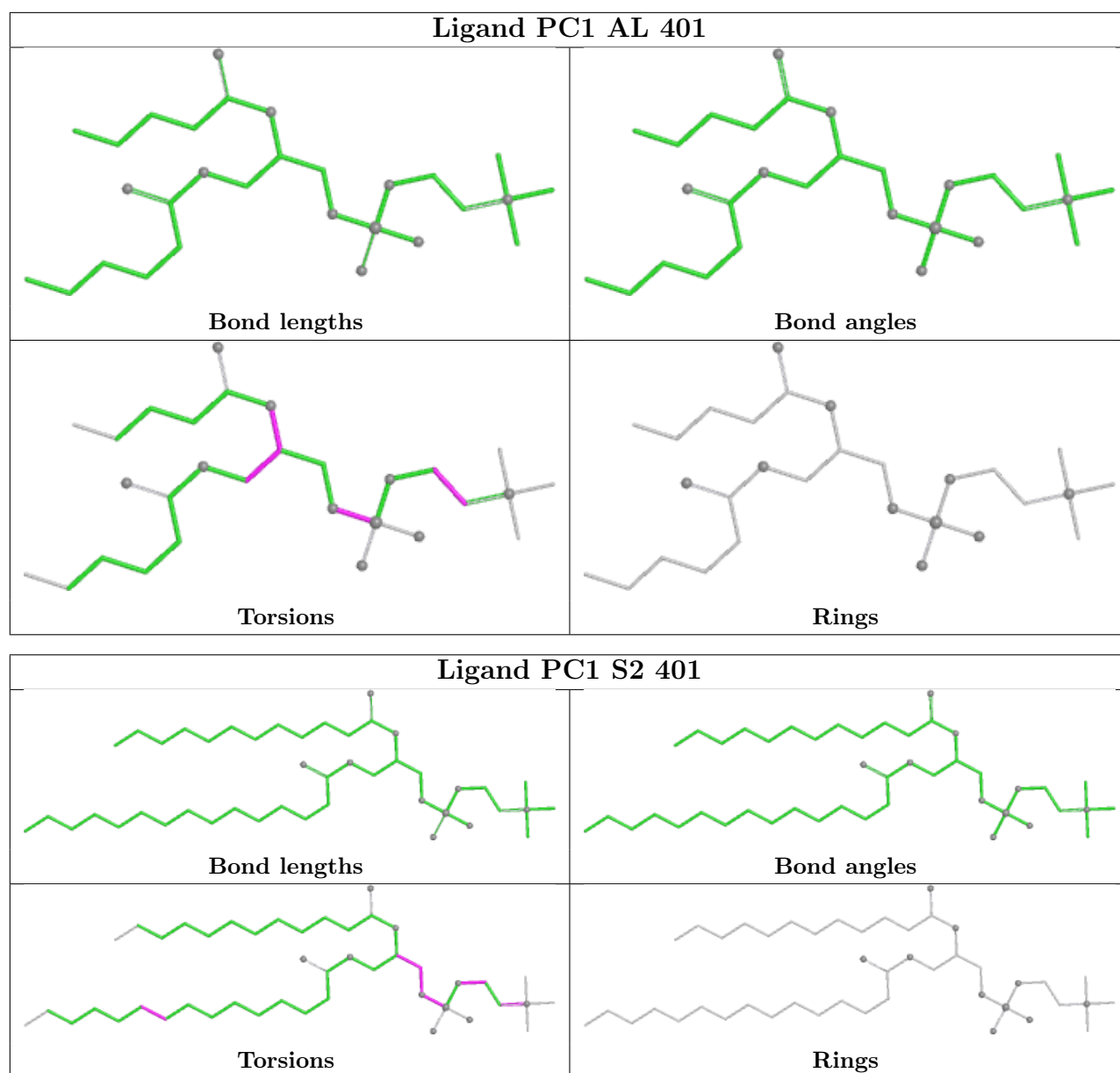
Mol	Chain	Res	Type	Atoms
35	A9	401	NAP	C5B-O5B-PA-O2A
35	A9	401	NAP	C5B-O5B-PA-O3
35	A9	401	NAP	O4D-C1D-N1N-C2N
35	A9	401	NAP	O4D-C1D-N1N-C6N

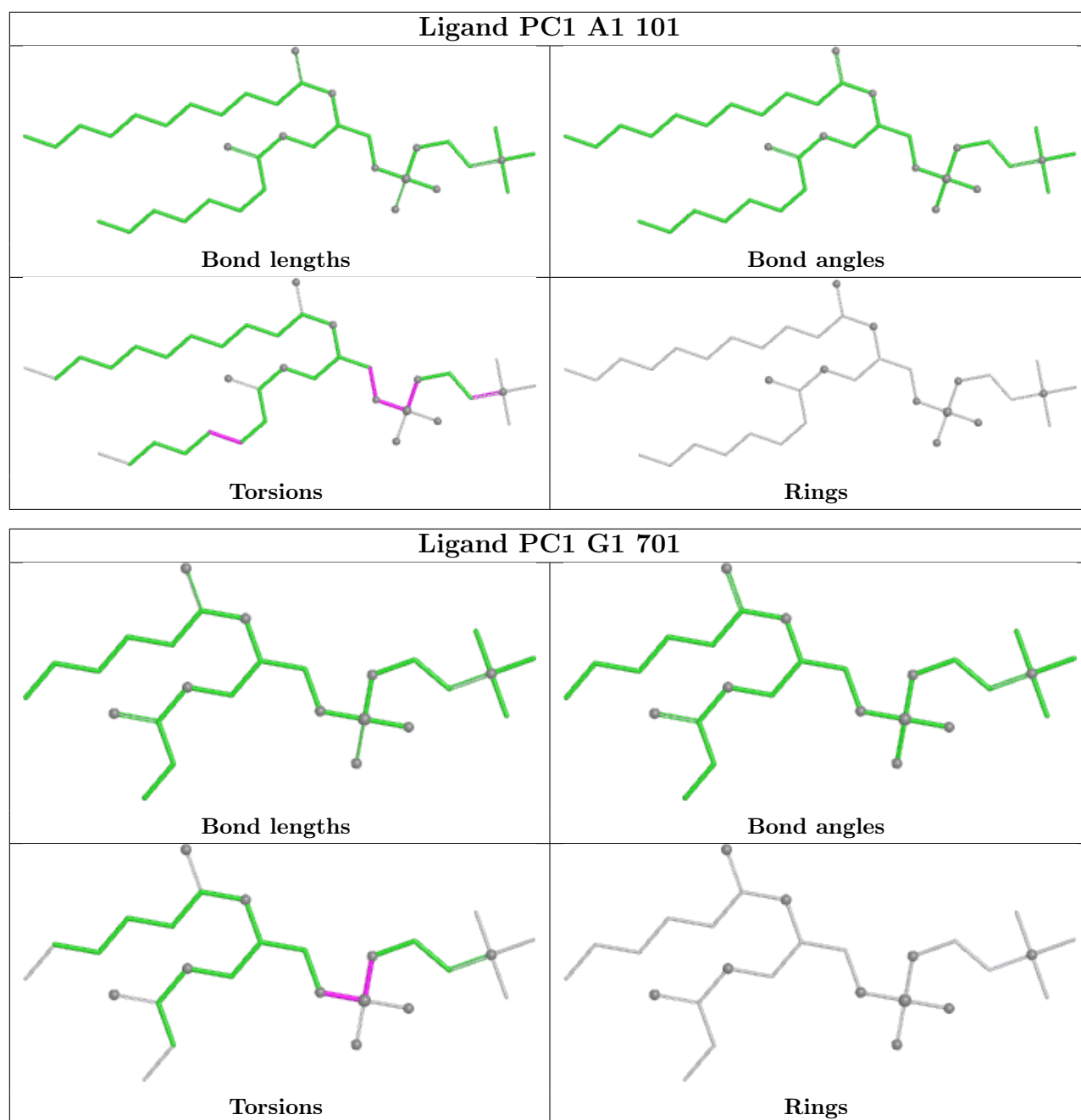
There are no ring outliers.

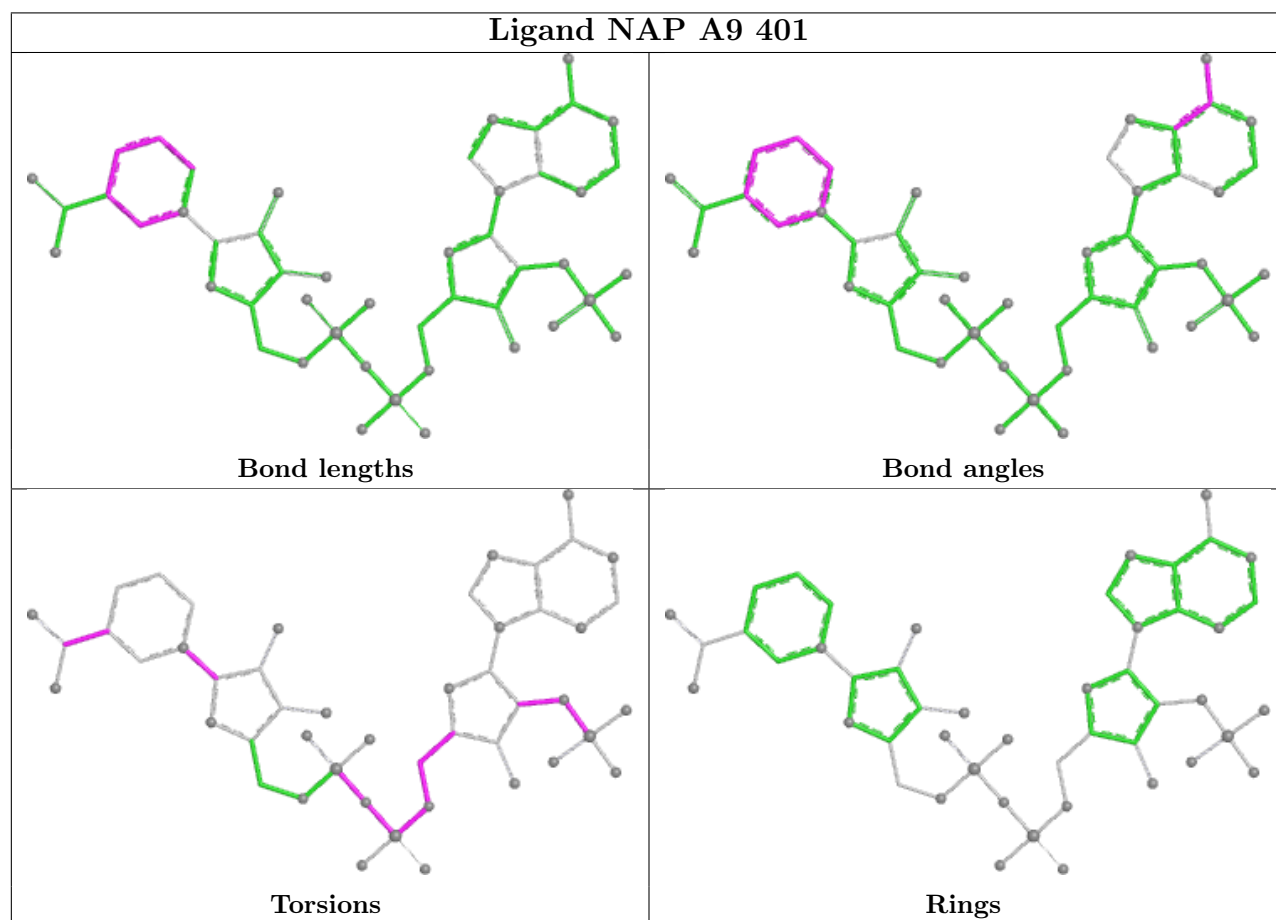
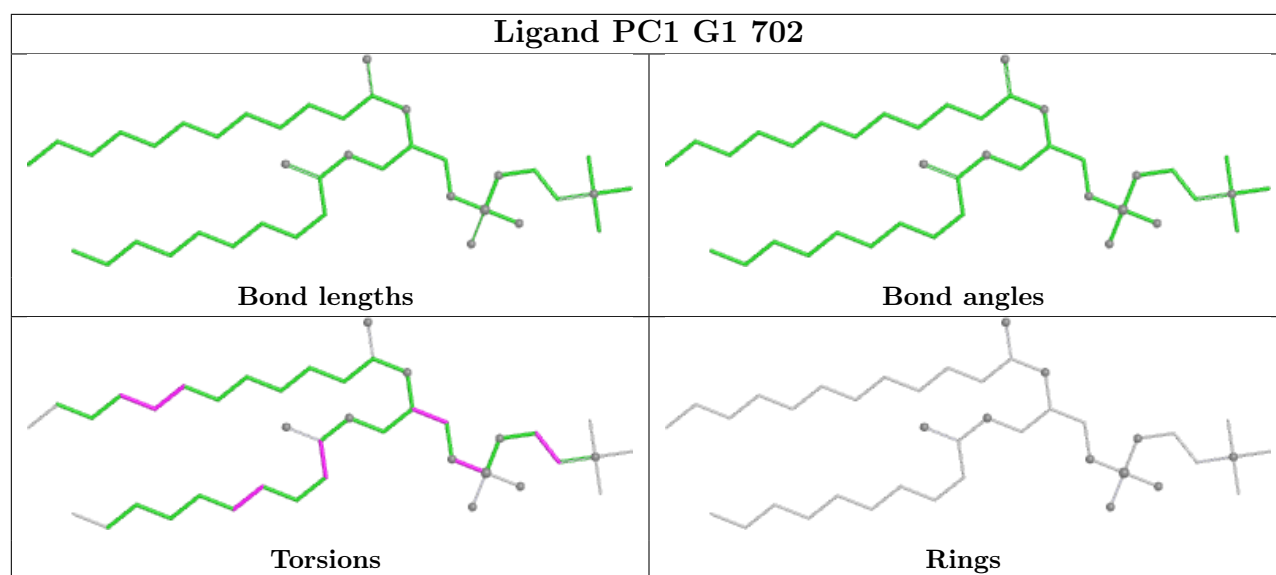
13 monomers are involved in 38 short contacts:

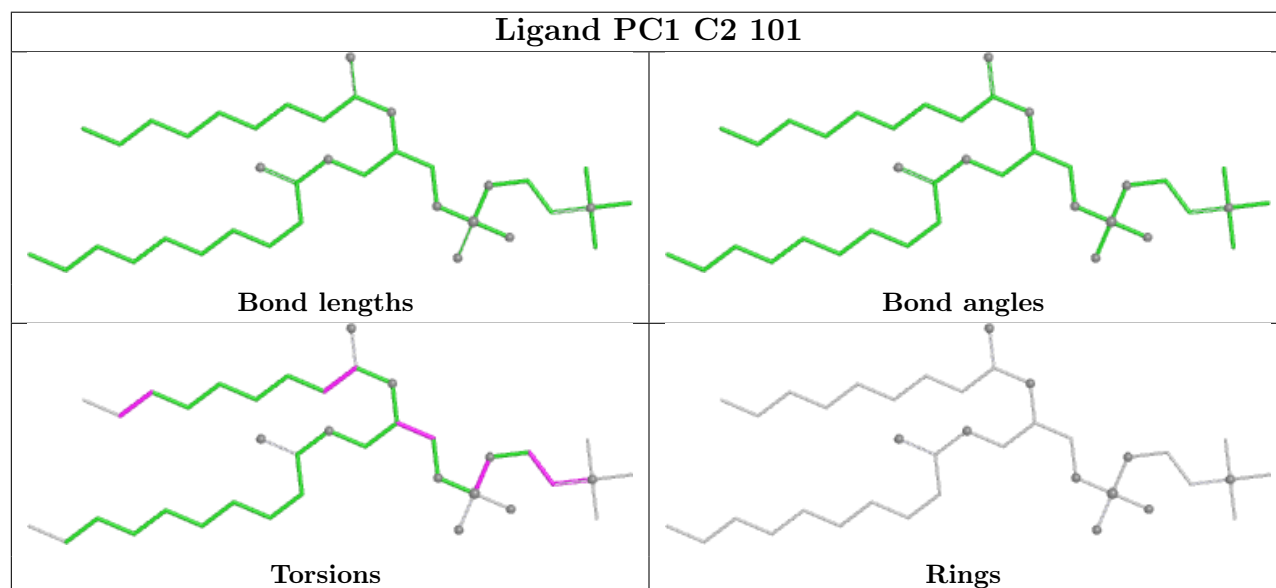
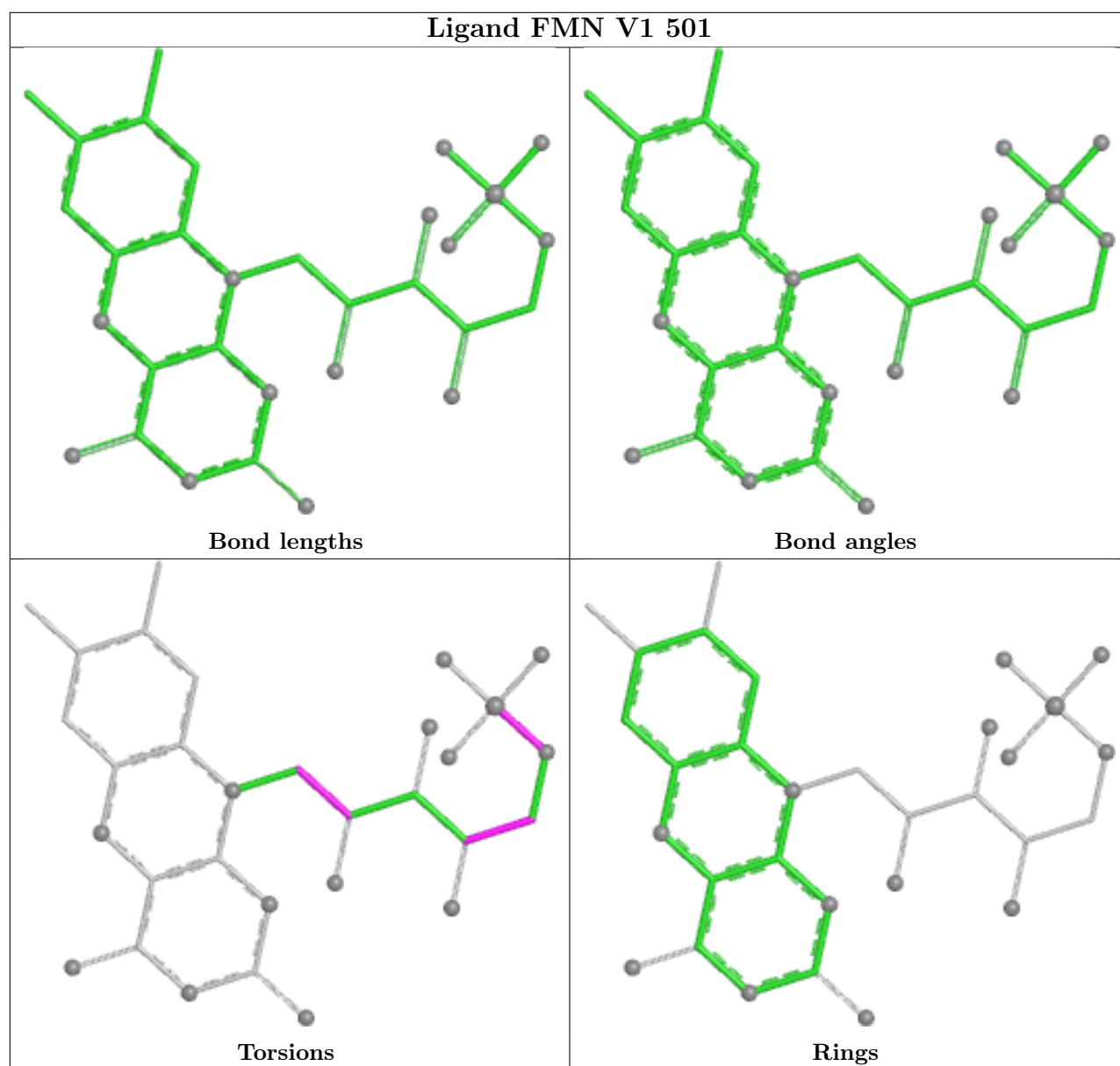
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	AL	401	PC1	2	0
36	S2	401	PC1	1	0
36	A1	101	PC1	1	0
36	G1	701	PC1	3	0
37	S1	802	SF4	5	0
37	S8	302	SF4	2	0
37	S7	301	SF4	2	0
37	S1	801	SF4	1	0
36	G1	702	PC1	5	0
35	A9	401	NAP	7	0
40	V1	501	FMN	3	0
36	C2	101	PC1	6	0
37	V1	500	SF4	3	0

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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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

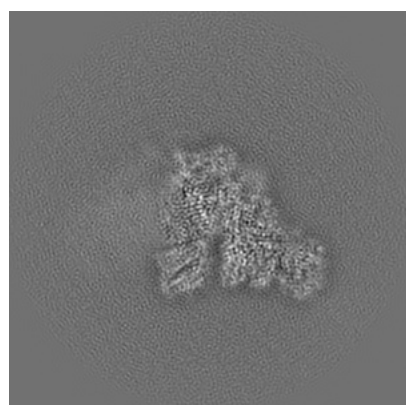
## 6 Map visualisation [i](#)

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.

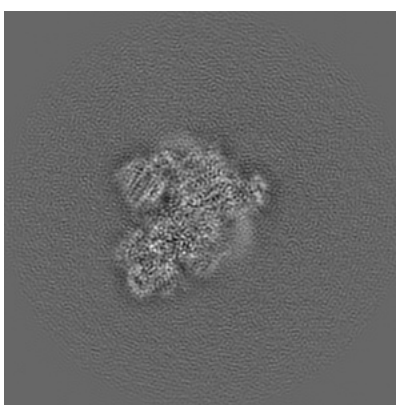
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

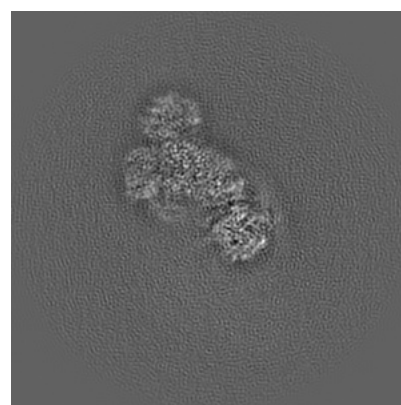
#### 6.1.1 Primary map



X



Y

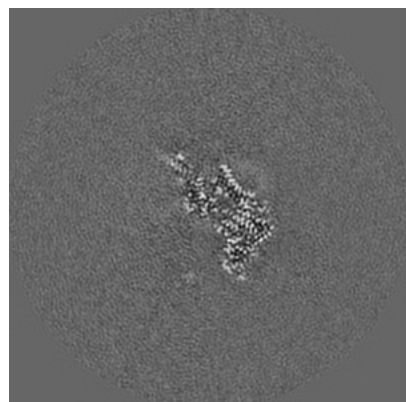


Z

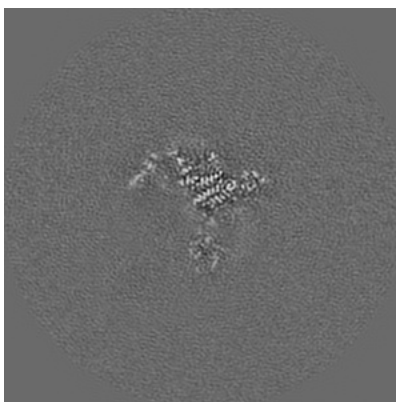
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

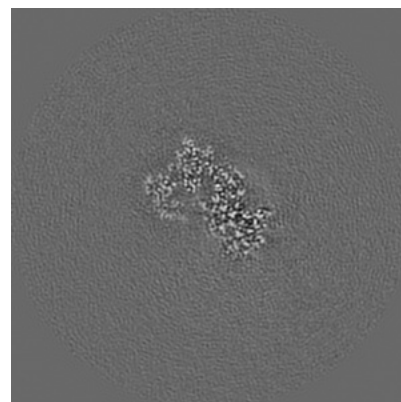
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

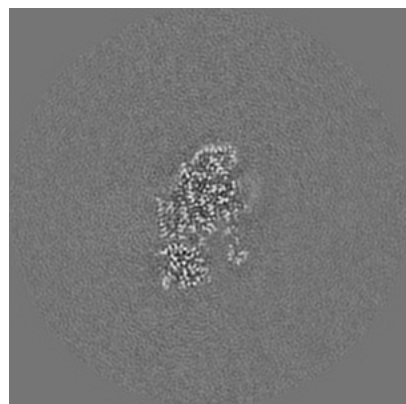


Z Index: 256

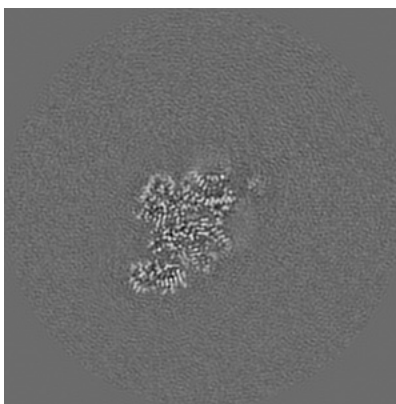
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

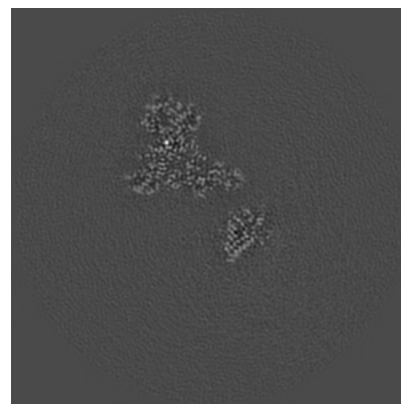
### 6.3.1 Primary map



X Index: 288



Y Index: 291

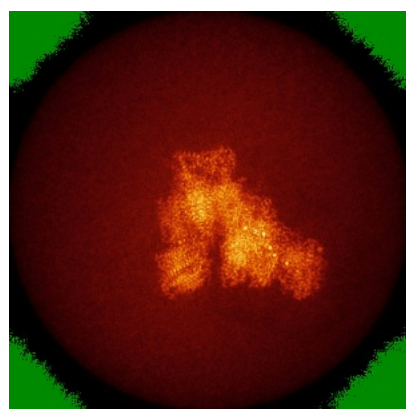


Z Index: 199

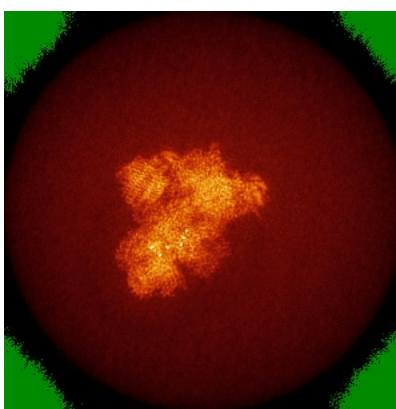
The images above show the largest variance slices of the map in three orthogonal directions.

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

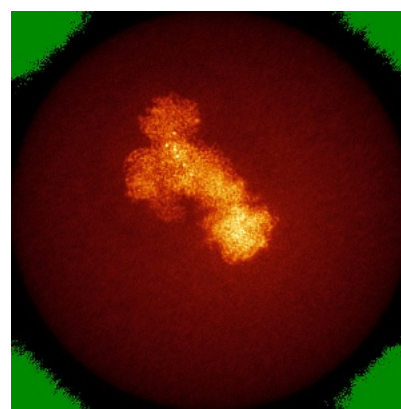
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

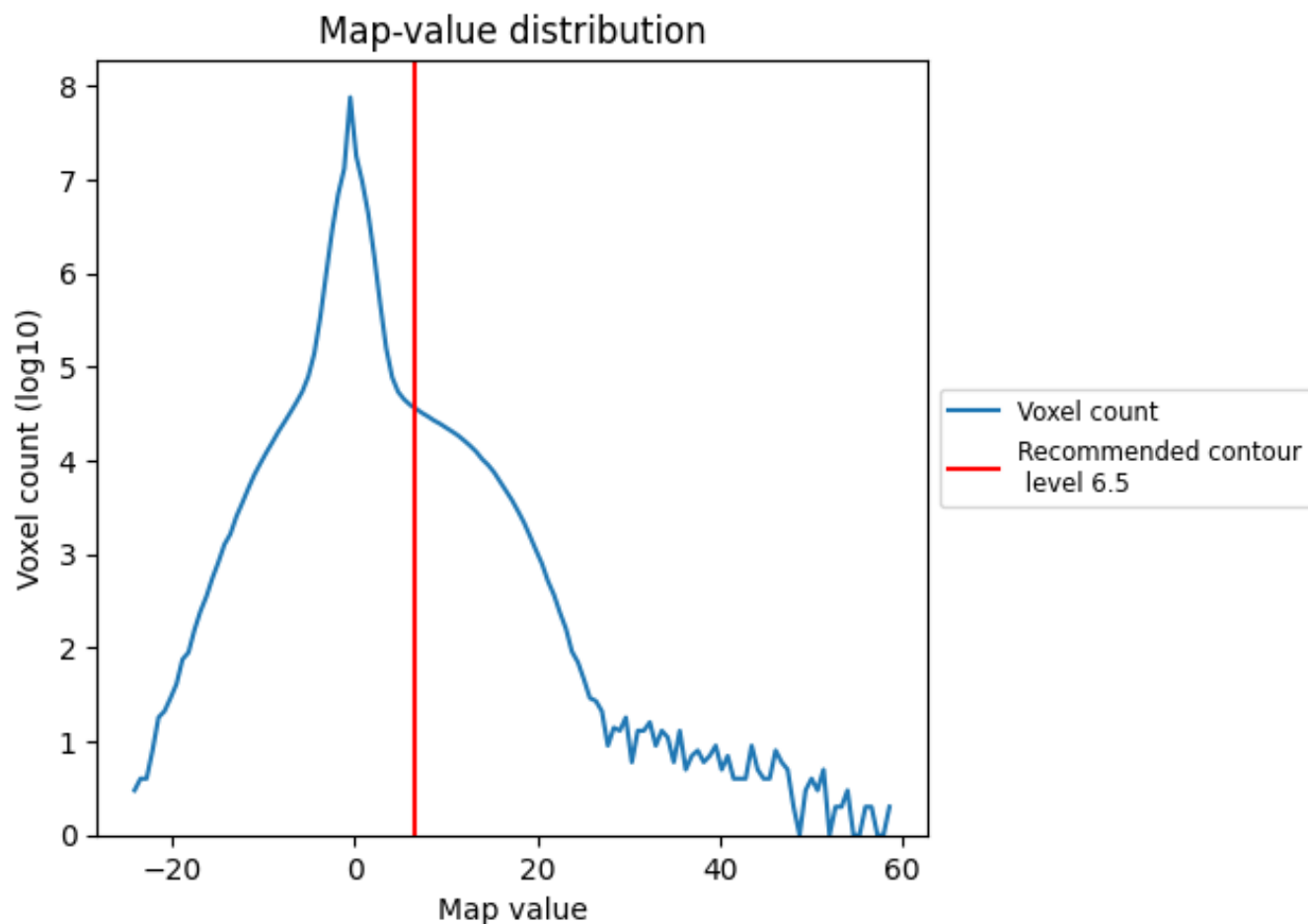
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

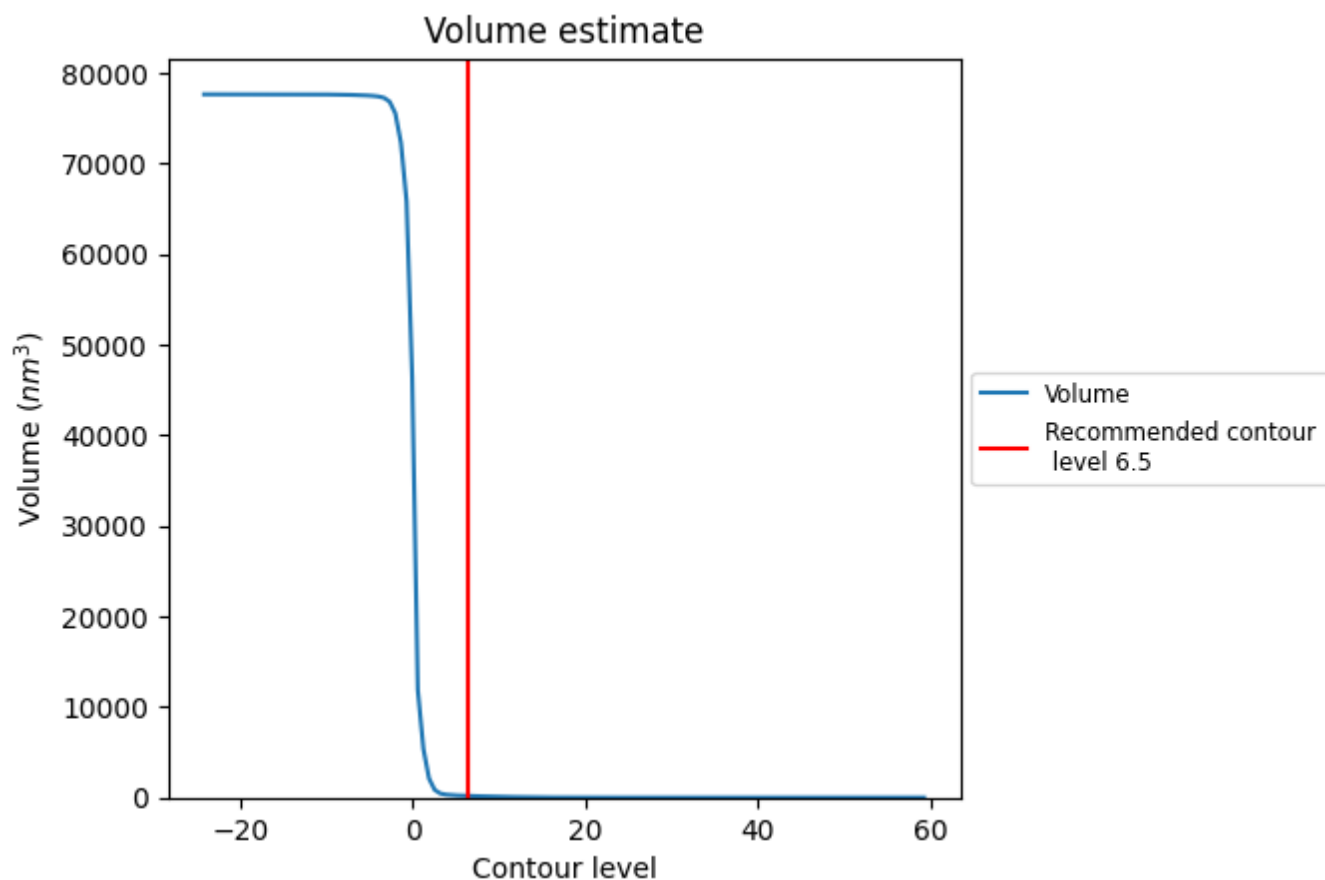
This section contains the results of statistical analysis of the map.

### 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.

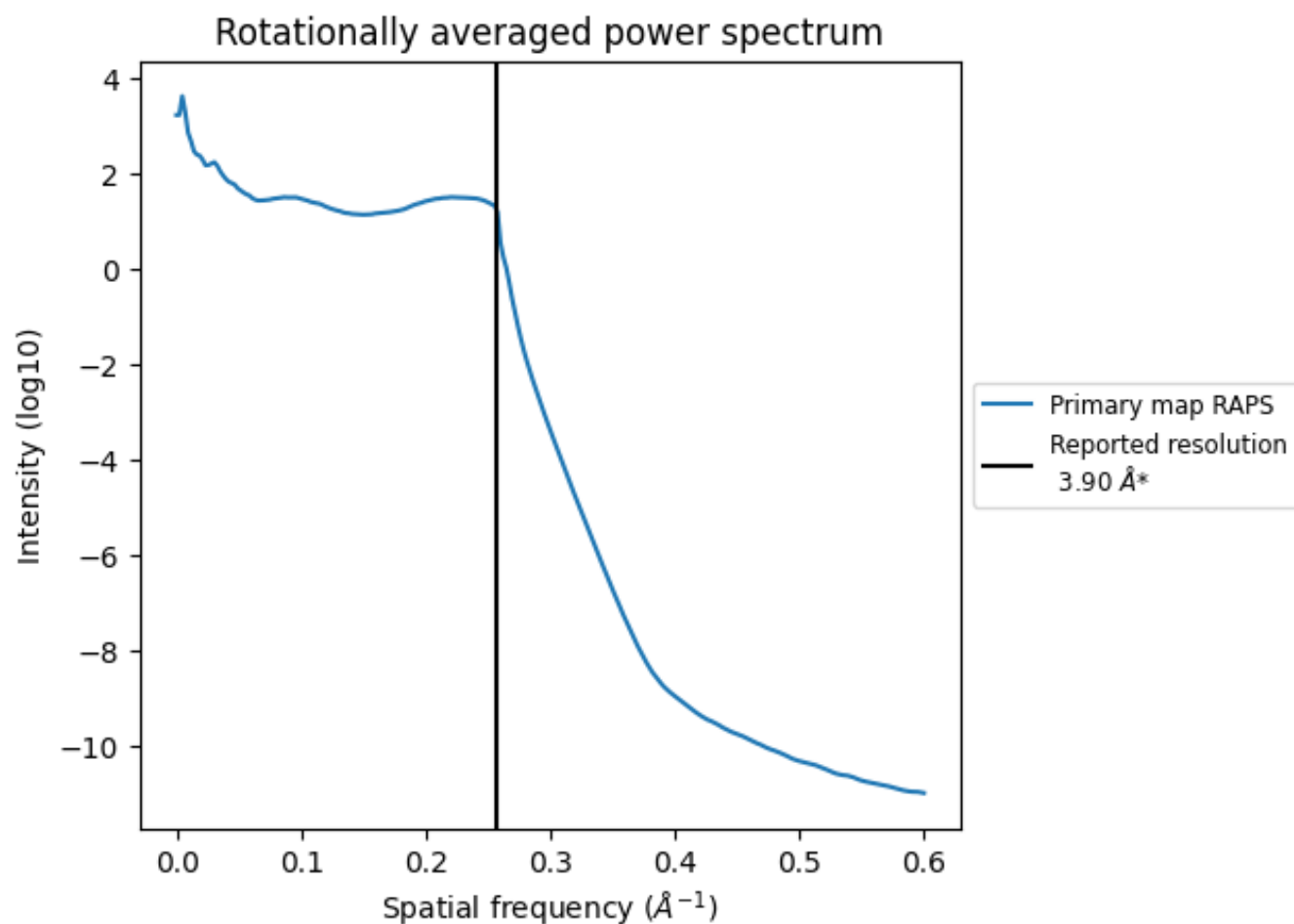
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 183  $\text{nm}^3$ ; 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

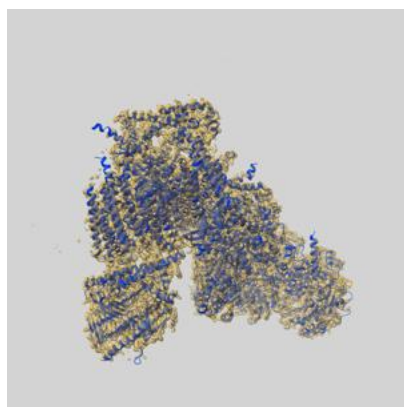
This section was not generated. No FSC curve or half-maps provided.



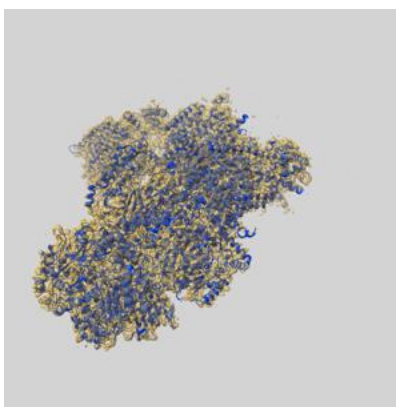
## 9 Map-model fit [i](#)

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

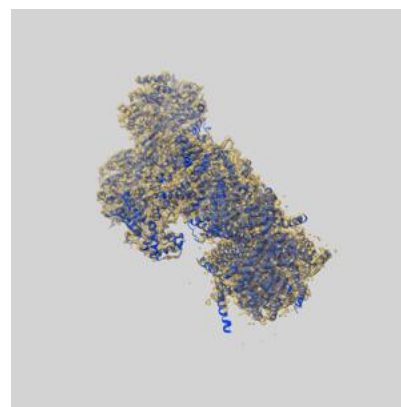
### 9.1 Map-model overlay [i](#)



X



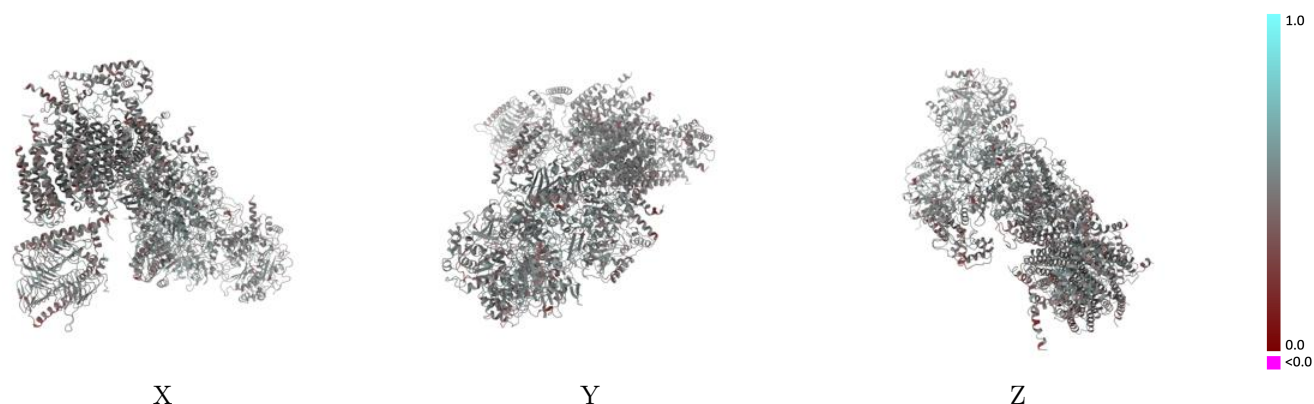
Y



Z

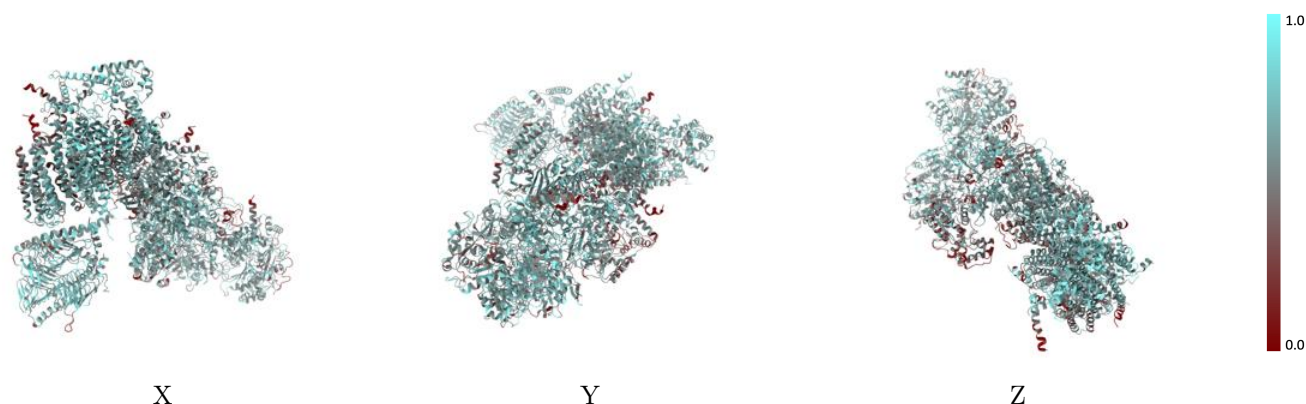
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



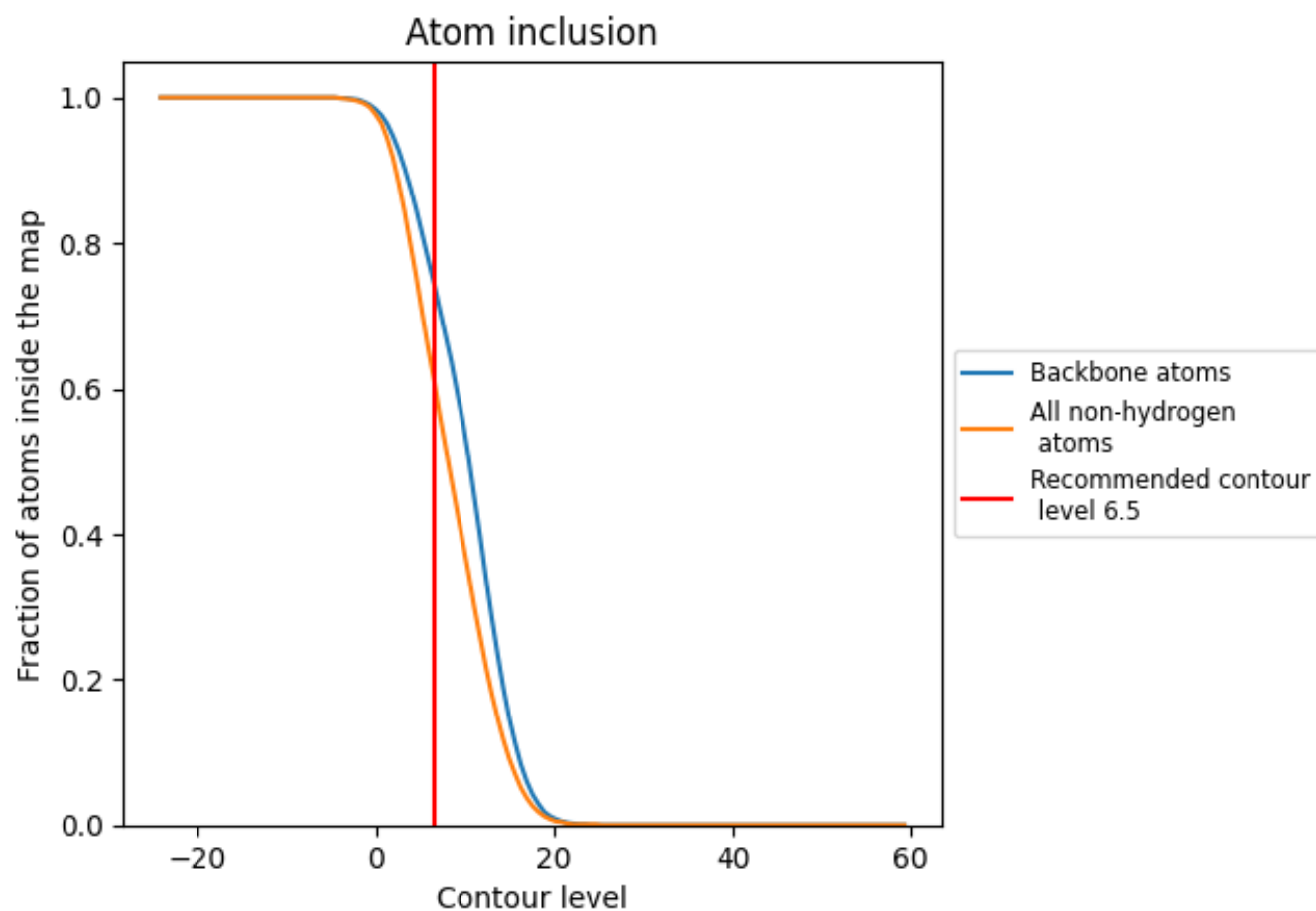
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 61% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6120	 0.4810
1M	 0.5890	 0.4750
2M	 0.5870	 0.4640
3M	 0.6040	 0.4740
4L	 0.6250	 0.4730
6M	 0.6400	 0.4780
A	 0.7110	 0.5560
A1	 0.5610	 0.4720
A2	 0.5950	 0.4680
A3	 0.5140	 0.4580
A5	 0.5780	 0.4620
A6	 0.6460	 0.4890
A7	 0.4880	 0.4730
A8	 0.6610	 0.4600
A9	 0.4300	 0.4610
AL	 0.4860	 0.4810
AM	 0.5930	 0.4560
B	 0.6960	 0.5260
C	 0.4790	 0.4170
C2	 0.5880	 0.4650
G1	 0.6610	 0.4660
G2	 0.6570	 0.4670
L2	 0.6870	 0.4910
P2	 0.6700	 0.4890
S1	 0.6450	 0.4970
S2	 0.6630	 0.5070
S3	 0.6580	 0.5050
S4	 0.6850	 0.5190
S5	 0.7060	 0.4770
S6	 0.6610	 0.4950
S7	 0.6410	 0.5000
S8	 0.6420	 0.5050
V1	 0.5990	 0.4860
V2	 0.5970	 0.4750
X1	 0.7140	 0.4720

