wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2026 – 04:57 PM UTC

PDB ID	:	3IAS / pdb_00003ias
Title	:	Crystal structure of the hydrophilic domain of respiratory complex I from Thermus thermophilus, oxidized, 4 mol/ASU, re-refined to 3.15 angstrom resolution
Authors	:	Sazanov, L.A.; Berrisford, J.M.
Deposited on	:	2009-07-14
Resolution	:	3.15 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

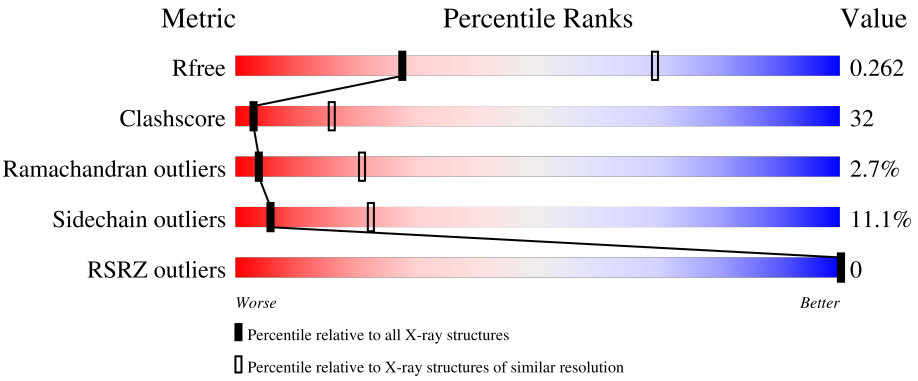
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	438	49% 42% 8%
1	A	438	49% 43% 8%
1	J	438	48% 43% 8%
1	S	438	49% 42% 8%

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Mol	Chain	Length	Quality of chain
2	2	181	52% 38% 7%
2	B	181	55% 36% 7%
2	K	181	53% 37% 7%
2	T	181	52% 38% 8%
3	3	783	46% 42% 8%
3	C	783	46% 42% 8%
3	L	783	46% 42% 8%
3	U	783	45% 42% 8%
4	4	409	37% 44% 11% 8%
4	D	409	37% 44% 11% 8%
4	M	409	38% 44% 10% 8%
4	V	409	35% 48% 9% 8%
5	5	207	41% 42% 12% 5%
5	E	207	40% 43% 12% 5%
5	N	207	41% 43% 11% 5%
5	W	207	38% 45% 12% 5%
6	6	181	34% 37% 9% 20%
6	F	181	34% 38% 9% 20%
6	O	181	34% 39% 7% 20%
6	X	181	31% 39% 9% 20%
7	9	182	45% 34% 6% 15%
7	G	182	47% 33% 5% 15%
7	P	182	45% 35% 5% 15%
7	Y	182	46% 34% 5% 15%
8	7	129	59% 34% 5%

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Mol	Chain	Length	Quality of chain
8	H	129	55% 37% 5%
8	Q	129	53% 40% 5%
8	Z	129	56% 39%

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
9	SF4	6	182	-	-	X	-
9	SF4	F	182	-	-	X	-
9	SF4	O	182	-	-	X	-
9	SF4	X	182	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 75028 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	A	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	J	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	S	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	B	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	K	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	T	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	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	C	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	L	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	U	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	D	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	M	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	V	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	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	E	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	N	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	W	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	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	F	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	O	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	X	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	G	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	P	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

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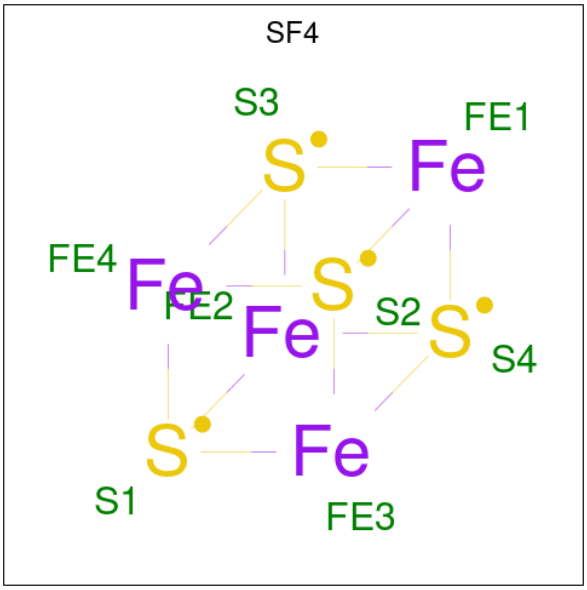
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Y	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

- 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	H	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	Q	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	Z	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	1	1	Total	Fe	S		0	0
			8	4	4			
9	3	1	Total	Fe	S		0	0
			8	4	4			
9	3	1	Total	Fe	S		0	0
			8	4	4			
9	3	1	Total	Fe	S		0	0
			8	4	4			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	6	1	Total Fe S 8 4 4	0	0
9	9	1	Total Fe S 8 4 4	0	0
9	9	1	Total Fe S 8 4 4	0	0
9	A	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	F	1	Total Fe S 8 4 4	0	0
9	G	1	Total Fe S 8 4 4	0	0
9	G	1	Total Fe S 8 4 4	0	0
9	J	1	Total Fe S 8 4 4	0	0
9	L	1	Total Fe S 8 4 4	0	0
9	L	1	Total Fe S 8 4 4	0	0
9	L	1	Total Fe S 8 4 4	0	0
9	O	1	Total Fe S 8 4 4	0	0
9	P	1	Total Fe S 8 4 4	0	0
9	P	1	Total Fe S 8 4 4	0	0
9	S	1	Total Fe S 8 4 4	0	0
9	U	1	Total Fe S 8 4 4	0	0
9	U	1	Total Fe S 8 4 4	0	0
9	U	1	Total Fe S 8 4 4	0	0

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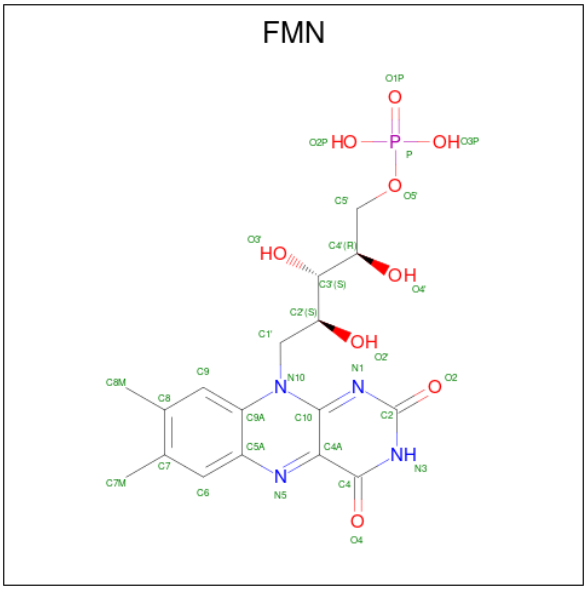
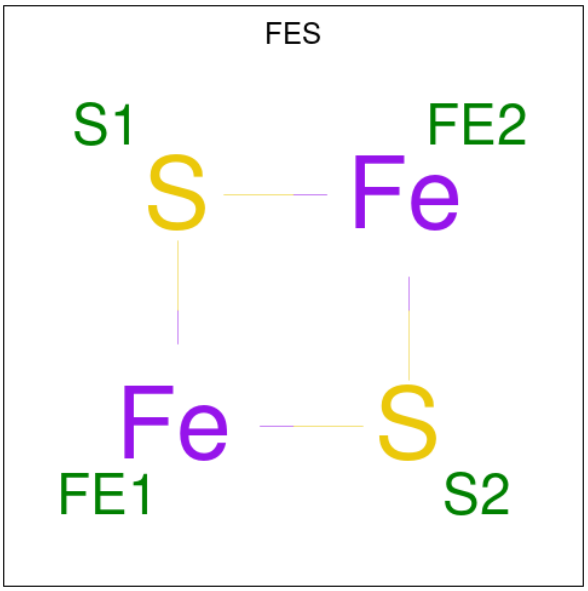
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	X	1	Total Fe S 8 4 4	0	0
9	Y	1	Total Fe S 8 4 4	0	0
9	Y	1	Total Fe S 8 4 4	0	0

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	1	1	Total C N O P 31 17 4 9 1	0	0
10	A	1	Total C N O P 31 17 4 9 1	0	0
10	J	1	Total C N O P 31 17 4 9 1	0	0
10	S	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	2	1	Total Fe S 4 2 2	0	0
11	3	1	Total Fe S 4 2 2	0	0
11	B	1	Total Fe S 4 2 2	0	0
11	C	1	Total Fe S 4 2 2	0	0
11	K	1	Total Fe S 4 2 2	0	0
11	L	1	Total Fe S 4 2 2	0	0
11	T	1	Total Fe S 4 2 2	0	0
11	U	1	Total Fe S 4 2 2	0	0

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	2	1	Total Ca 1 1	0	0
12	3	2	Total Ca 2 2	0	0
12	9	1	Total Ca 1 1	0	0
12	B	1	Total Ca 1 1	0	0

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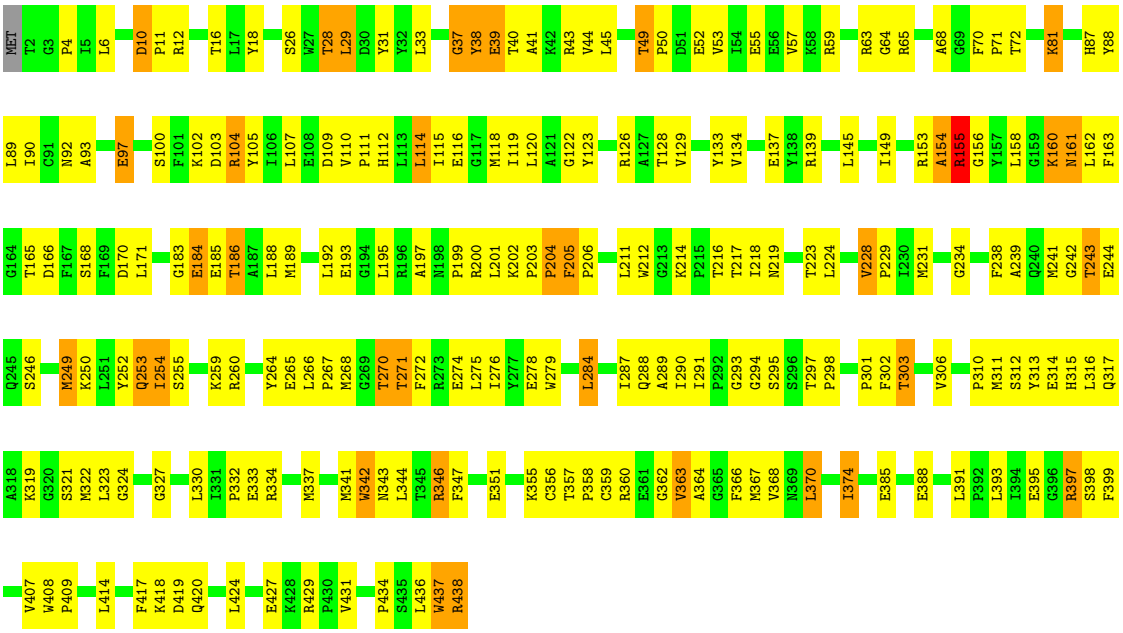
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total Ca 1 1	0	0
12	G	1	Total Ca 1 1	0	0
12	H	1	Total Ca 1 1	0	0
12	K	1	Total Ca 1 1	0	0
12	L	2	Total Ca 2 2	0	0
12	P	1	Total Ca 1 1	0	0
12	T	1	Total Ca 1 1	0	0
12	U	1	Total Ca 1 1	0	0
12	Y	1	Total Ca 1 1	0	0
12	Z	1	Total Ca 1 1	0	0

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 and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

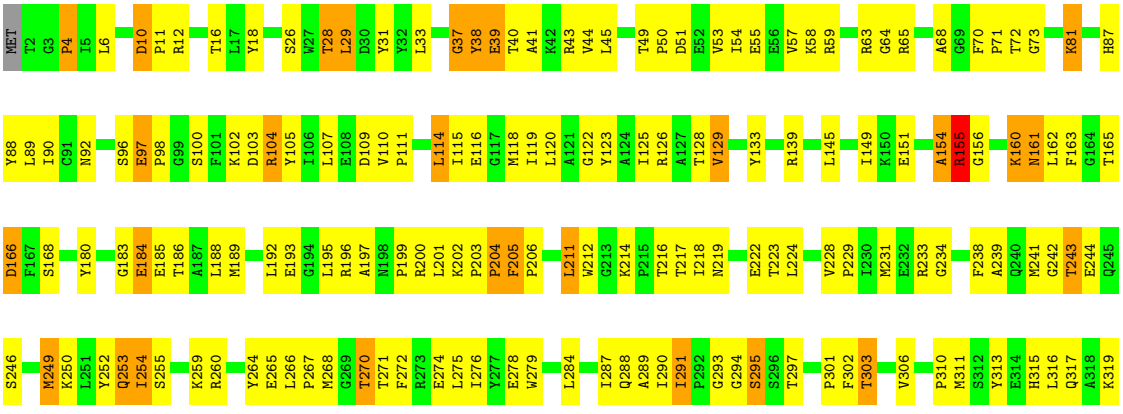
• Molecule 1: NADH-quinone oxidoreductase subunit 1

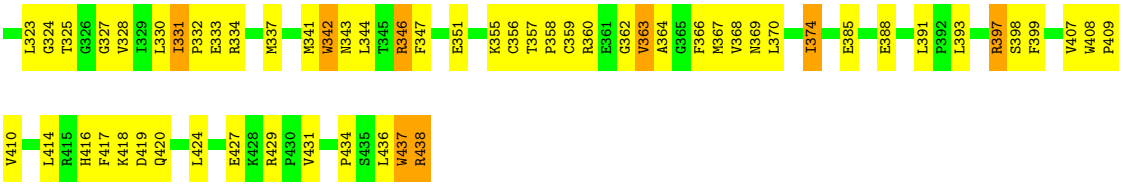
Chain 1:



• Molecule 1: NADH-quinone oxidoreductase subunit 1

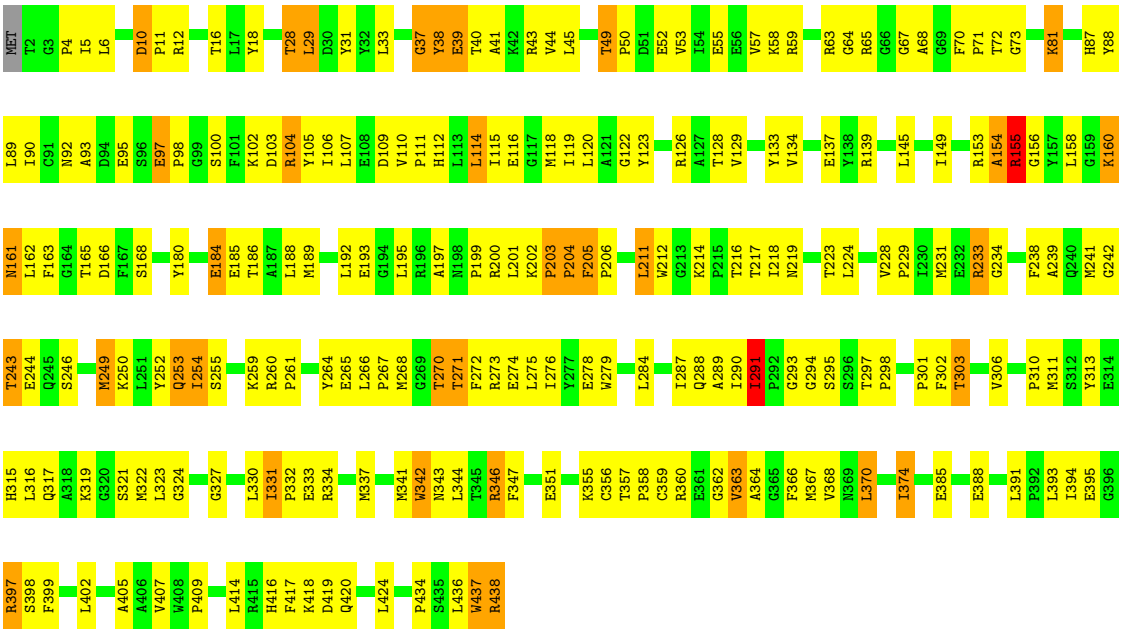
Chain A:





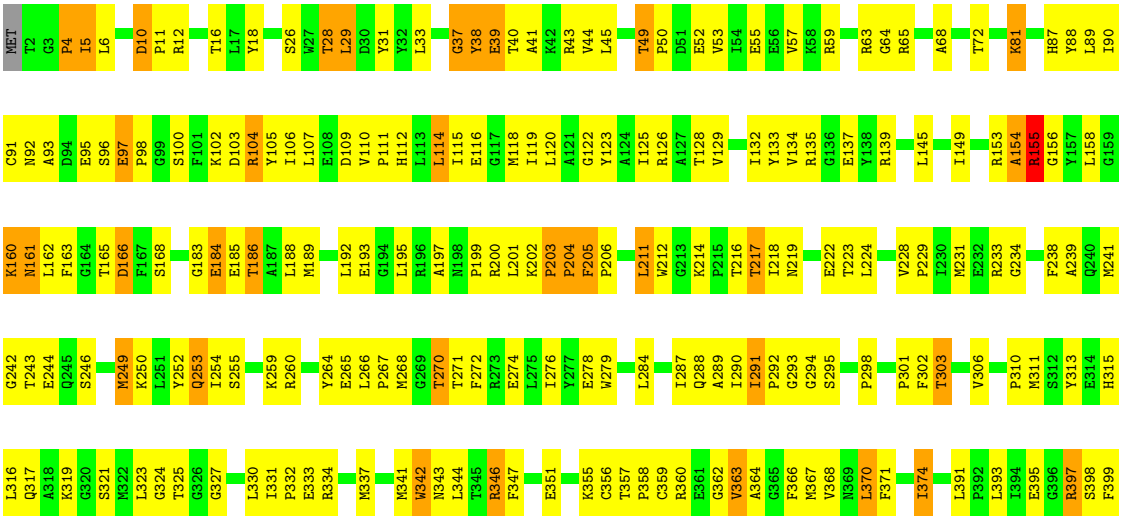
• Molecule 1: NADH-quinone oxidoreductase subunit 1

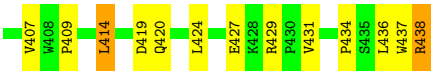
Chain J:



• Molecule 1: NADH-quinone oxidoreductase subunit 1

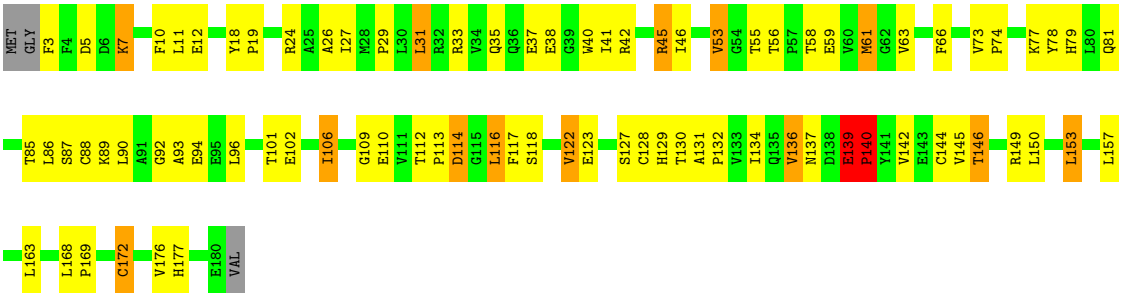
Chain S:





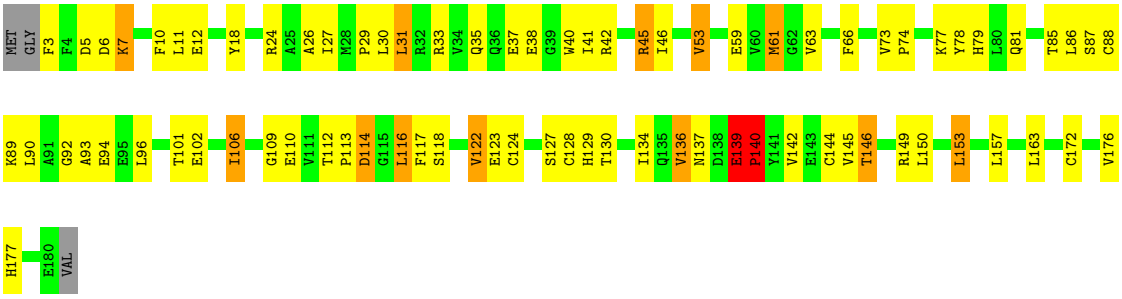
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:



• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain B:

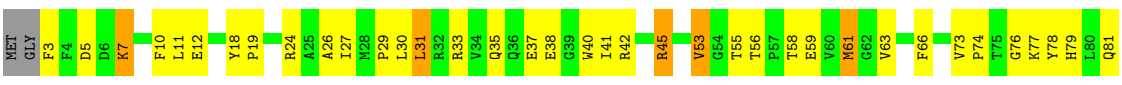


• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain K:

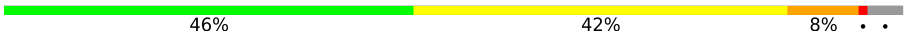
• Molecule 2: NADH-quinone oxidoreductase subunit 2

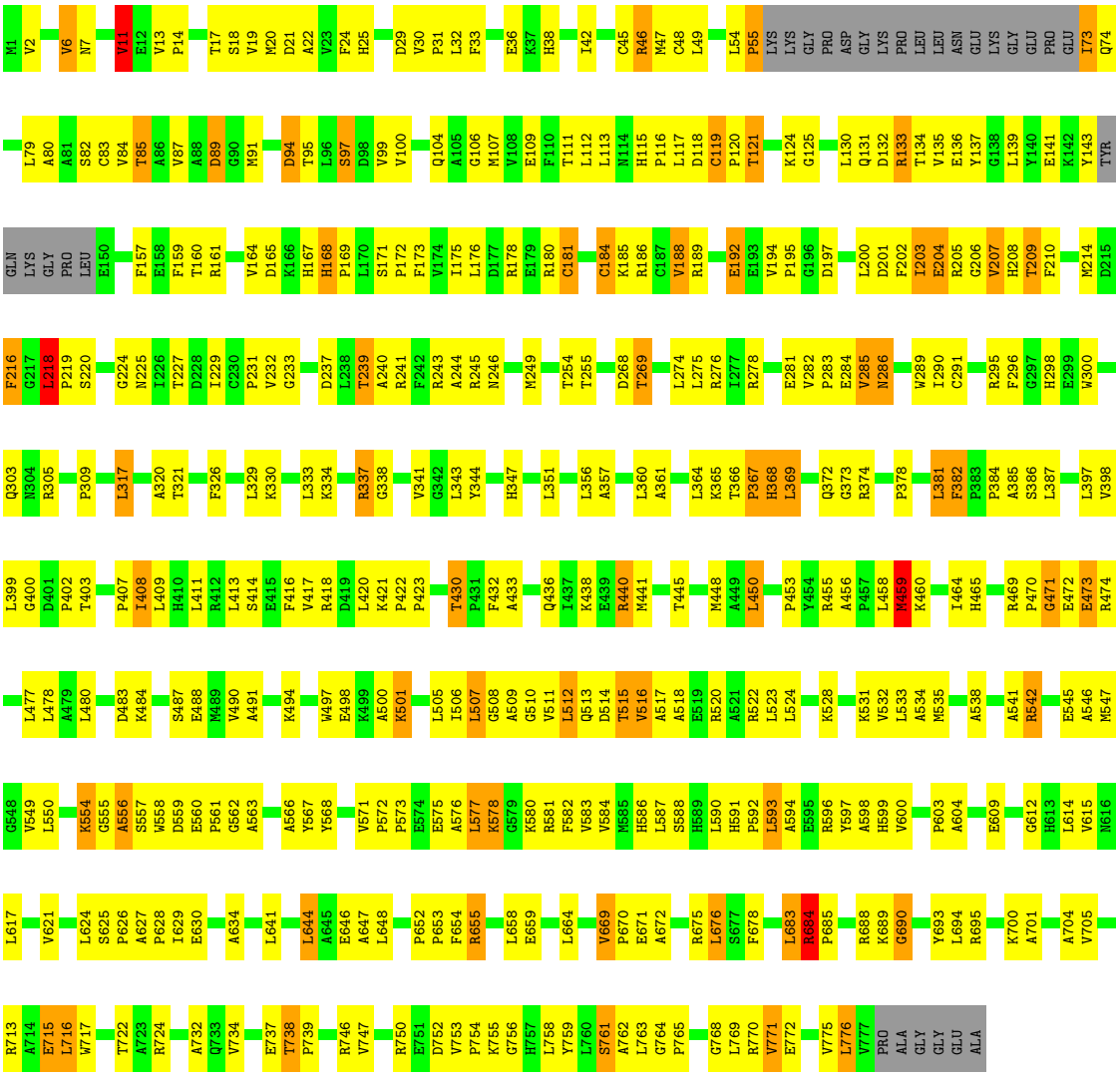
Chain T:



• Molecule 3: NADH-quinone oxidoreductase subunit 3

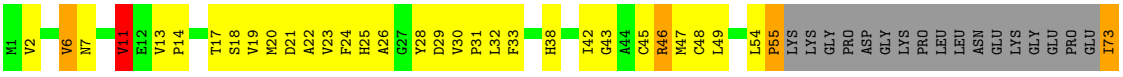
Chain 3:

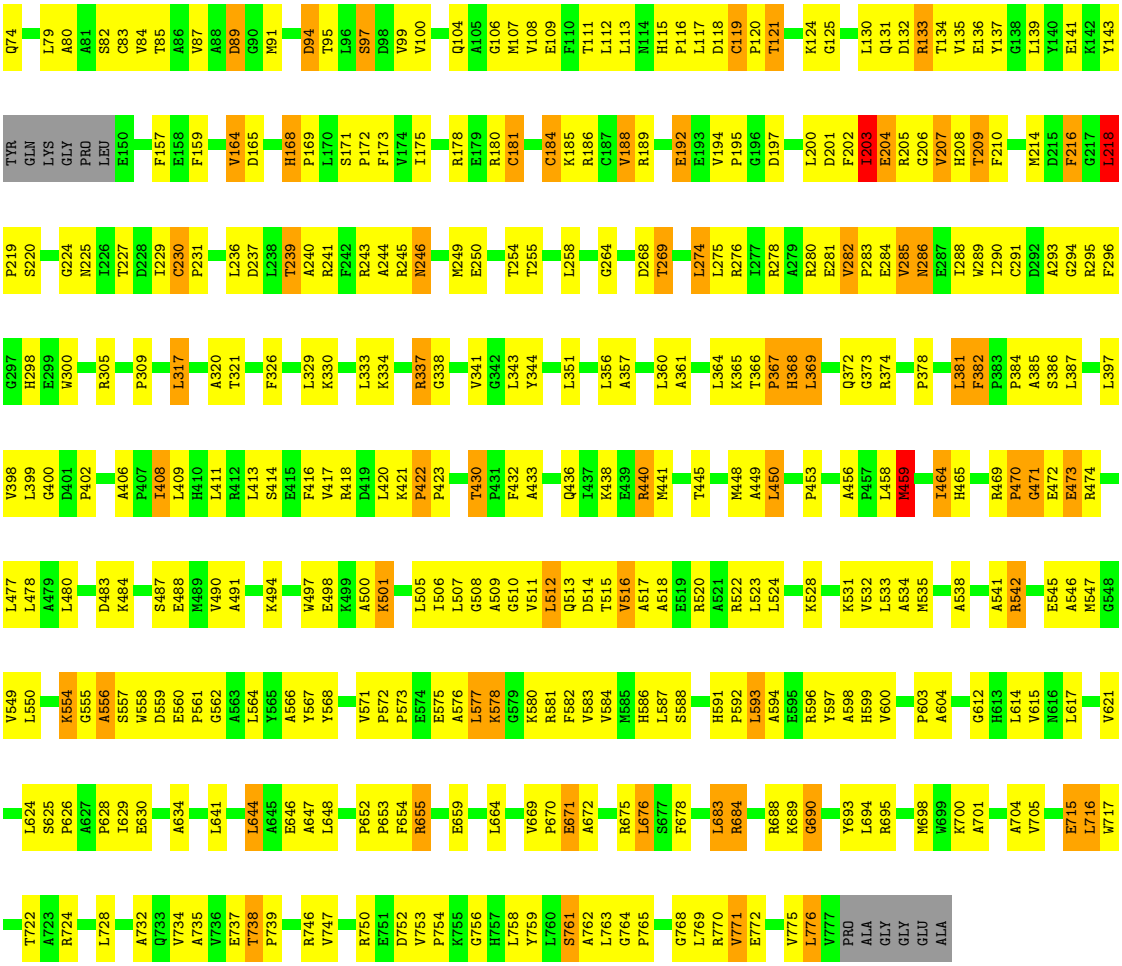




• Molecule 3: NADH-quinone oxidoreductase subunit 3

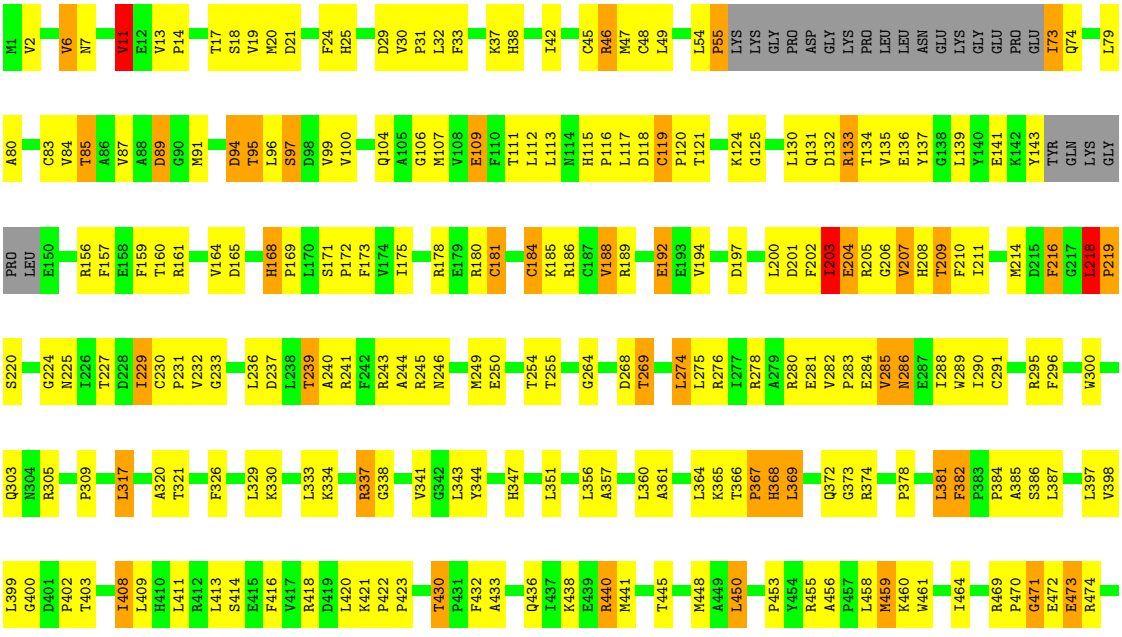
Chain C:

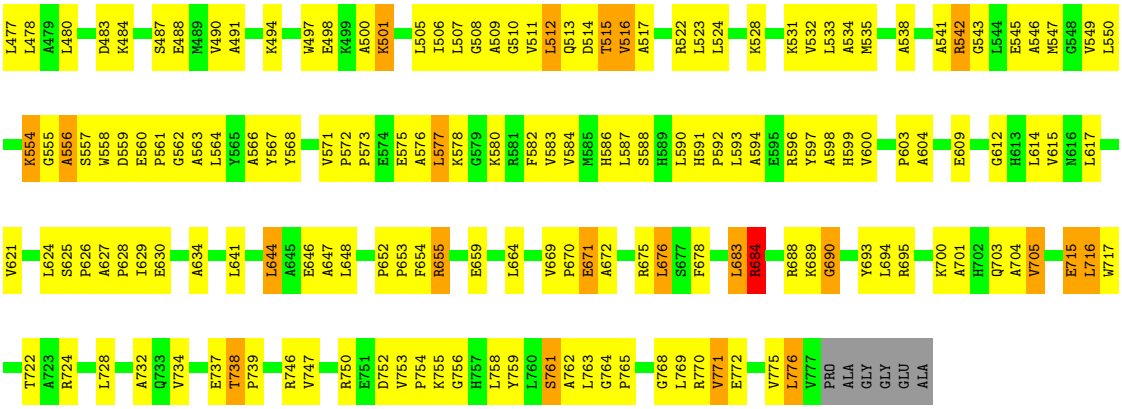




• Molecule 3: NADH-quinone oxidoreductase subunit 3

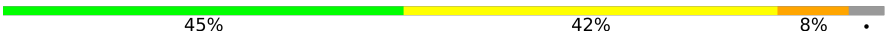
Chain L:

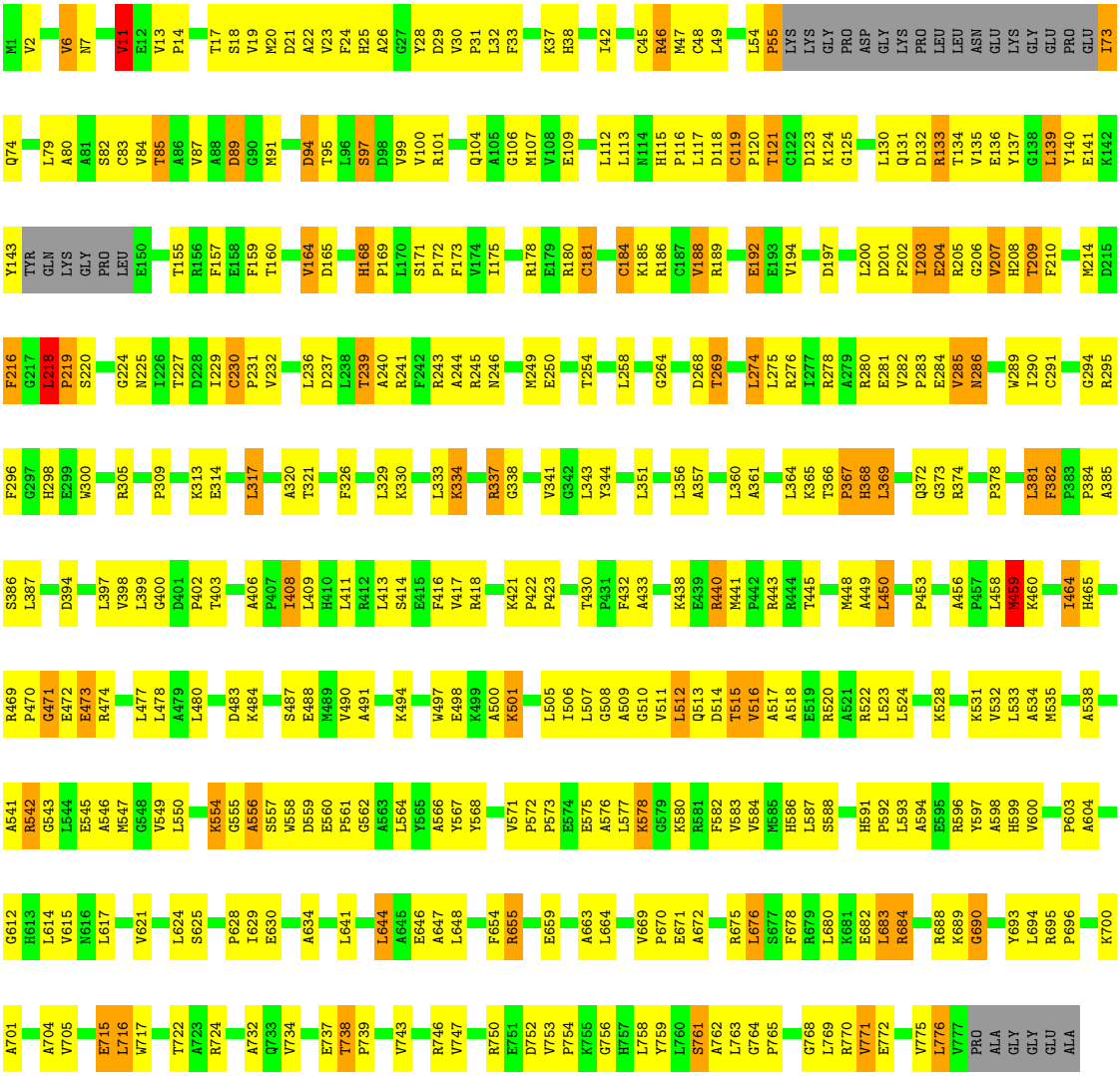




• Molecule 3: NADH-quinone oxidoreductase subunit 3

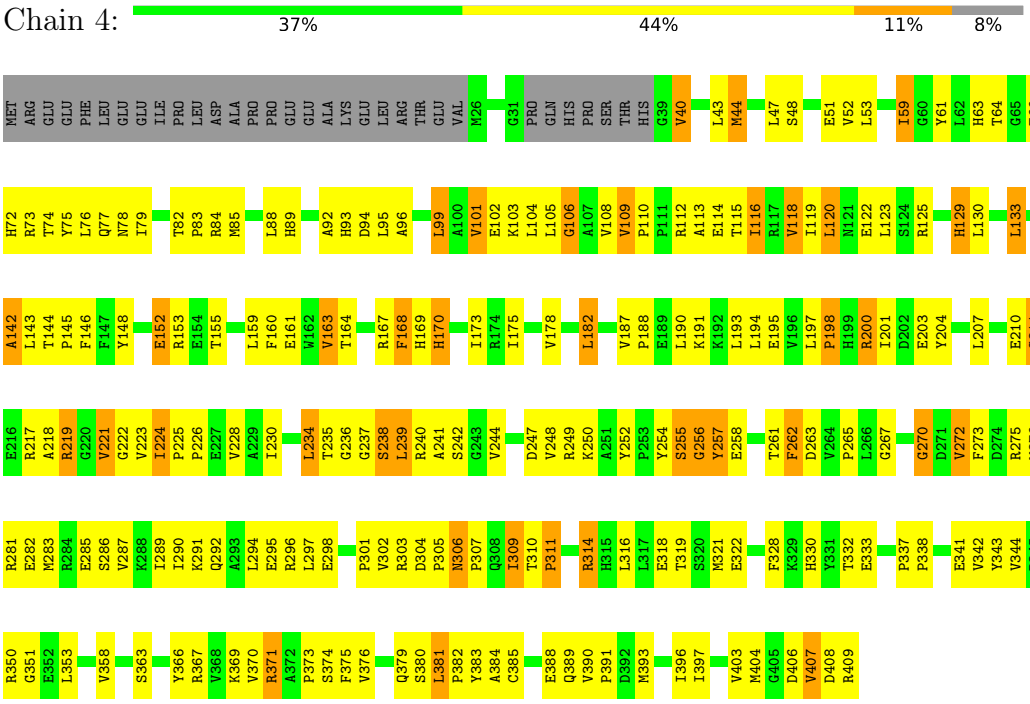
Chain U:





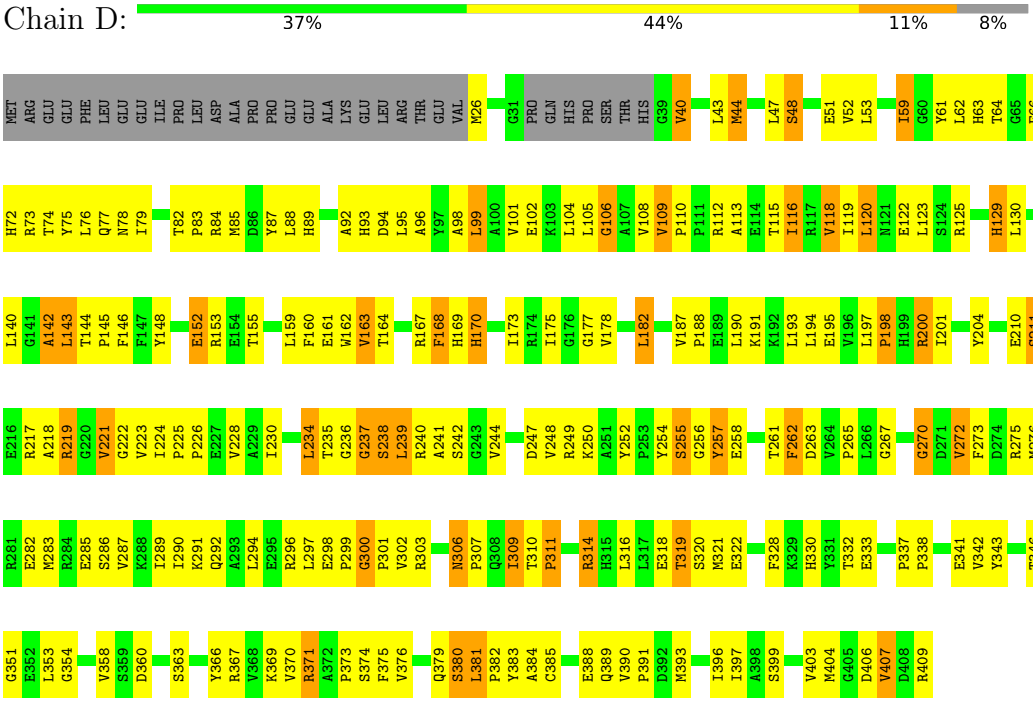
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4:



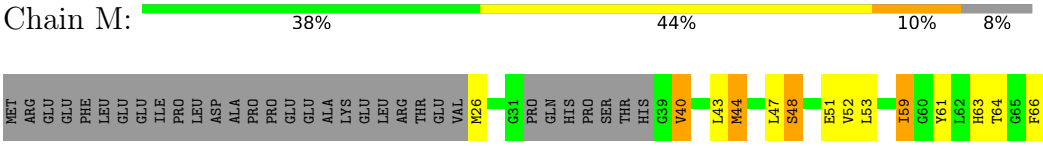
• Molecule 4: NADH-quinone oxidoreductase subunit 4

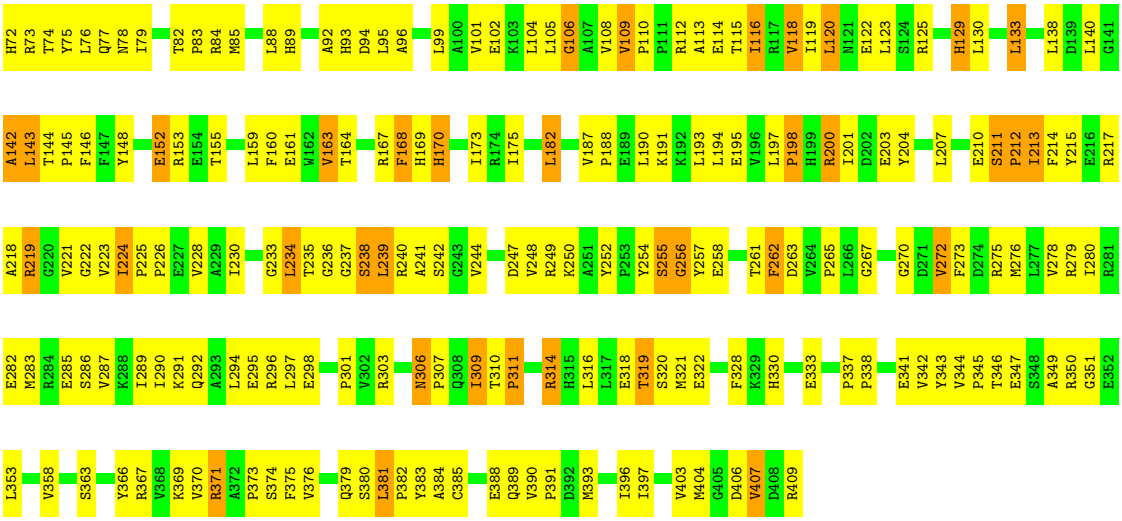
Chain D:



• Molecule 4: NADH-quinone oxidoreductase subunit 4

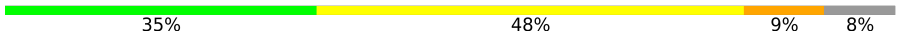
Chain M:

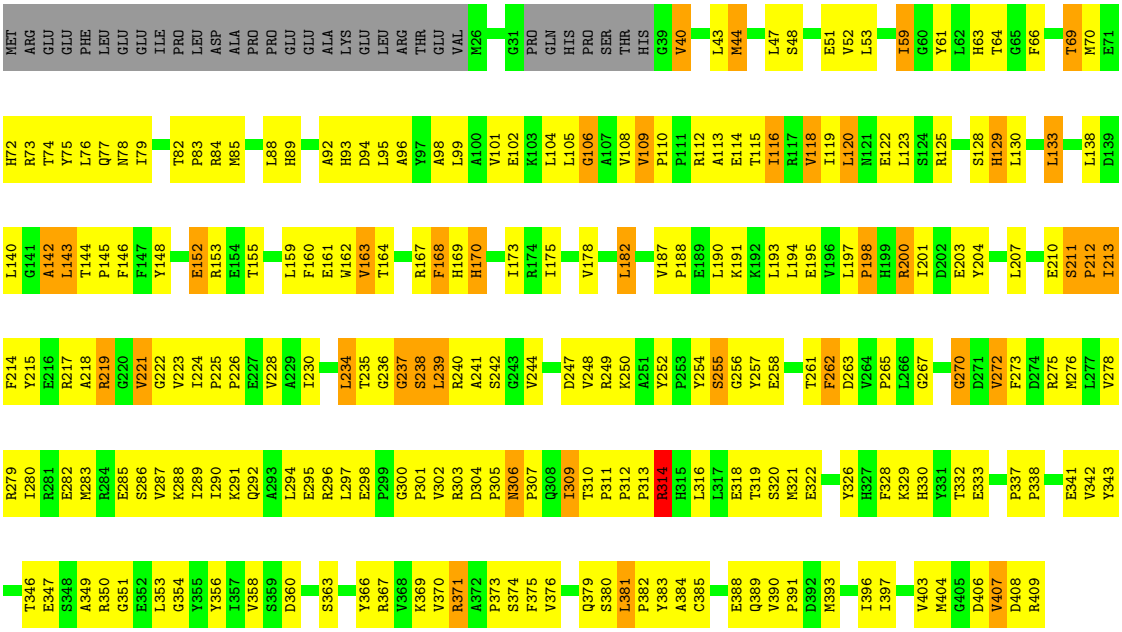




• Molecule 4: NADH-quinone oxidoreductase subunit 4

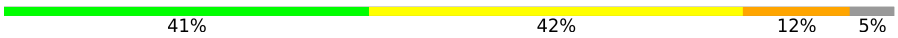
Chain V:

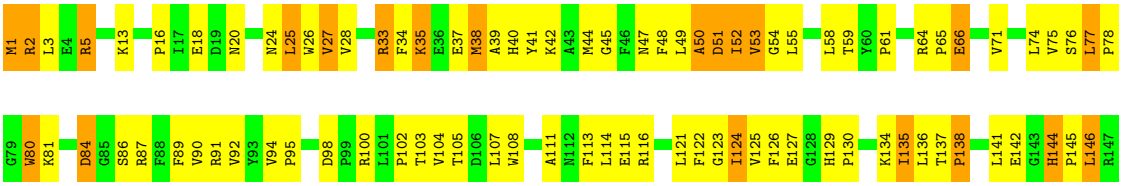


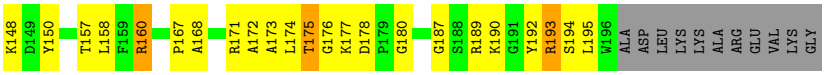


• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5:

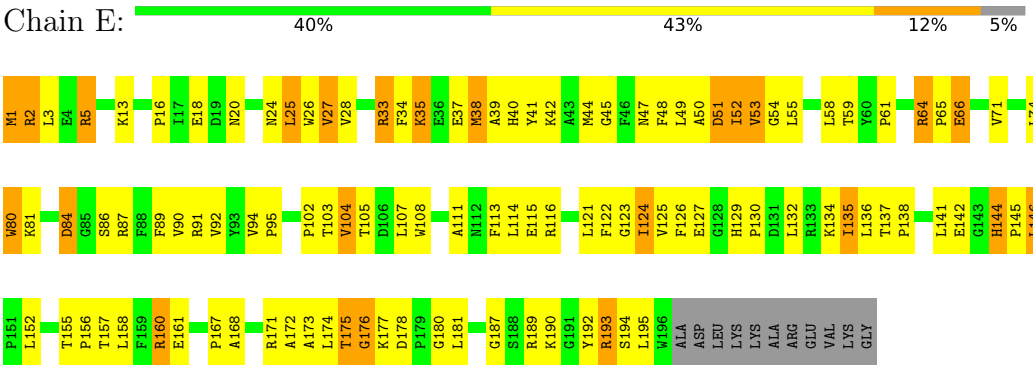






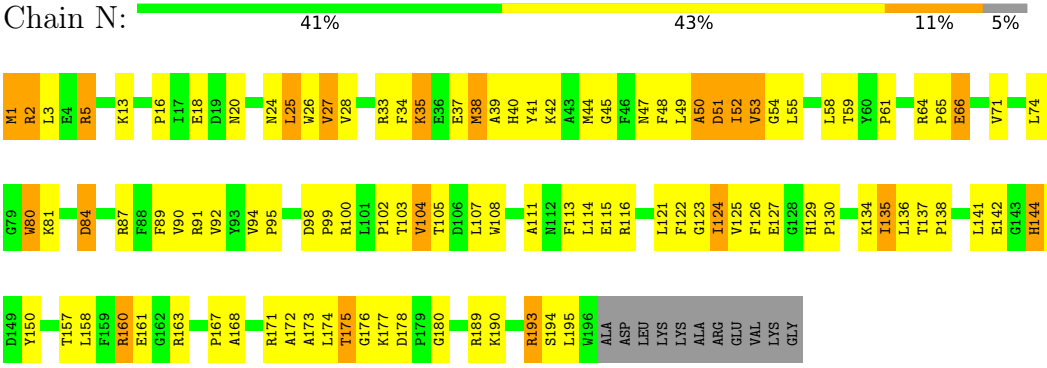
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain E:



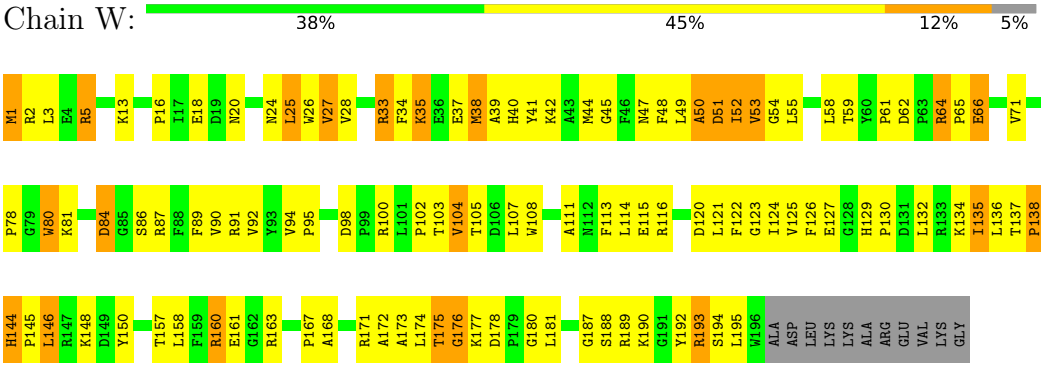
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain N:



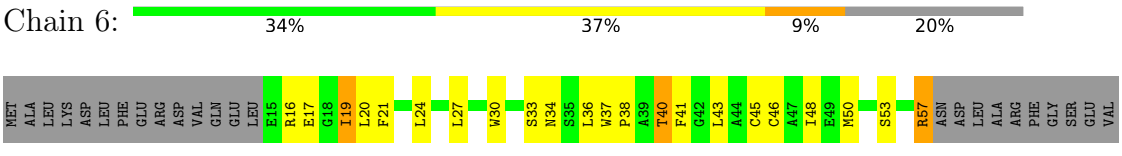
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain W:



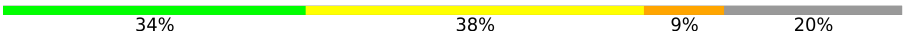
• Molecule 6: NADH-quinone oxidoreductase subunit 6

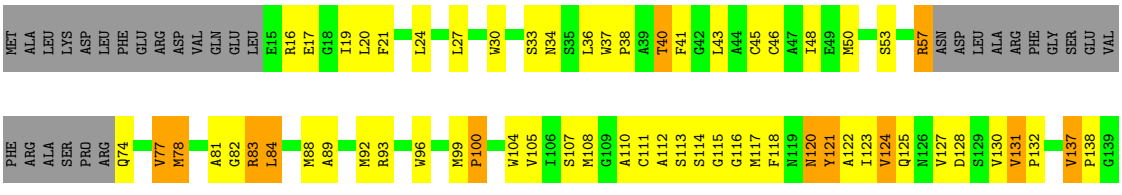
Chain 6:

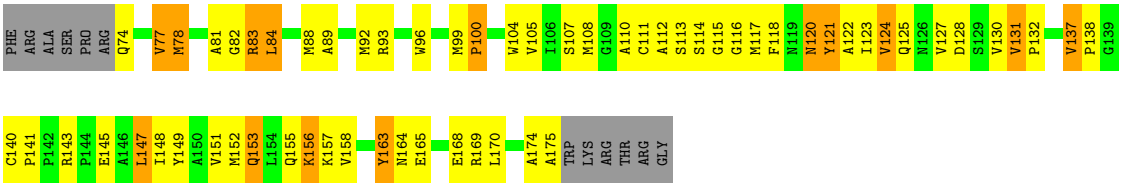


• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain F:

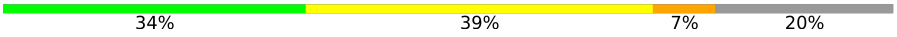


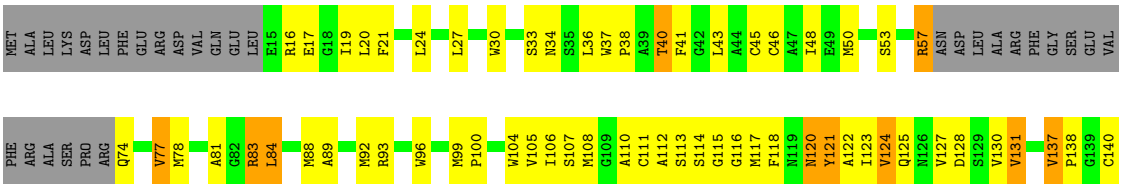


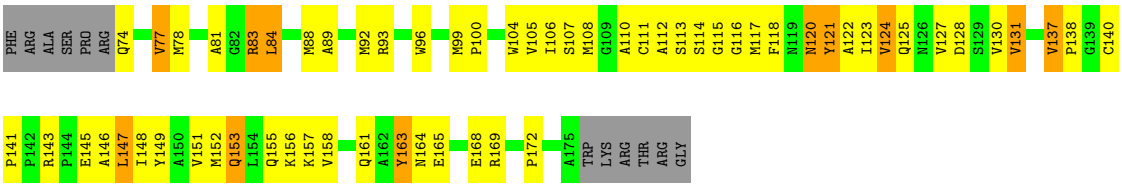


• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain O:

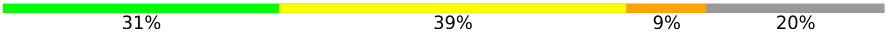


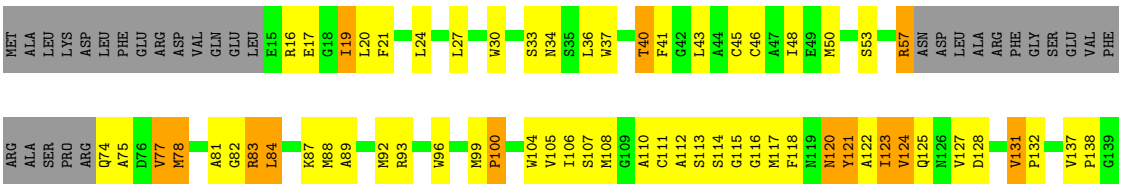


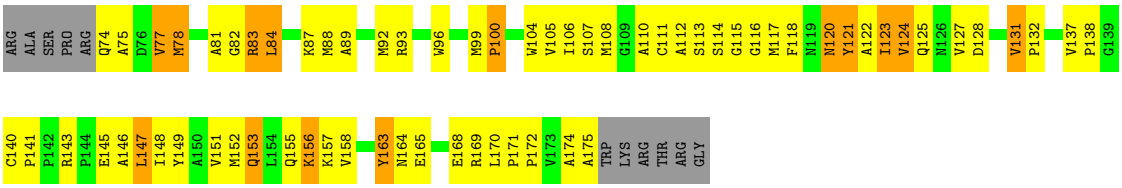


• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain X:

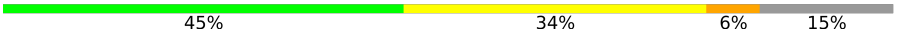


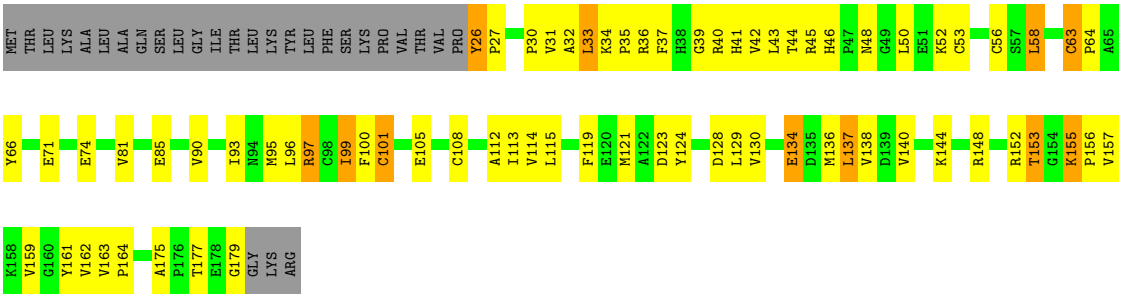




• Molecule 7: NADH-quinone oxidoreductase subunit 9

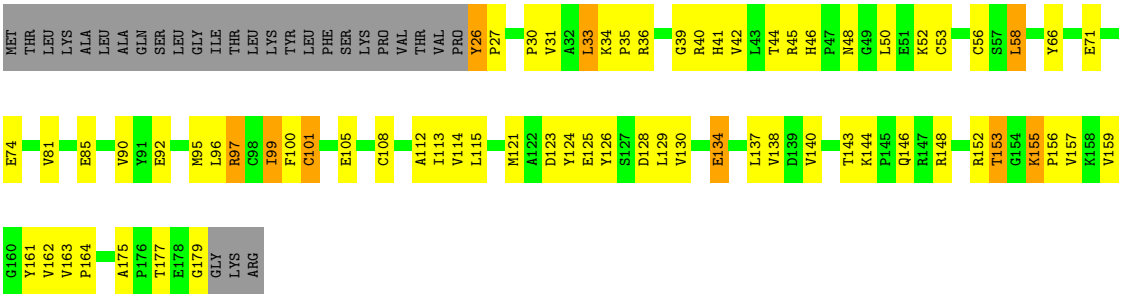
Chain 9:





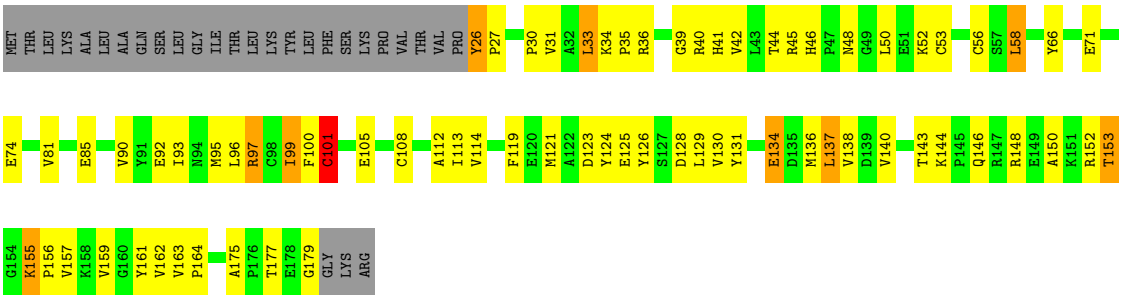
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain G:



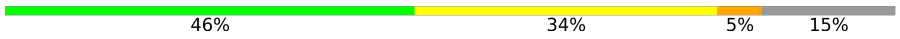
• Molecule 7: NADH-quinone oxidoreductase subunit 9

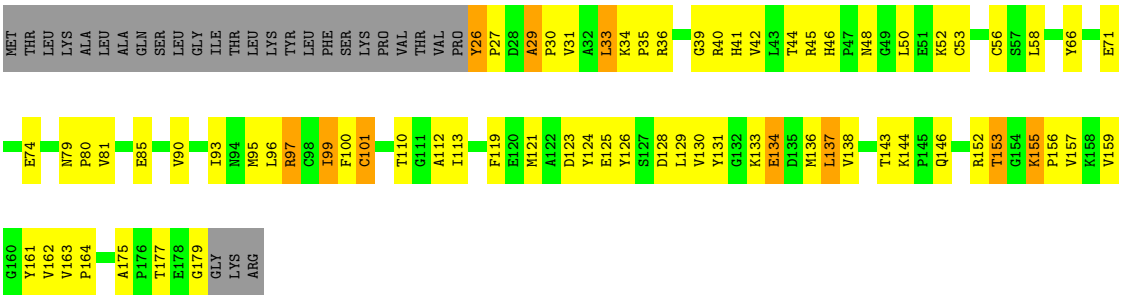
Chain P:



• Molecule 7: NADH-quinone oxidoreductase subunit 9

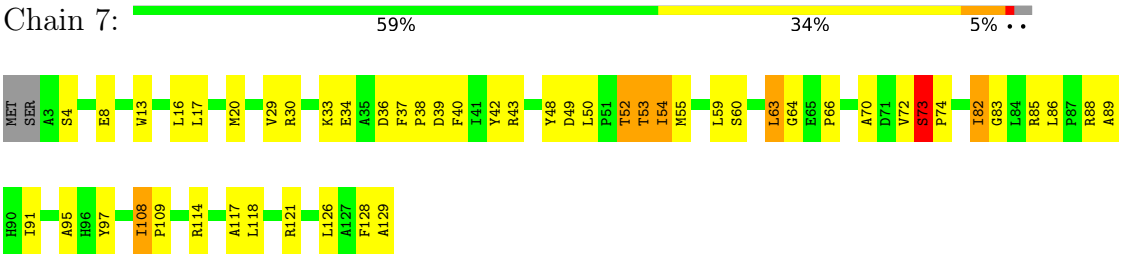
Chain Y:





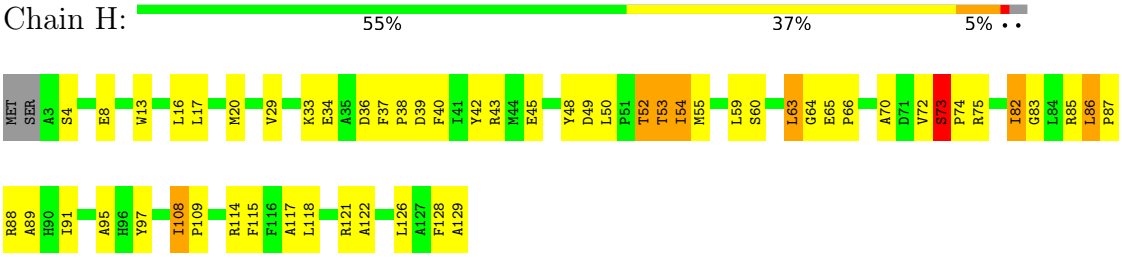
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:



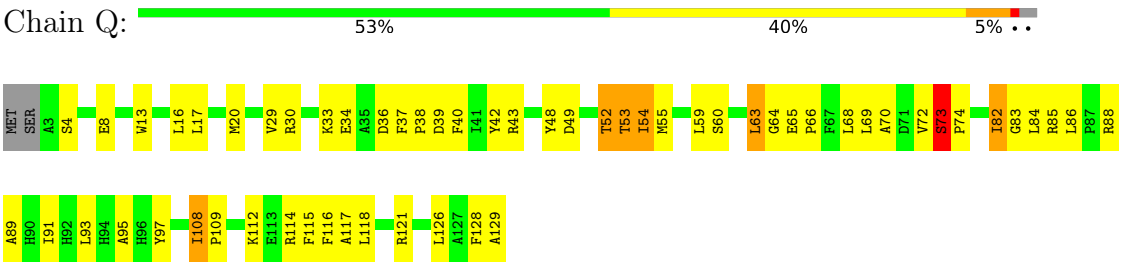
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain H:



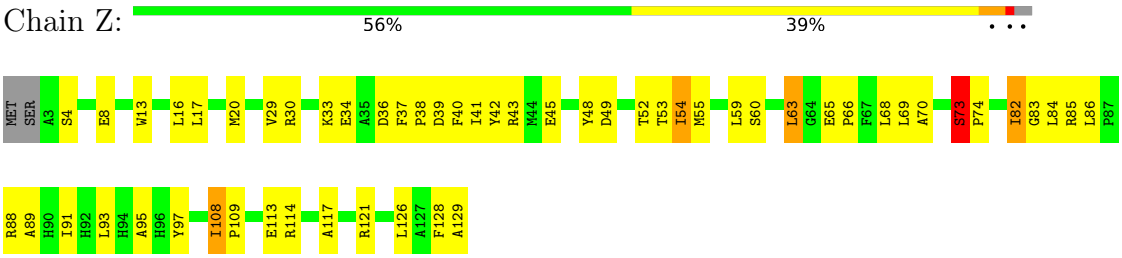
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain Q:



• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.08Å 266.11Å 201.73Å 90.00° 104.71° 90.00°	Depositor
Resolution (Å)	29.98 – 3.15 29.98 – 3.15	Depositor EDS
% Data completeness (in resolution range)	82.5 (29.98-3.15) 82.5 (29.98-3.15)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.237 , 0.270 0.232 , 0.262	Depositor DCC
R_{free} test set	4194 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	75028	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, CA, FES, 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	0.55	0/3506	0.93	6/4745 (0.1%)
1	A	0.51	0/3506	0.94	8/4745 (0.2%)
1	J	0.57	0/3506	0.93	9/4745 (0.2%)
1	S	0.50	0/3506	0.94	6/4745 (0.1%)
2	2	0.55	0/1439	0.97	9/1953 (0.5%)
2	B	0.49	0/1439	0.95	6/1953 (0.3%)
2	K	0.55	0/1439	0.95	11/1953 (0.6%)
2	T	0.52	0/1439	0.95	9/1953 (0.5%)
3	3	0.54	0/6019	0.98	24/8163 (0.3%)
3	C	0.51	0/6019	0.98	27/8163 (0.3%)
3	L	0.50	0/6019	0.97	21/8163 (0.3%)
3	U	0.51	0/6019	0.97	22/8163 (0.3%)
4	4	0.52	0/3089	0.94	12/4197 (0.3%)
4	D	0.52	0/3089	0.94	9/4197 (0.2%)
4	M	0.56	0/3089	0.95	11/4197 (0.3%)
4	V	0.50	0/3089	0.94	8/4197 (0.2%)
5	5	0.50	0/1656	1.00	11/2246 (0.5%)
5	E	0.48	0/1656	1.03	12/2246 (0.5%)
5	N	0.51	0/1656	1.03	13/2246 (0.6%)
5	W	0.46	0/1656	1.01	13/2246 (0.6%)
6	6	0.57	0/1137	1.01	5/1542 (0.3%)
6	F	0.59	0/1137	1.01	5/1542 (0.3%)
6	O	0.55	0/1137	0.99	3/1542 (0.2%)
6	X	0.53	0/1137	0.99	3/1542 (0.2%)
7	9	0.57	0/1224	0.96	4/1663 (0.2%)
7	G	0.57	0/1224	0.97	2/1663 (0.1%)
7	P	0.55	0/1224	0.97	3/1663 (0.2%)
7	Y	0.52	0/1224	0.97	4/1663 (0.2%)
8	7	0.51	0/1059	0.97	5/1429 (0.3%)
8	H	0.50	0/1059	0.96	7/1429 (0.5%)
8	Q	0.51	0/1059	0.96	5/1429 (0.3%)
8	Z	0.48	0/1059	0.94	6/1429 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.52	0/76516	0.96	299/103752 (0.3%)

There are no bond length outliers.

The worst 5 of 299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	184	CYS	N-CA-C	-10.00	98.11	110.41
3	3	184	CYS	N-CA-C	-9.44	98.80	110.41
3	L	184	CYS	N-CA-C	-9.39	98.86	110.41
3	C	430	THR	CA-C-N	9.35	129.11	119.76
3	C	430	THR	C-N-CA	9.35	129.11	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	211	0
1	A	3417	0	3388	217	0
1	J	3417	0	3388	218	0
1	S	3417	0	3388	205	0
2	2	1406	0	1373	75	0
2	B	1406	0	1373	79	0
2	K	1406	0	1373	77	0
2	T	1406	0	1373	79	0
3	3	5880	0	5911	370	0
3	C	5880	0	5911	370	0
3	L	5880	0	5911	373	0
3	U	5880	0	5911	386	0
4	4	3011	0	3000	271	0
4	D	3011	0	3000	288	0
4	M	3011	0	3000	263	0
4	V	3011	0	3000	290	0
5	5	1607	0	1574	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1607	0	1574	122	0
5	N	1607	0	1574	110	0
5	W	1607	0	1574	131	0
6	6	1113	0	1121	111	0
6	F	1113	0	1121	111	0
6	O	1113	0	1121	110	0
6	X	1113	0	1121	116	0
7	9	1193	0	1160	77	0
7	G	1193	0	1160	77	0
7	P	1193	0	1160	77	0
7	Y	1193	0	1160	74	0
8	7	1031	0	1029	50	0
8	H	1031	0	1029	58	0
8	Q	1031	0	1029	55	0
8	Z	1031	0	1029	50	0
9	1	8	0	0	0	0
9	3	24	0	0	3	0
9	6	8	0	0	2	0
9	9	16	0	0	2	0
9	A	8	0	0	1	0
9	C	24	0	0	1	0
9	F	8	0	0	3	0
9	G	16	0	0	2	0
9	J	8	0	0	0	0
9	L	24	0	0	3	0
9	O	8	0	0	2	0
9	P	16	0	0	2	0
9	S	8	0	0	0	0
9	U	24	0	0	2	0
9	X	8	0	0	3	0
9	Y	16	0	0	0	0
10	1	31	0	19	7	0
10	A	31	0	19	6	0
10	J	31	0	19	8	0
10	S	31	0	19	6	0
11	2	4	0	0	1	0
11	3	4	0	0	0	0
11	B	4	0	0	1	0
11	C	4	0	0	1	0
11	K	4	0	0	1	0
11	L	4	0	0	0	0
11	T	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	U	4	0	0	0	0
12	2	1	0	0	0	0
12	3	2	0	0	0	0
12	9	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
12	K	1	0	0	0	0
12	L	2	0	0	0	0
12	P	1	0	0	0	0
12	T	1	0	0	0	0
12	U	1	0	0	0	0
12	Y	1	0	0	0	0
12	Z	1	0	0	0	0
All	All	75028	0	74300	4758	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 32.

The worst 5 of 4758 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:D:188:PRO:HB3	3:U:724:ARG:CD	1.63	1.27
3:C:46:ARG:HG2	3:C:46:ARG:HH11	1.05	1.19
3:C:474:ARG:NH2	3:C:516:VAL:HG21	1.62	1.13
6:X:145:GLU:HG2	7:Y:31:VAL:HG21	1.31	1.11
4:D:188:PRO:CB	3:U:724:ARG:HD2	1.81	1.11

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%)	366 (84%)	59 (14%)	10 (2%)	5 24
1	A	435/438 (99%)	359 (82%)	65 (15%)	11 (2%)	4 22
1	J	435/438 (99%)	363 (83%)	62 (14%)	10 (2%)	5 24
1	S	435/438 (99%)	362 (83%)	62 (14%)	11 (2%)	4 22
2	2	176/181 (97%)	147 (84%)	26 (15%)	3 (2%)	7 30
2	B	176/181 (97%)	145 (82%)	28 (16%)	3 (2%)	7 30
2	K	176/181 (97%)	145 (82%)	29 (16%)	2 (1%)	11 39
2	T	176/181 (97%)	147 (84%)	27 (15%)	2 (1%)	11 39
3	3	748/783 (96%)	628 (84%)	96 (13%)	24 (3%)	3 17
3	C	748/783 (96%)	632 (84%)	93 (12%)	23 (3%)	3 18
3	L	748/783 (96%)	630 (84%)	93 (12%)	25 (3%)	3 17
3	U	748/783 (96%)	633 (85%)	93 (12%)	22 (3%)	3 20
4	4	373/409 (91%)	319 (86%)	44 (12%)	10 (3%)	4 21
4	D	373/409 (91%)	320 (86%)	41 (11%)	12 (3%)	3 17
4	M	373/409 (91%)	319 (86%)	44 (12%)	10 (3%)	4 21
4	V	373/409 (91%)	319 (86%)	42 (11%)	12 (3%)	3 17
5	5	194/207 (94%)	162 (84%)	21 (11%)	11 (6%)	1 9
5	E	194/207 (94%)	160 (82%)	23 (12%)	11 (6%)	1 9
5	N	194/207 (94%)	160 (82%)	23 (12%)	11 (6%)	1 9
5	W	194/207 (94%)	157 (81%)	26 (13%)	11 (6%)	1 9
6	6	141/181 (78%)	121 (86%)	17 (12%)	3 (2%)	5 26
6	F	141/181 (78%)	120 (85%)	18 (13%)	3 (2%)	5 26
6	O	141/181 (78%)	119 (84%)	21 (15%)	1 (1%)	18 49
6	X	141/181 (78%)	120 (85%)	18 (13%)	3 (2%)	5 26
7	9	152/182 (84%)	127 (84%)	23 (15%)	2 (1%)	9 36
7	G	152/182 (84%)	128 (84%)	22 (14%)	2 (1%)	9 36
7	P	152/182 (84%)	128 (84%)	22 (14%)	2 (1%)	9 36
7	Y	152/182 (84%)	130 (86%)	20 (13%)	2 (1%)	9 36
8	7	125/129 (97%)	114 (91%)	11 (9%)	0	100 100
8	H	125/129 (97%)	115 (92%)	10 (8%)	0	100 100
8	Q	125/129 (97%)	115 (92%)	10 (8%)	0	100 100
8	Z	125/129 (97%)	114 (91%)	11 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9376/10040 (93%)	7924 (84%)	1200 (13%)	252 (3%)	4 21

5 of 252 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
1	1	68	ALA
1	1	81	LYS
1	1	160	LYS
1	1	234	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 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%)	318 (90%)	37 (10%)	7 24
1	A	355/356 (100%)	320 (90%)	35 (10%)	7 27
1	J	355/356 (100%)	316 (89%)	39 (11%)	6 23
1	S	355/356 (100%)	318 (90%)	37 (10%)	7 24
2	2	150/152 (99%)	131 (87%)	19 (13%)	4 18
2	B	150/152 (99%)	131 (87%)	19 (13%)	4 18
2	K	150/152 (99%)	131 (87%)	19 (13%)	4 18
2	T	150/152 (99%)	133 (89%)	17 (11%)	5 21
3	3	607/628 (97%)	541 (89%)	66 (11%)	6 23
3	C	607/628 (97%)	541 (89%)	66 (11%)	6 23
3	L	607/628 (97%)	538 (89%)	69 (11%)	5 21
3	U	607/628 (97%)	541 (89%)	66 (11%)	6 23
4	4	325/355 (92%)	288 (89%)	37 (11%)	5 21
4	D	325/355 (92%)	288 (89%)	37 (11%)	5 21
4	M	325/355 (92%)	288 (89%)	37 (11%)	5 21
4	V	325/355 (92%)	288 (89%)	37 (11%)	5 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	5	167/175 (95%)	147 (88%)	20 (12%)	5 20
5	E	167/175 (95%)	146 (87%)	21 (13%)	4 18
5	N	167/175 (95%)	147 (88%)	20 (12%)	5 20
5	W	167/175 (95%)	147 (88%)	20 (12%)	5 20
6	6	118/149 (79%)	103 (87%)	15 (13%)	4 18
6	F	118/149 (79%)	102 (86%)	16 (14%)	3 16
6	O	118/149 (79%)	103 (87%)	15 (13%)	4 18
6	X	118/149 (79%)	101 (86%)	17 (14%)	3 14
7	9	126/150 (84%)	111 (88%)	15 (12%)	5 20
7	G	126/150 (84%)	112 (89%)	14 (11%)	6 22
7	P	126/150 (84%)	111 (88%)	15 (12%)	5 20
7	Y	126/150 (84%)	112 (89%)	14 (11%)	6 22
8	7	104/106 (98%)	96 (92%)	8 (8%)	12 37
8	H	104/106 (98%)	96 (92%)	8 (8%)	12 37
8	Q	104/106 (98%)	96 (92%)	8 (8%)	12 37
8	Z	104/106 (98%)	97 (93%)	7 (7%)	15 42
All	All	7808/8284 (94%)	6938 (89%)	870 (11%)	6 22

5 of 870 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	363	VAL
4	M	143	LEU
4	V	239	LEU
2	K	45	ARG
1	J	346	ARG

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

Mol	Chain	Res	Type
6	O	155	GLN
4	V	169	HIS
1	S	86	GLN
3	U	428	HIS
5	W	129	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 16 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
11	FES	K	182	2	0,4,4	-	-	-		
9	SF4	9	183	7	0,12,12	-	-	-		
9	SF4	9	184	7	0,12,12	-	-	-		
10	FMN	S	440	-	33,33,33	1.19	3 (9%)	48,50,50	1.94	14 (29%)
11	FES	2	182	2	0,4,4	-	-	-		
9	SF4	F	182	6	0,12,12	-	-	-		
9	SF4	L	786	3	0,12,12	-	-	-		
11	FES	C	787	3	0,4,4	-	-	-		
9	SF4	J	439	1	0,12,12	-	-	-		
11	FES	U	787	3	0,4,4	-	-	-		
9	SF4	L	784	3	0,12,12	-	-	-		
9	SF4	U	785	3	0,12,12	-	-	-		
9	SF4	U	786	3	0,12,12	-	-	-		
9	SF4	P	183	7	0,12,12	-	-	-		
9	SF4	P	184	7	0,12,12	-	-	-		
9	SF4	3	785	3	0,12,12	-	-	-		
9	SF4	A	439	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SF4	L	785	3	0,12,12	-	-	-		
9	SF4	3	784	3	0,12,12	-	-	-		
11	FES	B	182	2	0,4,4	-	-	-		
11	FES	3	787	3	0,4,4	-	-	-		
11	FES	L	787	3	0,4,4	-	-	-		
9	SF4	X	182	6	0,12,12	-	-	-		
9	SF4	6	182	6	0,12,12	-	-	-		
9	SF4	U	784	3	0,12,12	-	-	-		
9	SF4	C	786	3	0,12,12	-	-	-		
9	SF4	G	183	7	0,12,12	-	-	-		
9	SF4	C	784	3	0,12,12	-	-	-		
10	FMN	1	440	-	33,33,33	1.23	3 (9%)	48,50,50	2.07	13 (27%)
9	SF4	3	786	3	0,12,12	-	-	-		
9	SF4	O	182	6	0,12,12	-	-	-		
9	SF4	G	184	7	0,12,12	-	-	-		
9	SF4	Y	184	7	0,12,12	-	-	-		
10	FMN	A	440	-	33,33,33	1.25	4 (12%)	48,50,50	1.81	11 (22%)
9	SF4	C	785	3	0,12,12	-	-	-		
9	SF4	1	439	1	0,12,12	-	-	-		
9	SF4	S	439	1	0,12,12	-	-	-		
11	FES	T	182	2	0,4,4	-	-	-		
10	FMN	J	440	-	33,33,33	1.24	3 (9%)	48,50,50	1.73	11 (22%)
9	SF4	Y	183	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
11	FES	K	182	2	-	-	0/1/1/1
9	SF4	9	183	7	-	-	0/6/5/5
9	SF4	9	184	7	-	-	0/6/5/5
10	FMN	S	440	-	-	2/18/18/18	0/3/3/3
11	FES	2	182	2	-	-	0/1/1/1
9	SF4	F	182	6	-	-	0/6/5/5
9	SF4	L	786	3	-	-	0/6/5/5
11	FES	C	787	3	-	-	0/1/1/1
9	SF4	J	439	1	-	-	0/6/5/5
11	FES	U	787	3	-	-	0/1/1/1
9	SF4	L	784	3	-	-	0/6/5/5
9	SF4	U	785	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	U	786	3	-	-	0/6/5/5
9	SF4	P	183	7	-	-	0/6/5/5
9	SF4	P	184	7	-	-	0/6/5/5
9	SF4	3	785	3	-	-	0/6/5/5
9	SF4	A	439	1	-	-	0/6/5/5
9	SF4	3	784	3	-	-	0/6/5/5
9	SF4	L	785	3	-	-	0/6/5/5
11	FES	B	182	2	-	-	0/1/1/1
11	FES	3	787	3	-	-	0/1/1/1
11	FES	L	787	3	-	-	0/1/1/1
9	SF4	X	182	6	-	-	0/6/5/5
9	SF4	6	182	6	-	-	0/6/5/5
9	SF4	U	784	3	-	-	0/6/5/5
9	SF4	C	786	3	-	-	0/6/5/5
9	SF4	G	183	7	-	-	0/6/5/5
9	SF4	C	784	3	-	-	0/6/5/5
10	FMN	1	440	-	-	6/18/18/18	0/3/3/3
9	SF4	3	786	3	-	-	0/6/5/5
9	SF4	O	182	6	-	-	0/6/5/5
9	SF4	G	184	7	-	-	0/6/5/5
10	FMN	A	440	-	-	7/18/18/18	0/3/3/3
9	SF4	Y	184	7	-	-	0/6/5/5
9	SF4	C	785	3	-	-	0/6/5/5
9	SF4	1	439	1	-	-	0/6/5/5
9	SF4	S	439	1	-	-	0/6/5/5
11	FES	T	182	2	-	-	0/1/1/1
10	FMN	J	440	-	-	5/18/18/18	0/3/3/3
9	SF4	Y	183	7	-	-	0/6/5/5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	440	FMN	C4A-N5	4.15	1.39	1.30
10	1	440	FMN	C4A-N5	3.95	1.39	1.30
10	S	440	FMN	C4A-N5	3.84	1.39	1.30
10	J	440	FMN	C4A-N5	3.69	1.38	1.30
10	A	440	FMN	C10-N1	2.73	1.38	1.33

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	1	440	FMN	C5'-C4'-C3'	-8.32	96.52	112.22
10	S	440	FMN	C5'-C4'-C3'	-6.77	99.44	112.22
10	A	440	FMN	C1'-C2'-C3'	-6.27	92.66	109.66
10	J	440	FMN	C1'-C2'-C3'	-5.90	93.67	109.66
10	A	440	FMN	C5'-C4'-C3'	-5.25	102.32	112.22

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1	440	FMN	N10-C1'-C2'-O2'
10	1	440	FMN	N10-C1'-C2'-C3'
10	1	440	FMN	C1'-C2'-C3'-O3'
10	1	440	FMN	C1'-C2'-C3'-C4'
10	A	440	FMN	N10-C1'-C2'-O2'

There are no ring outliers.

29 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	182	FES	1	0
9	9	183	SF4	1	0
9	9	184	SF4	1	0
10	S	440	FMN	6	0
11	2	182	FES	1	0
9	F	182	SF4	3	0
9	L	786	SF4	1	0
11	C	787	FES	1	0
9	L	784	SF4	1	0
9	U	785	SF4	1	0
9	P	183	SF4	1	0
9	P	184	SF4	1	0
9	3	785	SF4	1	0
9	A	439	SF4	1	0
9	L	785	SF4	1	0
9	3	784	SF4	1	0
11	B	182	FES	1	0
9	X	182	SF4	3	0
9	6	182	SF4	2	0
9	U	784	SF4	1	0
9	G	183	SF4	1	0
10	1	440	FMN	7	0

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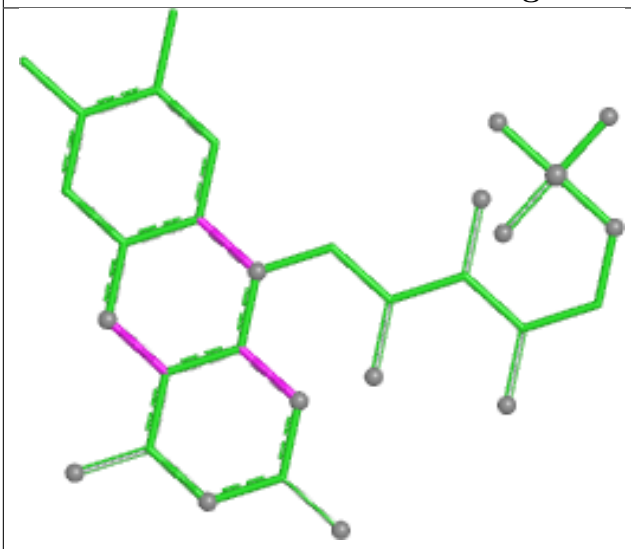
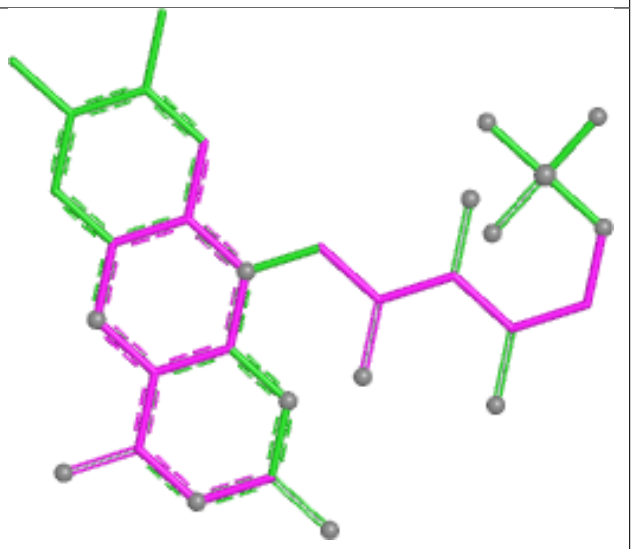
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	3	786	SF4	1	0
9	O	182	SF4	2	0
9	G	184	SF4	1	0
10	A	440	FMN	6	0
9	C	785	SF4	1	0
11	T	182	FES	1	0
10	J	440	FMN	8	0

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.

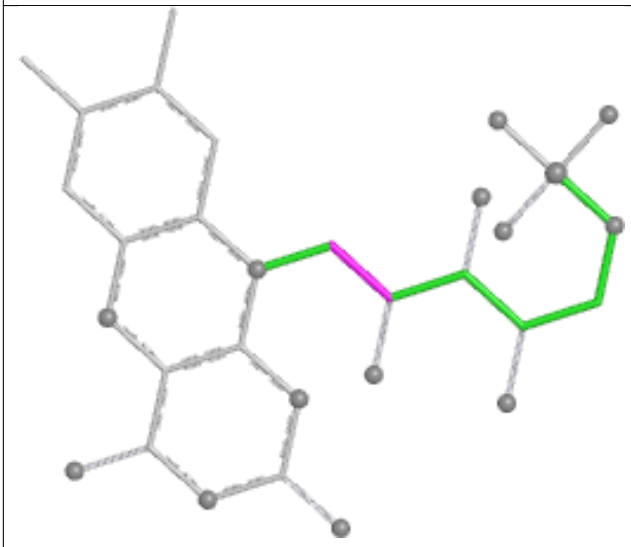
Ligand FMN S 440



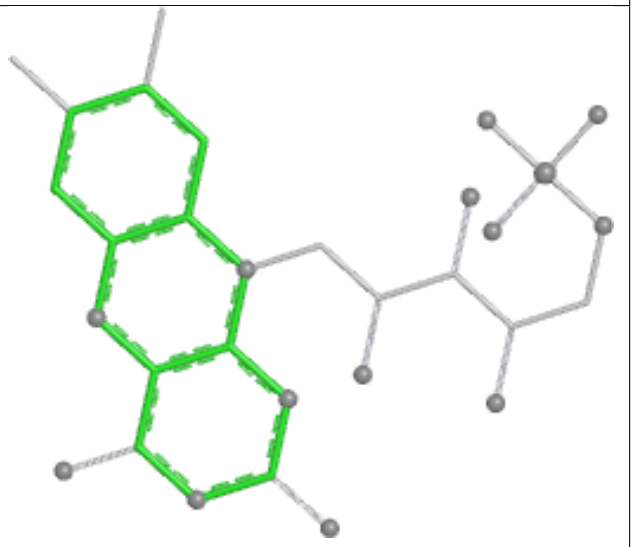
Bond lengths



Bond angles

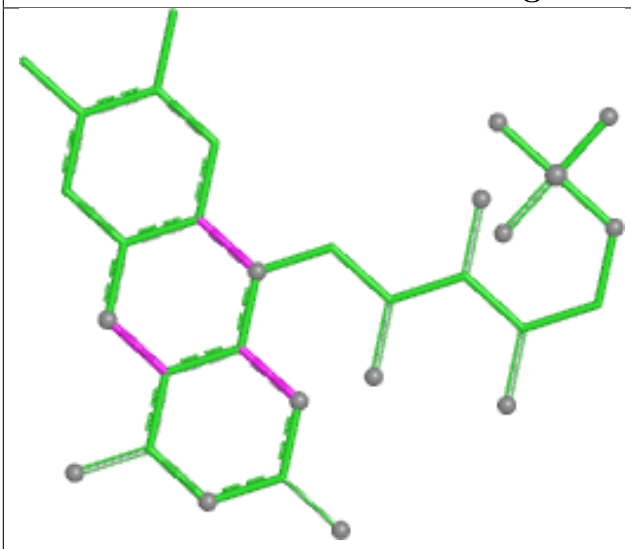


Torsions

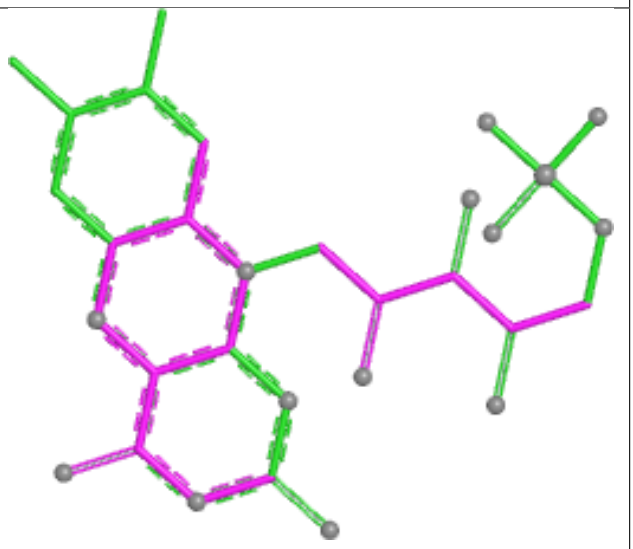


Rings

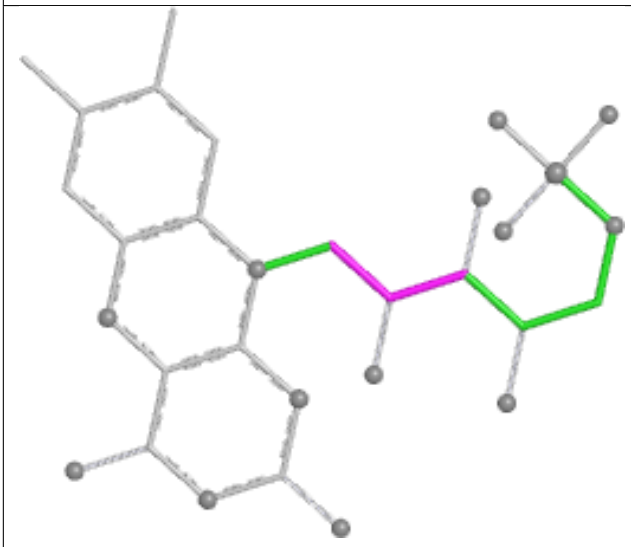
Ligand FMN 1 440



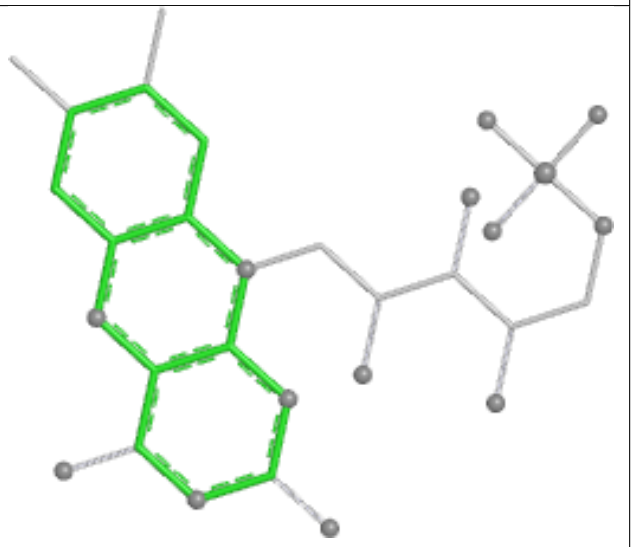
Bond lengths



Bond angles

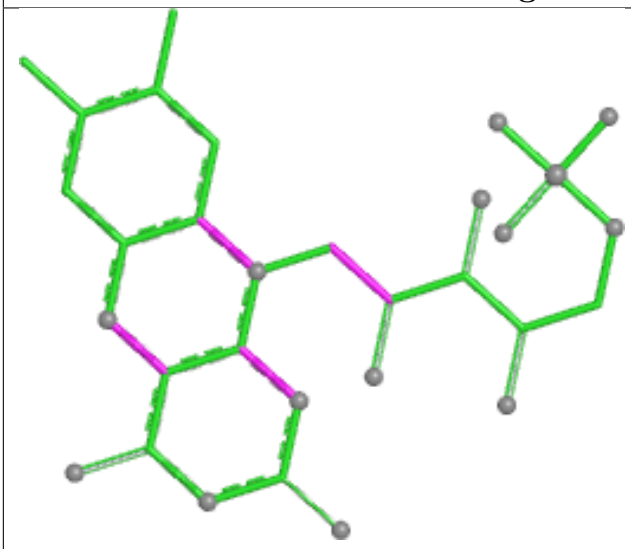


Torsions

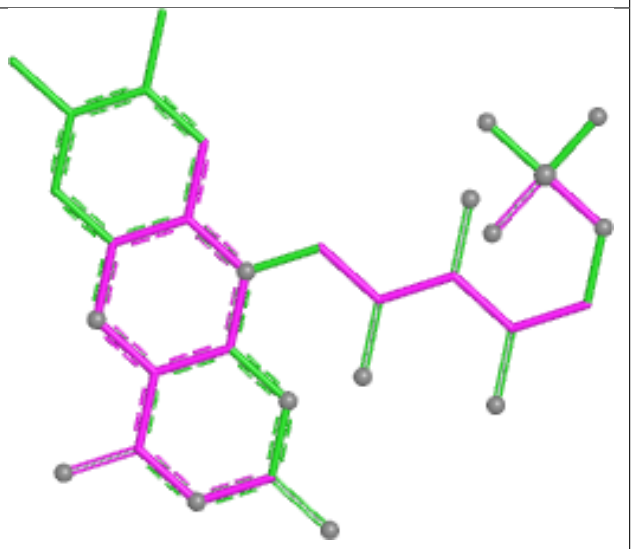


Rings

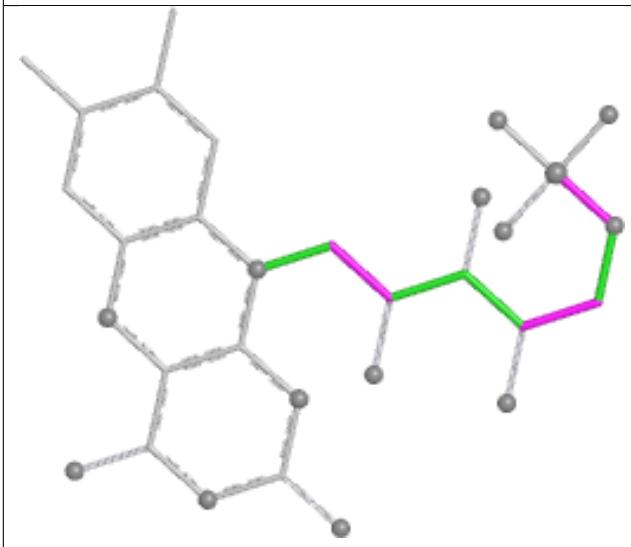
Ligand FMN A 440



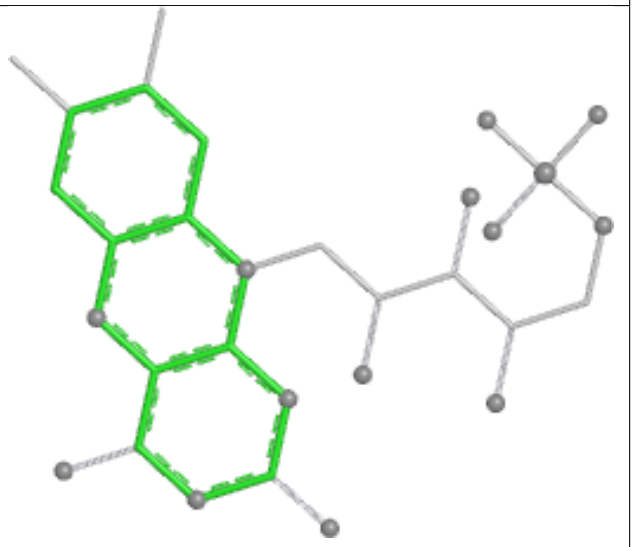
Bond lengths



Bond angles

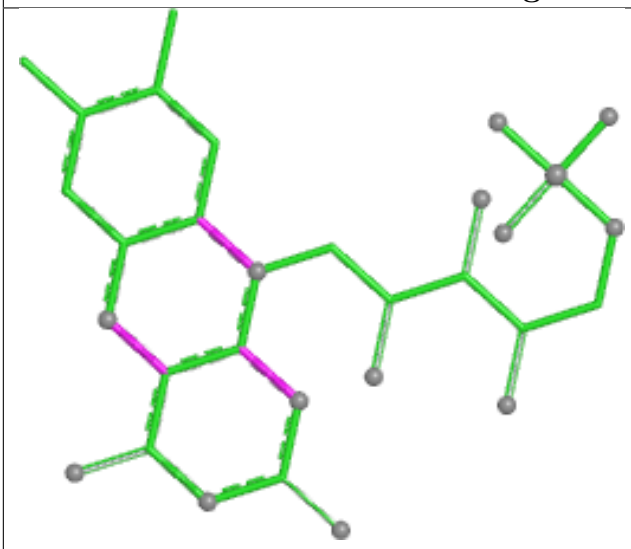


Torsions

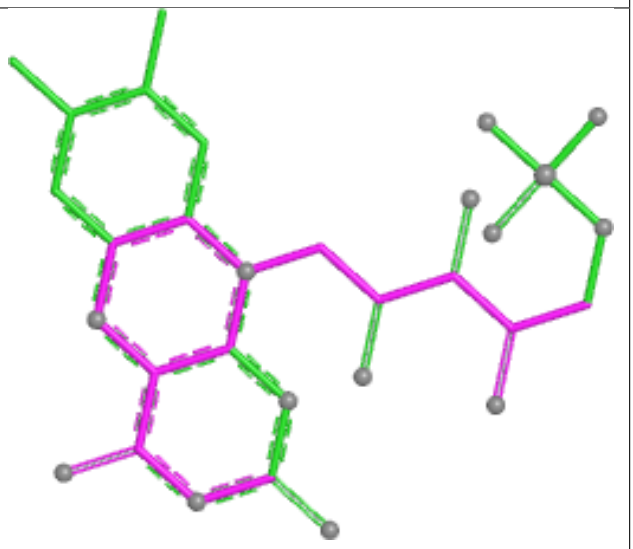


Rings

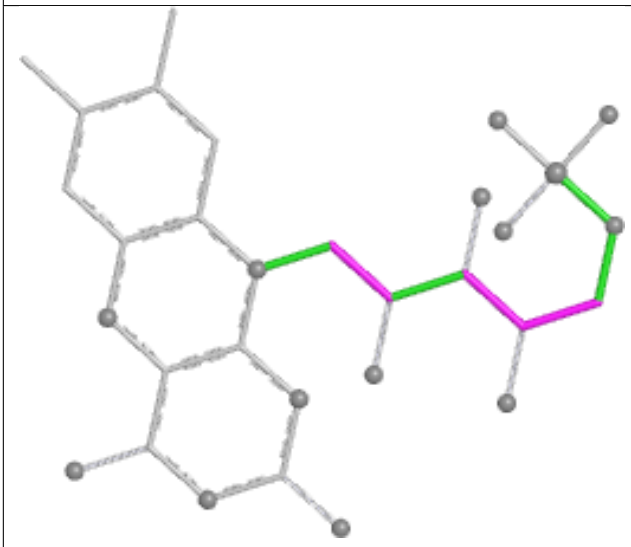
Ligand FMN J 440



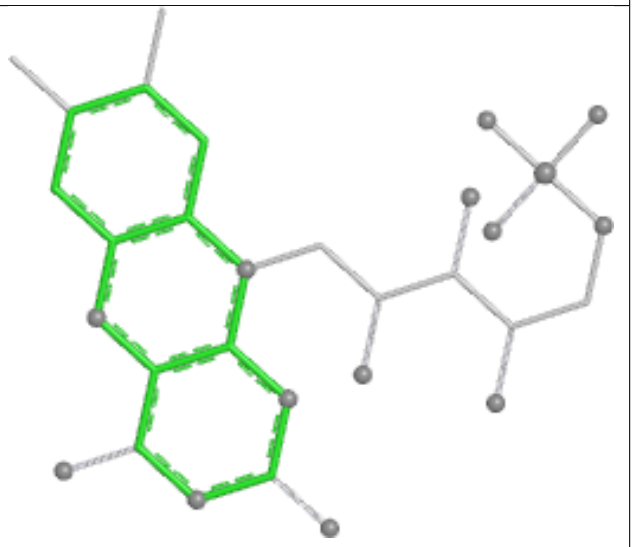
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1	437/438 (99%)	-1.75	0	100	100	38, 59, 83, 110	0
1	A	437/438 (99%)	-1.73	0	100	100	40, 60, 84, 110	0
1	J	437/438 (99%)	-1.73	0	100	100	39, 59, 83, 110	0
1	S	437/438 (99%)	-1.77	0	100	100	39, 60, 83, 111	0
2	2	178/181 (98%)	-1.74	0	100	100	43, 63, 93, 135	0
2	B	178/181 (98%)	-1.70	0	100	100	43, 64, 94, 134	0
2	K	178/181 (98%)	-1.73	0	100	100	43, 63, 93, 136	0
2	T	178/181 (98%)	-1.75	0	100	100	43, 64, 94, 134	0
3	3	754/783 (96%)	-1.71	0	100	100	36, 74, 112, 133	0
3	C	754/783 (96%)	-1.72	0	100	100	36, 75, 113, 134	0
3	L	754/783 (96%)	-1.69	0	100	100	37, 75, 114, 133	0
3	U	754/783 (96%)	-1.72	0	100	100	36, 75, 113, 134	0
4	4	377/409 (92%)	-1.68	0	100	100	38, 78, 112, 129	0
4	D	377/409 (92%)	-1.72	0	100	100	38, 77, 112, 129	0
4	M	377/409 (92%)	-1.68	0	100	100	38, 78, 112, 129	0
4	V	377/409 (92%)	-1.67	0	100	100	39, 78, 112, 130	0
5	5	196/207 (94%)	-1.66	0	100	100	50, 83, 120, 132	0
5	E	196/207 (94%)	-1.67	0	100	100	51, 83, 120, 132	0
5	N	196/207 (94%)	-1.68	0	100	100	50, 83, 120, 132	0
5	W	196/207 (94%)	-1.61	0	100	100	52, 84, 120, 133	0
6	6	145/181 (80%)	-1.69	0	100	100	51, 71, 104, 125	0
6	F	145/181 (80%)	-1.64	0	100	100	49, 71, 105, 125	0
6	O	145/181 (80%)	-1.62	0	100	100	50, 71, 105, 125	0
6	X	145/181 (80%)	-1.61	0	100	100	51, 72, 105, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
7	9	154/182 (84%)	-1.78	0	100	100	37, 59, 96, 136	0
7	G	154/182 (84%)	-1.74	0	100	100	37, 58, 95, 135	0
7	P	154/182 (84%)	-1.79	0	100	100	37, 59, 95, 136	0
7	Y	154/182 (84%)	-1.72	0	100	100	37, 60, 96, 136	0
8	7	127/129 (98%)	-1.79	0	100	100	49, 66, 101, 119	0
8	H	127/129 (98%)	-1.78	0	100	100	48, 66, 101, 120	0
8	Q	127/129 (98%)	-1.76	0	100	100	48, 66, 102, 120	0
8	Z	127/129 (98%)	-1.77	0	100	100	48, 67, 101, 119	0
All	All	9472/10040 (94%)	-1.71	0	100	100	36, 69, 111, 136	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CA	T	202	1/1	0.97	0.03	100,100,100,100	0
12	CA	B	202	1/1	0.98	0.02	108,108,108,108	0
10	FMN	A	440	31/31	0.99	0.04	48,60,64,66	0
10	FMN	J	440	31/31	0.99	0.04	42,53,60,63	0
9	SF4	6	182	8/8	1.00	0.01	24,37,69,69	0
9	SF4	9	183	8/8	1.00	0.01	12,19,45,48	0
9	SF4	9	184	8/8	1.00	0.01	7,27,44,48	0
9	SF4	A	439	8/8	1.00	0.01	13,26,49,50	0
9	SF4	C	784	8/8	1.00	0.01	13,18,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SF4	C	785	8/8	1.00	0.01	12,22,39,40	0
9	SF4	C	786	8/8	1.00	0.01	21,34,56,59	0
9	SF4	F	182	8/8	1.00	0.01	18,31,51,62	0
9	SF4	G	183	8/8	1.00	0.01	11,18,42,46	0
9	SF4	G	184	8/8	1.00	0.01	12,15,39,39	0
9	SF4	J	439	8/8	1.00	0.01	8,25,43,44	0
9	SF4	L	784	8/8	1.00	0.01	11,17,34,42	0
9	SF4	L	785	8/8	1.00	0.02	11,18,39,39	0
9	SF4	L	786	8/8	1.00	0.01	30,39,61,62	0
9	SF4	O	182	8/8	1.00	0.01	18,27,54,59	0
9	SF4	P	183	8/8	1.00	0.01	10,16,42,46	0
9	SF4	P	184	8/8	1.00	0.02	1,19,41,41	0
9	SF4	S	439	8/8	1.00	0.01	19,27,49,51	0
9	SF4	U	784	8/8	1.00	0.01	15,26,43,43	0
9	SF4	U	785	8/8	1.00	0.02	19,27,43,43	0
9	SF4	U	786	8/8	1.00	0.01	21,33,51,58	0
9	SF4	X	182	8/8	1.00	0.01	39,56,81,89	0
9	SF4	Y	183	8/8	1.00	0.01	17,35,53,57	0
9	SF4	Y	184	8/8	1.00	0.01	19,29,51,57	0
10	FMN	1	440	31/31	1.00	0.03	48,54,62,68	0
9	SF4	1	439	8/8	1.00	0.01	13,24,43,45	0
9	SF4	3	784	8/8	1.00	0.01	12,16,36,38	0
10	FMN	S	440	31/31	1.00	0.02	53,60,65,66	0
11	FES	2	182	4/4	1.00	0.01	11,18,41,42	0
11	FES	3	787	4/4	1.00	0.01	17,20,34,47	0
11	FES	B	182	4/4	1.00	0.01	15,29,43,48	0
11	FES	C	787	4/4	1.00	0.01	22,23,31,43	0
11	FES	K	182	4/4	1.00	0.01	14,22,42,44	0
11	FES	L	787	4/4	1.00	0.01	16,17,33,41	0
11	FES	T	182	4/4	1.00	0.02	18,26,47,47	0
11	FES	U	787	4/4	1.00	0.01	22,28,34,45	0
12	CA	2	202	1/1	1.00	0.03	58,58,58,58	0
12	CA	3	788	1/1	1.00	0.01	43,43,43,43	0
12	CA	3	789	1/1	1.00	0.01	50,50,50,50	0
12	CA	9	201	1/1	1.00	0.05	37,37,37,37	0
9	SF4	3	785	8/8	1.00	0.01	8,18,36,38	0
12	CA	C	788	1/1	1.00	0.01	46,46,46,46	0
12	CA	G	201	1/1	1.00	0.02	43,43,43,43	0
12	CA	H	203	1/1	1.00	0.03	55,55,55,55	0
12	CA	K	202	1/1	1.00	0.03	66,66,66,66	0
12	CA	L	788	1/1	1.00	0.01	50,50,50,50	0
12	CA	L	789	1/1	1.00	0.01	62,62,62,62	0

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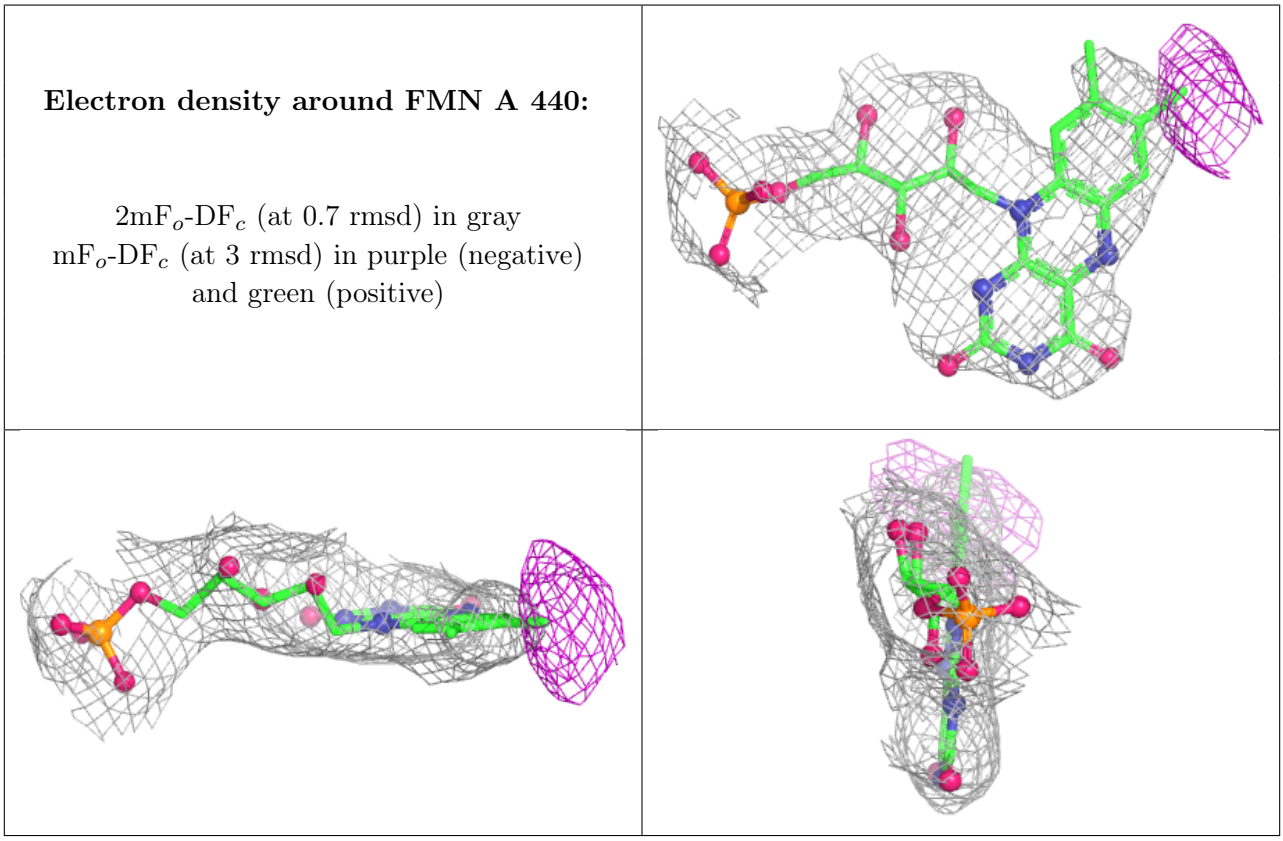
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CA	P	201	1/1	1.00	0.04	40,40,40,40	0
9	SF4	3	786	8/8	1.00	0.01	16,27,50,50	0
12	CA	U	788	1/1	1.00	0.01	50,50,50,50	0
12	CA	Y	201	1/1	1.00	0.03	41,41,41,41	0
12	CA	Z	203	1/1	1.00	0.03	60,60,60,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

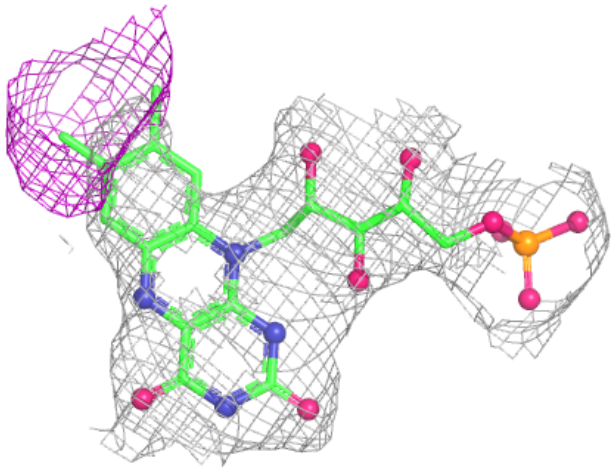
Electron density around FMN A 440:

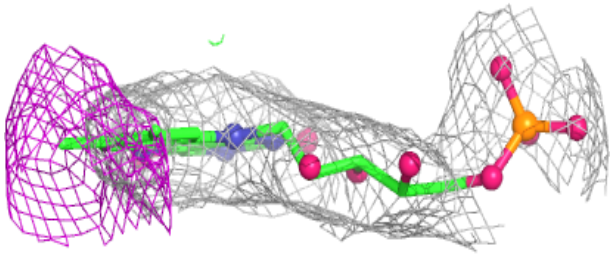
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

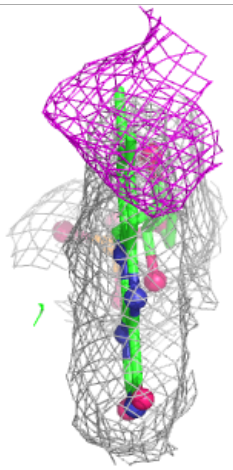


Electron density around FMN J 440:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

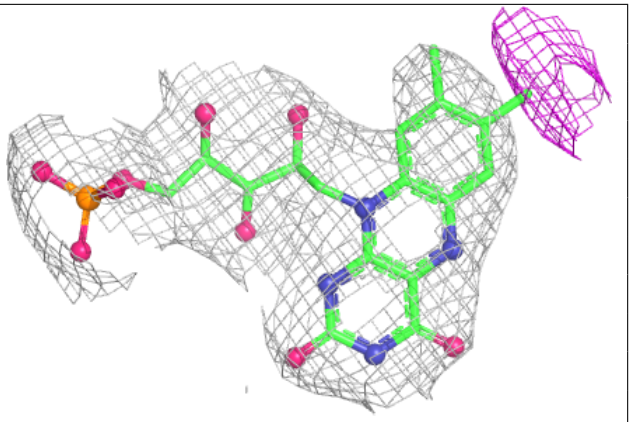


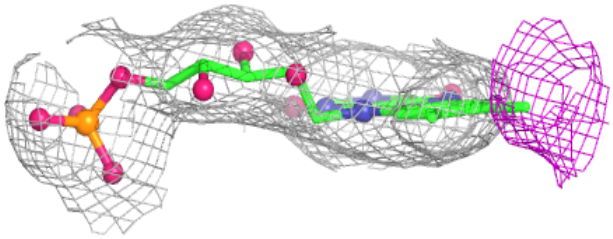


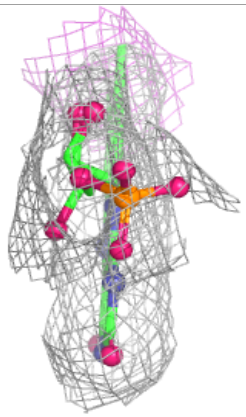


Electron density around FMN 1 440:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

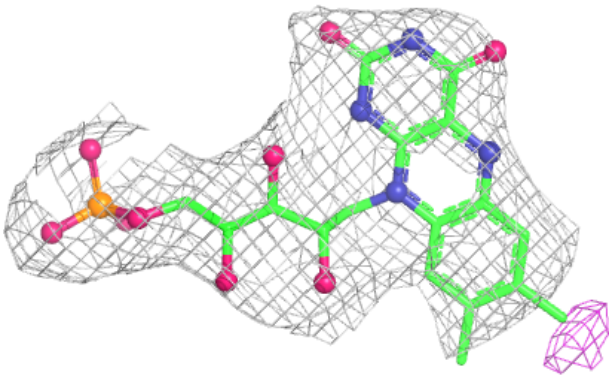


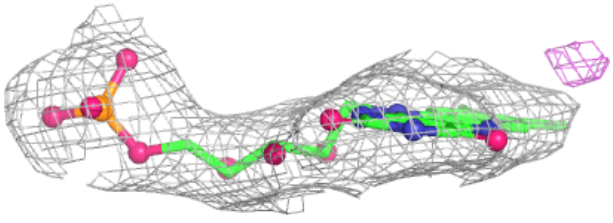


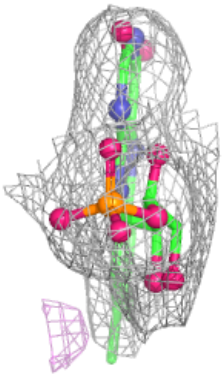


Electron density around FMN S 440:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.