



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2023 – 02:25 PM EDT

PDB ID : 6I0D  
Title : Respiratory complex I from *Thermus thermophilus* with bound Decyl-Ubiquinone  
Authors : Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.  
Deposited on : 2018-10-25  
Resolution : 3.60 Å (reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

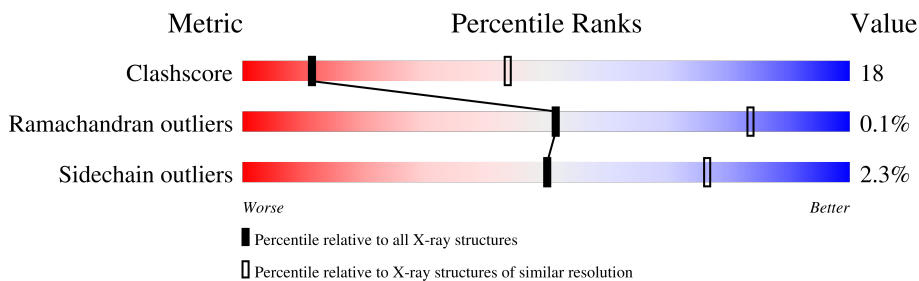
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	
1	B	438	
2	2	181	
2	C	181	
3	3	783	
3	D	783	
4	4	409	
4	E	409	

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Mol	Chain	Length	Quality of chain
5	5	207	63% 30% 5%
5	F	207	61% 33% 5%
6	6	181	51% 38% 8%
6	G	181	43% 46% 8%
7	9	182	58% 39% ..
7	O	182	64% 35% ..
8	7	129	64% 34% ..
8	I	129	68% 30% .
9	W	131	78% 18% ..
9	X	131	72% 24% ..
10	A	119	55% 41% ..
10	P	119	59% 37% ..
11	J	176	60% 30% 9%
11	R	176	60% 30% 9%
12	K	95	72% 27% .
12	S	95	77% 22% .
13	L	606	66% 34%
13	T	606	62% 37%
14	M	469	60% 38%
14	U	469	63% 36%
15	N	427	62% 37%
15	V	427	63% 37%
16	H	365	52% 39% 5%
16	Q	365	51% 43% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	3	803	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	B	501	-	-	X	-
17	SF4	D	803	-	-	X	-
17	SF4	O	201	-	-	X	-
18	FMN	1	502	-	-	X	-
18	FMN	B	502	-	-	X	-
19	FES	D	804	-	-	X	-

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 74132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	437	3417	2180	595	624	18	0	0	0
1	B	437	3417	2180	595	624	18	0	0	0

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	178	1406	895	238	265	8	0	0	0
2	C	178	1406	895	238	265	8	0	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	756	5895	3754	1057	1053	31	0	0	0
3	D	756	5895	3754	1057	1053	31	0	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	384	3067	1975	522	559	11	0	0	0
4	E	384	3067	1975	522	559	11	0	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	5	196	Total 1607	C 1043	N 273	O 288	S 3	0	0	0
5	F	196	Total 1607	C 1043	N 273	O 288	S 3	0	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	6	166	Total 1289	C 815	N 235	O 226	S 13	0	0	0
6	G	166	Total 1289	C 815	N 235	O 226	S 13	0	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	9	180	Total 1388	C 890	N 232	O 255	S 11	0	0	0
7	O	180	Total 1388	C 890	N 232	O 255	S 11	0	0	0

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	7	127	Total 1031	C 664	N 183	O 181	S 3	0	0	0
8	I	127	Total 1031	C 664	N 183	O 181	S 3	0	0	0

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	W	127	Total 967	C 623	N 165	O 175	S 4	0	0	0
9	X	127	Total 967	C 623	N 165	O 175	S 4	0	0	0

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	A	117	Total 910	C 624	N 138	O 144	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	P	117	Total	C	N	O	S	0	0	0
			910	624	138	144	4			

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	160	Total	C	N	O	S	0	0	0
			1183	806	183	191	3			
11	R	160	Total	C	N	O	S	0	0	0
			1183	806	183	191	3			

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	95	Total	C	N	O	S	0	0	0
			703	456	118	126	3			
12	S	95	Total	C	N	O	S	0	0	0
			703	456	118	126	3			

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	605	Total	C	N	O	S	0	0	0
			4604	3089	740	756	19			
13	T	605	Total	C	N	O	S	0	0	0
			4604	3089	740	756	19			

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	467	Total	C	N	O	S	0	0	0
			3489	2363	546	572	8			
14	U	467	Total	C	N	O	S	0	0	0
			3489	2363	546	572	8			

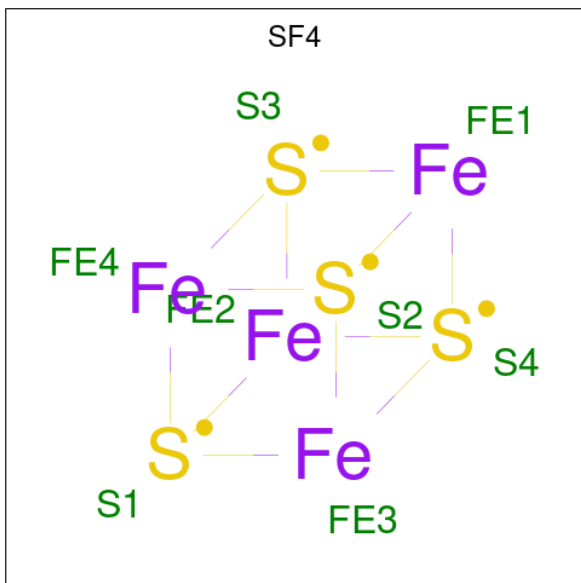
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	427	Total	C	N	O	S	0	0	0
			3154	2125	505	518	6			
15	V	427	Total	C	N	O	S	0	0	0
			3154	2125	505	518	6			

- Molecule 16 is a protein called NADH-quinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	H	353	Total 2838	C 1943	N 431	O 457	S 7	0	0	0
16	Q	353	Total 2838	C 1943	N 431	O 457	S 7	0	0	0

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	Fe S			
17	1	1	Total 8	Fe 4	S 4	0	0
17	3	1	Total 8	Fe 4	S 4	0	0
17	3	1	Total 8	Fe 4	S 4	0	0
17	3	1	Total 8	Fe 4	S 4	0	0
17	6	1	Total 8	Fe 4	S 4	0	0
17	9	1	Total 8	Fe 4	S 4	0	0
17	9	1	Total 8	Fe 4	S 4	0	0
17	B	1	Total 8	Fe 4	S 4	0	0
17	D	1	Total 8	Fe 4	S 4	0	0

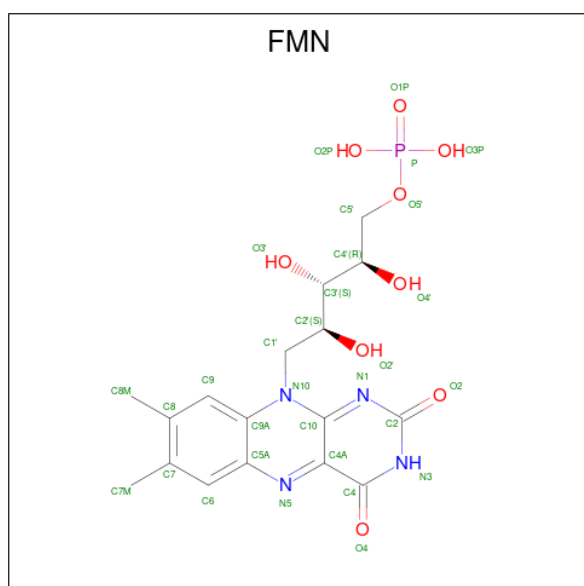
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	G	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 18 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).



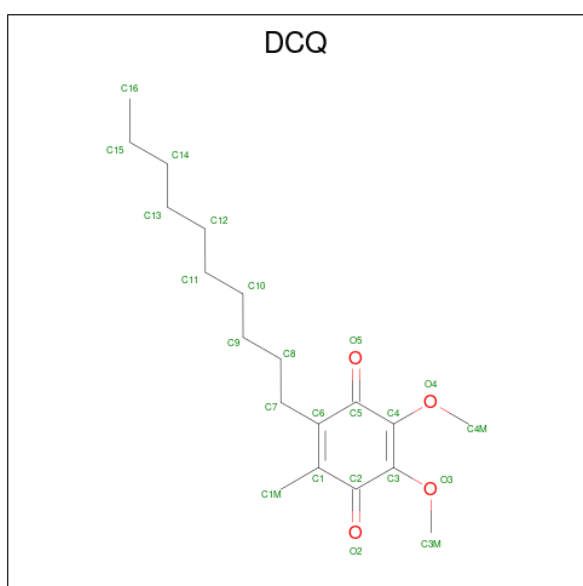
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
18	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	2	1	Total	Fe	S	0	0
			4	2	2		
19	3	1	Total	Fe	S	0	0
			4	2	2		
19	C	1	Total	Fe	S	0	0
			4	2	2		
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: C<sub>19</sub>H<sub>30</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
20	4	1	Total	C	O	0	0
			23	19	4		
20	E	1	Total	C	O	0	0
			23	19	4		

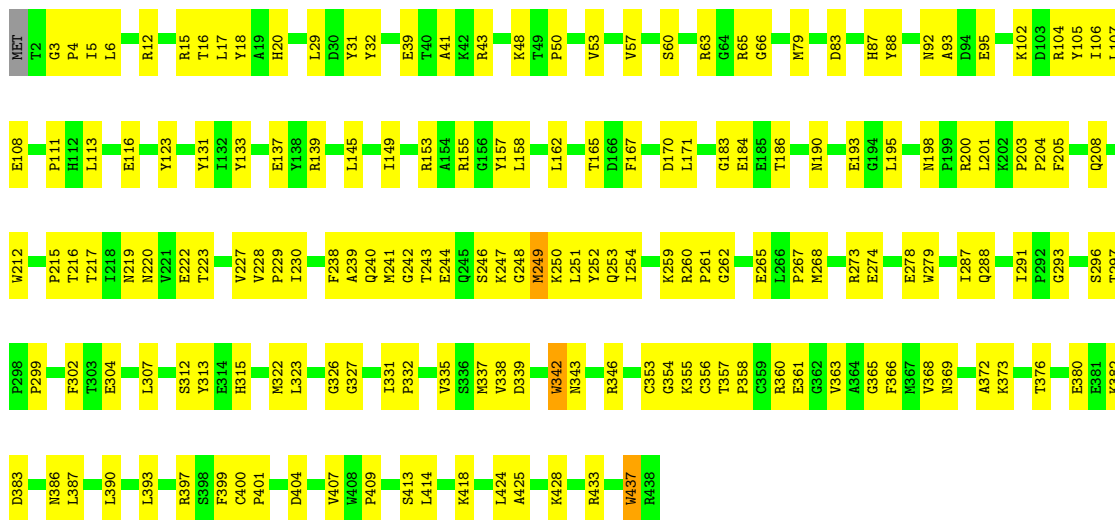
### 3 Residue-property plots

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

Note EDS failed to run properly.

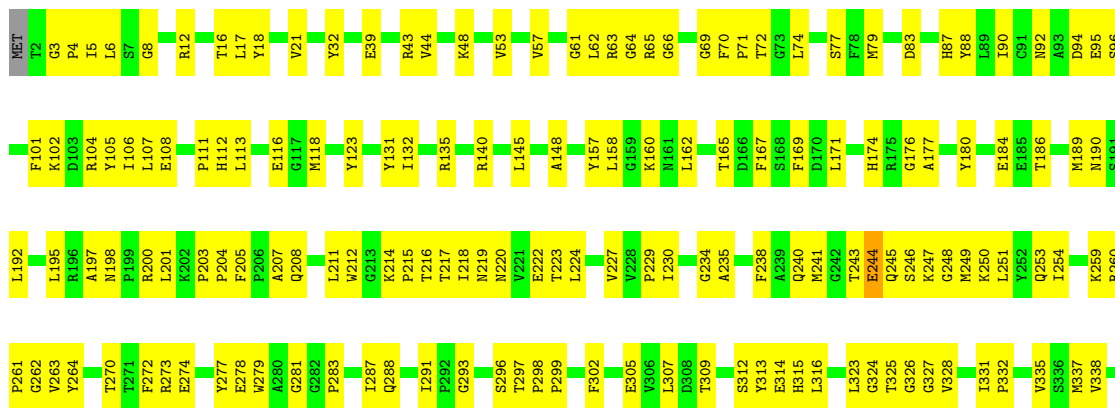
- Molecule 1: NADH-quinone oxidoreductase subunit 1

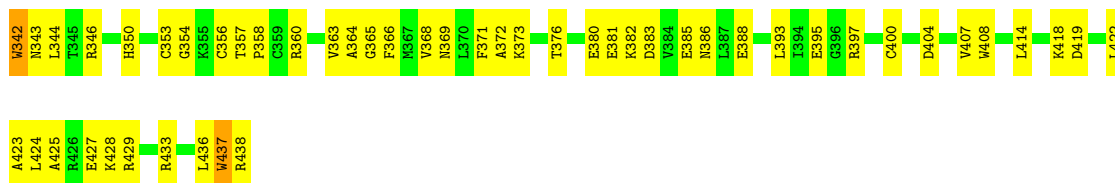
Chain 1: 



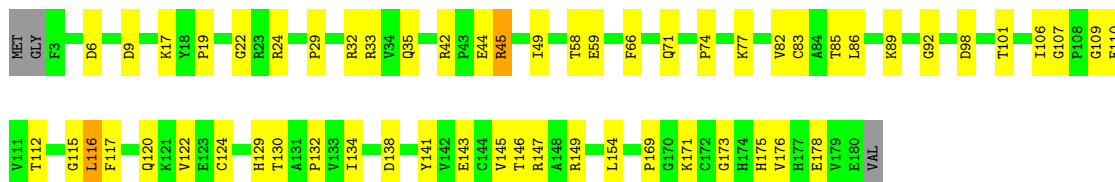
- Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain B: 

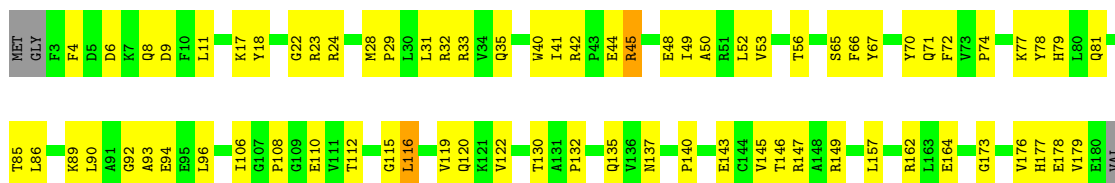




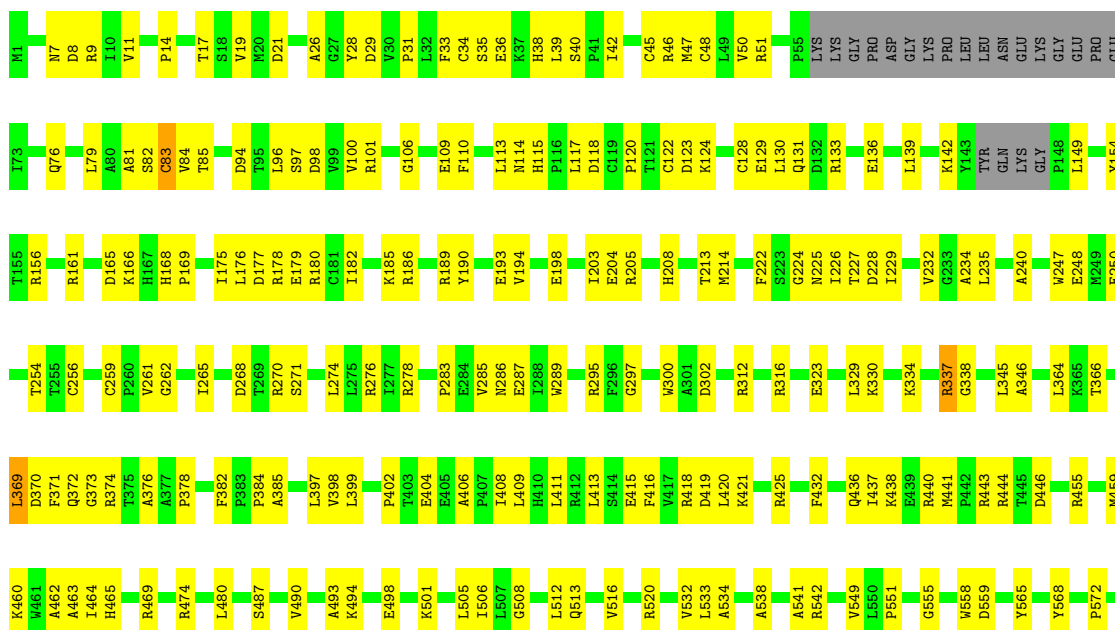
• Molecule 2: NADH-quinone oxidoreductase subunit 2

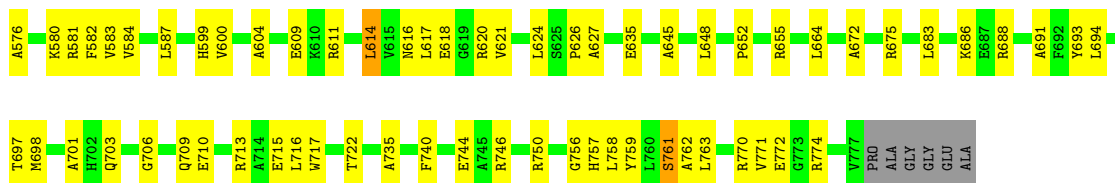


• Molecule 2: NADH-quinone oxidoreductase subunit 2



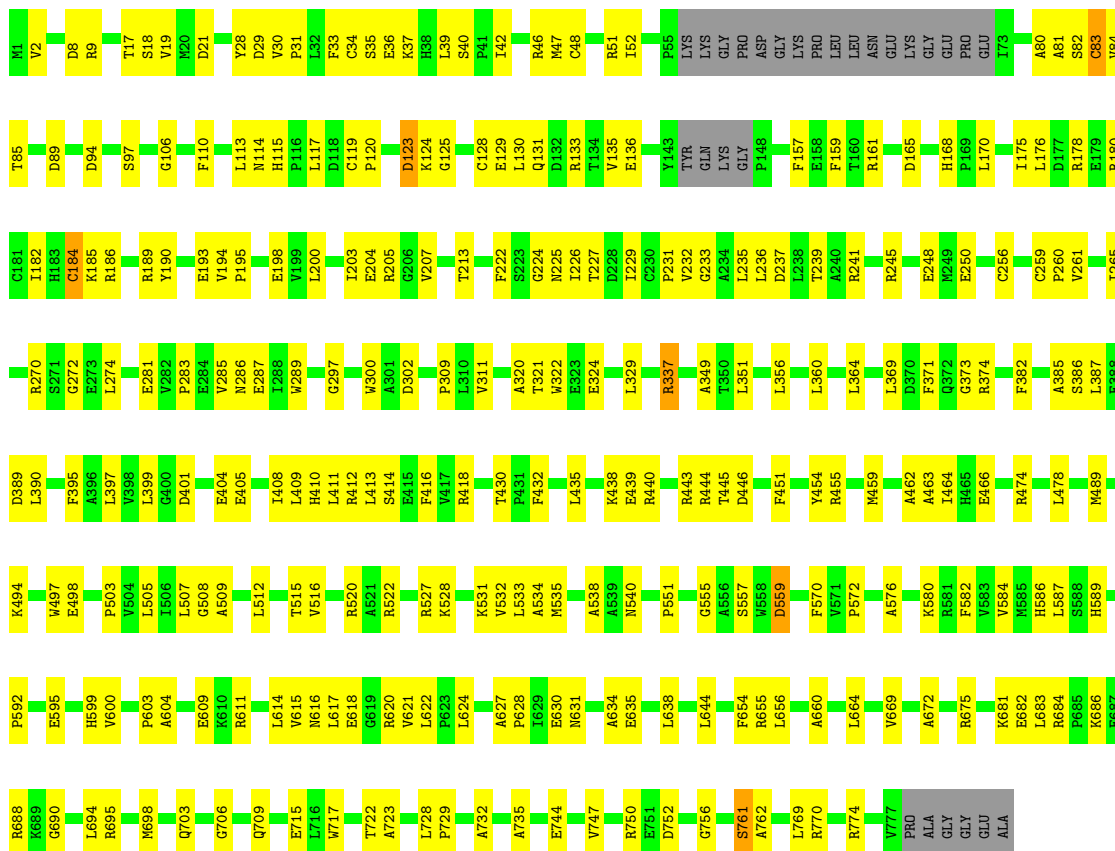
• Molecule 3: NADH-quinone oxidoreductase subunit 3





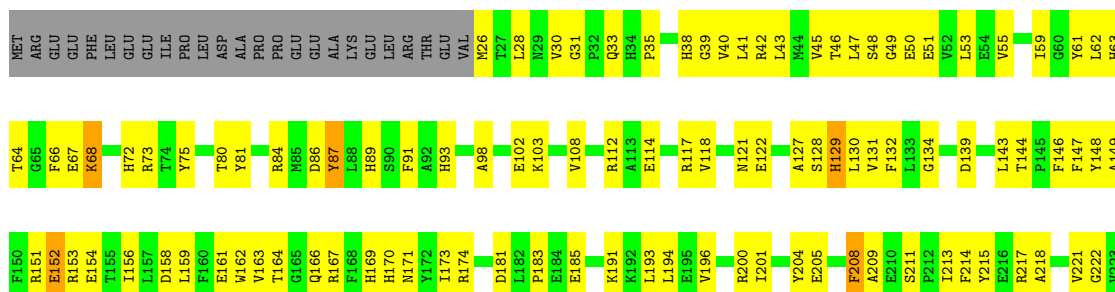
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D: 62% 34%



• Molecule 4: NADH-quinone oxidoreductase subunit 4

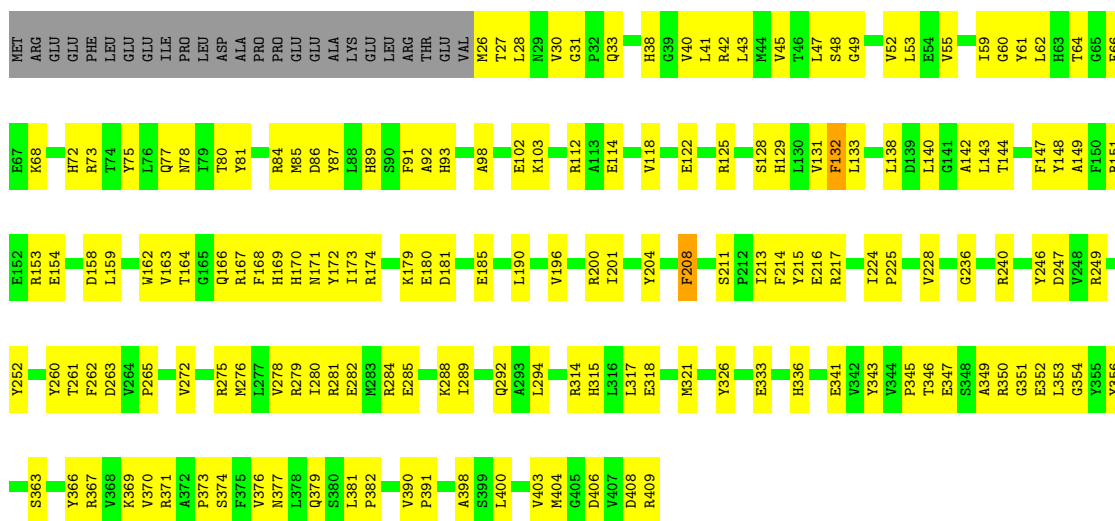
Chain 4: 48% 44% 6%





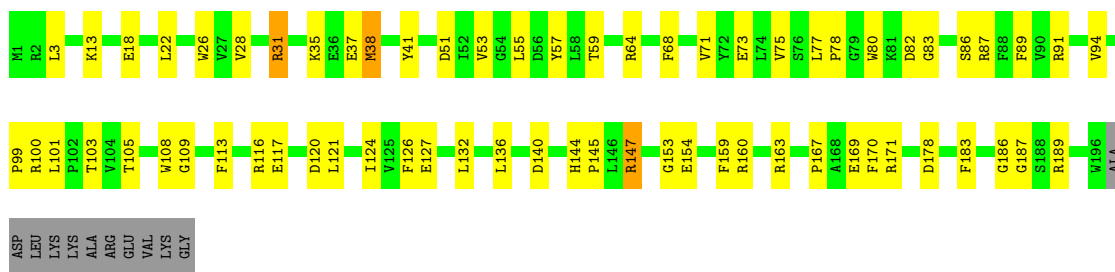
- Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E: 54% 40% 6%



- Molecule 5: NADH-quinone oxidoreductase subunit 5

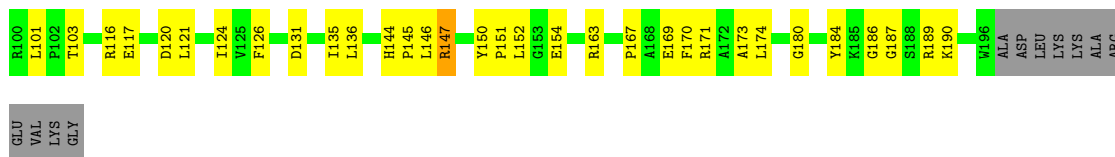
Chain 5: 63% 30% 5%



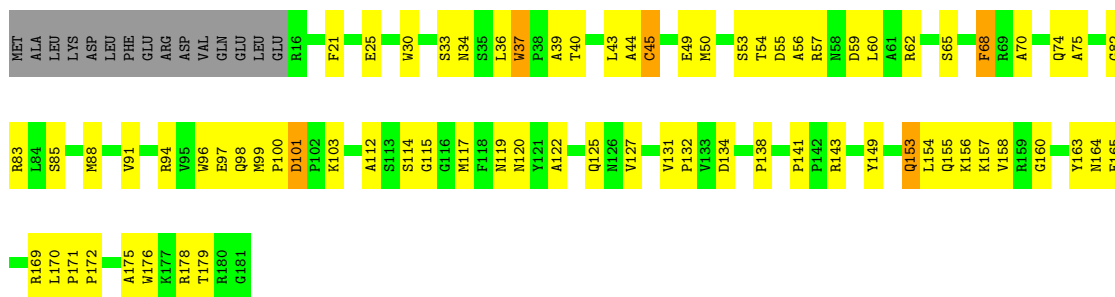
- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F: 61% 33% 5%





• Molecule 6: NADH-quinone oxidoreductase subunit 6



• Molecule 6: NADH-quinone oxidoreductase subunit 6



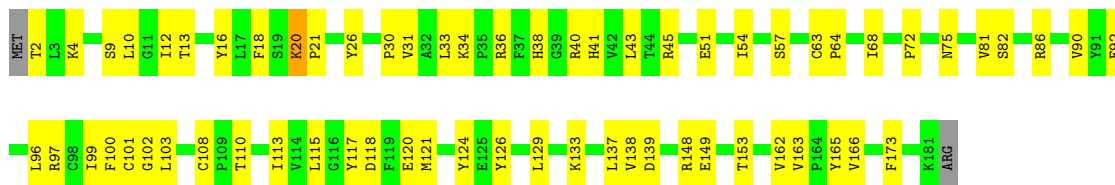
• Molecule 7: NADH-quinone oxidoreductase subunit 9



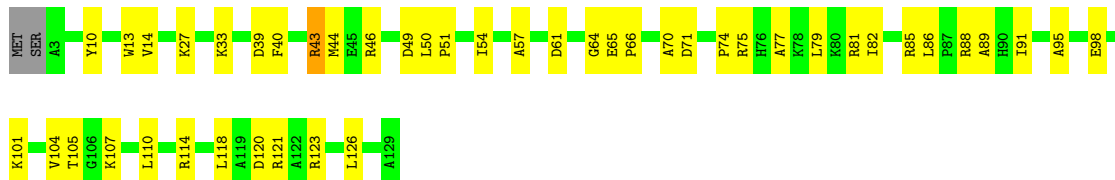
• Molecule 7: NADH-quinone oxidoreductase subunit 9



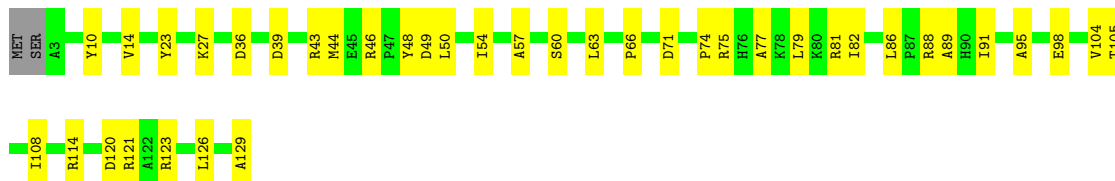




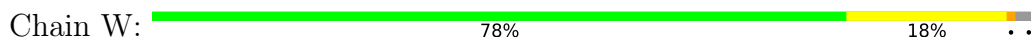
- Molecule 8: NADH-quinone oxidoreductase subunit 15



- Molecule 8: NADH-quinone oxidoreductase subunit 15



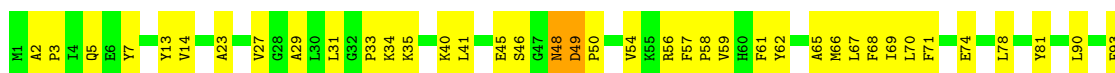
- Molecule 9: NADH-quinone oxidoreductase subunit 16



- Molecule 9: NADH-quinone oxidoreductase subunit 16



- Molecule 10: NADH-quinone oxidoreductase subunit 7





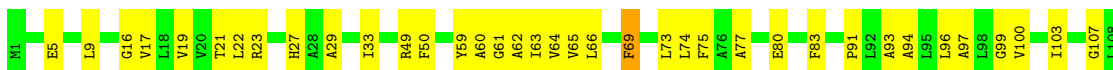
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P: 59% 37%



- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J: 60% 30% 9%



- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R: 60% 30% 9%



- Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K: 72% 27%



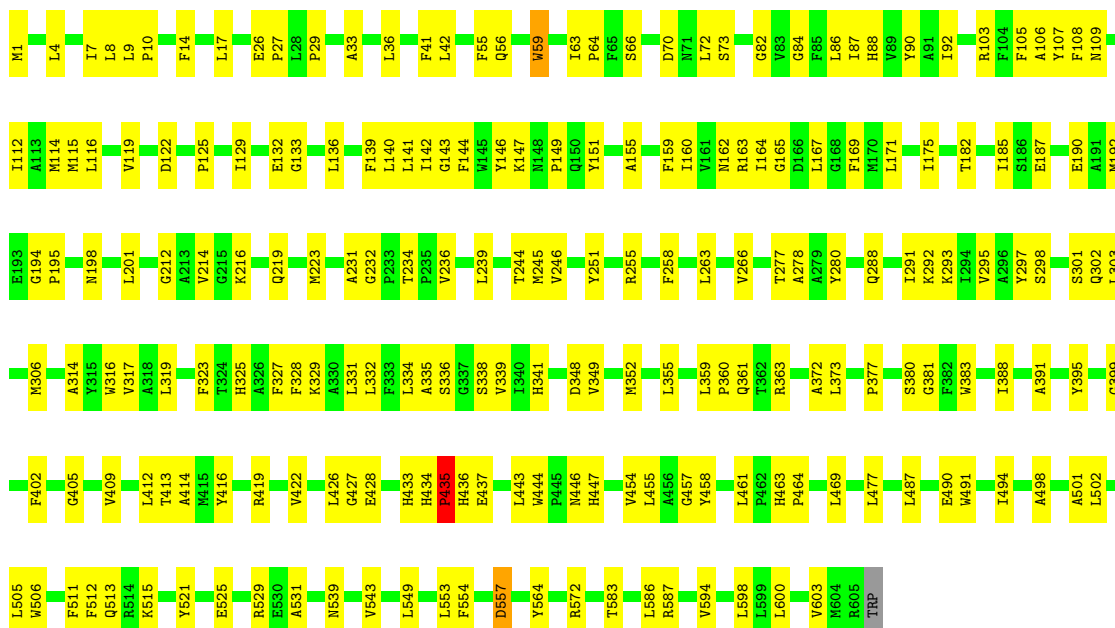
- Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S: 77% 22%



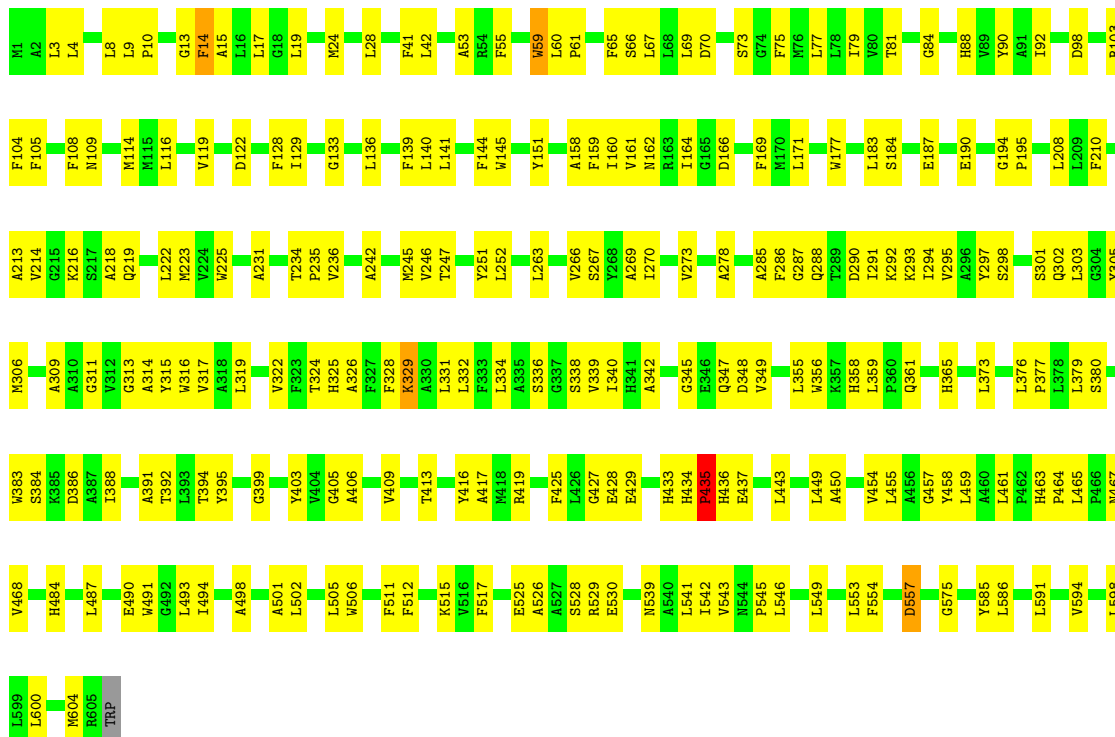
- Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:  66% 34%



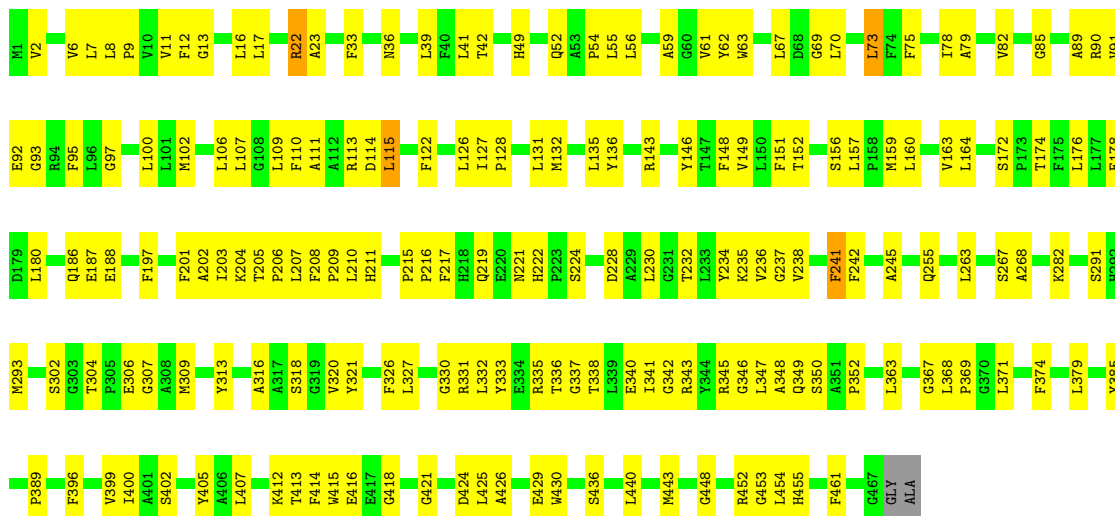
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain T:  62% 37%

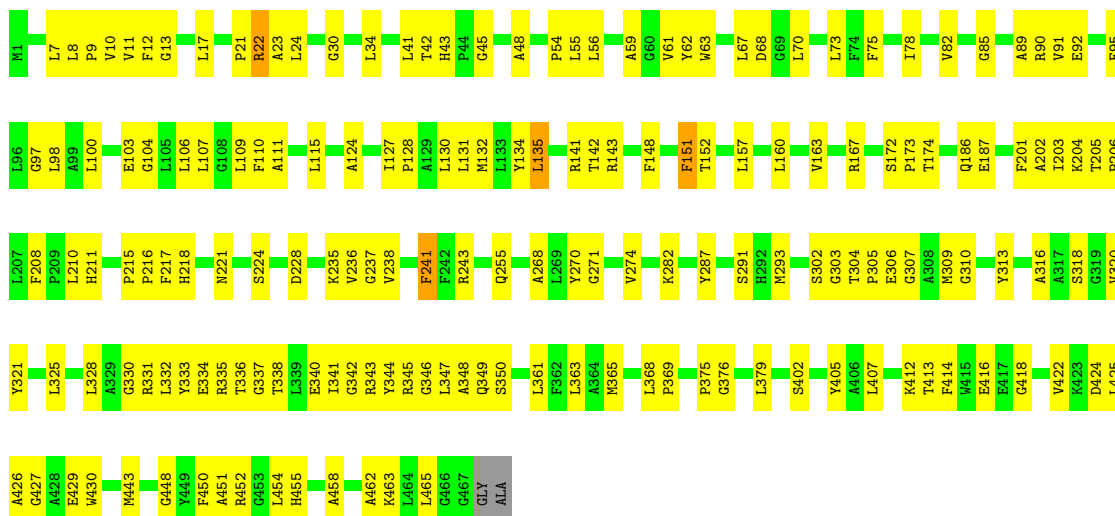


• Molecule 14: NADH-quinone oxidoreductase subunit 13

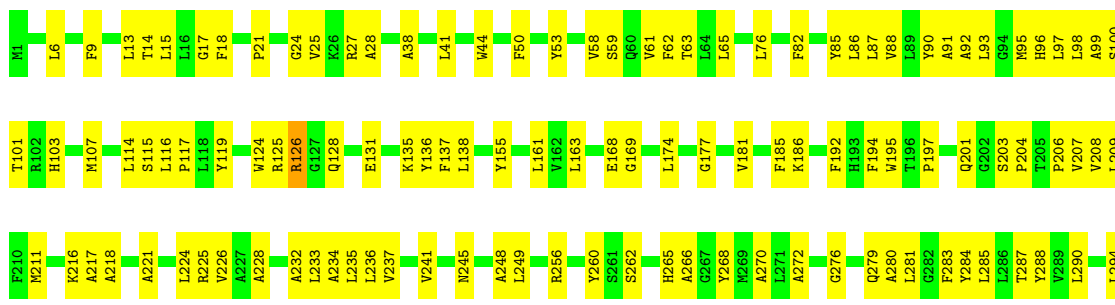
Chain M:  60% 38%

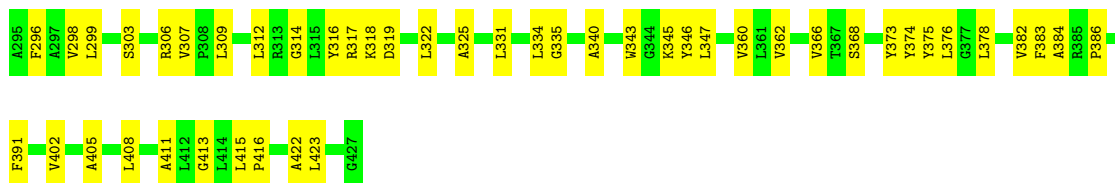


• Molecule 14: NADH-quinone oxidoreductase subunit 13



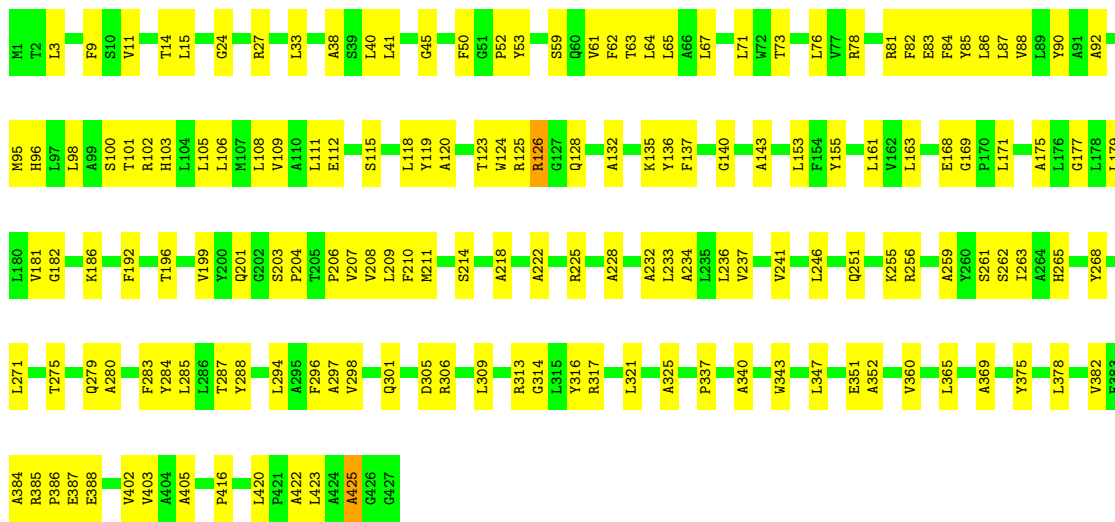
• Molecule 15: NADH-quinone oxidoreductase subunit 14





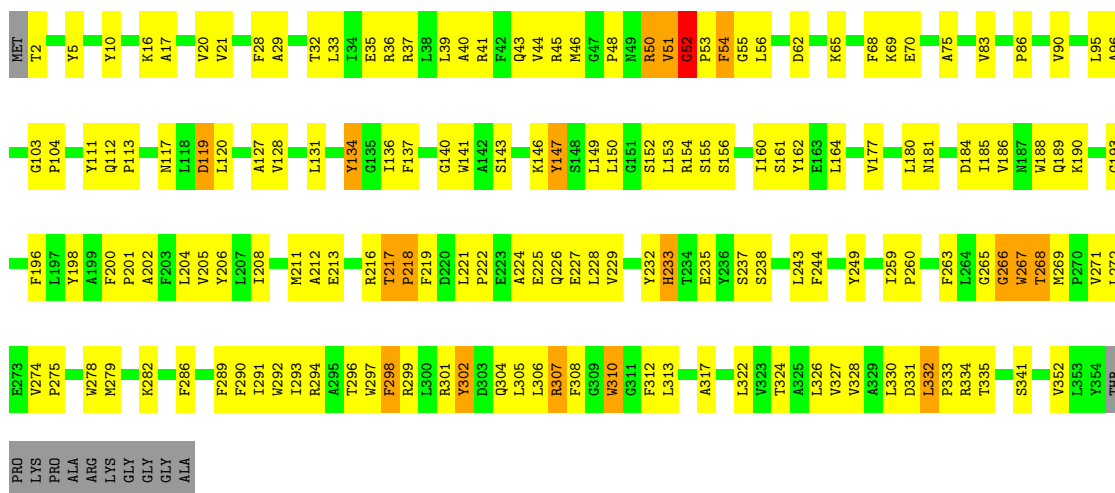
- Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V: 63% 37%



- Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H: 52% 39% 5%



- Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q: 51% 43% ..

MET	T2
Y5	
D8	
M12	
K16	
A17	
V21	
F28	
M31	
T32	
L33	
E35	
R36	
R37	
L38	
L39	
A40	
R41	
F42	
Q43	
V44	
R45	
M46	
G47	
P48	
N49	
R50	
V51	
G52	
P53	
F54	
L56	
L60	
I64	
K65	
K69	
I72	
P86	
L95	
A96	
L99	
I100	
P101	
S107	
Y111	
P113	
W114	
D119	
L120	
G121	
L122	
L123	
Y124	
L125	
V128	
L131	
Y134	
W141	
A142	
S143	
K146	
Y147	
S148	
L149	
L150	
L153	
R154	
S155	
S156	
A157	
S158	
L159	
I160	
Y162	
E163	
L164	
G165	
L166	
G167	
L168	
A169	
L170	
V174	
V177	
G178	
S179	
L180	
I185	
V186	
Q189	
K190	
G193	
G265	
L195	
F196	
P200	
P201	
L204	
V205	
I208	
M211	
A212	
E213	
A214	
A215	
R216	
T217	
P218	
F219	
D220	
L221	
P222	
E223	
A224	
E225	
Q226	
E227	
L228	
V229	
G230	
G231	
Y232	
H233	
T234	
E235	
Y236	
S237	
S238	
I239	
K240	
F244	
Y249	
I250	
H251	
A255	
S256	
A257	
L258	
I259	
P260	
T261	
L262	
F264	
L264	
G266	
W267	
T268	
M269	
P270	
V271	
L272	
E273	
V274	
P275	
Y276	
F280	
L281	
K282	
F286	
L287	
F288	
F289	
F290	
I291	
W292	
I293	
R294	
A295	
T296	
W297	
F298	
R299	
L300	
R301	
Y302	
D303	
Q304	
L305	
L306	
R307	
W310	
F314	
P315	
L316	
A317	
W320	
T324	
A325	
L326	
V327	
V328	
D331	
L332	
P333	
R334	
T335	
Y336	
S341	
L348	
Y354	
THR	
PRO	
LYS	
PRO	
ALA	
ARG	
LYS	
GLY	
GLY	
GLY	
ALA	

## 4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.70Å 328.00Å 260.90Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60	Depositor
% Data completeness (in resolution range)	76.5 (29.87-3.60)	Depositor
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.56Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.214 , 0.225	Depositor
Wilson B-factor (Å <sup>2</sup> )	81.1	Xtrriage
Anisotropy	0.034	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$	Xtrriage
Estimated twinning fraction	0.337 for h,-k,-h-l	Xtrriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 137833 reflections	Xtrriage
Total number of atoms	74132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: FMN, FES, DCQ, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.27	0/3506	0.47	1/4745 (0.0%)
1	B	0.26	0/3506	0.48	1/4745 (0.0%)
2	2	0.28	0/1439	0.45	0/1953
2	C	0.27	0/1439	0.47	0/1953
3	3	0.28	0/6035	0.52	2/8185 (0.0%)
3	D	0.28	0/6035	0.50	1/8185 (0.0%)
4	4	0.28	0/3150	0.48	0/4284
4	E	0.28	0/3150	0.48	0/4284
5	5	0.28	0/1656	0.49	0/2246
5	F	0.28	0/1656	0.48	0/2246
6	6	0.30	0/1319	0.53	0/1786
6	G	0.30	0/1319	0.54	0/1786
7	9	0.31	0/1423	0.52	0/1933
7	O	0.31	0/1423	0.51	0/1933
8	7	0.27	0/1059	0.49	0/1429
8	I	0.26	0/1059	0.48	0/1429
9	W	0.27	0/985	0.49	0/1335
9	X	0.26	0/985	0.46	0/1335
10	A	0.29	0/940	0.49	0/1280
10	P	0.30	0/940	0.53	1/1280 (0.1%)
11	J	0.28	0/1206	0.45	0/1649
11	R	0.27	0/1206	0.45	0/1649
12	K	0.28	0/710	0.45	0/962
12	S	0.28	0/710	0.46	0/962
13	L	0.26	0/4741	0.45	0/6460
13	T	0.26	0/4741	0.44	0/6460
14	M	0.27	0/3591	0.47	0/4896
14	U	0.27	0/3591	0.47	0/4896
15	N	0.27	0/3238	0.43	0/4434
15	V	0.27	0/3238	0.42	0/4434
16	H	0.29	0/2935	0.52	0/4014
16	Q	0.29	0/2935	0.51	0/4014



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.28	0/75866	0.48	6/103182 (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
7	9	0	2
7	O	0	2
12	K	0	1
12	S	0	1
13	L	0	1
13	T	0	1
16	H	0	4
16	Q	0	3
All	All	0	15

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	559	ASP	C-N-CA	-6.26	106.06	121.70
10	P	67	LEU	CA-CB-CG	6.00	129.09	115.30
1	1	296	SER	C-N-CA	-5.78	107.25	121.70
3	3	614	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	296	SER	C-N-CA	-5.27	108.53	121.70

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	20	LYS	Peptide
7	9	21	PRO	Peptide
16	H	52	GLY	Peptide
12	K	50	GLY	Peptide
13	L	435	PRO	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	1	3417	0	3388	127	0
1	B	3417	0	3389	162	0
2	2	1406	0	1373	49	0
2	C	1406	0	1373	62	0
3	3	5895	0	5931	192	0
3	D	5895	0	5931	193	0
4	4	3067	0	3049	181	0
4	E	3067	0	3049	172	0
5	5	1607	0	1574	66	0
5	F	1607	0	1574	61	0
6	6	1289	0	1298	75	0
6	G	1289	0	1298	88	0
7	9	1388	0	1383	74	0
7	O	1388	0	1383	57	0
8	7	1031	0	1029	38	0
8	I	1031	0	1029	30	0
9	W	967	0	1010	21	0
9	X	967	0	1010	26	0
10	A	910	0	939	59	0
10	P	910	0	939	59	0
11	J	1183	0	1286	61	0
11	R	1183	0	1286	52	0
12	K	703	0	747	26	0
12	S	703	0	747	23	0
13	L	4604	0	4734	153	0
13	T	4604	0	4734	157	0
14	M	3489	0	3606	136	0
14	U	3489	0	3606	126	0
15	N	3154	0	3343	111	0
15	V	3154	0	3343	114	0
16	H	2838	0	2903	157	0
16	Q	2838	0	2903	165	0
17	1	8	0	0	0	0
17	3	24	0	0	3	0
17	6	8	0	0	1	0
17	9	16	0	0	3	0
17	B	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	24	0	0	2	0
17	G	8	0	0	0	0
17	O	16	0	0	3	0
18	1	31	0	19	9	0
18	B	31	0	19	9	0
19	2	4	0	0	0	0
19	3	4	0	0	1	0
19	C	4	0	0	0	0
19	D	4	0	0	2	0
20	4	23	0	30	4	0
20	E	23	0	30	4	0
All	All	74132	0	75285	2642	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 18.

The worst 5 of 2642 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)
4:4:162:TRP:CE2	7:9:34:LYS:HD2	1.87	1.09
12:S:28:PHE:CZ	12:S:68:VAL:HA	1.91	1.05
12:S:28:PHE:HZ	12:S:68:VAL:HA	1.16	1.04
4:E:138:LEU:CD1	4:E:143:LEU:HD23	1.89	1.02
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.45	0.97

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	435/438 (99%)	408 (94%)	27 (6%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	435/438 (99%)	407 (94%)	28 (6%)	0	100	100
2	2	176/181 (97%)	165 (94%)	11 (6%)	0	100	100
2	C	176/181 (97%)	165 (94%)	11 (6%)	0	100	100
3	3	750/783 (96%)	695 (93%)	55 (7%)	0	100	100
3	D	750/783 (96%)	698 (93%)	52 (7%)	0	100	100
4	4	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
4	E	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
5	5	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
5	F	194/207 (94%)	180 (93%)	14 (7%)	0	100	100
6	6	164/181 (91%)	149 (91%)	15 (9%)	0	100	100
6	G	164/181 (91%)	152 (93%)	12 (7%)	0	100	100
7	9	178/182 (98%)	170 (96%)	8 (4%)	0	100	100
7	O	178/182 (98%)	169 (95%)	9 (5%)	0	100	100
8	7	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
8	I	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
9	W	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
9	X	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
10	A	115/119 (97%)	103 (90%)	12 (10%)	0	100	100
10	P	115/119 (97%)	104 (90%)	11 (10%)	0	100	100
11	J	158/176 (90%)	146 (92%)	12 (8%)	0	100	100
11	R	158/176 (90%)	145 (92%)	13 (8%)	0	100	100
12	K	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
12	S	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
13	L	603/606 (100%)	562 (93%)	40 (7%)	1 (0%)	47	79
13	T	603/606 (100%)	568 (94%)	34 (6%)	1 (0%)	47	79
14	M	465/469 (99%)	436 (94%)	29 (6%)	0	100	100
14	U	465/469 (99%)	439 (94%)	26 (6%)	0	100	100
15	N	425/427 (100%)	399 (94%)	26 (6%)	0	100	100
15	V	425/427 (100%)	397 (93%)	27 (6%)	1 (0%)	47	79
16	H	351/365 (96%)	302 (86%)	43 (12%)	6 (2%)	9	45
16	Q	351/365 (96%)	307 (88%)	39 (11%)	5 (1%)	11	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9478/9796 (97%)	8820 (93%)	644 (7%)	14 (0%)	51 83

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL
16	H	44	VAL
16	Q	51	VAL
16	H	268	THR
16	Q	44	VAL

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	355/356 (100%)	347 (98%)	8 (2%)	50 76
1	B	355/356 (100%)	346 (98%)	9 (2%)	47 75
2	2	150/152 (99%)	144 (96%)	6 (4%)	31 65
2	C	150/152 (99%)	145 (97%)	5 (3%)	38 69
3	3	609/628 (97%)	597 (98%)	12 (2%)	55 79
3	D	609/628 (97%)	600 (98%)	9 (2%)	65 84
4	4	332/355 (94%)	325 (98%)	7 (2%)	53 78
4	E	332/355 (94%)	329 (99%)	3 (1%)	78 90
5	5	167/175 (95%)	162 (97%)	5 (3%)	41 71
5	F	167/175 (95%)	164 (98%)	3 (2%)	59 81
6	6	135/149 (91%)	126 (93%)	9 (7%)	16 50
6	G	135/149 (91%)	125 (93%)	10 (7%)	13 46
7	9	148/150 (99%)	146 (99%)	2 (1%)	67 85
7	O	148/150 (99%)	146 (99%)	2 (1%)	67 85
8	7	104/106 (98%)	103 (99%)	1 (1%)	76 88
8	I	104/106 (98%)	103 (99%)	1 (1%)	76 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	99/101 (98%)	98 (99%)	1 (1%)	76	88
9	X	99/101 (98%)	98 (99%)	1 (1%)	76	88
10	A	90/92 (98%)	87 (97%)	3 (3%)	38	69
10	P	90/92 (98%)	86 (96%)	4 (4%)	28	63
11	J	118/130 (91%)	115 (98%)	3 (2%)	47	75
11	R	118/130 (91%)	115 (98%)	3 (2%)	47	75
12	K	71/71 (100%)	70 (99%)	1 (1%)	67	85
12	S	71/71 (100%)	69 (97%)	2 (3%)	43	72
13	L	453/454 (100%)	443 (98%)	10 (2%)	52	77
13	T	453/454 (100%)	444 (98%)	9 (2%)	55	79
14	M	332/332 (100%)	325 (98%)	7 (2%)	53	78
14	U	332/332 (100%)	326 (98%)	6 (2%)	59	81
15	N	302/302 (100%)	298 (99%)	4 (1%)	69	86
15	V	302/302 (100%)	297 (98%)	5 (2%)	60	82
16	H	293/300 (98%)	282 (96%)	11 (4%)	33	66
16	Q	293/300 (98%)	285 (97%)	8 (3%)	44	73
All	All	7516/7706 (98%)	7346 (98%)	170 (2%)	50	76

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	262	PHE
13	T	59	TRP
6	G	37	TRP
7	O	38	HIS
13	T	557	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	129	HIS
14	U	221	ASN
6	G	120	ASN
11	R	55	GLN
15	V	277	ASN

### 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](#)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	SF4	D	801	3	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.37	11 (22%)
17	SF4	9	201	7	0,12,12	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
20	DCQ	E	501	-	23,23,23	0.18	0	26,29,29	0.86	1 (3%)
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	O	202	7	0,12,12	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
20	DCQ	4	501	-	23,23,23	0.22	0	26,29,29	0.84	1 (3%)
17	SF4	6	201	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	FMN	1	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.37	12 (25%)
17	SF4	G	201	6	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	O	201	7	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
17	SF4	D	801	3	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
19	FES	3	804	3	-	-	0/1/1/1
20	DCQ	E	501	-	-	4/14/38/38	0/1/1/1
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
20	DCQ	4	501	-	-	4/14/38/38	0/1/1/1
17	SF4	D	802	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4A-N5	3.82	1.38	1.30
18	B	502	FMN	C4A-N5	3.70	1.37	1.30
18	B	502	FMN	C10-N1	2.54	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C10-N1	2.51	1.38	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	502	FMN	C4-N3-C2	-3.34	119.47	125.64
18	1	502	FMN	C4-N3-C2	-3.26	119.62	125.64
18	B	502	FMN	C5'-C4'-C3'	-2.90	106.61	112.20
18	B	502	FMN	C4A-C4-N3	2.81	120.32	113.19
18	B	502	FMN	C4A-C10-N1	-2.80	118.22	124.73

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

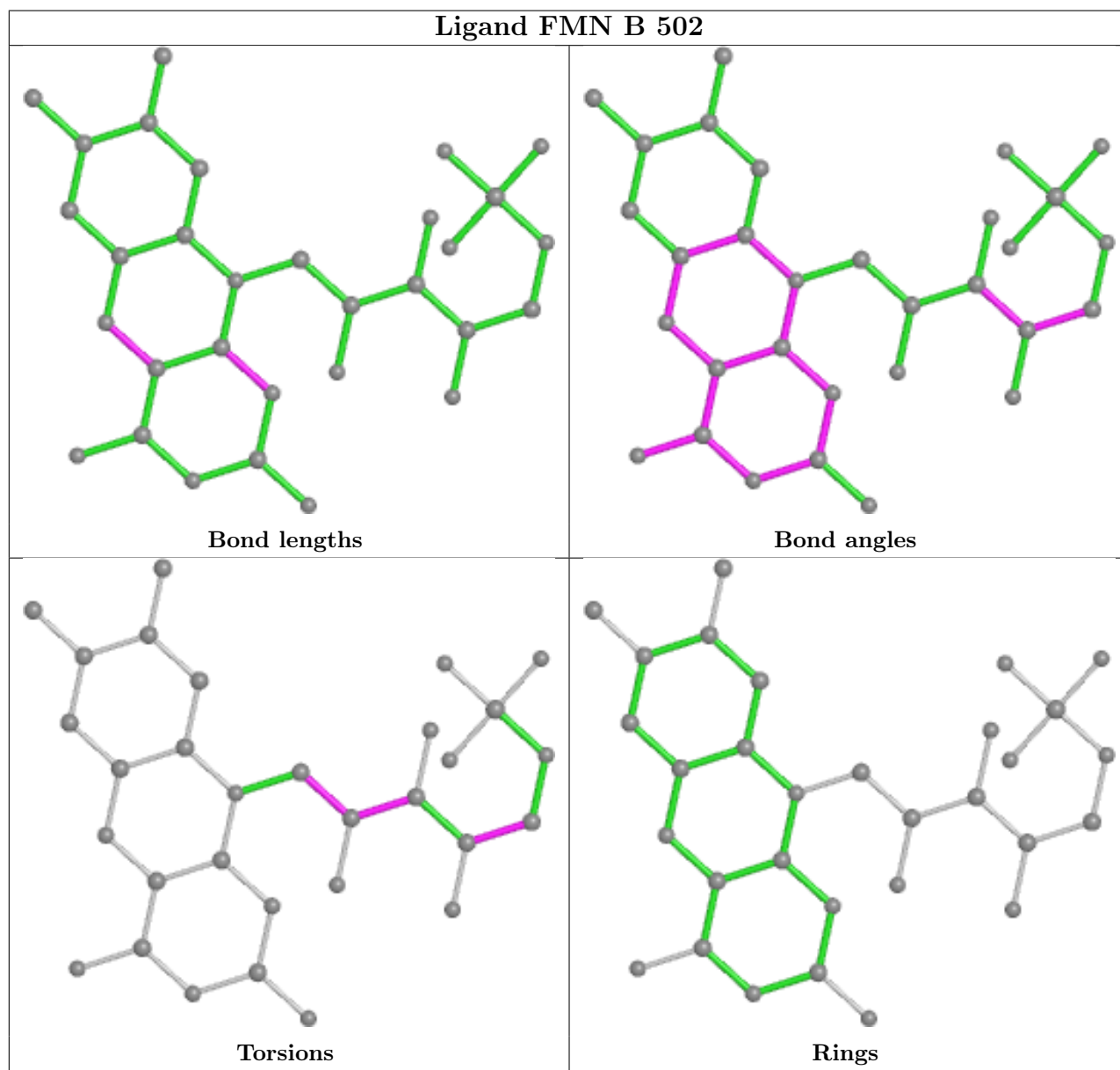
Mol	Chain	Res	Type	Atoms
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	N10-C1'-C2'-C3'
18	1	502	FMN	C1'-C2'-C3'-O3'
18	1	502	FMN	C1'-C2'-C3'-C4'
18	1	502	FMN	C3'-C4'-C5'-O5'

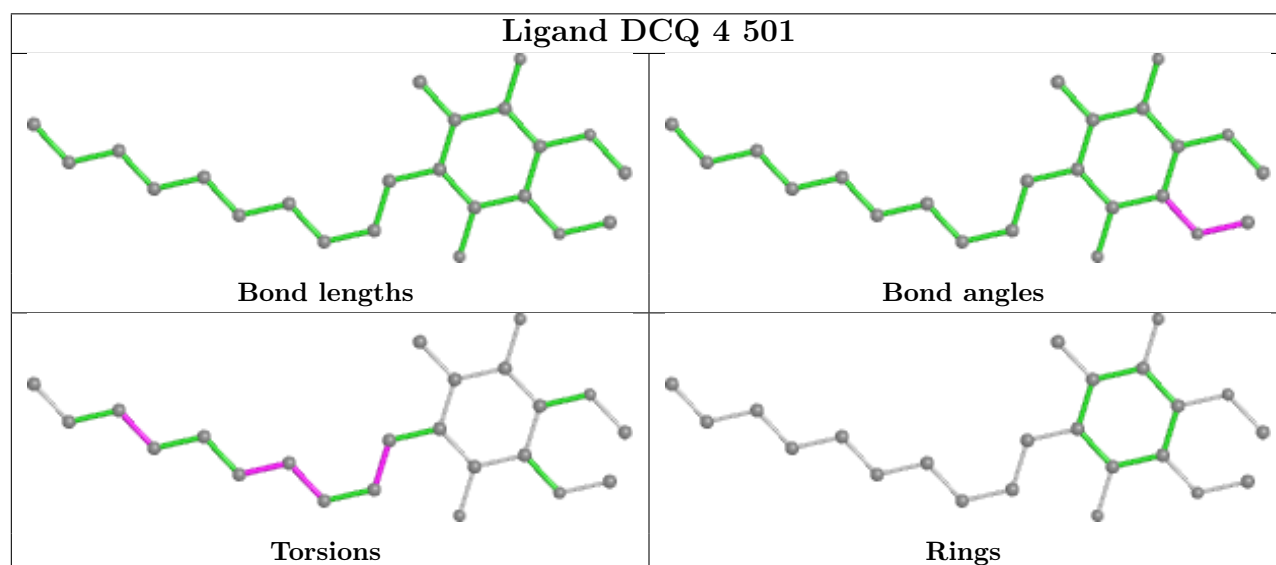
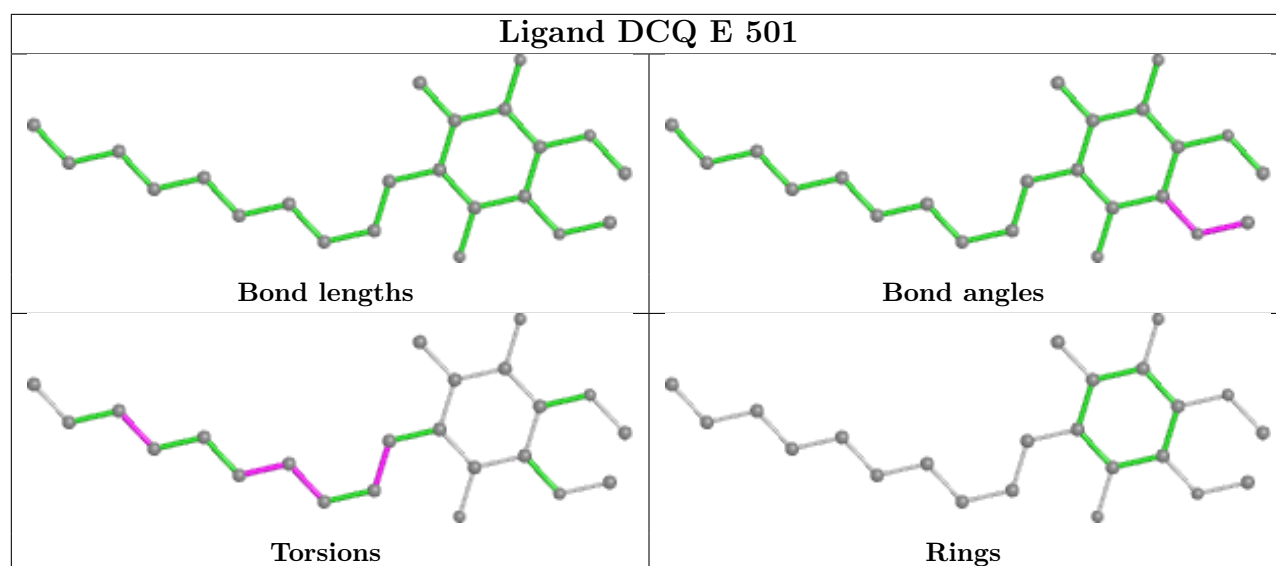
There are no ring outliers.

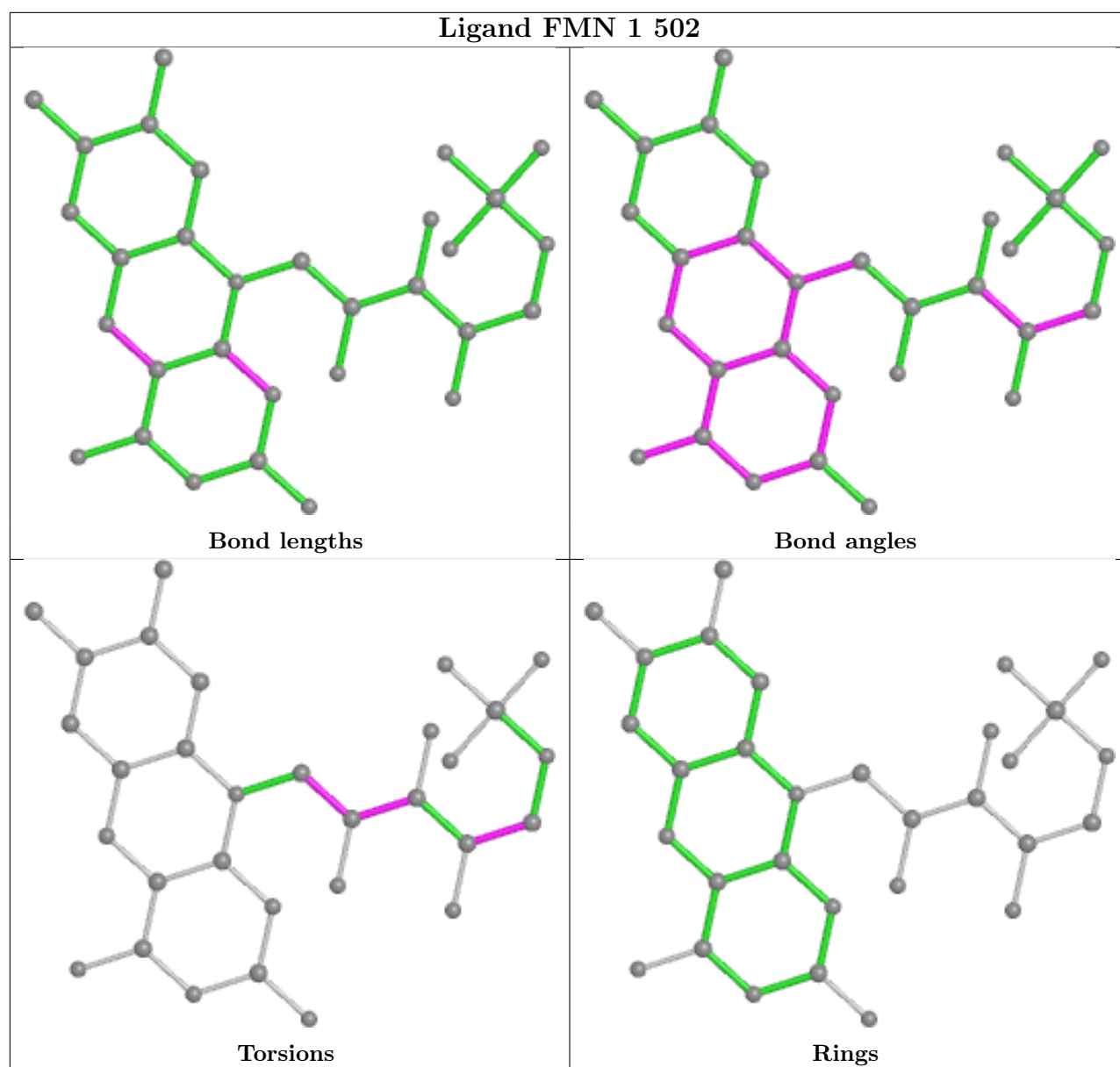
15 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	502	FMN	9	0
17	9	201	SF4	2	0
17	D	803	SF4	2	0
19	3	804	FES	1	0
17	B	501	SF4	3	0
20	E	501	DCQ	4	0
17	O	202	SF4	1	0
17	3	803	SF4	2	0
17	3	801	SF4	1	0
19	D	804	FES	2	0
20	4	501	DCQ	4	0
17	6	201	SF4	1	0
18	1	502	FMN	9	0
17	9	202	SF4	1	0
17	O	201	SF4	2	0

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







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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.