wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2020 – 10:43 AM BST

PDB ID	:	6Y11
Title	:	Respiratory complex I from Thermus thermophilus
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2020-02-10
Resolution	:	3.11 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

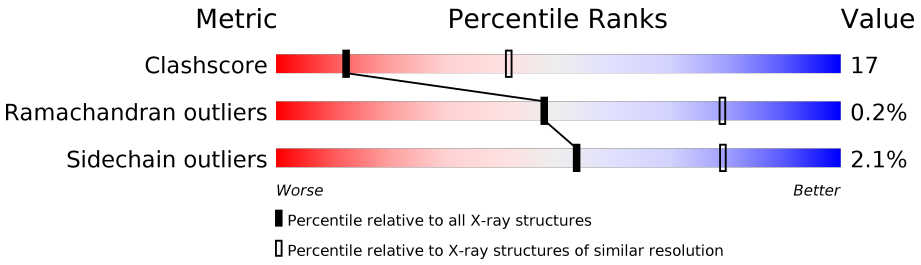
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 on the lower 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	67% 31% •
1	B	438	62% 37% •
2	2	181	71% 25% • •
2	C	181	66% 31% • •
3	3	783	65% 31% •
3	D	783	64% 31% • •
4	4	409	55% 38% • 6%
4	E	409	56% 37% • 6%

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Mol	Chain	Length	Quality of chain
5	5	207	57% 37% • 5%
5	F	207	62% 32% • 5%
6	6	181	54% 34% • 8%
6	G	181	43% 47% • 8%
7	9	182	55% 42% •••
7	O	182	60% 37% ••
8	7	129	66% 32% ••
8	I	129	64% 33% ••
9	W	131	79% 18% •
9	X	131	71% 26% •
10	A	119	58% 39% ••
10	P	119	54% 43% ••
11	J	176	61% 30% • 9%
11	R	176	58% 32% • 9%
12	K	95	63% 37%
12	S	95	64% 35% •
13	L	606	67% 33% •
13	T	606	66% 33% •
14	M	469	58% 41%
14	U	469	62% 37%
15	N	427	68% 32%
15	V	427	71% 29%
16	H	365	49% 44% ••
16	Q	365	44% 50% ••

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	1	501	-	-	X	-
17	SF4	6	201	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	B	501	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	201	-	-	X	-
17	SF4	O	202	-	-	X	-
19	FES	3	804	-	-	X	-
19	FES	C	201	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 74086 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
1	1	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	B	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called DUF3197 domain-containing protein.

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

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

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

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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			

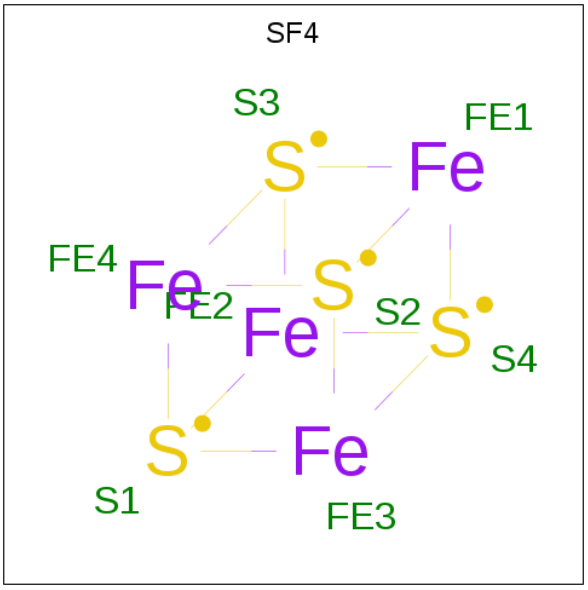
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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
16	H	353	Total	C	N	O	S	0	0	0
			2838	1943	431	457	7			
16	Q	353	Total	C	N	O	S	0	0	0
			2838	1943	431	457	7			

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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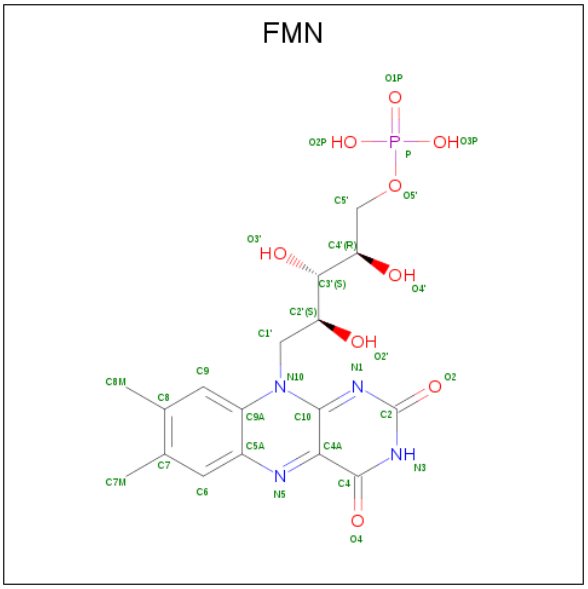
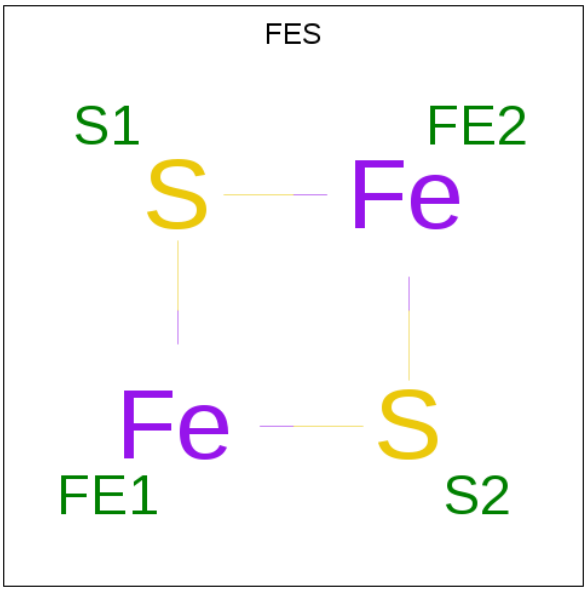
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total Fe S 8 4 4	0	0
17	D	1	Total Fe S 8 4 4	0	0
17	G	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0

- Molecule 18 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

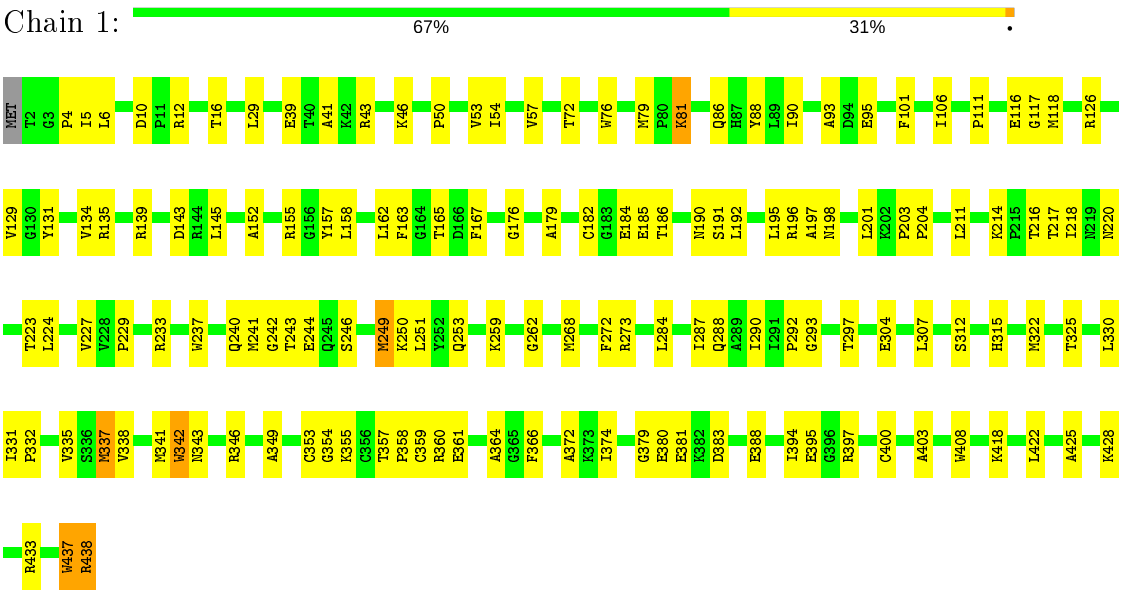
3 Residue-property plots (i)

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

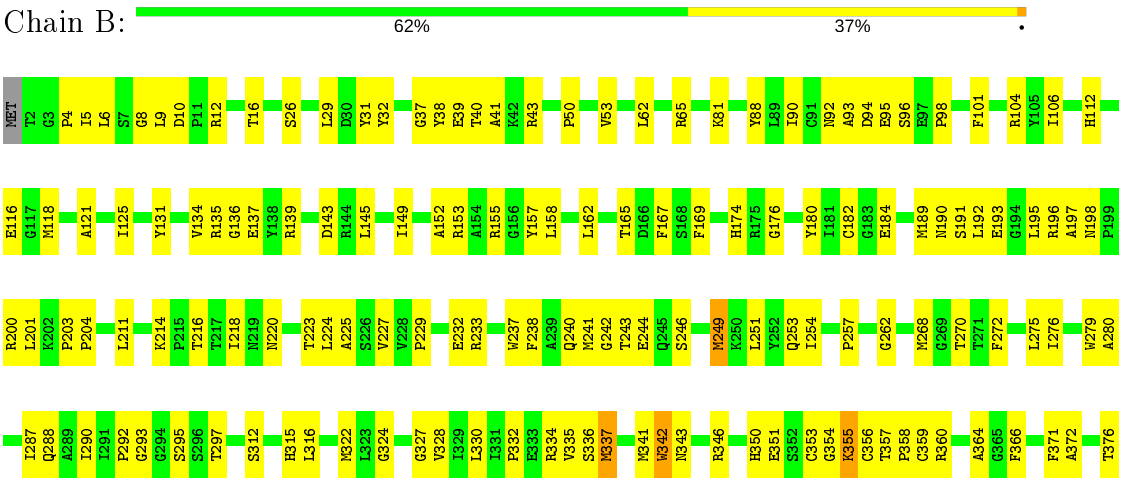
- Molecule 1: NADH-quinone oxidoreductase subunit 1

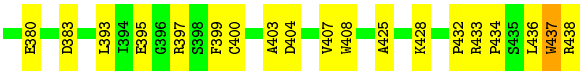
Chain 1:



- Molecule 1: NADH-quinone oxidoreductase subunit 1

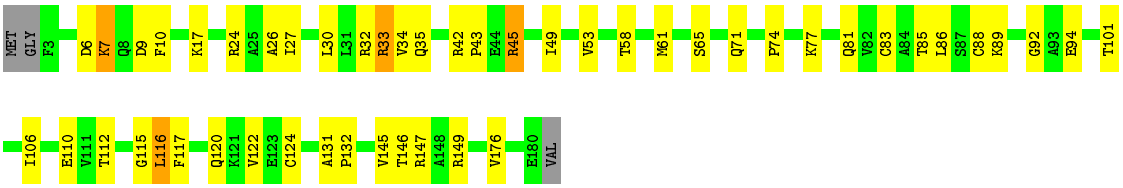
Chain B:





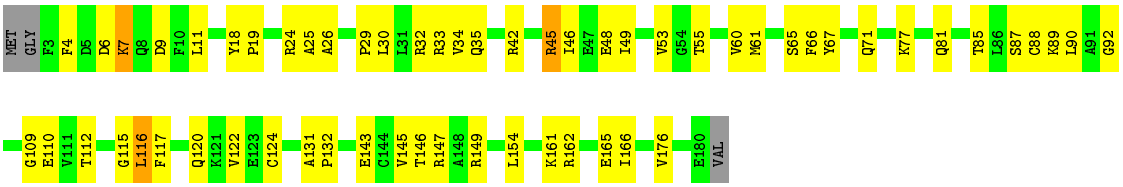
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:



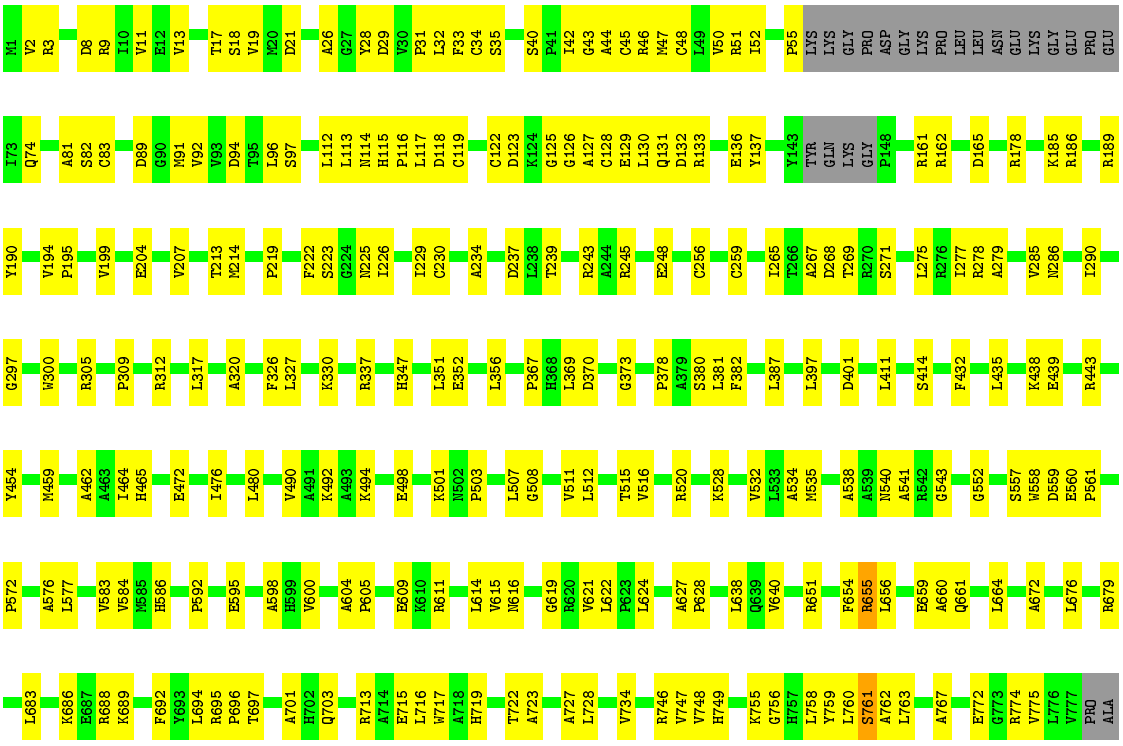
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain C:



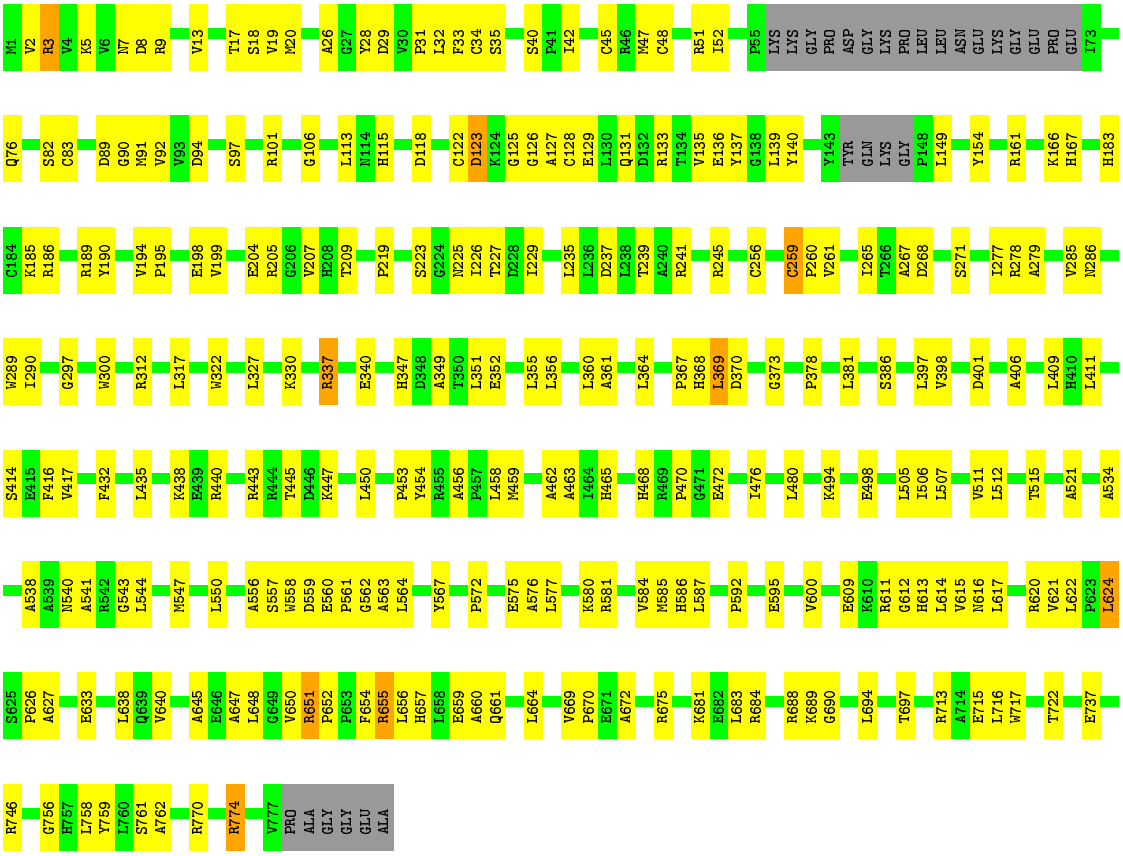
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3:



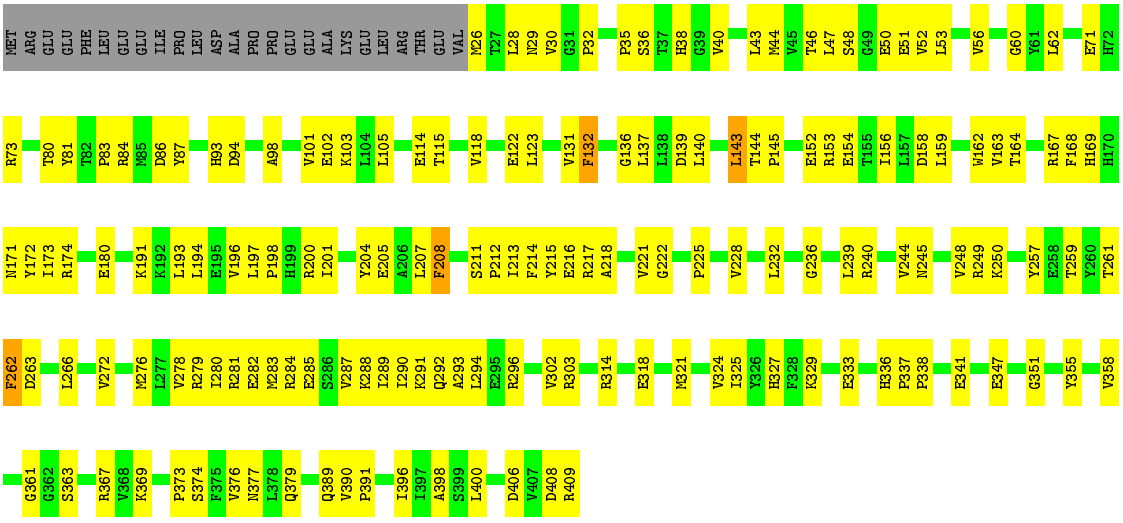
- Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D:



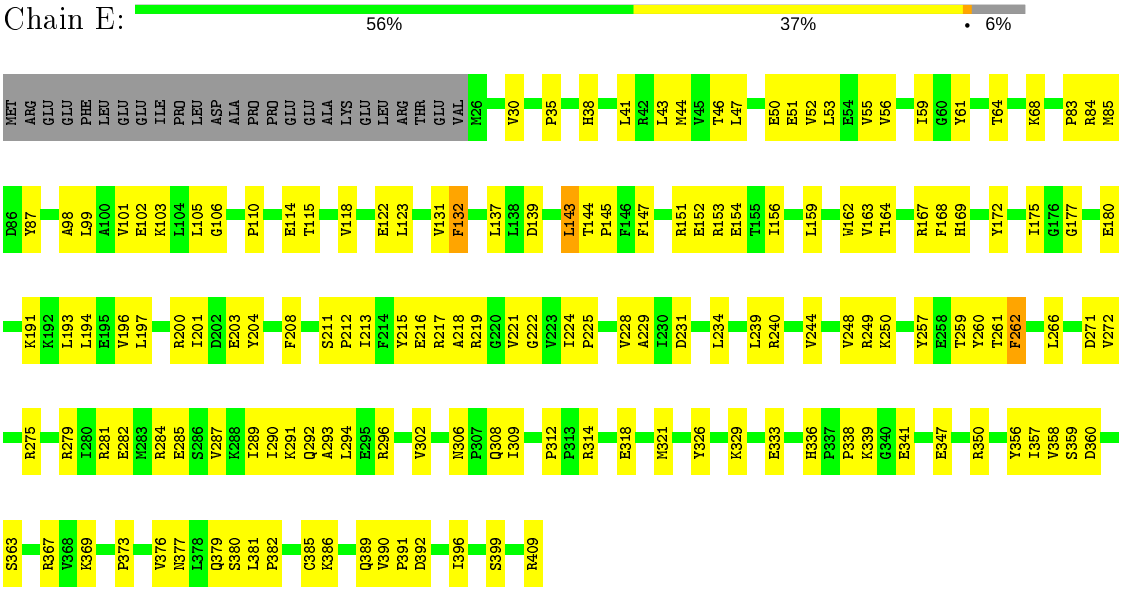
- Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4:



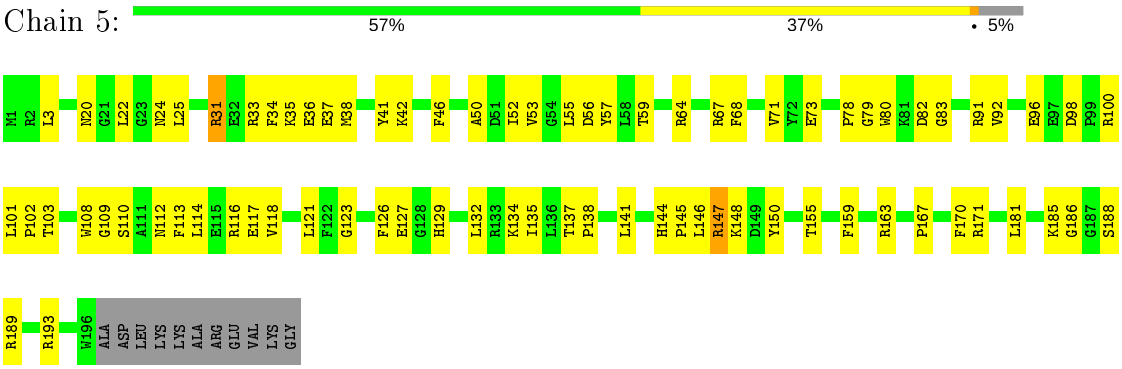
- Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E:



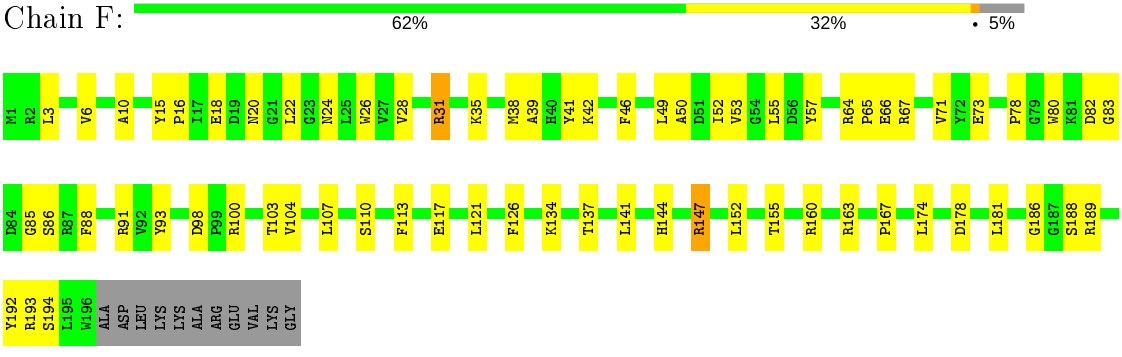
- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5:



- Molecule 5: NADH-quinone oxidoreductase subunit 5

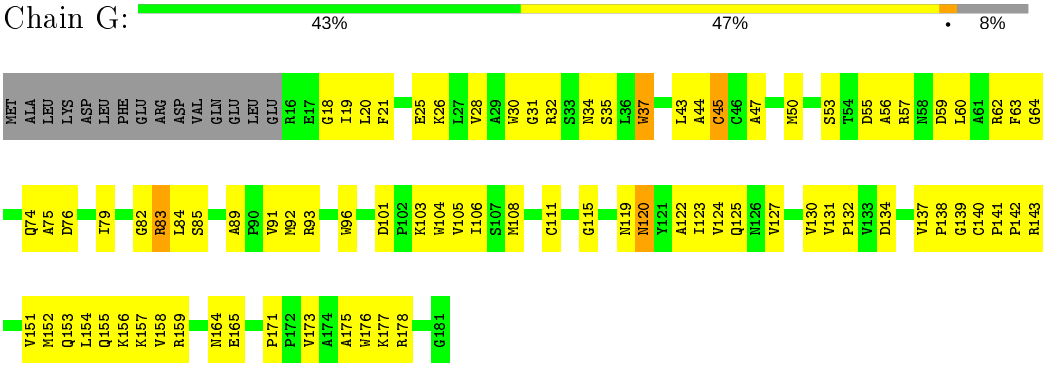
Chain F:



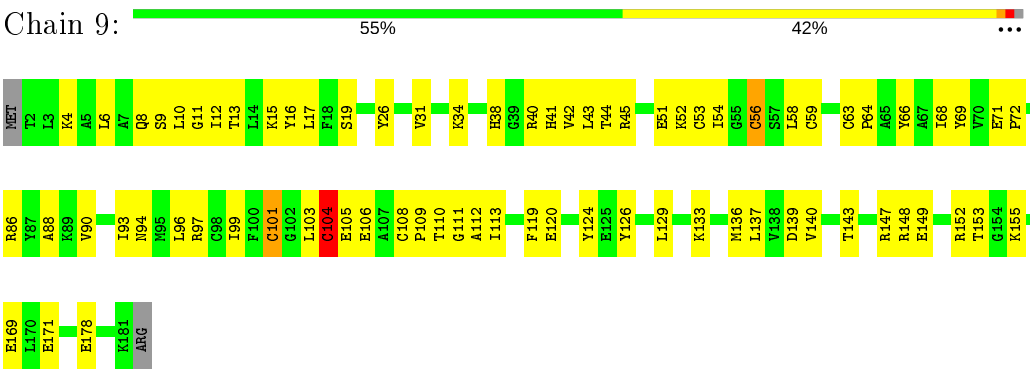
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6:

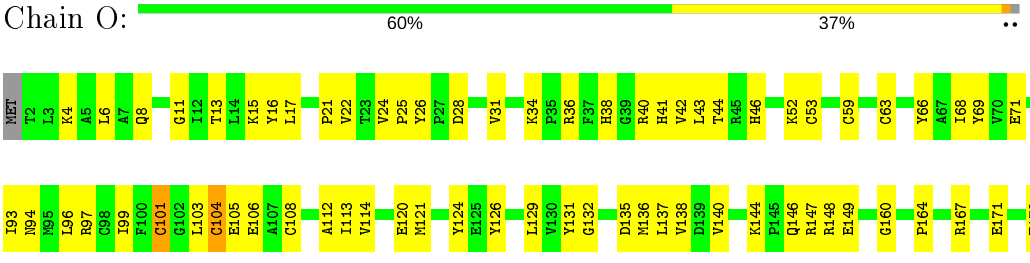
• Molecule 6: NADH-quinone oxidoreductase subunit 6



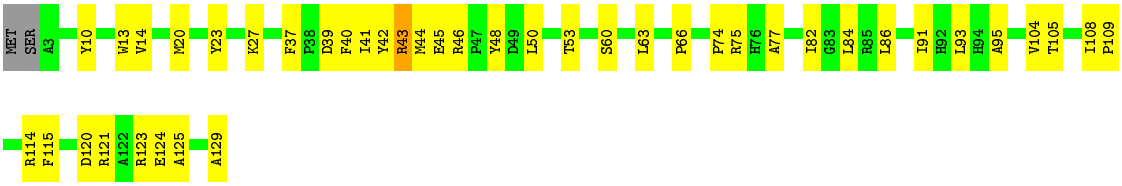
• Molecule 7: NADH-quinone oxidoreductase subunit 9



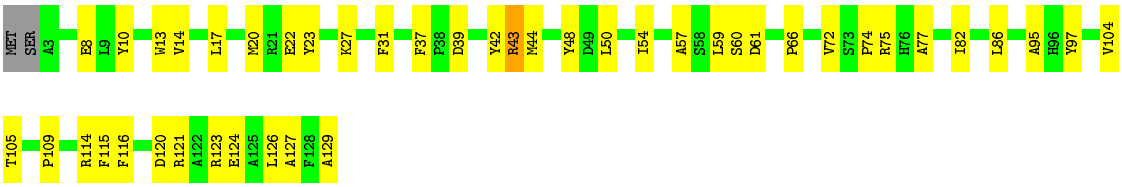
• Molecule 7: NADH-quinone oxidoreductase subunit 9



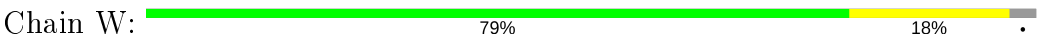
• Molecule 8: NADH-quinone oxidoreductase subunit 15

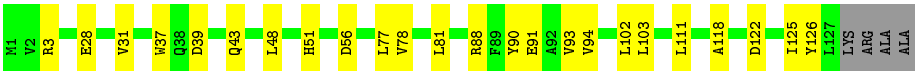


• Molecule 8: NADH-quinone oxidoreductase subunit 15

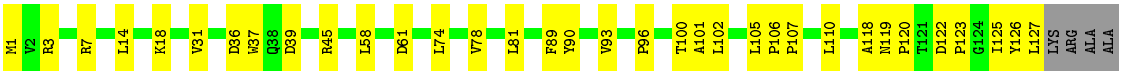


• Molecule 9: DUF3197 domain-containing protein

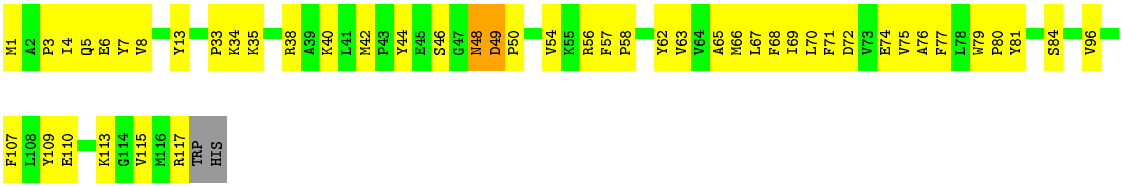




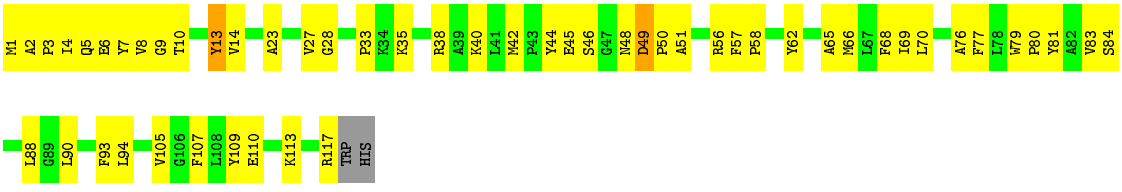
• Molecule 9: DUF3197 domain-containing protein



• Molecule 10: NADH-quinone oxidoreductase subunit 7

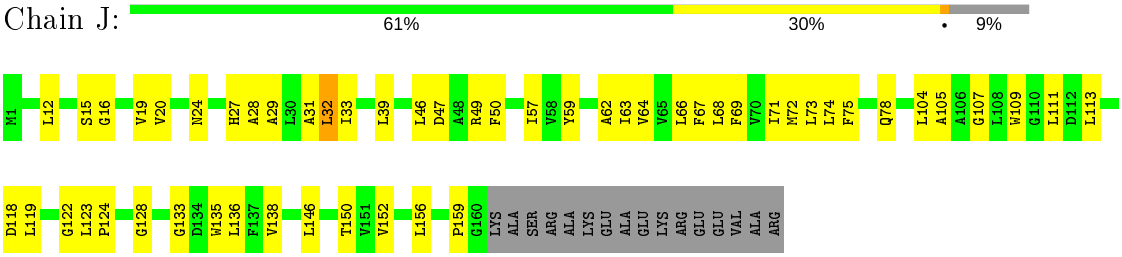


• Molecule 10: NADH-quinone oxidoreductase subunit 7



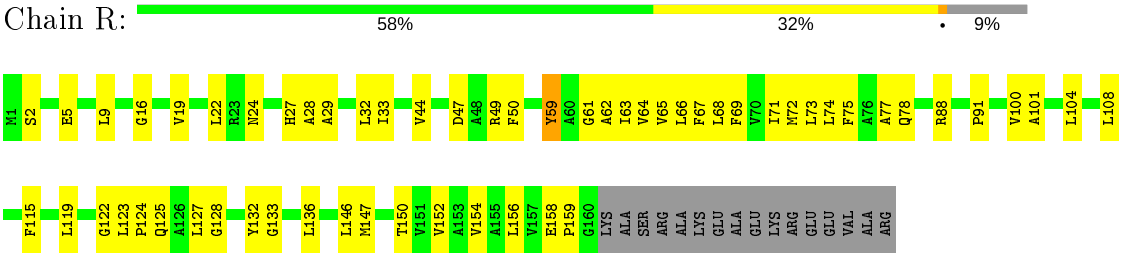
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



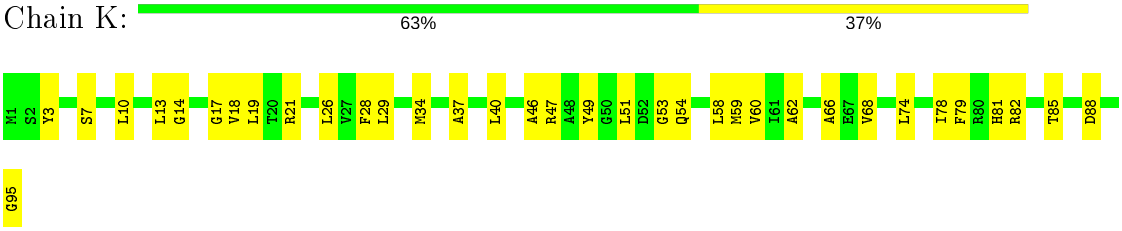
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



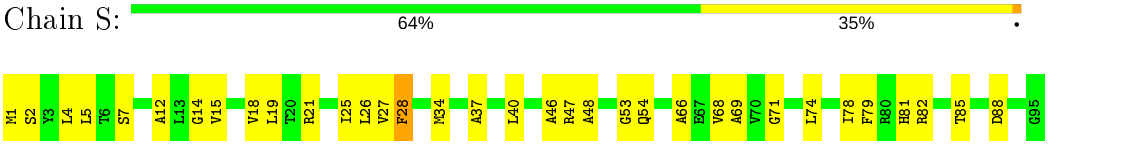
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



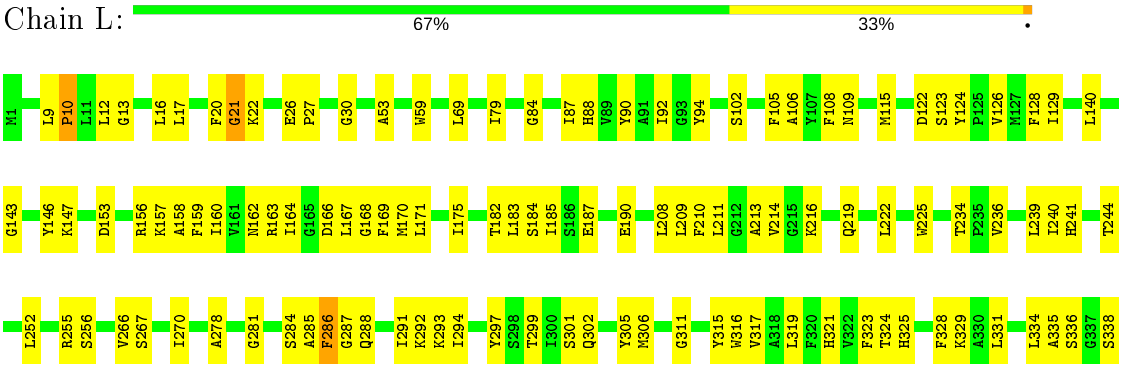
• Molecule 12: NADH-quinone oxidoreductase subunit 11

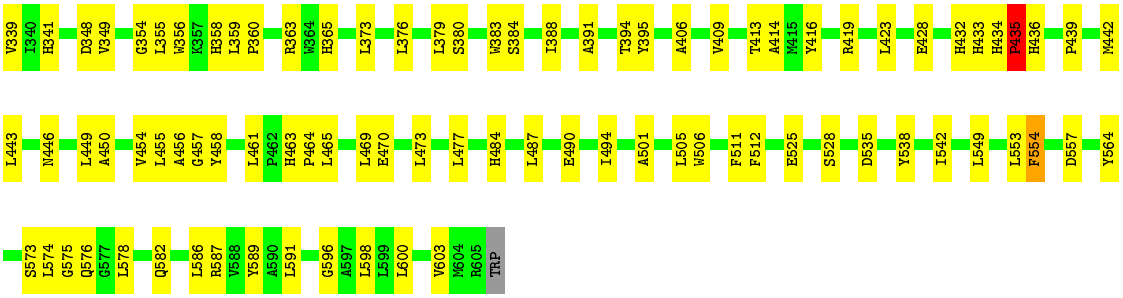
Chain S:



• Molecule 13: NADH-quinone oxidoreductase subunit 12

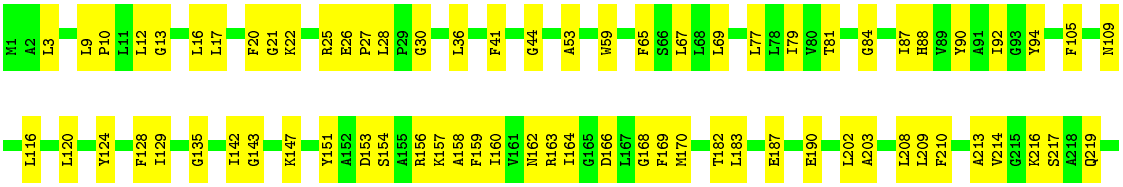
Chain L:

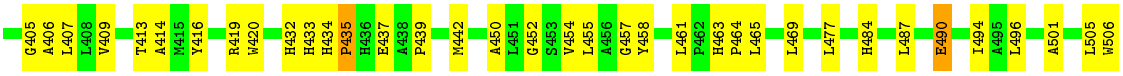




• Molecule 13: NADH-quinone oxidoreductase subunit 12

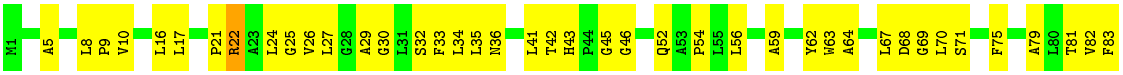
Chain T:

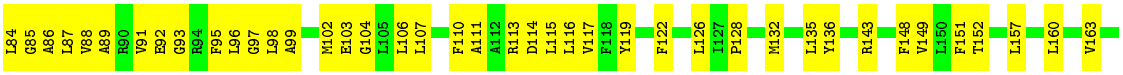


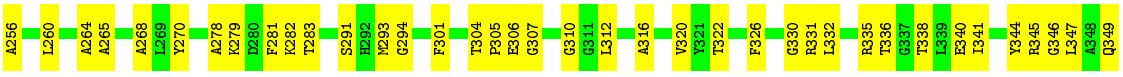


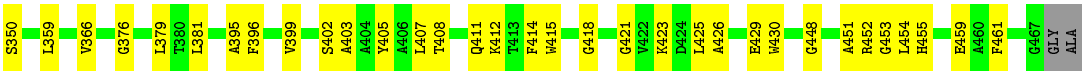
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain M:



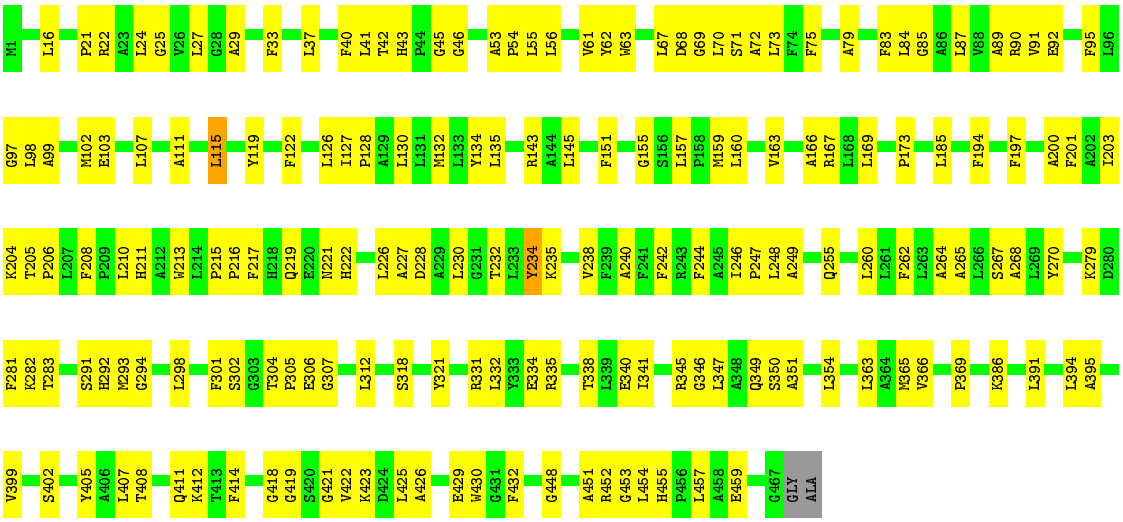






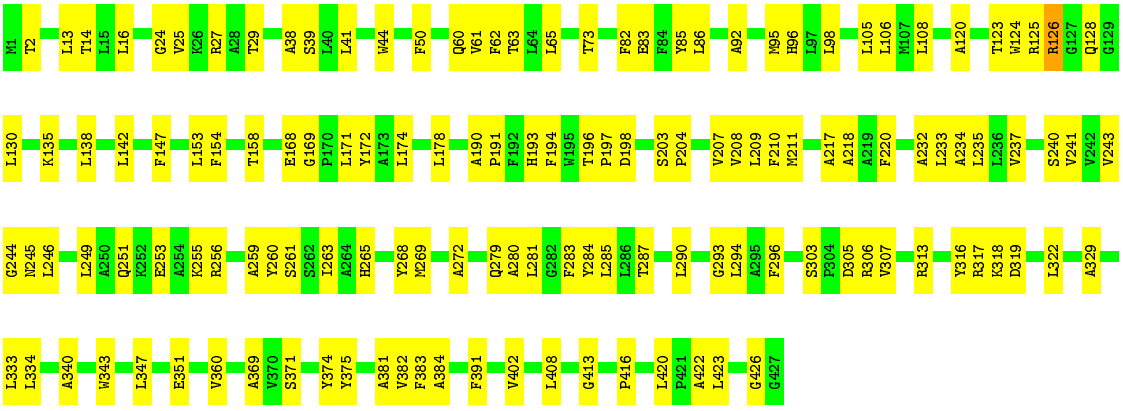
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U:



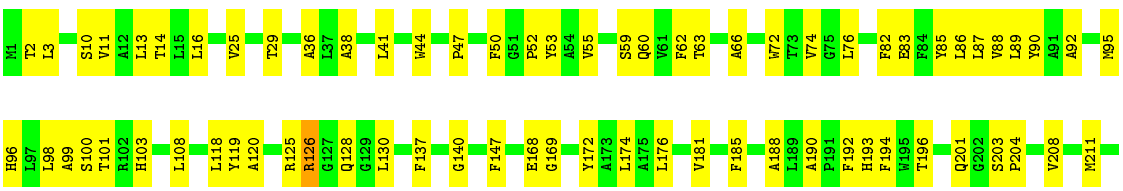
• Molecule 15: NADH-quinone oxidoreductase subunit 14

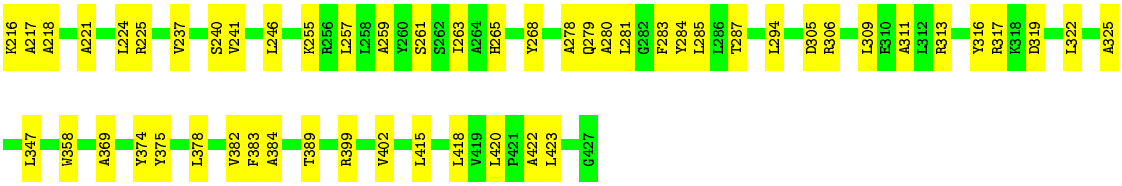
Chain N:



• Molecule 15: NADH-quinone oxidoreductase subunit 14

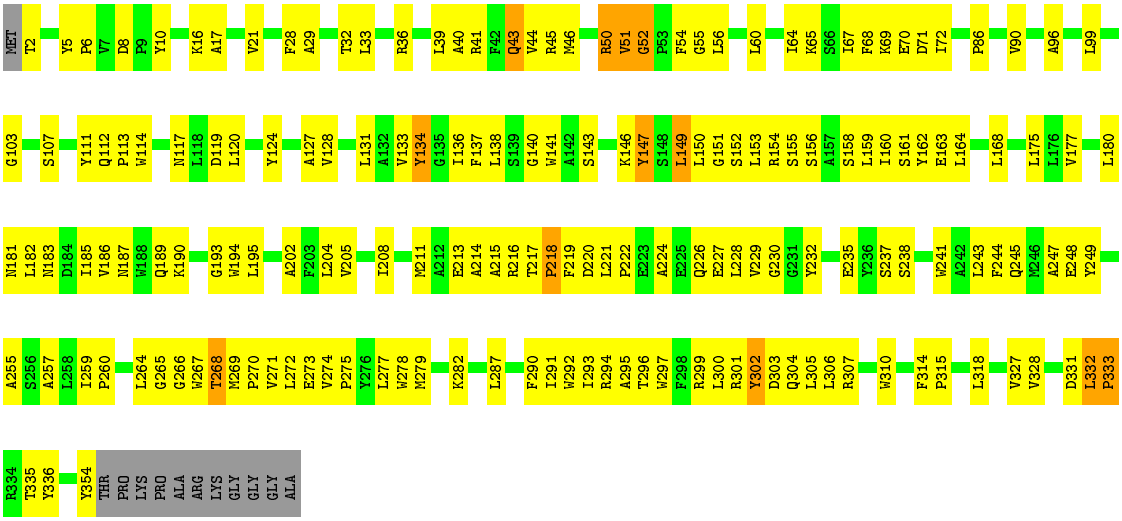
Chain V:





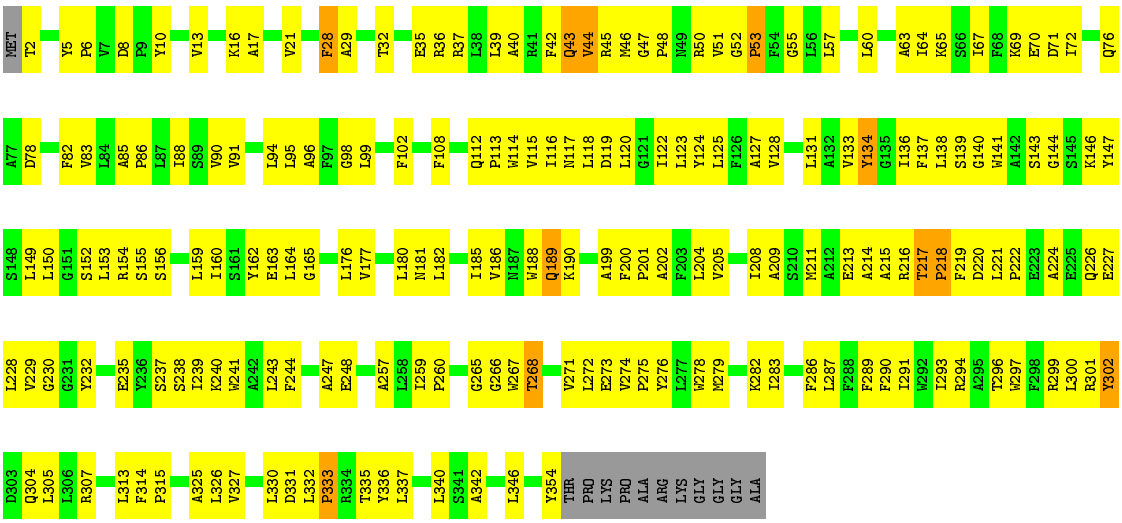
• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H:



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:



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, α, β, γ	96.28Å 340.89Å 263.30Å 90.00° 100.57° 90.00°	Depositor
Resolution (Å)	58.67 – 3.11	Depositor
% Data completeness (in resolution range)	90.0 (58.67-3.11)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.229	Depositor
Wilson B-factor (Å^2)	91.2	Xtriage
Anisotropy	0.025	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.420 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -h,-k,h+l	Depositor
Outliers	0 of 268255 reflections	Xtriage
Total number of atoms	74086	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, 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	#$\|Z\|>5$
1	1	0.34	0/3506	0.48	0/4745
1	B	0.36	0/3506	0.48	0/4745
2	2	0.33	0/1439	0.48	0/1953
2	C	0.34	0/1439	0.48	0/1953
3	3	0.38	0/6035	0.53	1/8185 (0.0%)
3	D	0.39	1/6035 (0.0%)	0.54	1/8185 (0.0%)
4	4	0.36	0/3150	0.51	0/4284
4	E	0.36	0/3150	0.51	0/4284
5	5	0.38	0/1656	0.52	0/2246
5	F	0.40	0/1656	0.52	0/2246
6	6	0.40	0/1319	0.55	0/1786
6	G	0.43	0/1319	0.55	0/1786
7	9	0.55	3/1423 (0.2%)	0.57	0/1933
7	O	0.50	1/1423 (0.1%)	0.55	0/1933
8	7	0.32	0/1059	0.49	0/1429
8	I	0.35	0/1059	0.50	0/1429
9	W	0.36	0/985	0.49	0/1335
9	X	0.35	0/985	0.50	0/1335
10	A	0.37	0/940	0.51	0/1280
10	P	0.38	0/940	0.53	0/1280
11	J	0.31	0/1206	0.48	0/1649
11	R	0.31	0/1206	0.50	0/1649
12	K	0.31	0/710	0.44	0/962
12	S	0.30	0/710	0.45	0/962
13	L	0.33	0/4741	0.49	1/6460 (0.0%)
13	T	0.33	0/4741	0.48	1/6460 (0.0%)
14	M	0.34	0/3591	0.51	0/4896
14	U	0.32	0/3591	0.50	0/4896
15	N	0.33	0/3238	0.46	0/4434
15	V	0.33	0/3238	0.47	0/4434
16	H	0.39	0/2935	0.56	0/4014
16	Q	0.40	0/2935	0.56	0/4014

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.37	5/75866 (0.0%)	0.51	4/103182 (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	O	0	1
13	L	0	1
13	T	0	1
16	H	0	5
16	Q	0	3
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	101	CYS	CB-SG	-6.99	1.70	1.82
7	9	104	CYS	CB-SG	-5.75	1.72	1.81
7	O	101	CYS	CB-SG	-5.55	1.72	1.81
3	D	624	LEU	C-N	-5.32	1.21	1.34
7	9	56	CYS	CB-SG	-5.14	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	369	LEU	CA-CB-CG	5.81	128.66	115.30
3	3	369	LEU	CA-CB-CG	5.34	127.58	115.30
13	T	574	LEU	CB-CG-CD2	5.29	120.00	111.00
13	L	574	LEU	CB-CG-CD2	5.16	119.77	111.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
16	H	43	GLN	Peptide
16	H	52	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	3389	97	0
1	B	3417	0	3388	123	0
2	2	1406	0	1373	41	0
2	C	1406	0	1373	49	0
3	3	5895	0	5930	165	0
3	D	5895	0	5930	186	0
4	4	3067	0	3049	153	0
4	E	3067	0	3049	143	0
5	5	1607	0	1574	70	0
5	F	1607	0	1574	62	0
6	6	1289	0	1298	71	0
6	G	1289	0	1298	89	0
7	9	1388	0	1383	84	0
7	O	1388	0	1383	70	0
8	7	1031	0	1029	42	0
8	I	1031	0	1029	37	0
9	W	967	0	1010	17	0
9	X	967	0	1010	24	0
10	A	910	0	939	52	0
10	P	910	0	939	61	0
11	J	1183	0	1286	51	0
11	R	1183	0	1286	57	0
12	K	703	0	747	36	0
12	S	703	0	747	31	0
13	L	4604	0	4734	159	0
13	T	4604	0	4734	146	0
14	M	3489	0	3606	138	0
14	U	3489	0	3606	124	0
15	N	3154	0	3343	104	0
15	V	3154	0	3343	85	0
16	H	2838	0	2903	173	0
16	Q	2838	0	2903	184	0
17	1	8	0	0	2	0
17	3	24	0	0	2	0
17	6	8	0	0	3	0
17	9	16	0	0	9	0
17	B	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	24	0	0	1	0
17	G	8	0	0	3	0
17	O	16	0	0	6	0
18	1	31	0	19	3	0
18	B	31	0	19	4	0
19	2	4	0	0	1	0
19	3	4	0	0	2	0
19	C	4	0	0	2	0
19	D	4	0	0	0	0
All	All	74086	0	75223	2529	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 17.

The worst 5 of 2529 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:E:85:MET:HE2	4:E:409:ARG:HG3	1.33	1.10
6:G:140:CYS:SG	7:O:99:ILE:HD11	1.93	1.08
4:E:47:LEU:CD1	4:E:51:GLU:O	2.00	1.08
7:9:108:CYS:HA	17:9:202:SF4:S3	1.99	1.02
3:D:115:HIS:HB3	4:E:321:MET:HE3	1.45	0.98

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%)	413 (95%)	22 (5%)	0	100	100
1	B	435/438 (99%)	410 (94%)	25 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	176/181 (97%)	168 (96%)	8 (4%)	0	100	100
2	C	176/181 (97%)	167 (95%)	9 (5%)	0	100	100
3	3	750/783 (96%)	708 (94%)	42 (6%)	0	100	100
3	D	750/783 (96%)	710 (95%)	40 (5%)	0	100	100
4	4	382/409 (93%)	361 (94%)	21 (6%)	0	100	100
4	E	382/409 (93%)	362 (95%)	20 (5%)	0	100	100
5	5	194/207 (94%)	185 (95%)	9 (5%)	0	100	100
5	F	194/207 (94%)	186 (96%)	8 (4%)	0	100	100
6	6	164/181 (91%)	152 (93%)	12 (7%)	0	100	100
6	G	164/181 (91%)	150 (92%)	14 (8%)	0	100	100
7	9	178/182 (98%)	169 (95%)	9 (5%)	0	100	100
7	O	178/182 (98%)	171 (96%)	7 (4%)	0	100	100
8	7	125/129 (97%)	118 (94%)	7 (6%)	0	100	100
8	I	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
9	W	125/131 (95%)	122 (98%)	3 (2%)	0	100	100
9	X	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
10	A	115/119 (97%)	105 (91%)	10 (9%)	0	100	100
10	P	115/119 (97%)	106 (92%)	9 (8%)	0	100	100
11	J	158/176 (90%)	148 (94%)	10 (6%)	0	100	100
11	R	158/176 (90%)	150 (95%)	8 (5%)	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%)	567 (94%)	34 (6%)	2 (0%)	41	73
13	T	603/606 (100%)	574 (95%)	27 (4%)	2 (0%)	41	73
14	M	465/469 (99%)	440 (95%)	25 (5%)	0	100	100
14	U	465/469 (99%)	447 (96%)	18 (4%)	0	100	100
15	N	425/427 (100%)	409 (96%)	16 (4%)	0	100	100
15	V	425/427 (100%)	407 (96%)	18 (4%)	0	100	100
16	H	351/365 (96%)	312 (89%)	33 (9%)	6 (2%)	9	36
16	Q	351/365 (96%)	308 (88%)	38 (11%)	5 (1%)	11	40
All	All	9478/9796 (97%)	8942 (94%)	521 (6%)	15 (0%)	47	79

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL
16	H	44	VAL
16	H	50	ARG
16	Q	44	VAL
13	L	435	PRO

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%)	344 (97%)	11 (3%)	40	70
1	B	355/356 (100%)	344 (97%)	11 (3%)	40	70
2	2	150/152 (99%)	144 (96%)	6 (4%)	31	65
2	C	150/152 (99%)	144 (96%)	6 (4%)	31	65
3	3	609/628 (97%)	599 (98%)	10 (2%)	62	84
3	D	609/628 (97%)	602 (99%)	7 (1%)	73	89
4	4	332/355 (94%)	328 (99%)	4 (1%)	71	88
4	E	332/355 (94%)	326 (98%)	6 (2%)	59	82
5	5	167/175 (95%)	165 (99%)	2 (1%)	71	88
5	F	167/175 (95%)	165 (99%)	2 (1%)	71	88
6	6	135/149 (91%)	125 (93%)	10 (7%)	13	42
6	G	135/149 (91%)	128 (95%)	7 (5%)	23	55
7	9	148/150 (99%)	146 (99%)	2 (1%)	67	86
7	O	148/150 (99%)	146 (99%)	2 (1%)	67	86
8	7	104/106 (98%)	103 (99%)	1 (1%)	76	90
8	I	104/106 (98%)	103 (99%)	1 (1%)	76	90
9	W	99/101 (98%)	97 (98%)	2 (2%)	55	80
9	X	99/101 (98%)	98 (99%)	1 (1%)	76	90
10	A	90/92 (98%)	87 (97%)	3 (3%)	38	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	P	90/92 (98%)	88 (98%)	2 (2%)	52 78
11	J	118/130 (91%)	115 (98%)	3 (2%)	47 75
11	R	118/130 (91%)	116 (98%)	2 (2%)	60 83
12	K	71/71 (100%)	69 (97%)	2 (3%)	43 73
12	S	71/71 (100%)	70 (99%)	1 (1%)	67 86
13	L	453/454 (100%)	445 (98%)	8 (2%)	59 82
13	T	453/454 (100%)	444 (98%)	9 (2%)	55 80
14	M	332/332 (100%)	325 (98%)	7 (2%)	53 79
14	U	332/332 (100%)	326 (98%)	6 (2%)	59 82
15	N	302/302 (100%)	298 (99%)	4 (1%)	69 87
15	V	302/302 (100%)	298 (99%)	4 (1%)	69 87
16	H	293/300 (98%)	283 (97%)	10 (3%)	37 69
16	Q	293/300 (98%)	287 (98%)	6 (2%)	55 80
All	All	7516/7706 (98%)	7358 (98%)	158 (2%)	53 79

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	N	50	PHE
1	B	342	TRP
14	U	255	GLN
15	N	126	ARG
16	H	245	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
16	H	187	ASN
2	C	71	GLN
16	Q	112	GLN
16	H	304	GLN
1	B	35	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

20 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	3	801	3	0,12,12	0.00	-	-		
17	SF4	O	201	7	0,12,12	0.00	-	-		
19	FES	C	201	2	0,4,4	0.00	-	-		
17	SF4	3	802	3	0,12,12	0.00	-	-		
17	SF4	O	202	7	0,12,12	0.00	-	-		
18	FMN	1	502	-	31,33,33	1.60	4 (12%)	40,50,50	1.74	6 (15%)
19	FES	D	804	3	0,4,4	0.00	-	-		
17	SF4	B	501	1	0,12,12	0.00	-	-		
17	SF4	3	803	3	0,12,12	0.00	-	-		
17	SF4	6	201	6	0,12,12	0.00	-	-		
17	SF4	9	201	7	0,12,12	0.00	-	-		
17	SF4	D	803	3	0,12,12	0.00	-	-		
17	SF4	1	501	1	0,12,12	0.00	-	-		
17	SF4	G	201	6	0,12,12	0.00	-	-		
19	FES	2	201	2	0,4,4	0.00	-	-		
17	SF4	D	801	3	0,12,12	0.00	-	-		
19	FES	3	804	3	0,4,4	0.00	-	-		
17	SF4	9	202	7	0,12,12	0.00	-	-		
17	SF4	D	802	3	0,12,12	0.00	-	-		
18	FMN	B	502	-	31,33,33	1.46	4 (12%)	40,50,50	1.60	6 (15%)

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	3	801	3	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
18	FMN	1	502	-	-	7/18/18/18	0/3/3/3
19	FES	D	804	3	-	-	0/1/1/1
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	G	201	6	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	D	801	3	-	-	0/6/5/5
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
18	FMN	B	502	-	-	6/18/18/18	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C10-N1	4.81	1.39	1.33
18	B	502	FMN	C10-N1	4.26	1.38	1.33
18	1	502	FMN	C4A-N5	3.78	1.38	1.33
18	B	502	FMN	C4A-N5	3.65	1.38	1.33
18	1	502	FMN	C4-N3	3.46	1.39	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	502	FMN	C4-N3-C2	6.72	120.82	115.14
18	B	502	FMN	C4-N3-C2	6.46	120.60	115.14
18	1	502	FMN	C5A-C9A-N10	4.26	120.80	117.72
18	1	502	FMN	C4A-N5-C5A	4.03	120.80	116.77
18	B	502	FMN	C5A-C9A-N10	3.47	120.23	117.72

There are no chirality outliers.

5 of 13 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	C3'-C4'-C5'-O5'
18	1	502	FMN	O4'-C4'-C5'-O5'
18	B	502	FMN	N10-C1'-C2'-O2'

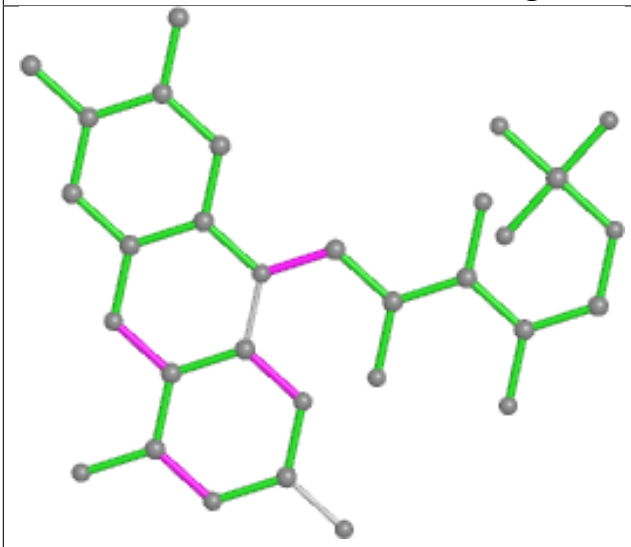
There are no ring outliers.

16 monomers are involved in 40 short contacts:

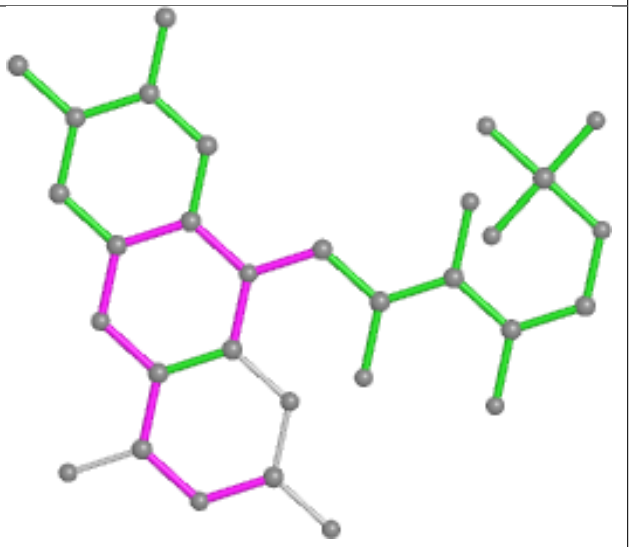
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	801	SF4	1	0
17	O	201	SF4	3	0
19	C	201	FES	2	0
17	O	202	SF4	3	0
18	1	502	FMN	3	0
17	B	501	SF4	2	0
17	3	803	SF4	1	0
17	6	201	SF4	3	0
17	9	201	SF4	3	0
17	1	501	SF4	2	0
17	G	201	SF4	3	0
19	2	201	FES	1	0
17	D	801	SF4	1	0
19	3	804	FES	2	0
17	9	202	SF4	6	0
18	B	502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

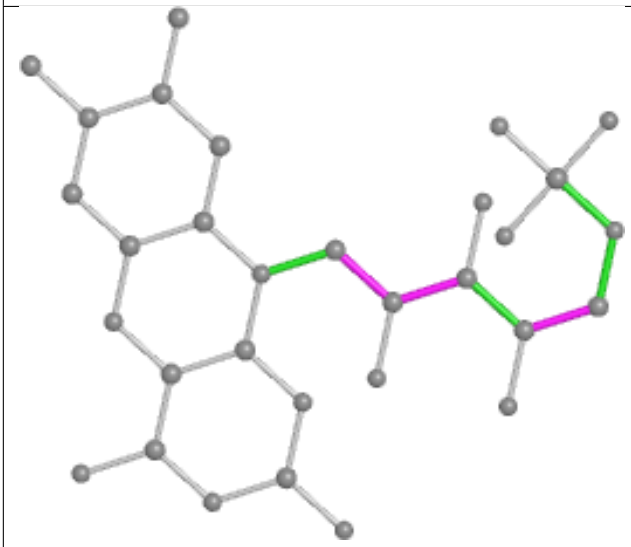
Ligand FMN 1 502



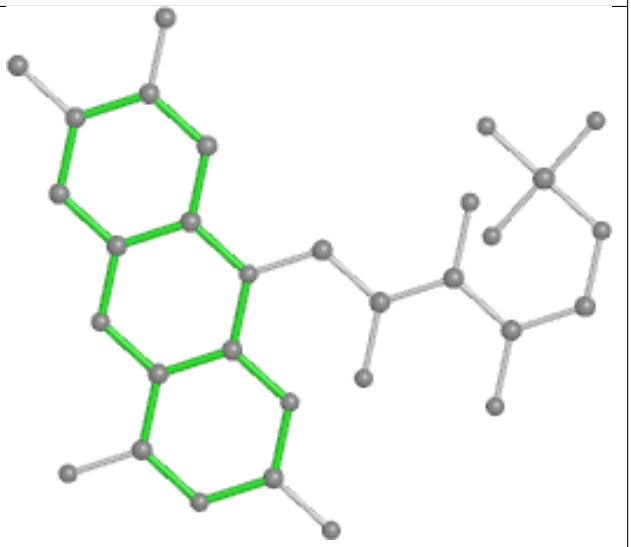
Bond lengths



Bond angles

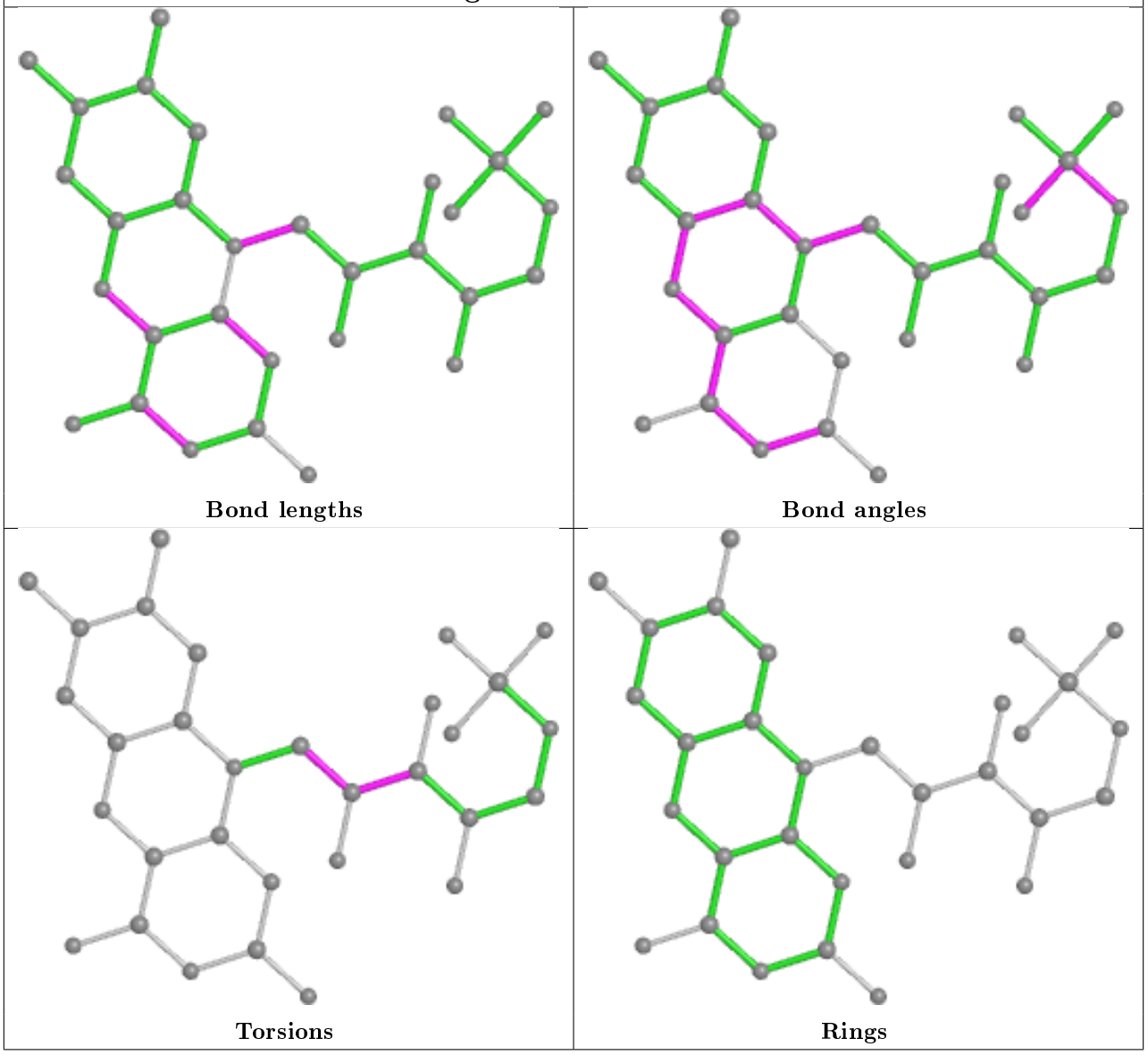


Torsions



Rings

Ligand FMN B 502



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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