wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2020 – 11:19 PM BST

PDB ID	:	2FUG
Title	:	Crystal structure of the hydrophilic domain of respiratory complex I from Thermus thermophilus
Authors	:	Sazanov, L.A.; Hinchliffe, P.
Deposited on	:	2006-01-26
Resolution	:	3.30 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 (i)) were used in the production of this report:

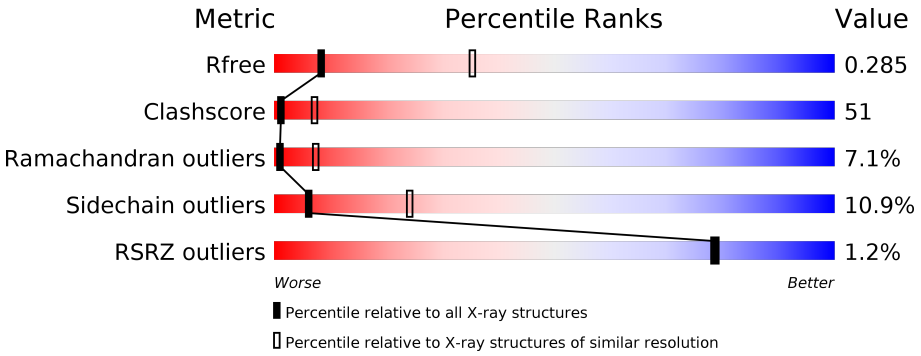
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.30 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.



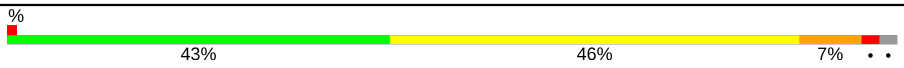
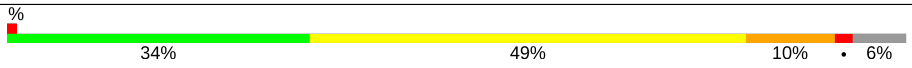
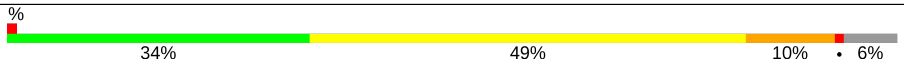
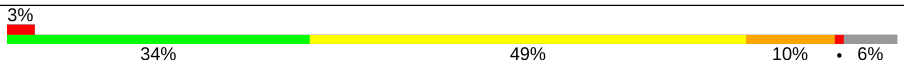
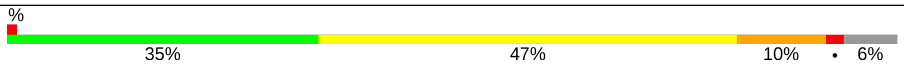
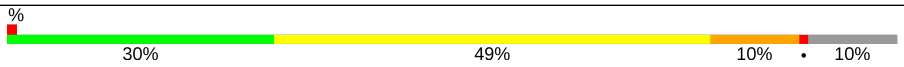
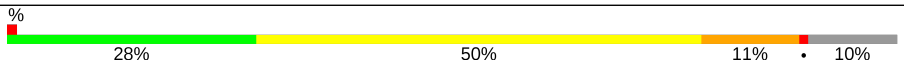
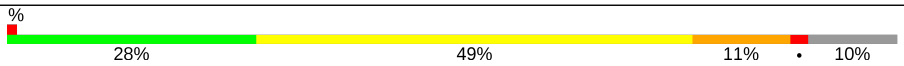
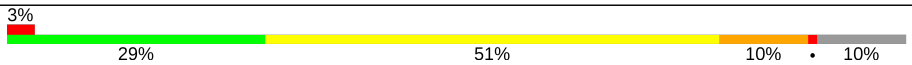
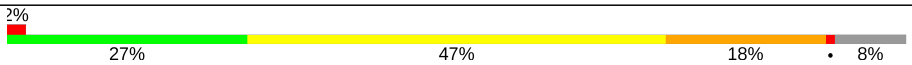
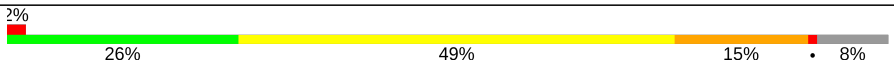
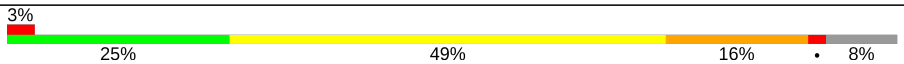
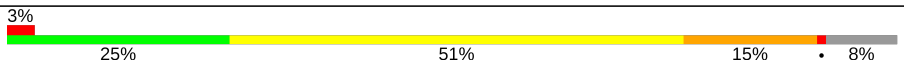
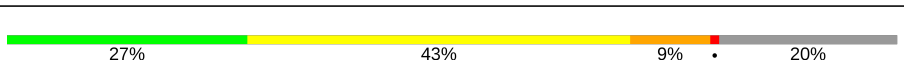
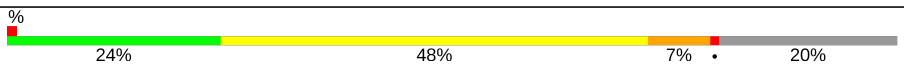
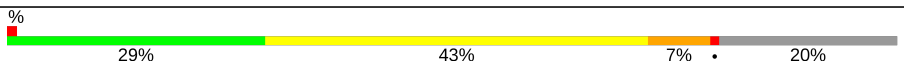
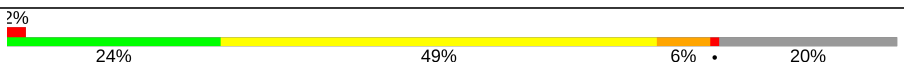
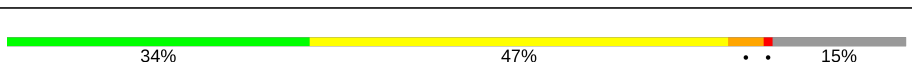
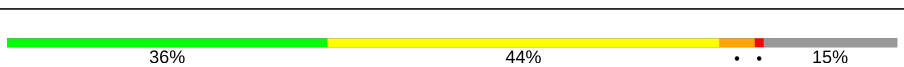
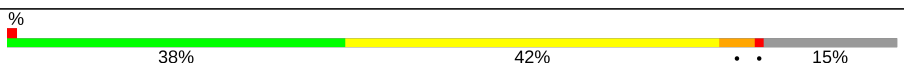
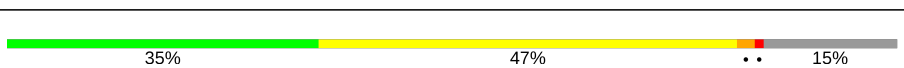
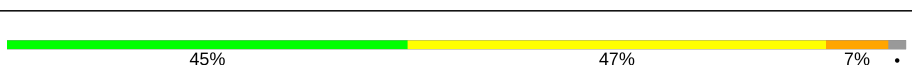
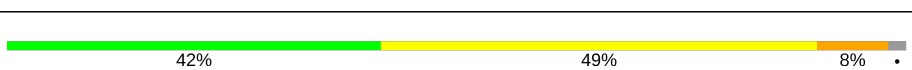
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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% 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	40% 49% 9%
1	A	438	40% 49% 9%
1	J	438	41% 47% 10%
1	S	438	40% 48% 10%
2	2	181	41% 48% 8%
2	B	181	45% 45% 7%

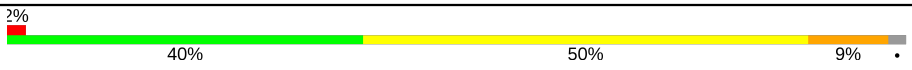
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	181	
2	T	181	
3	3	783	
3	C	783	
3	L	783	
3	U	783	
4	4	409	
4	D	409	
4	M	409	
4	V	409	
5	5	207	
5	E	207	
5	N	207	
5	W	207	
6	6	181	
6	F	181	
6	O	181	
6	X	181	
7	9	182	
7	G	182	
7	P	182	
7	Y	182	
8	7	129	
8	H	129	
8	Q	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	Z	129	

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
10	FES	2	182	-	-	X	-
10	FES	B	182	-	-	X	-
10	FES	K	182	-	-	X	-
9	SF4	3	786	-	-	X	-
9	SF4	C	786	-	-	X	-
9	SF4	L	786	-	-	X	-
9	SF4	U	786	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 73916 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 chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			
1	A	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			
1	J	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			
1	S	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			

- Molecule 2 is a protein called NADH-quinone oxidoreductase chain 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 chain 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			
3	C	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			
3	L	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			
3	U	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			
4	D	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			
4	M	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			
4	V	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			
5	E	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			
5	N	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			
5	W	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	F	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	O	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	X	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			

- Molecule 7 is a protein called NADH-quinone oxidoreductase chain 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			

Continued on next page...

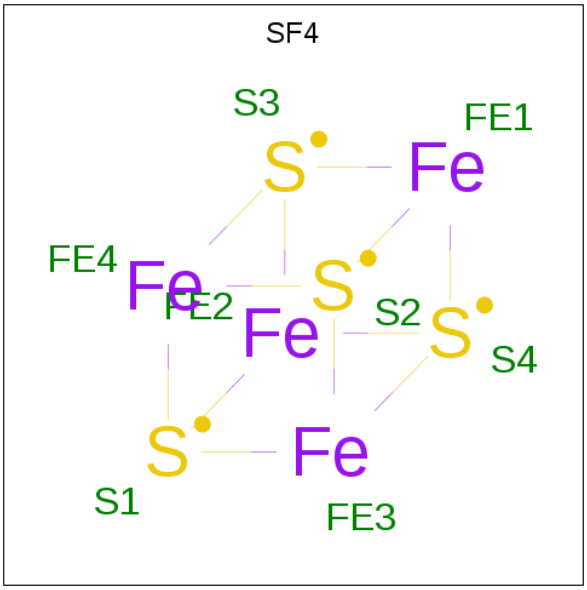
Continued from previous page...

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 conserved hypothetical protein.

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 (three-letter code: 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		

Continued on next page...

Continued from previous page...

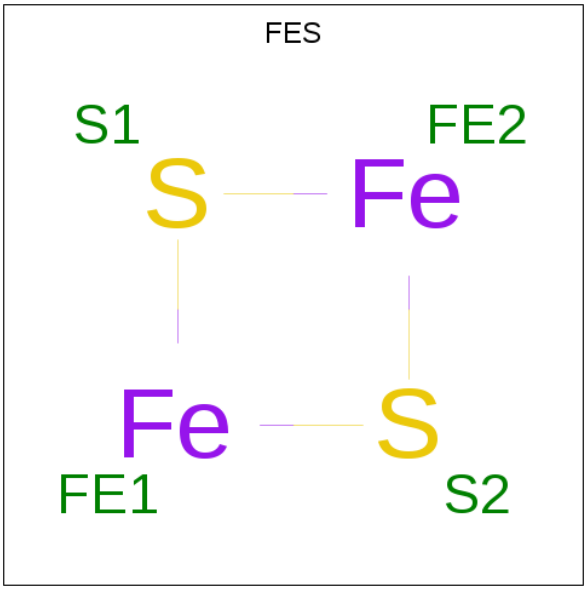
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	6	1	Total Fe S 8 4 4	0	0
9	9	1	Total Fe S 8 4 4	0	0
9	9	1	Total Fe S 8 4 4	0	0
9	A	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	F	1	Total Fe S 8 4 4	0	0
9	G	1	Total Fe S 8 4 4	0	0
9	G	1	Total Fe S 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

Continued on next page...

Continued from previous page...

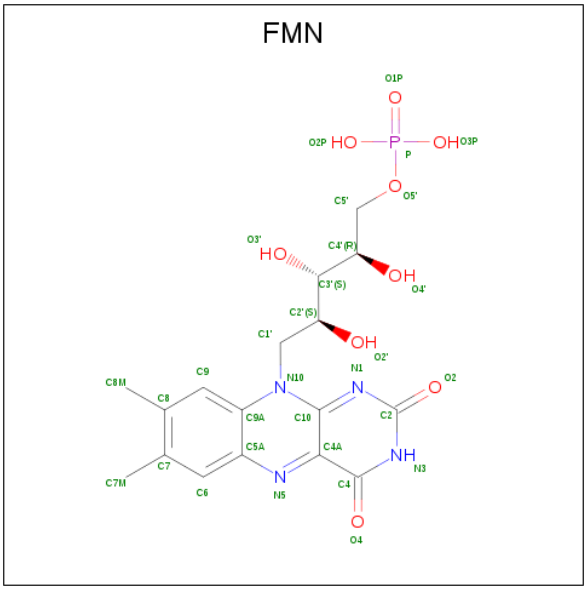
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	X	1	Total Fe S 8 4 4	0	0
9	Y	1	Total Fe S 8 4 4	0	0
9	Y	1	Total Fe S 8 4 4	0	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	2	1	Total Fe S 4 2 2	0	0
10	3	1	Total Fe S 4 2 2	0	0
10	B	1	Total Fe S 4 2 2	0	0
10	C	1	Total Fe S 4 2 2	0	0
10	K	1	Total Fe S 4 2 2	0	0
10	L	1	Total Fe S 4 2 2	0	0
10	T	1	Total Fe S 4 2 2	0	0
10	U	1	Total Fe S 4 2 2	0	0

- Molecule 11 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



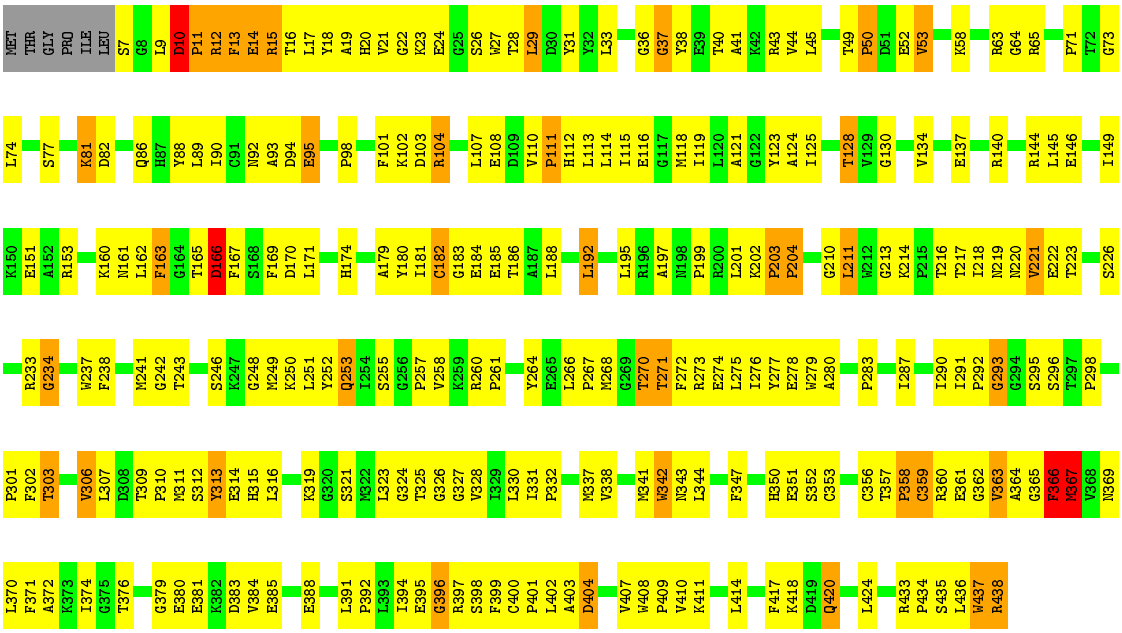
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	7	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
11	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
11	Q	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
11	Z	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

3 Residue-property plots (i)

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

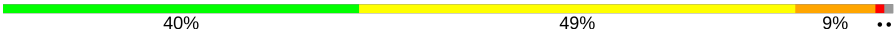
- Molecule 1: NADH-quinone oxidoreductase chain 1

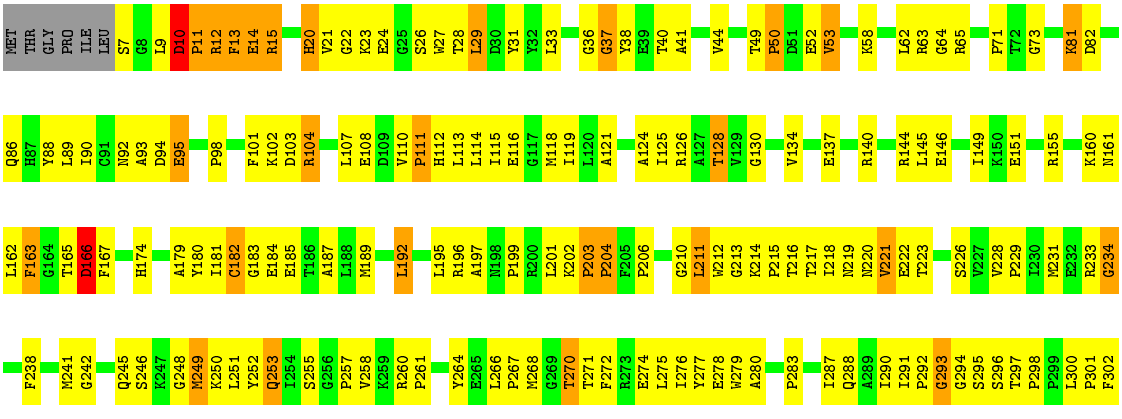
Chain 1:

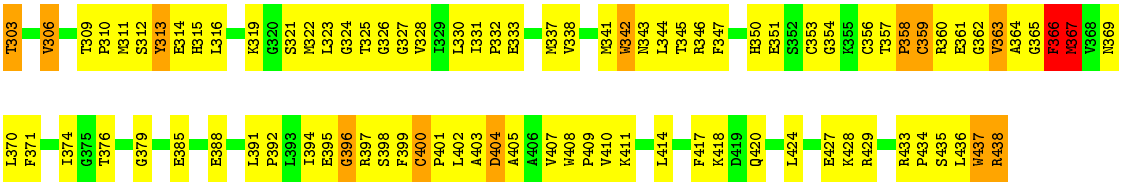


- Molecule 1: NADH-quinone oxidoreductase chain 1

Chain A:

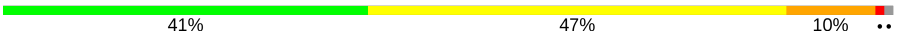


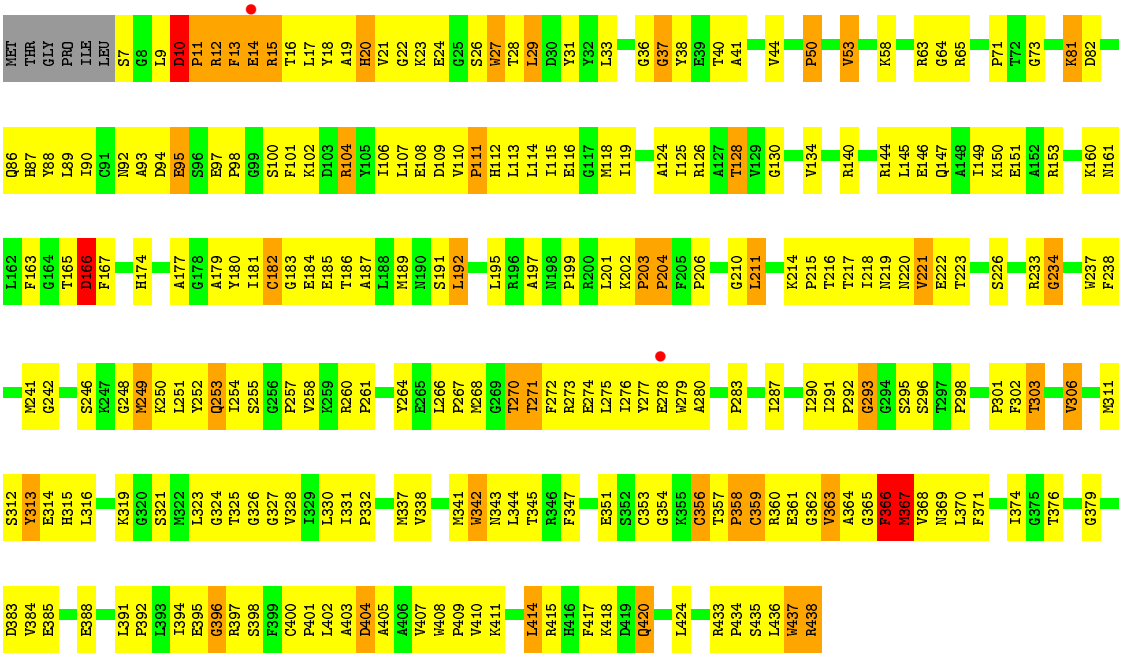




• Molecule 1: NADH-quinone oxidoreductase chain 1

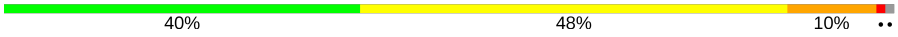
Chain J:

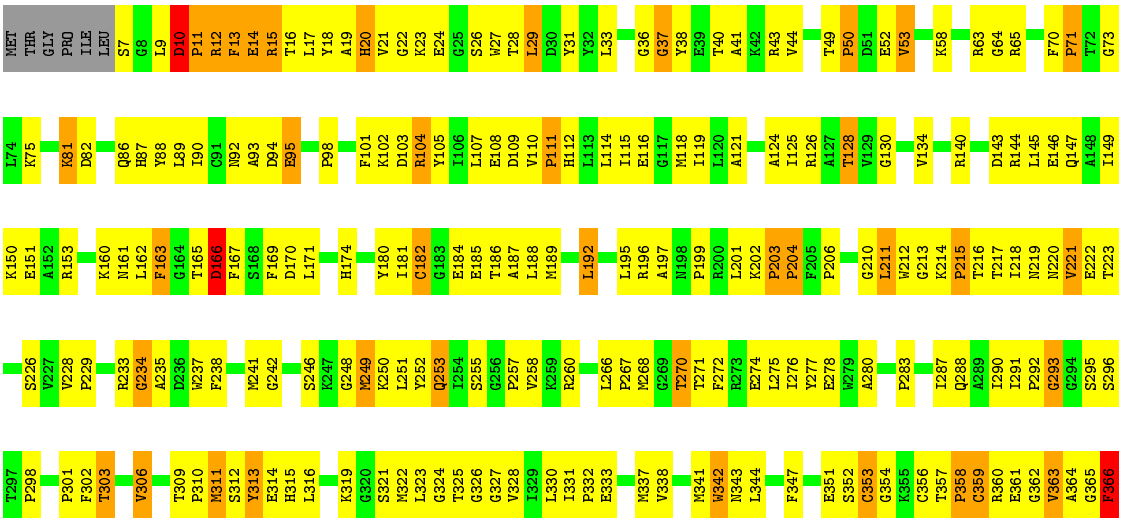


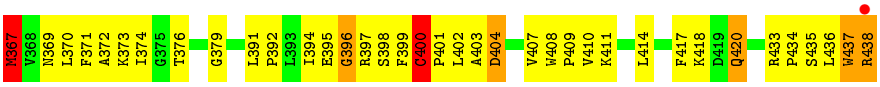


• Molecule 1: NADH-quinone oxidoreductase chain 1

Chain S:

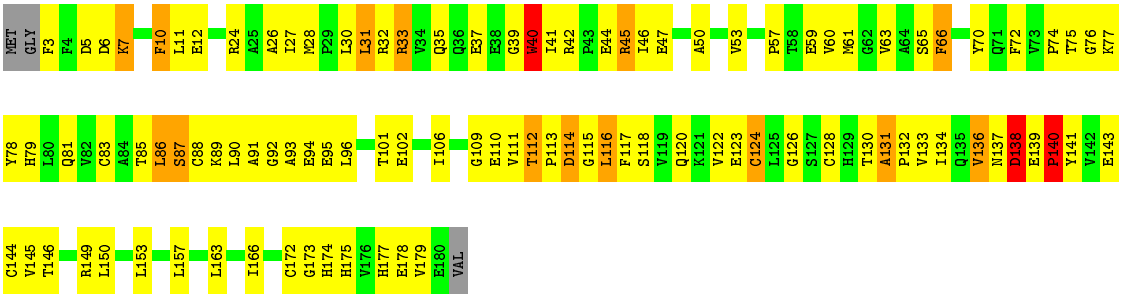






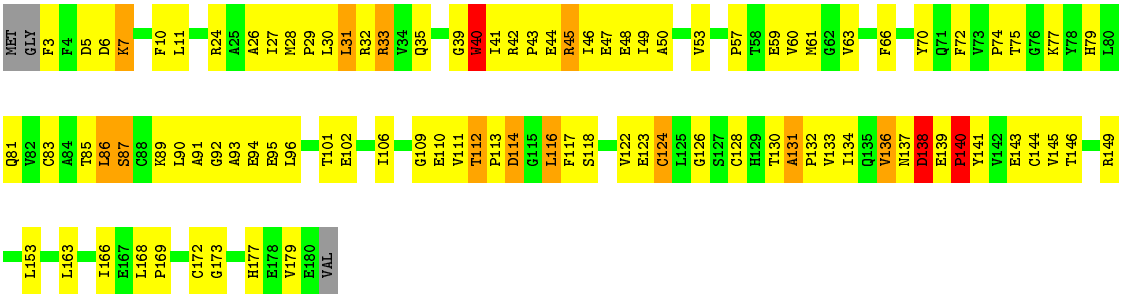
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain 2:



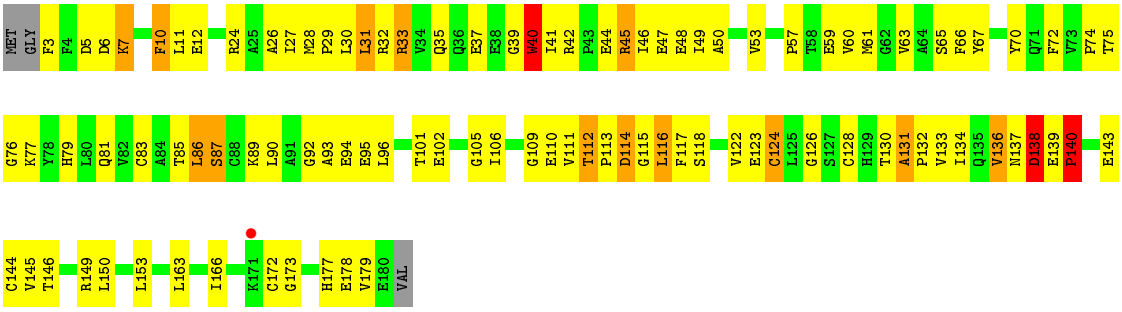
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain B:



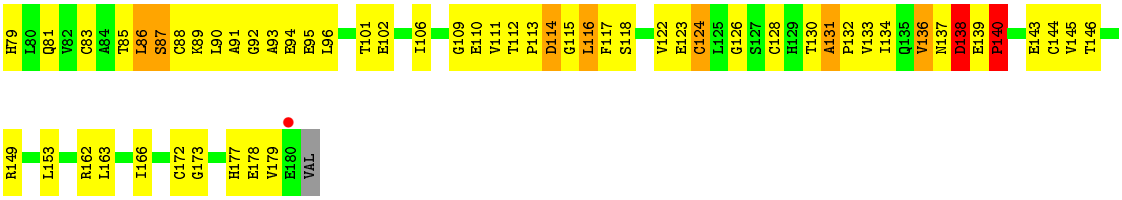
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain K:



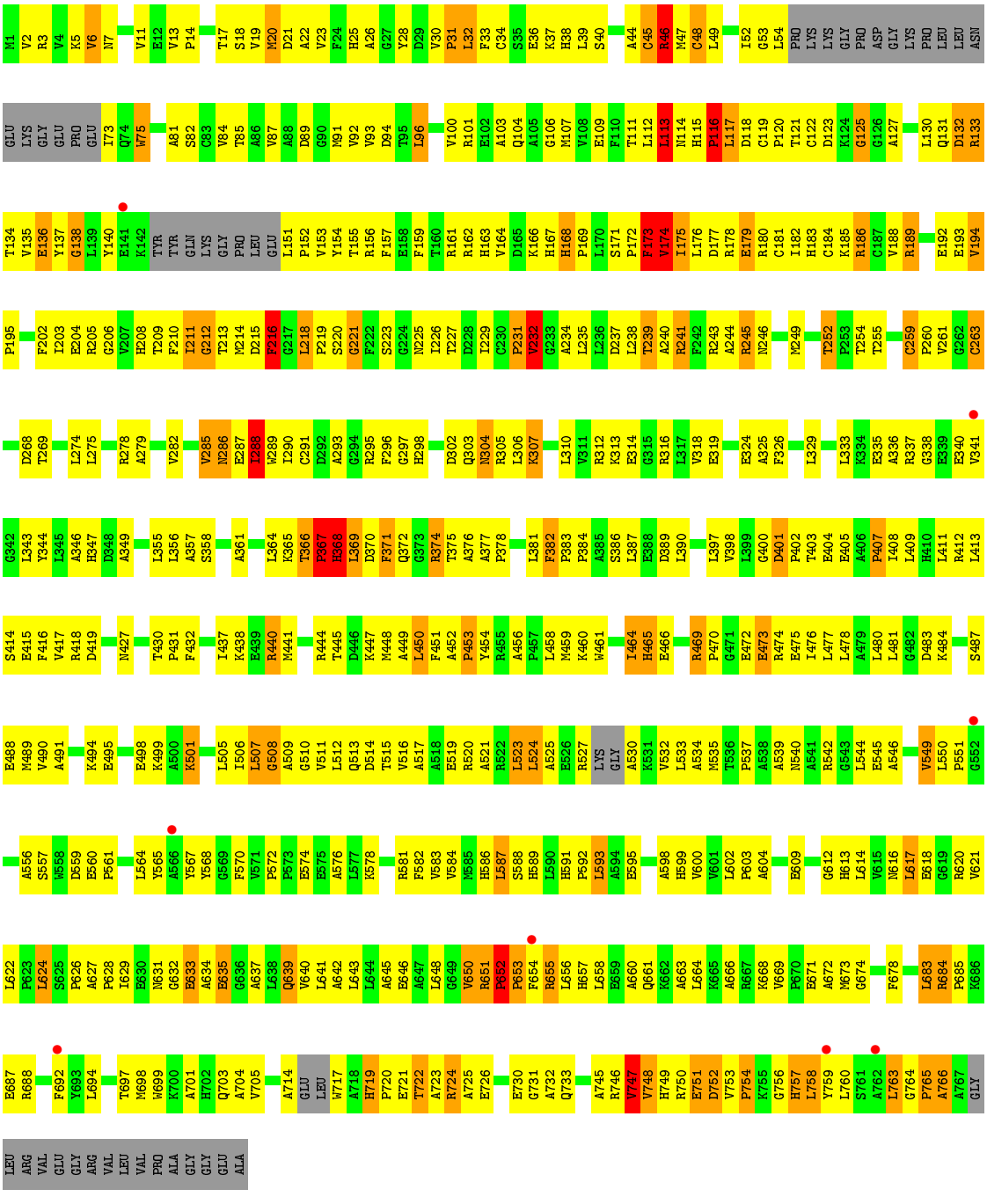
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain T:



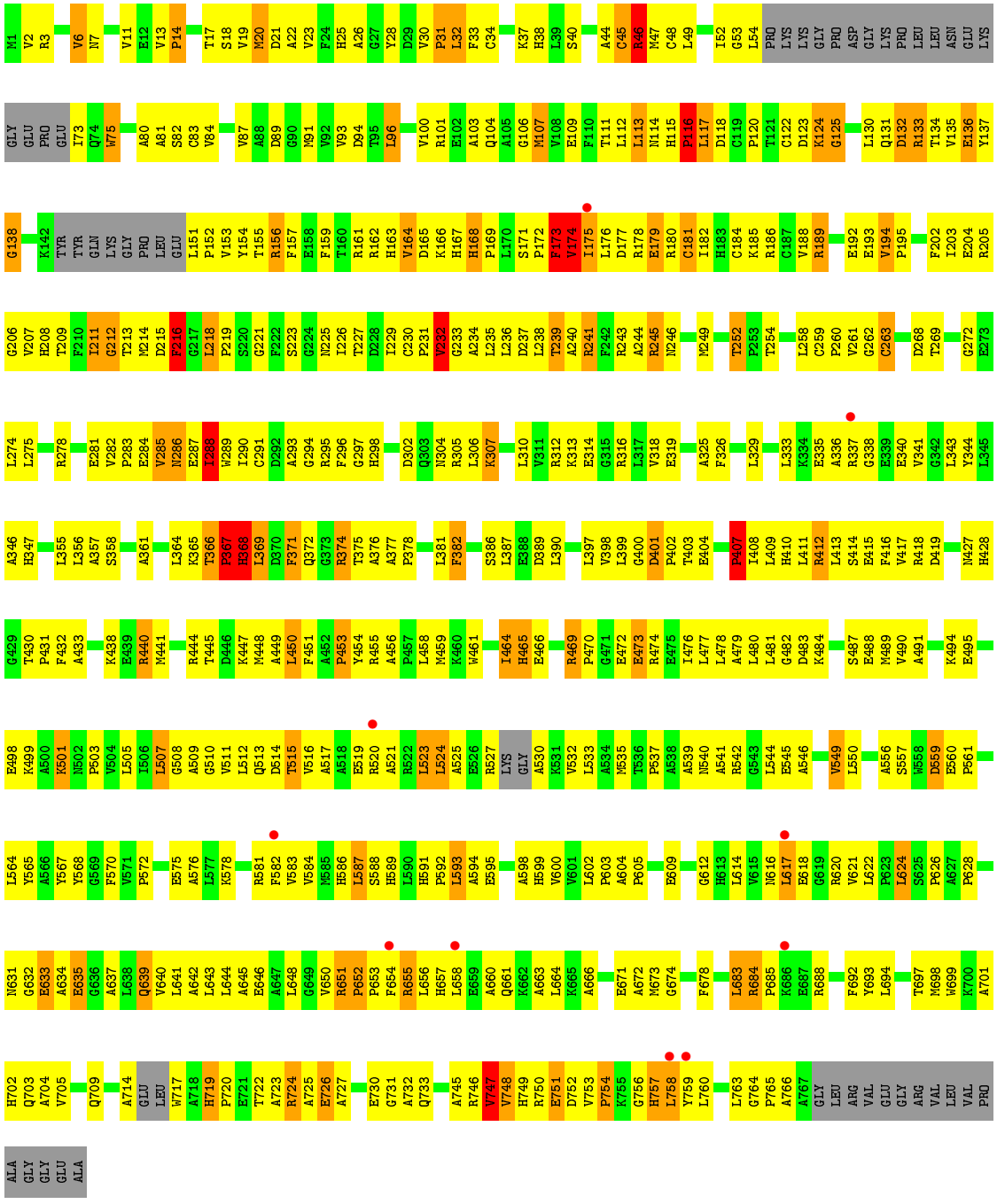
• Molecule 3: NADH-quinone oxidoreductase chain 3

Chain 3:



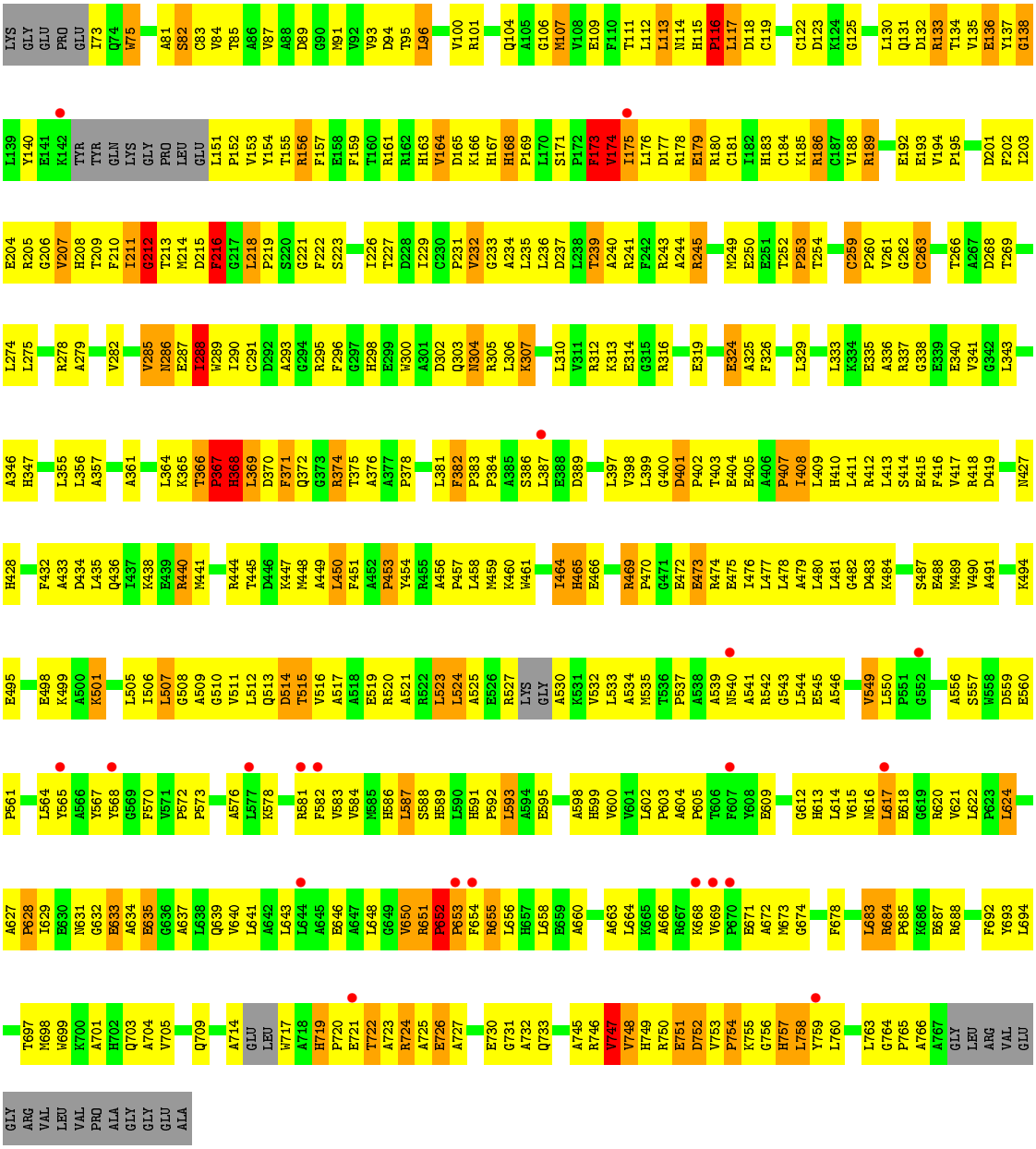
• Molecule 3: NADH-quinone oxidoreductase chain 3

Chain C:

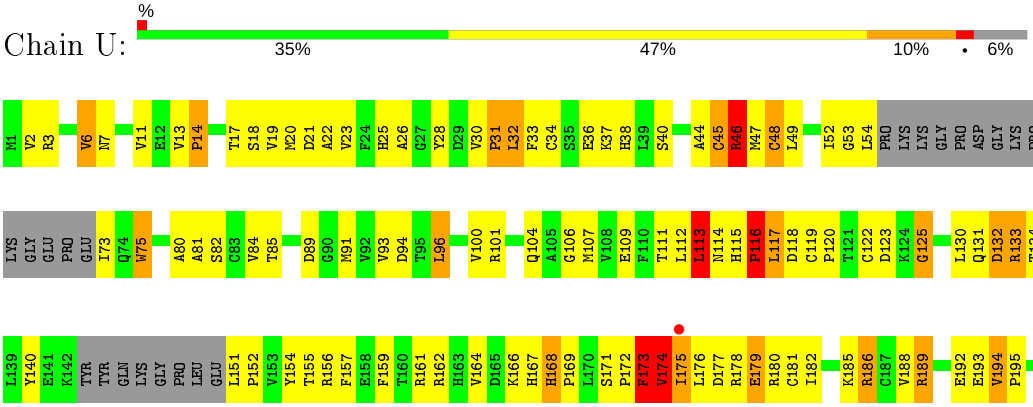


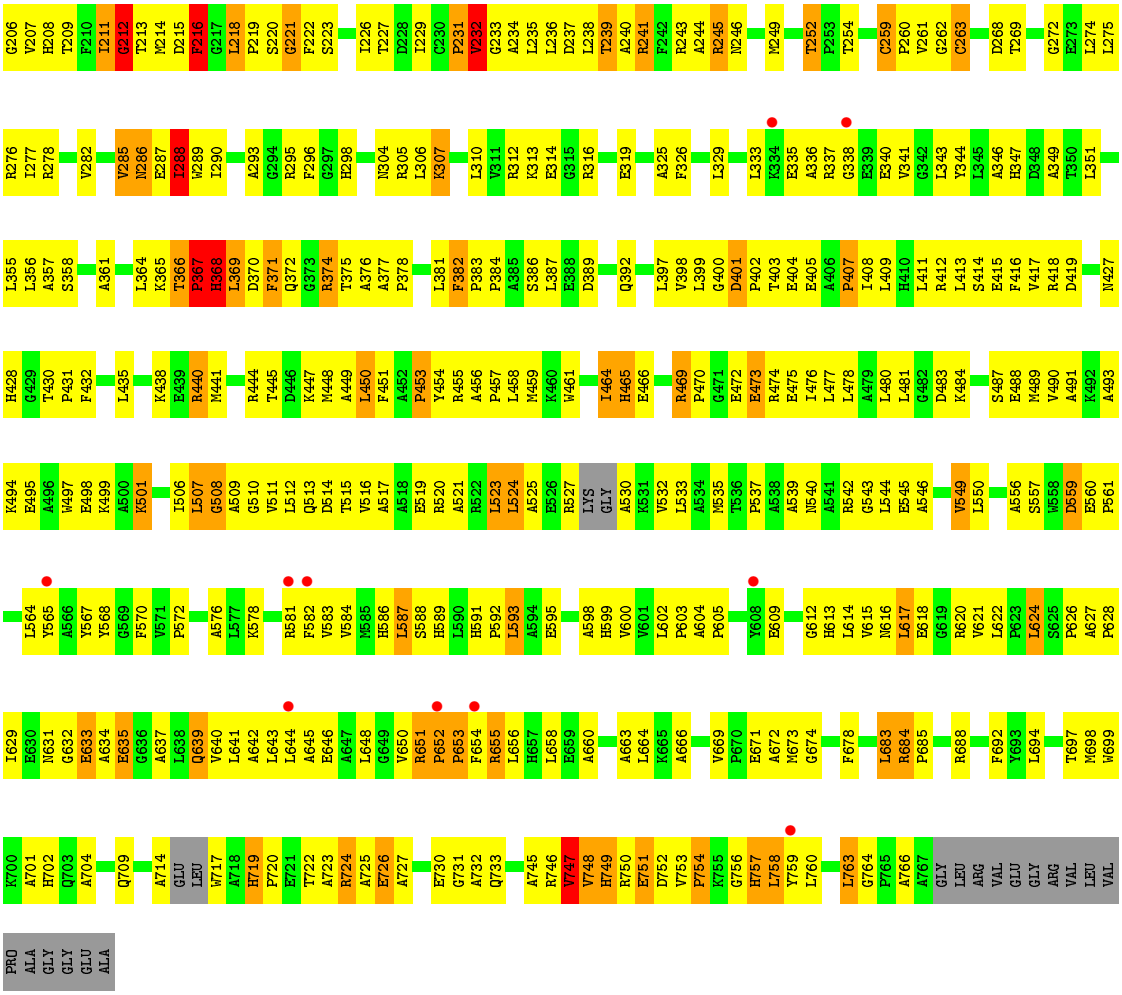
• Molecule 3: NADH-quinone oxidoreductase chain 3

Chain L:



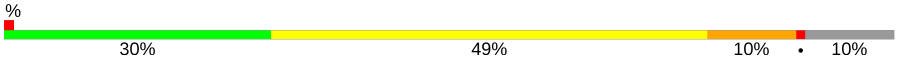
• Molecule 3: NADH-quinone oxidoreductase chain 3

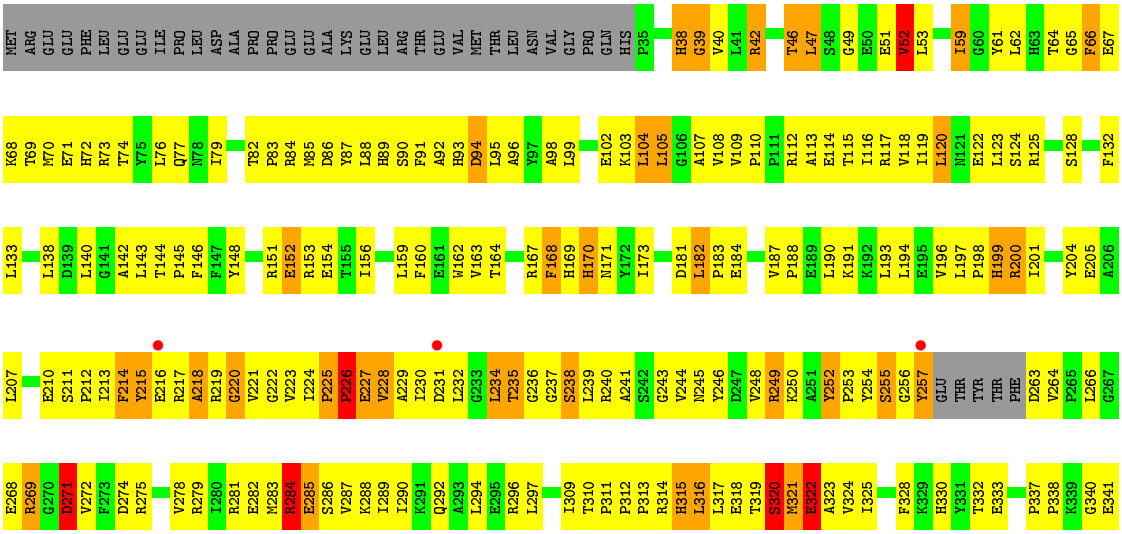


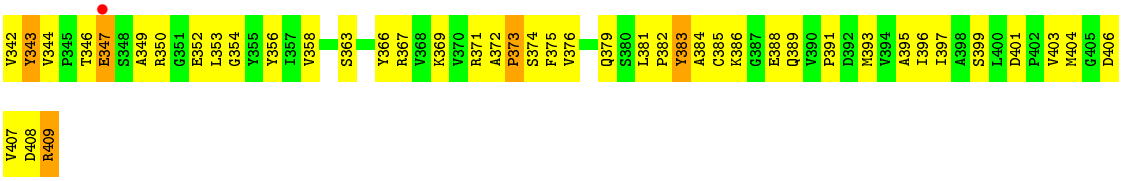


• Molecule 4: NADH-quinone oxidoreductase chain 4

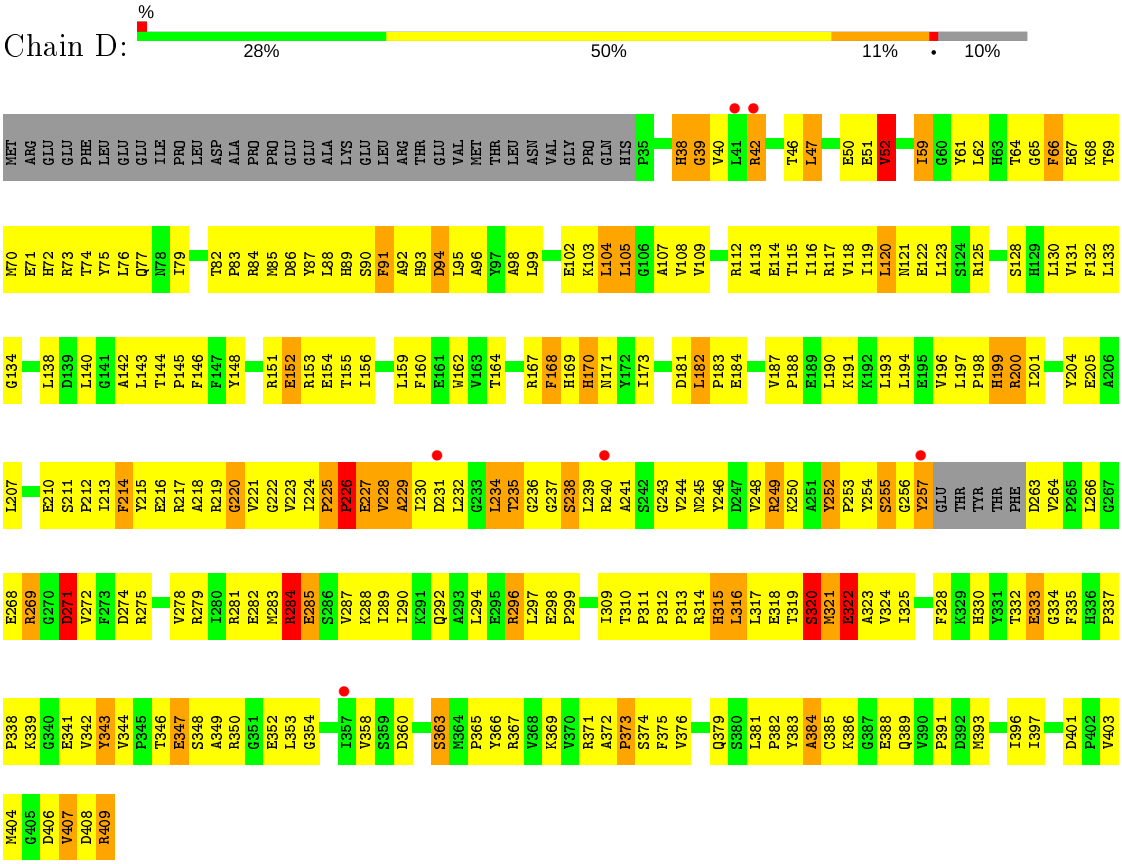
Chain 4:



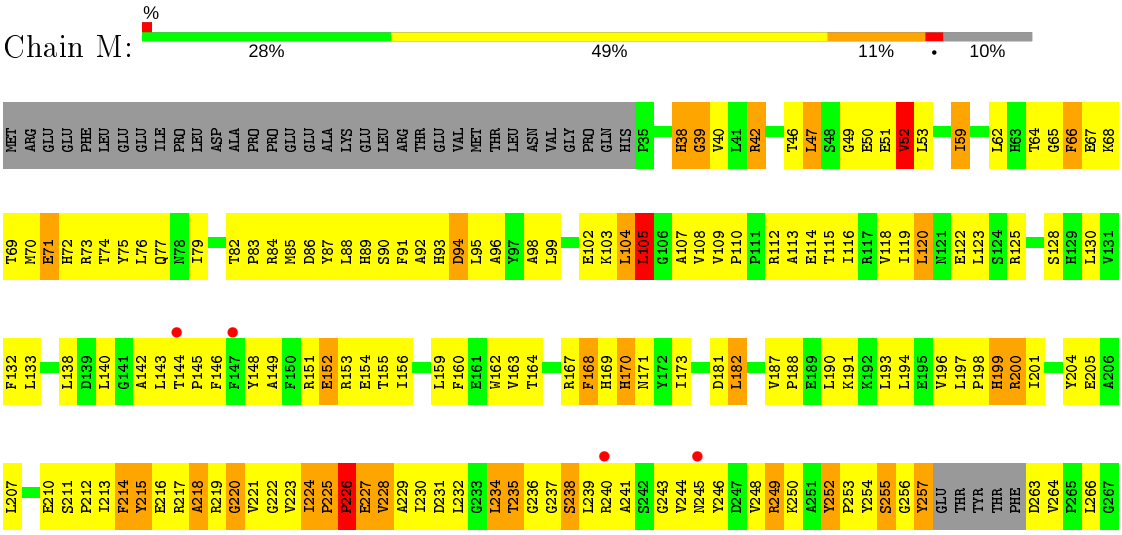


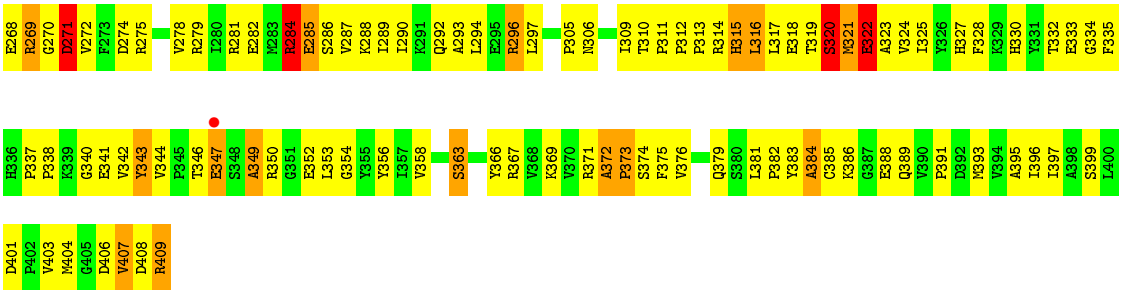


• Molecule 4: NADH-quinone oxidoreductase chain 4



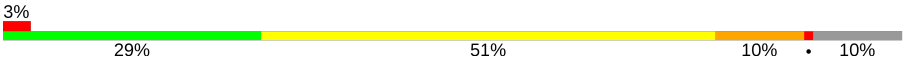
• Molecule 4: NADH-quinone oxidoreductase chain 4

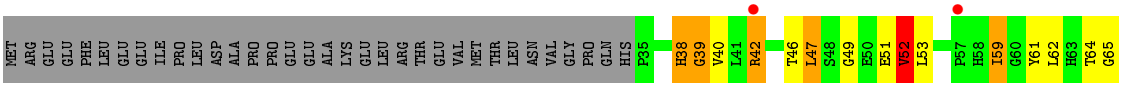


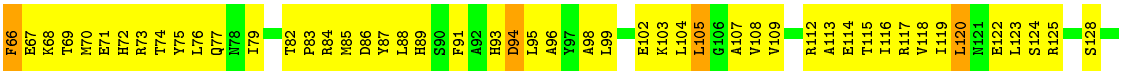


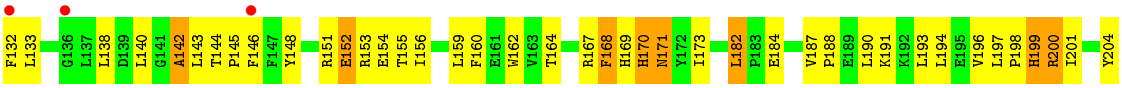
• Molecule 4: NADH-quinone oxidoreductase chain 4

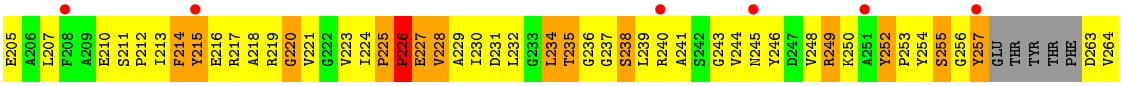
Chain V:

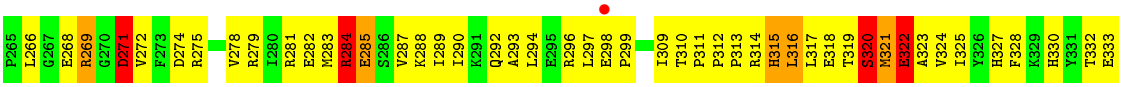


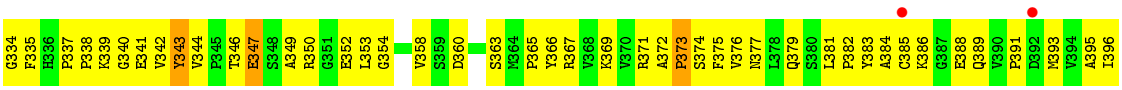


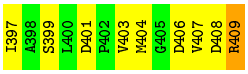






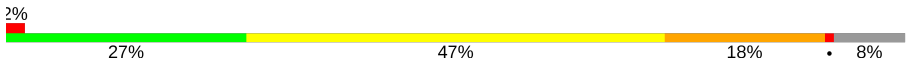


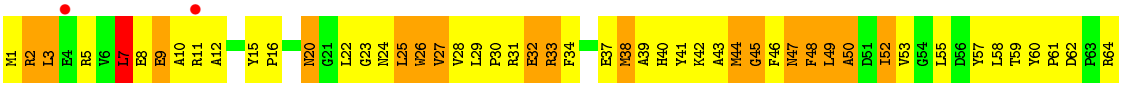


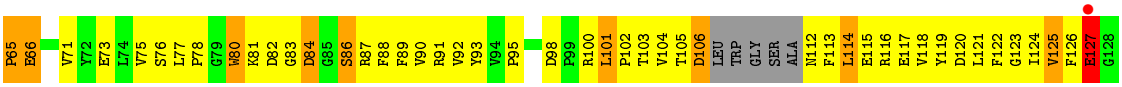


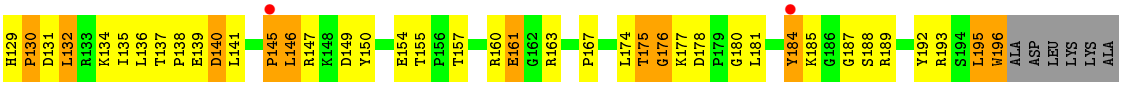
• Molecule 5: NADH-quinone oxidoreductase chain 5

Chain 5:





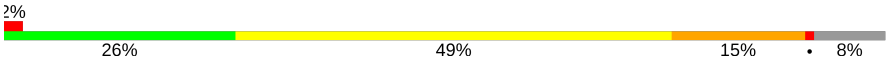




ARG GLU VAL LYS GLY

• Molecule 5: NADH-quinone oxidoreductase chain 5

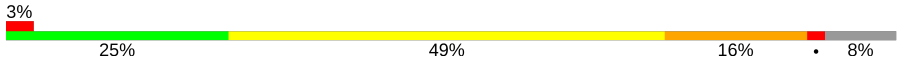
Chain E:

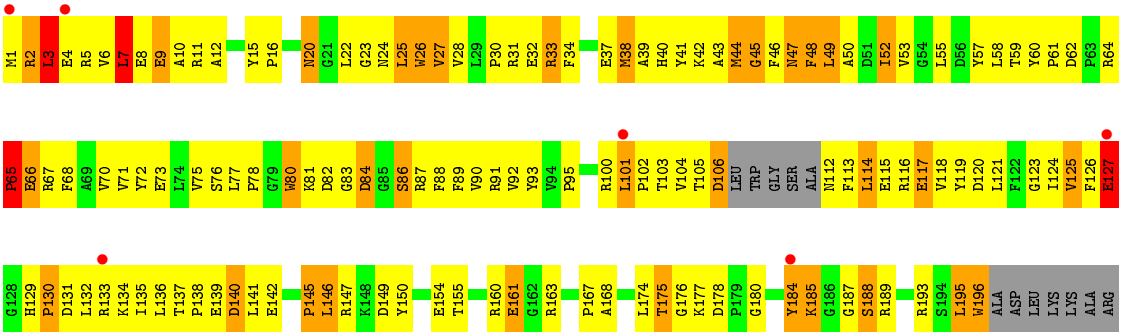


LYS GLY

• Molecule 5: NADH-quinone oxidoreductase chain 5

Chain N:

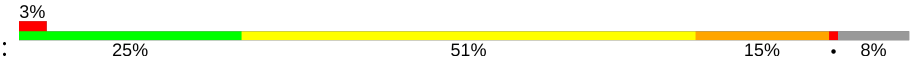


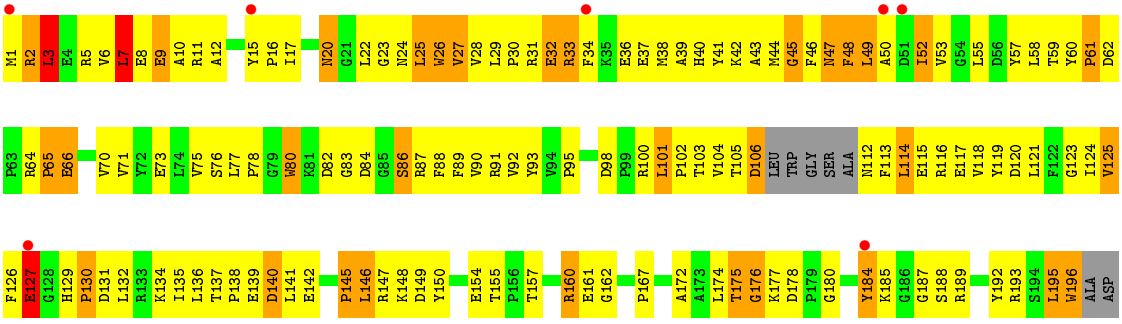


GLU VAL LYS GLY

• Molecule 5: NADH-quinone oxidoreductase chain 5

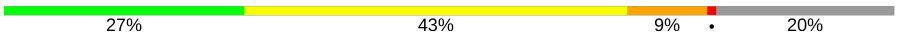
Chain W:

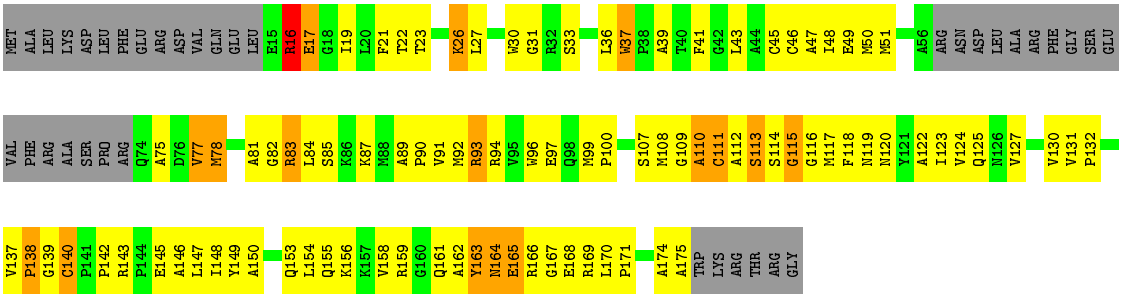




- Molecule 6: NADH-quinone oxidoreductase chain 6

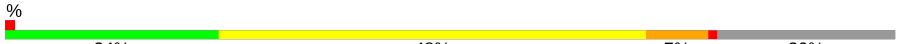
Chain 6:

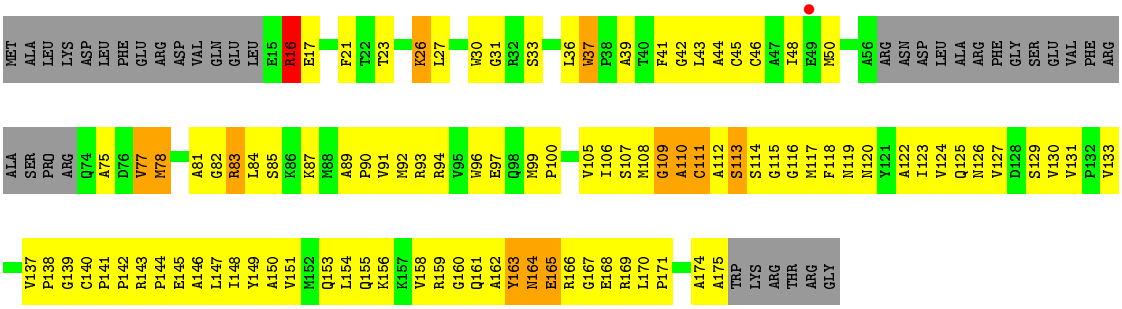




- Molecule 6: NADH-quinone oxidoreductase chain 6

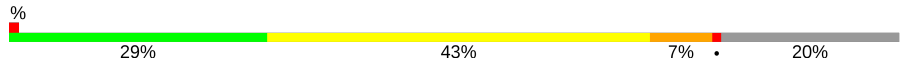
Chain F:

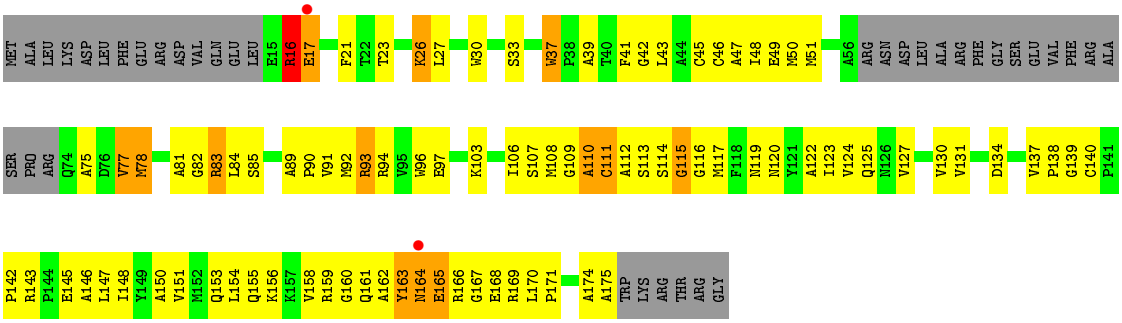




- Molecule 6: NADH-quinone oxidoreductase chain 6

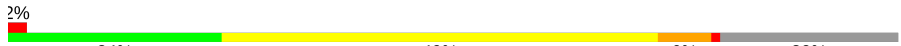
Chain O:

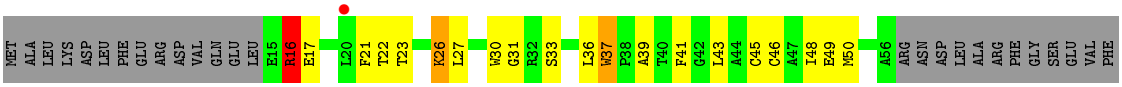


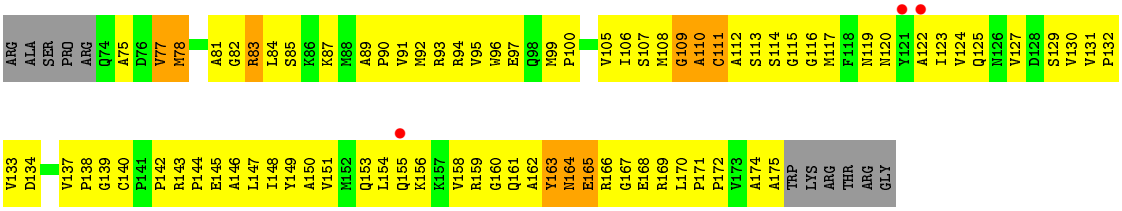


- Molecule 6: NADH-quinone oxidoreductase chain 6

Chain X:

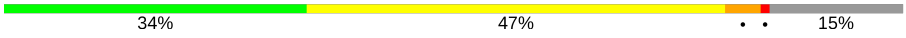


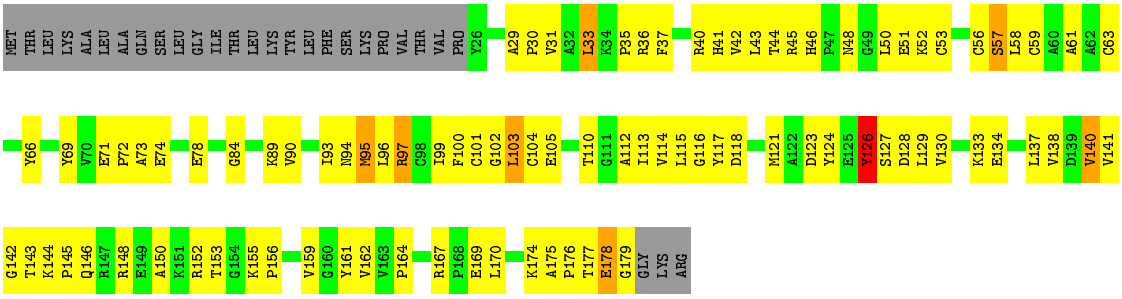




• Molecule 7: NADH-quinone oxidoreductase chain 9

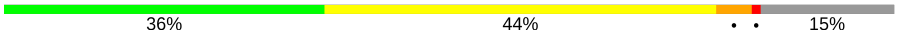
Chain 9:

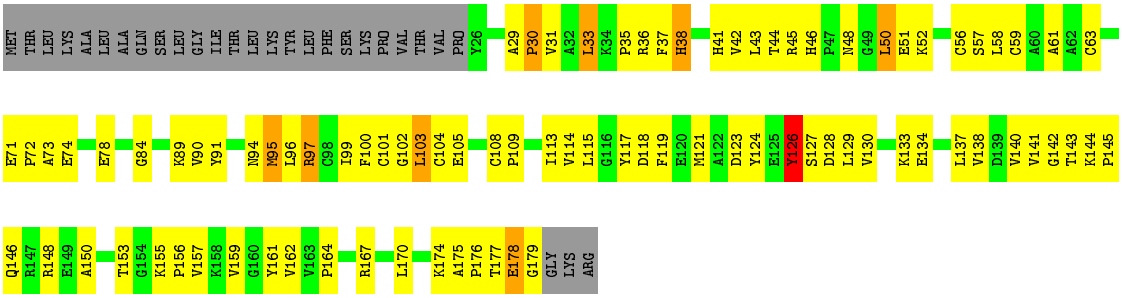




• Molecule 7: NADH-quinone oxidoreductase chain 9

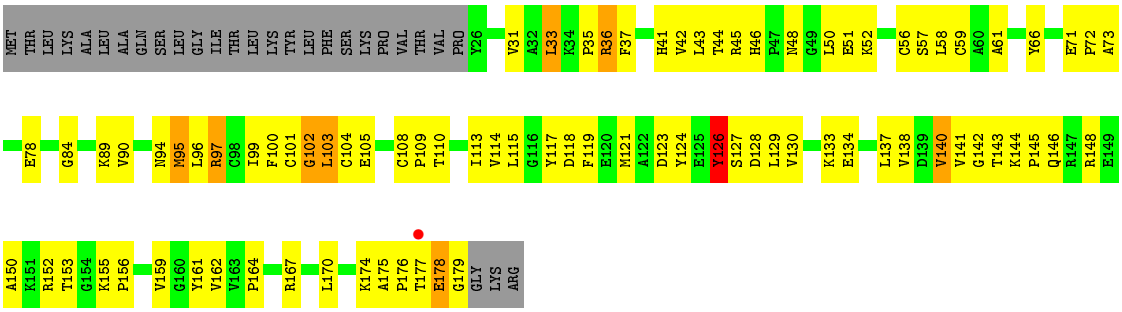
Chain G:





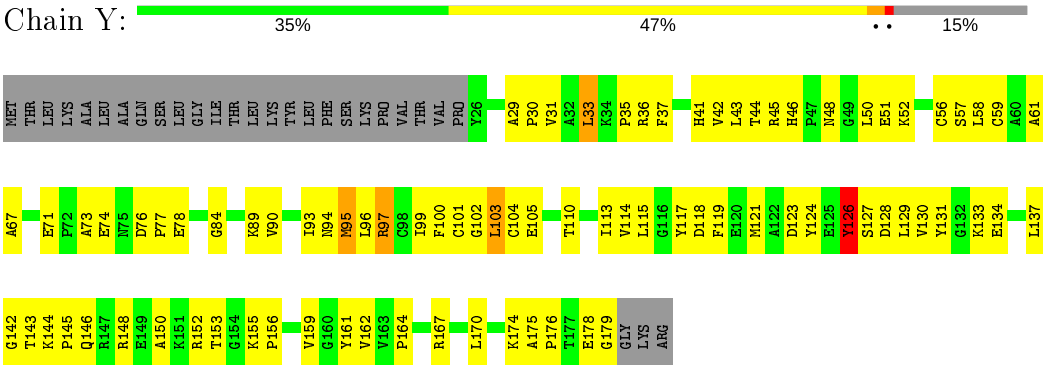
• Molecule 7: NADH-quinone oxidoreductase chain 9

Chain P:



• Molecule 7: NADH-quinone oxidoreductase chain 9

Chain Y:



- Molecule 8: conserved hypothetical protein

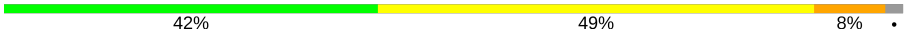
Chain 7:

- Molecule 8: conserved hypothetical protein

Chain H:

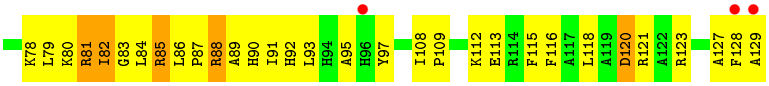
- Molecule 8: conserved hypothetical protein

Chain Q:



- Molecule 8: conserved hypothetical protein

Chain Z:


K78
L79
K80
R81
I82
G83
L84
R85
L86
P87
R88
A89
H90
I91
H92
L93
H94
A95
H96
Y97
I108
P109
K112
E113
R114
F115
F116
A117
L118
A119
D120
R121
A122
R123
A127
F128
A129

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)	20.00 – 3.30 29.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.30) 95.3 (29.99-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.298 0.251 , 0.285	Depositor DCC
R_{free} test set	3935 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	79.6	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	73916	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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, 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	0.47	0/3471	0.71	1/4696 (0.0%)
1	A	0.45	0/3471	0.70	1/4696 (0.0%)
1	J	0.48	1/3471 (0.0%)	0.70	1/4696 (0.0%)
1	S	0.44	1/3471 (0.0%)	0.69	1/4696 (0.0%)
2	2	0.47	0/1439	0.69	1/1953 (0.1%)
2	B	0.42	0/1439	0.68	0/1953
2	K	0.46	0/1439	0.70	1/1953 (0.1%)
2	T	0.42	0/1439	0.67	0/1953
3	3	0.46	1/5881 (0.0%)	0.73	7/7974 (0.1%)
3	C	0.45	1/5881 (0.0%)	0.72	6/7974 (0.1%)
3	L	0.44	1/5881 (0.0%)	0.73	8/7974 (0.1%)
3	U	0.44	1/5881 (0.0%)	0.72	6/7974 (0.1%)
4	4	0.46	0/3031	0.76	3/4118 (0.1%)
4	D	0.45	0/3031	0.76	3/4118 (0.1%)
4	M	0.47	0/3031	0.76	5/4118 (0.1%)
4	V	0.41	0/3031	0.73	2/4118 (0.0%)
5	5	0.43	0/1616	0.76	0/2189
5	E	0.45	0/1616	0.77	0/2189
5	N	0.46	0/1616	0.77	1/2189 (0.0%)
5	W	0.40	0/1616	0.74	0/2189
6	6	0.47	0/1126	0.77	2/1528 (0.1%)
6	F	0.49	0/1126	0.77	2/1528 (0.1%)
6	O	0.47	0/1126	0.77	2/1528 (0.1%)
6	X	0.43	0/1126	0.75	2/1528 (0.1%)
7	9	0.49	0/1224	0.72	0/1663
7	G	0.52	0/1224	0.75	1/1663 (0.1%)
7	P	0.47	0/1224	0.72	0/1663
7	Y	0.44	0/1224	0.70	0/1663
8	7	0.41	0/1059	0.70	0/1429
8	H	0.43	0/1059	0.71	0/1429
8	Q	0.44	0/1059	0.71	0/1429
8	Z	0.40	0/1059	0.69	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.45	6/75388 (0.0%)	0.73	56/102200 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	9	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	CYS	CB-SG	7.59	1.95	1.82
1	J	356	CYS	CB-SG	-6.43	1.71	1.82
3	U	181	CYS	CB-SG	6.33	1.93	1.82
3	L	181	CYS	CB-SG	6.06	1.92	1.82
3	3	181	CYS	CB-SG	5.82	1.92	1.82

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	221	GLY	N-CA-C	-7.56	94.20	113.10
3	C	221	GLY	N-CA-C	-7.31	94.82	113.10
3	L	221	GLY	N-CA-C	-7.19	95.12	113.10
3	3	221	GLY	N-CA-C	-6.92	95.80	113.10
4	D	322	GLU	N-CA-C	-6.92	92.32	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	69	TYR	Sidechain

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	3383	0	3349	268	0
1	A	3383	0	3349	267	0
1	J	3383	0	3349	272	0
1	S	3383	0	3349	268	0
2	2	1406	0	1373	145	0
2	B	1406	0	1373	137	0
2	K	1406	0	1373	142	0
2	T	1406	0	1373	133	0
3	3	5746	0	5767	594	0
3	C	5746	0	5767	588	0
3	L	5746	0	5767	592	1
3	U	5746	0	5767	605	1
4	4	2953	0	2944	436	0
4	D	2953	0	2944	432	0
4	M	2953	0	2944	433	0
4	V	2953	0	2944	433	0
5	5	1570	0	1539	247	0
5	E	1570	0	1539	251	0
5	N	1570	0	1539	250	0
5	W	1570	0	1539	248	0
6	6	1102	0	1108	147	0
6	F	1102	0	1108	148	0
6	O	1102	0	1108	131	0
6	X	1102	0	1108	141	0
7	9	1193	0	1160	112	0
7	G	1193	0	1160	103	0
7	P	1193	0	1160	98	0
7	Y	1193	0	1160	109	0
8	7	1031	0	1029	73	0
8	H	1031	0	1029	85	0
8	Q	1031	0	1029	88	0
8	Z	1031	0	1029	84	0
9	1	8	0	0	0	0
9	3	24	0	0	3	0
9	6	8	0	0	1	0
9	9	16	0	0	2	0
9	A	8	0	0	0	0
9	C	24	0	0	3	0
9	F	8	0	0	1	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	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	16	0	0	1	0
9	S	8	0	0	0	0
9	U	24	0	0	3	0
9	X	8	0	0	1	0
9	Y	16	0	0	2	0
10	2	4	0	0	2	0
10	3	4	0	0	1	0
10	B	4	0	0	2	0
10	C	4	0	0	1	0
10	K	4	0	0	2	0
10	L	4	0	0	1	0
10	T	4	0	0	1	0
10	U	4	0	0	0	0
11	7	31	0	19	5	0
11	H	31	0	19	5	0
11	Q	31	0	19	7	0
11	Z	31	0	19	6	0
All	All	73916	0	73152	7497	1

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 51.

The worst 5 of 7497 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)
2:K:139:GLU:HB2	2:K:140:PRO:HD2	1.25	1.19
4:M:249:ARG:HB3	4:M:249:ARG:HH11	1.08	1.18
1:S:10:ASP:HB3	1:S:11:PRO:HD2	1.19	1.17
1:S:11:PRO:HB3	1:S:270:THR:HB	1.26	1.17
1:J:11:PRO:HB3	1:J:270:THR:HB	1.20	1.17

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:MET:N	3:U:498:GLU:OE2[2_645]	2.01	0.19

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	430/438 (98%)	332 (77%)	68 (16%)	30 (7%)	1 7
1	A	430/438 (98%)	330 (77%)	70 (16%)	30 (7%)	1 7
1	J	430/438 (98%)	331 (77%)	70 (16%)	29 (7%)	1 8
1	S	430/438 (98%)	332 (77%)	65 (15%)	33 (8%)	1 6
2	2	176/181 (97%)	144 (82%)	24 (14%)	8 (4%)	2 15
2	B	176/181 (97%)	142 (81%)	26 (15%)	8 (4%)	2 15
2	K	176/181 (97%)	145 (82%)	23 (13%)	8 (4%)	2 15
2	T	176/181 (97%)	144 (82%)	24 (14%)	8 (4%)	2 15
3	3	727/783 (93%)	559 (77%)	117 (16%)	51 (7%)	1 7
3	C	727/783 (93%)	564 (78%)	116 (16%)	47 (6%)	1 9
3	L	727/783 (93%)	567 (78%)	109 (15%)	51 (7%)	1 7
3	U	727/783 (93%)	565 (78%)	110 (15%)	52 (7%)	1 7
4	4	366/409 (90%)	277 (76%)	64 (18%)	25 (7%)	1 8
4	D	366/409 (90%)	283 (77%)	57 (16%)	26 (7%)	1 7
4	M	366/409 (90%)	274 (75%)	63 (17%)	29 (8%)	1 6
4	V	366/409 (90%)	280 (76%)	63 (17%)	23 (6%)	1 9
5	5	187/207 (90%)	128 (68%)	34 (18%)	25 (13%)	0 1
5	E	187/207 (90%)	126 (67%)	35 (19%)	26 (14%)	0 1
5	N	187/207 (90%)	123 (66%)	38 (20%)	26 (14%)	0 1
5	W	187/207 (90%)	123 (66%)	39 (21%)	25 (13%)	0 1
6	6	140/181 (77%)	99 (71%)	31 (22%)	10 (7%)	1 7
6	F	140/181 (77%)	99 (71%)	33 (24%)	8 (6%)	1 11
6	O	140/181 (77%)	101 (72%)	31 (22%)	8 (6%)	1 11
6	X	140/181 (77%)	100 (71%)	33 (24%)	7 (5%)	2 14
7	9	152/182 (84%)	119 (78%)	24 (16%)	9 (6%)	1 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	152/182 (84%)	117 (77%)	25 (16%)	10 (7%)	1 8
7	P	152/182 (84%)	121 (80%)	22 (14%)	9 (6%)	1 10
7	Y	152/182 (84%)	116 (76%)	27 (18%)	9 (6%)	1 10
8	7	125/129 (97%)	110 (88%)	10 (8%)	5 (4%)	3 18
8	H	125/129 (97%)	110 (88%)	10 (8%)	5 (4%)	3 18
8	Q	125/129 (97%)	108 (86%)	11 (9%)	6 (5%)	2 14
8	Z	125/129 (97%)	107 (86%)	12 (10%)	6 (5%)	2 14
All	All	9212/10040 (92%)	7076 (77%)	1484 (16%)	652 (7%)	1 7

5 of 652 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	14	GLU
1	1	28	THR
1	1	37	GLY
1	1	160	LYS
1	1	166	ASP

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	351/356 (99%)	320 (91%)	31 (9%)	10 33
1	A	351/356 (99%)	318 (91%)	33 (9%)	8 30
1	J	351/356 (99%)	320 (91%)	31 (9%)	10 33
1	S	351/356 (99%)	318 (91%)	33 (9%)	8 30
2	2	150/152 (99%)	129 (86%)	21 (14%)	3 16
2	B	150/152 (99%)	134 (89%)	16 (11%)	6 25
2	K	150/152 (99%)	130 (87%)	20 (13%)	4 17
2	T	150/152 (99%)	132 (88%)	18 (12%)	5 20
3	3	593/628 (94%)	524 (88%)	69 (12%)	5 22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	593/628 (94%)	518 (87%)	75 (13%)	4 19
3	L	593/628 (94%)	520 (88%)	73 (12%)	4 20
3	U	593/628 (94%)	522 (88%)	71 (12%)	5 20
4	4	319/355 (90%)	281 (88%)	38 (12%)	5 21
4	D	319/355 (90%)	281 (88%)	38 (12%)	5 21
4	M	319/355 (90%)	280 (88%)	39 (12%)	5 20
4	V	319/355 (90%)	282 (88%)	37 (12%)	5 22
5	5	164/175 (94%)	142 (87%)	22 (13%)	4 16
5	E	164/175 (94%)	142 (87%)	22 (13%)	4 16
5	N	164/175 (94%)	140 (85%)	24 (15%)	3 14
5	W	164/175 (94%)	144 (88%)	20 (12%)	5 20
6	6	117/149 (78%)	108 (92%)	9 (8%)	13 38
6	F	117/149 (78%)	109 (93%)	8 (7%)	16 44
6	O	117/149 (78%)	108 (92%)	9 (8%)	13 38
6	X	117/149 (78%)	109 (93%)	8 (7%)	16 44
7	9	126/150 (84%)	117 (93%)	9 (7%)	14 42
7	G	126/150 (84%)	117 (93%)	9 (7%)	14 42
7	P	126/150 (84%)	117 (93%)	9 (7%)	14 42
7	Y	126/150 (84%)	120 (95%)	6 (5%)	25 56
8	7	104/106 (98%)	93 (89%)	11 (11%)	6 25
8	H	104/106 (98%)	95 (91%)	9 (9%)	10 34
8	Q	104/106 (98%)	94 (90%)	10 (10%)	8 29
8	Z	104/106 (98%)	94 (90%)	10 (10%)	8 29
All	All	7696/8284 (93%)	6858 (89%)	838 (11%)	6 24

5 of 838 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	38	MET
2	K	172	CYS
4	V	210	GLU
5	E	175	THR
1	J	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	389	GLN
2	K	8	GLN
4	V	170	HIS
5	E	24	ASN
7	G	94	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

40 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	$\#\|Z\| > 2$
9	SF4	G	183	7	0,12,12	0.00	-	-		
9	SF4	L	784	3	0,12,12	0.00	-	-		
9	SF4	Y	184	7	0,12,12	0.00	-	-		
9	SF4	G	184	7	0,12,12	0.00	-	-		
9	SF4	U	786	3	0,12,12	0.00	-	-		
10	FES	C	787	3	0,4,4	0.00	-	-		
9	SF4	L	786	3	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SF4	3	784	3	0,12,12	0.00	-	-		
9	SF4	U	784	3	0,12,12	0.00	-	-		
10	FES	B	182	2	0,4,4	0.00	-	-		
10	FES	3	787	3	0,4,4	0.00	-	-		
11	FMN	H	500	-	31,33,33	2.36	7 (22%)	40,50,50	4.09	13 (32%)
9	SF4	3	785	3	0,12,12	0.00	-	-		
9	SF4	C	786	3	0,12,12	0.00	-	-		
11	FMN	Z	500	-	31,33,33	2.26	6 (19%)	40,50,50	4.08	12 (30%)
9	SF4	C	785	3	0,12,12	0.00	-	-		
9	SF4	O	182	6	0,12,12	0.00	-	-		
9	SF4	J	439	1	0,12,12	0.00	-	-		
11	FMN	Q	500	-	31,33,33	2.26	6 (19%)	40,50,50	4.12	12 (30%)
10	FES	L	787	3	0,4,4	0.00	-	-		
11	FMN	7	500	-	31,33,33	2.31	7 (22%)	40,50,50	4.14	13 (32%)
9	SF4	S	439	1	0,12,12	0.00	-	-		
9	SF4	P	183	7	0,12,12	0.00	-	-		
10	FES	2	182	2	0,4,4	0.00	-	-		
10	FES	T	182	2	0,4,4	0.00	-	-		
10	FES	K	182	2	0,4,4	0.00	-	-		
9	SF4	9	183	7	0,12,12	0.00	-	-		
9	SF4	A	439	1	0,12,12	0.00	-	-		
9	SF4	9	184	7	0,12,12	0.00	-	-		
9	SF4	Y	183	7	0,12,12	0.00	-	-		
9	SF4	L	785	3	0,12,12	0.00	-	-		
9	SF4	F	182	6	0,12,12	0.00	-	-		
9	SF4	P	184	7	0,12,12	0.00	-	-		
9	SF4	1	439	1	0,12,12	0.00	-	-		
9	SF4	C	784	3	0,12,12	0.00	-	-		
9	SF4	U	785	3	0,12,12	0.00	-	-		
10	FES	U	787	3	0,4,4	0.00	-	-		
9	SF4	X	182	6	0,12,12	0.00	-	-		
9	SF4	6	182	6	0,12,12	0.00	-	-		
9	SF4	3	786	3	0,12,12	0.00	-	-		

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
9	SF4	G	183	7	-	-	0/6/5/5
9	SF4	L	784	3	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	Y	184	7	-	-	0/6/5/5
9	SF4	G	184	7	-	-	0/6/5/5
9	SF4	U	786	3	-	-	0/6/5/5
10	FES	C	787	3	-	-	0/1/1/1
9	SF4	L	786	3	-	-	0/6/5/5
9	SF4	3	784	3	-	-	0/6/5/5
9	SF4	U	784	3	-	-	0/6/5/5
10	FES	B	182	2	-	-	0/1/1/1
10	FES	3	787	3	-	-	0/1/1/1
11	FMN	H	500	-	-	1/18/18/18	0/3/3/3
9	SF4	3	785	3	-	-	0/6/5/5
9	SF4	C	786	3	-	-	0/6/5/5
11	FMN	Z	500	-	-	1/18/18/18	0/3/3/3
9	SF4	C	785	3	-	-	0/6/5/5
9	SF4	O	182	6	-	-	0/6/5/5
9	SF4	J	439	1	-	-	0/6/5/5
11	FMN	Q	500	-	-	1/18/18/18	0/3/3/3
10	FES	L	787	3	-	-	0/1/1/1
11	FMN	7	500	-	-	1/18/18/18	0/3/3/3
9	SF4	S	439	1	-	-	0/6/5/5
9	SF4	P	183	7	-	-	0/6/5/5
10	FES	2	182	2	-	-	0/1/1/1
10	FES	T	182	2	-	-	0/1/1/1
10	FES	K	182	2	-	-	0/1/1/1
9	SF4	9	183	7	-	-	0/6/5/5
9	SF4	A	439	1	-	-	0/6/5/5
9	SF4	9	184	7	-	-	0/6/5/5
9	SF4	Y	183	7	-	-	0/6/5/5
9	SF4	L	785	3	-	-	0/6/5/5
9	SF4	F	182	6	-	-	0/6/5/5
9	SF4	P	184	7	-	-	0/6/5/5
9	SF4	1	439	1	-	-	0/6/5/5
9	SF4	C	784	3	-	-	0/6/5/5
9	SF4	U	785	3	-	-	0/6/5/5
10	FES	U	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	3	786	3	-	-	0/6/5/5

The worst 5 of 26 bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	500	FMN	C4A-C10	8.99	1.47	1.38
11	Q	500	FMN	C4A-C10	8.38	1.47	1.38
11	Z	500	FMN	C4A-C10	8.22	1.47	1.38
11	7	500	FMN	C4A-C10	7.96	1.46	1.38
11	Q	500	FMN	C4-C4A	5.29	1.50	1.41

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	7	500	FMN	C1'-N10-C9A	16.46	131.25	118.29
11	Z	500	FMN	C1'-N10-C9A	16.36	131.17	118.29
11	H	500	FMN	C1'-N10-C9A	16.34	131.15	118.29
11	Q	500	FMN	C1'-N10-C9A	16.32	131.14	118.29
11	7	500	FMN	C1'-N10-C10	-10.90	108.65	118.41

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	500	FMN	C2'-C1'-N10-C10
11	Q	500	FMN	C2'-C1'-N10-C10
11	Z	500	FMN	C2'-C1'-N10-C10
11	7	500	FMN	C2'-C1'-N10-C10

There are no ring outliers.

30 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	183	SF4	1	0
9	L	784	SF4	1	0
9	Y	184	SF4	1	0
9	G	184	SF4	1	0
9	U	786	SF4	2	0
10	C	787	FES	1	0
9	L	786	SF4	2	0
9	3	784	SF4	1	0
9	U	784	SF4	1	0
10	B	182	FES	2	0
10	3	787	FES	1	0

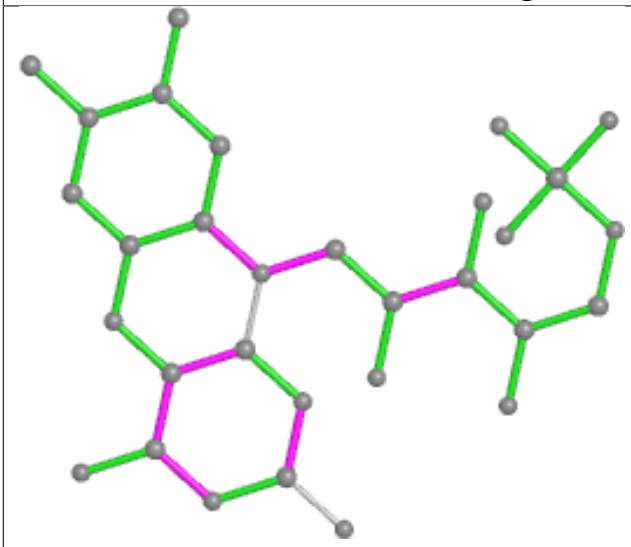
Continued on next page...

Continued from previous page...

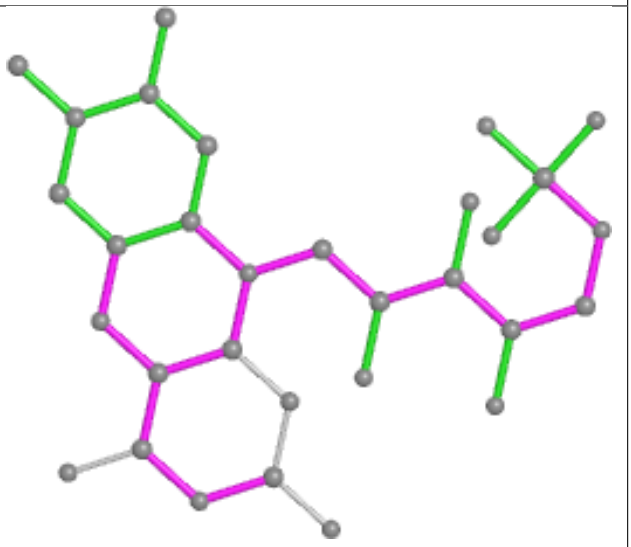
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	500	FMN	5	0
9	C	786	SF4	2	0
11	Z	500	FMN	6	0
9	O	182	SF4	1	0
11	Q	500	FMN	7	0
10	L	787	FES	1	0
11	7	500	FMN	5	0
10	2	182	FES	2	0
10	T	182	FES	1	0
10	K	182	FES	2	0
9	9	183	SF4	1	0
9	9	184	SF4	1	0
9	Y	183	SF4	1	0
9	F	182	SF4	1	0
9	P	184	SF4	1	0
9	C	784	SF4	1	0
9	X	182	SF4	1	0
9	6	182	SF4	1	0
9	3	786	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

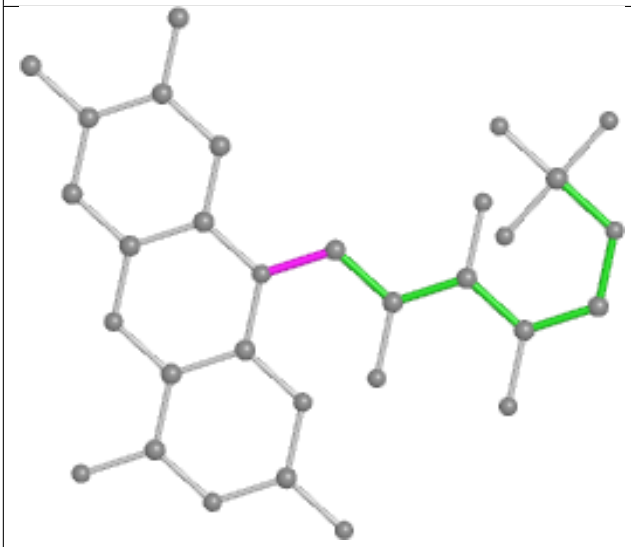
Ligand FMN H 500



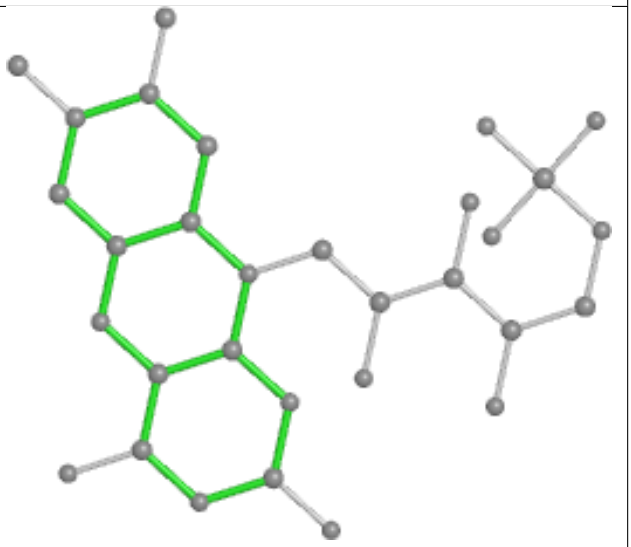
Bond lengths



Bond angles

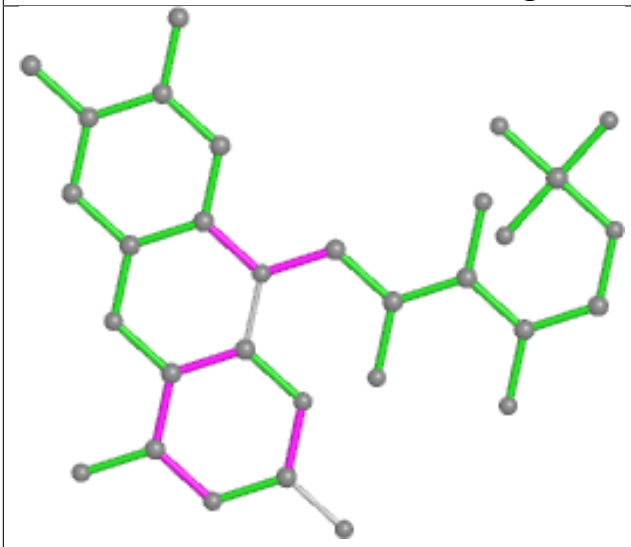


Torsions

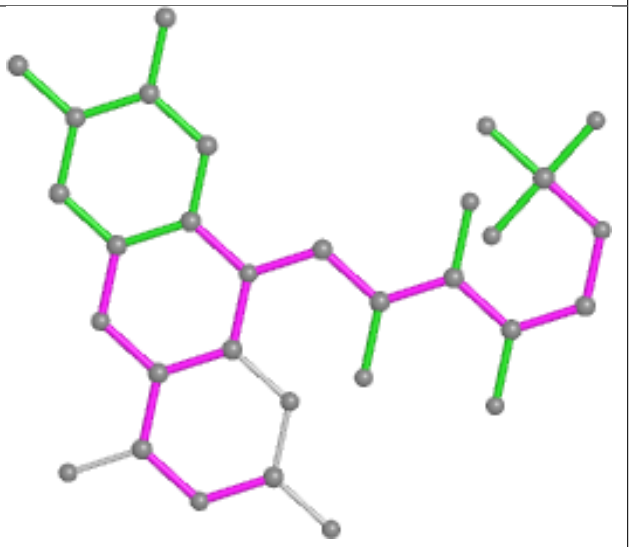


Rings

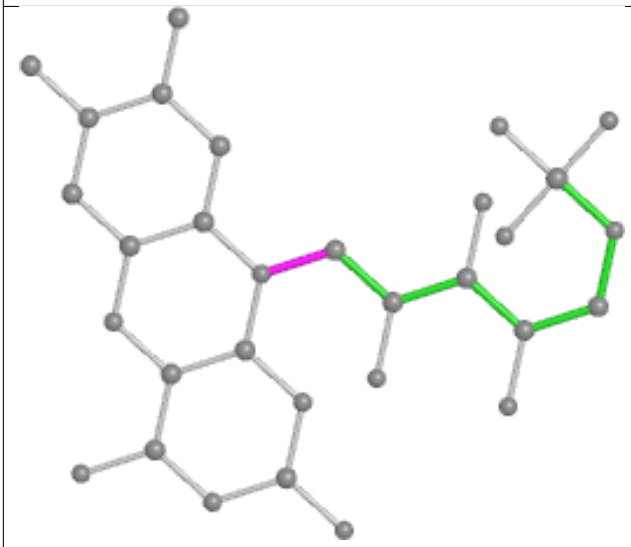
Ligand FMN Z 500



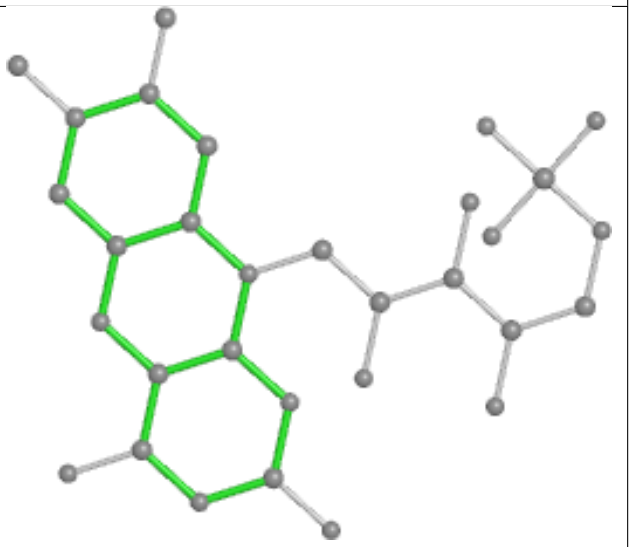
Bond lengths



Bond angles

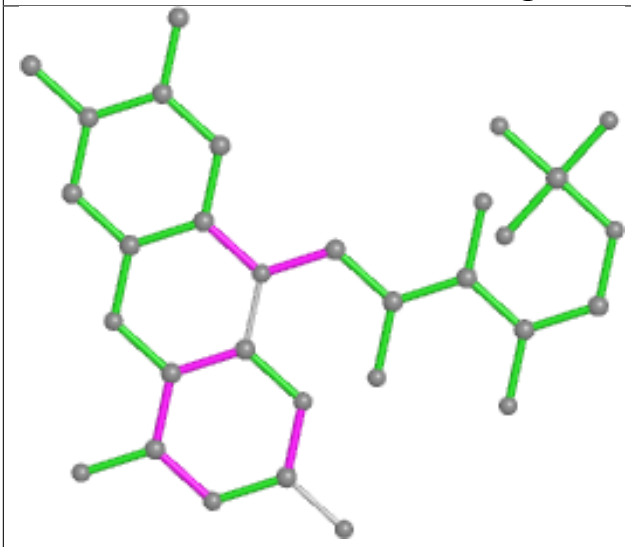


Torsions

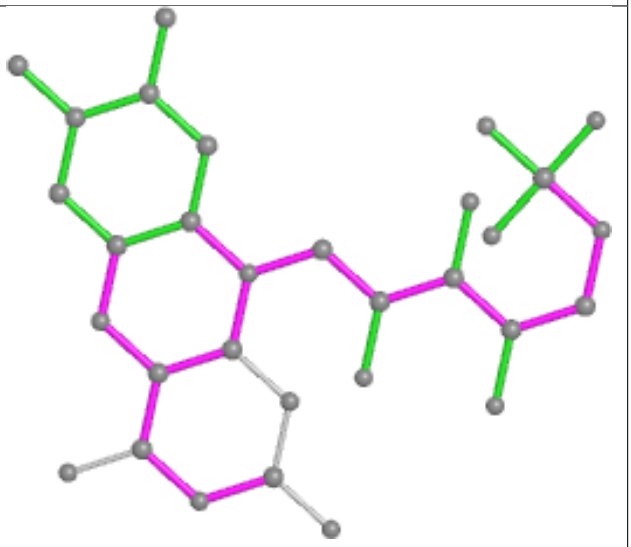


Rings

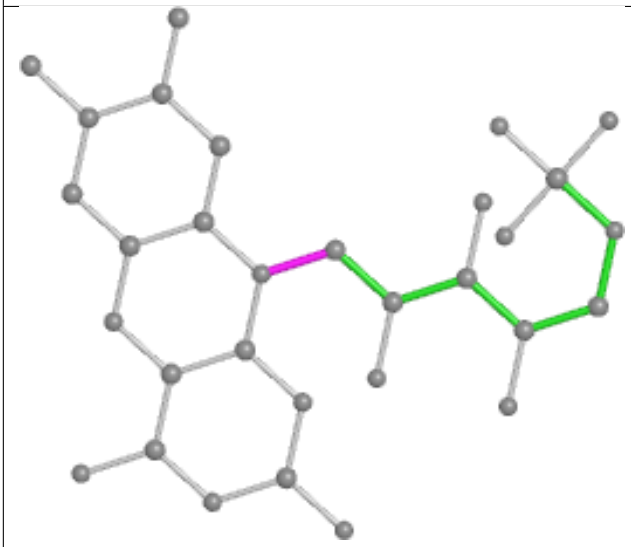
Ligand FMN Q 500



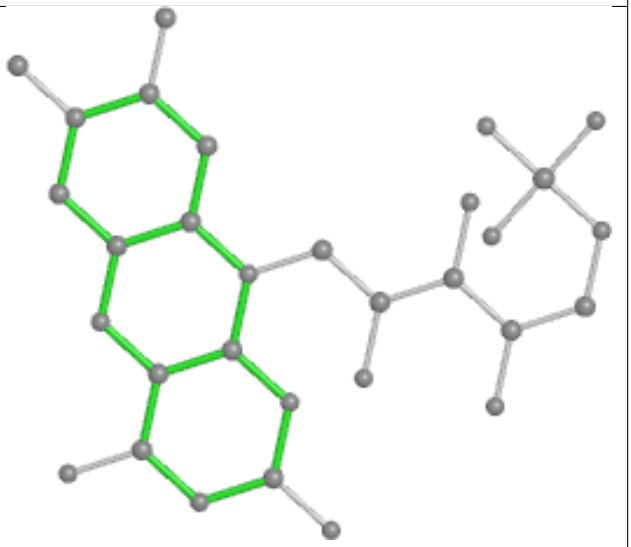
Bond lengths



Bond angles

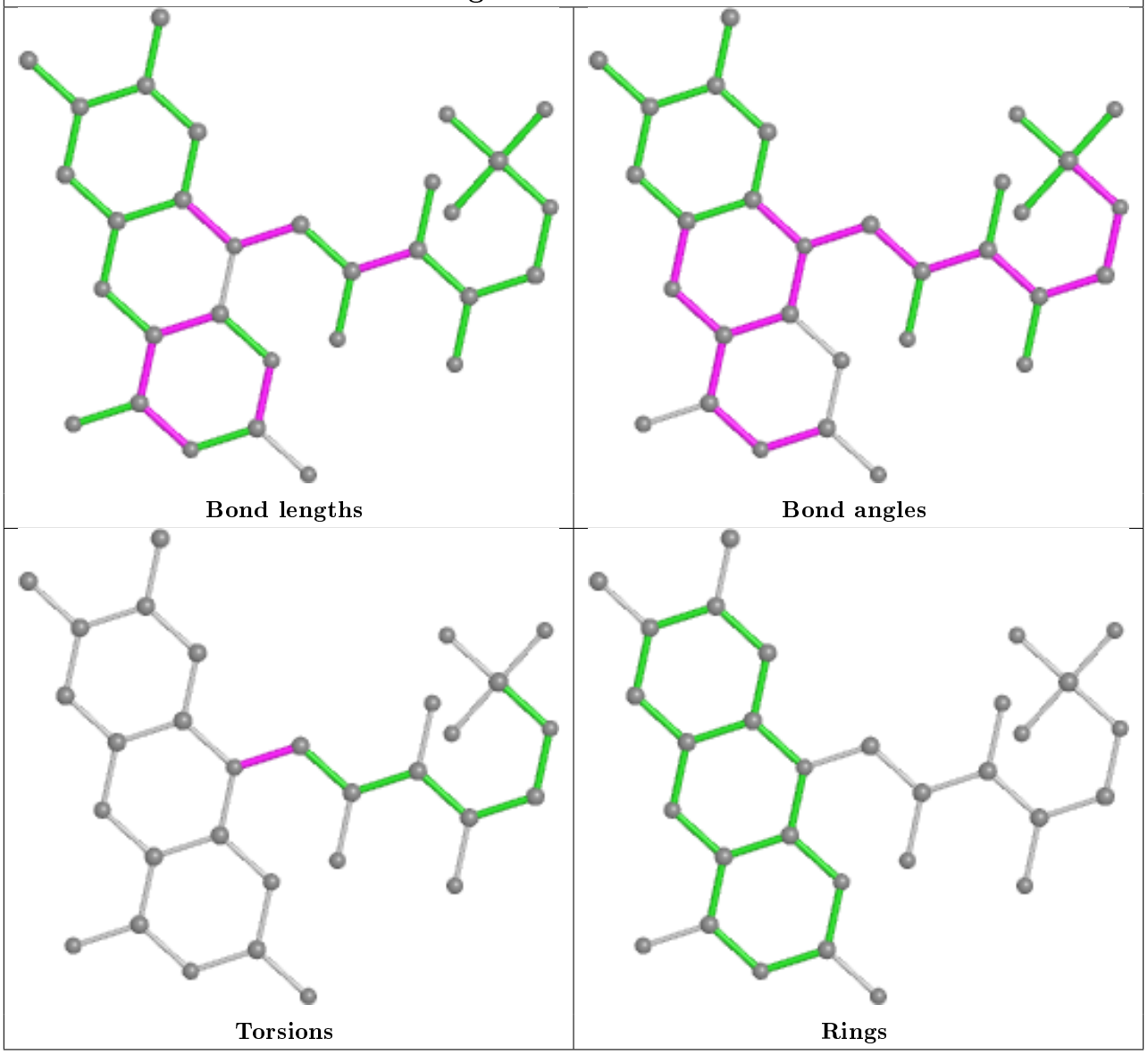


Torsions



Rings

Ligand FMN 7 500



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

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	432/438 (98%)	-0.14	0 100 100	14, 52, 90, 114	0
1	A	432/438 (98%)	-0.11	0 100 100	25, 57, 91, 115	0
1	J	432/438 (98%)	-0.13	2 (0%) 91 91	17, 52, 91, 113	0
1	S	432/438 (98%)	-0.16	1 (0%) 95 96	23, 58, 93, 115	0
2	2	178/181 (98%)	-0.15	0 100 100	26, 59, 98, 140	0
2	B	178/181 (98%)	-0.11	0 100 100	29, 64, 100, 141	0
2	K	178/181 (98%)	-0.08	1 (0%) 89 90	29, 60, 97, 143	0
2	T	178/181 (98%)	-0.20	1 (0%) 89 90	32, 66, 100, 146	0
3	3	737/783 (94%)	-0.02	8 (1%) 80 81	20, 65, 110, 130	0
3	C	737/783 (94%)	0.02	10 (1%) 75 75	23, 67, 111, 137	0
3	L	737/783 (94%)	0.10	20 (2%) 54 52	22, 69, 114, 137	0
3	U	737/783 (94%)	-0.00	11 (1%) 73 72	23, 68, 113, 135	0
4	4	370/409 (90%)	-0.00	4 (1%) 80 81	26, 67, 109, 167	0
4	D	370/409 (90%)	0.01	6 (1%) 72 70	26, 65, 109, 165	0
4	M	370/409 (90%)	0.02	5 (1%) 75 75	24, 65, 109, 158	0
4	V	370/409 (90%)	0.16	14 (3%) 40 37	32, 75, 113, 169	0
5	5	191/207 (92%)	-0.03	5 (2%) 56 53	35, 76, 112, 144	0
5	E	191/207 (92%)	0.02	4 (2%) 63 62	36, 76, 117, 138	0
5	N	191/207 (92%)	0.11	6 (3%) 49 48	36, 75, 114, 141	0
5	W	191/207 (92%)	0.15	7 (3%) 41 38	43, 83, 119, 143	0
6	6	144/181 (79%)	-0.05	0 100 100	34, 64, 110, 118	0
6	F	144/181 (79%)	0.01	1 (0%) 87 88	31, 62, 110, 119	0
6	O	144/181 (79%)	-0.01	2 (1%) 75 75	31, 62, 111, 116	0
6	X	144/181 (79%)	0.15	4 (2%) 53 51	45, 71, 113, 122	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	9	154/182 (84%)	-0.11	0 100 100	20, 56, 98, 118	0
7	G	154/182 (84%)	-0.11	0 100 100	26, 53, 95, 115	0
7	P	154/182 (84%)	-0.05	1 (0%) 89 90	26, 56, 96, 117	0
7	Y	154/182 (84%)	-0.05	0 100 100	31, 63, 100, 122	0
8	7	127/129 (98%)	-0.13	0 100 100	33, 62, 101, 116	0
8	H	127/129 (98%)	-0.12	0 100 100	35, 62, 102, 119	0
8	Q	127/129 (98%)	-0.01	0 100 100	32, 63, 104, 116	0
8	Z	127/129 (98%)	0.00	3 (2%) 59 56	34, 68, 105, 119	0
All	All	9332/10040 (92%)	-0.02	116 (1%) 79 78	14, 64, 109, 169	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	759	TYR	5.5
5	N	184	TYR	4.6
3	L	653	PRO	4.4
3	L	654	PHE	4.3
5	N	1	MET	4.3

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 monosaccharides 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, 95th 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
11	FMN	H	500	31/31	0.88	0.29	80,87,88,90	0
11	FMN	Q	500	31/31	0.90	0.29	79,86,88,91	0

Continued on next page...

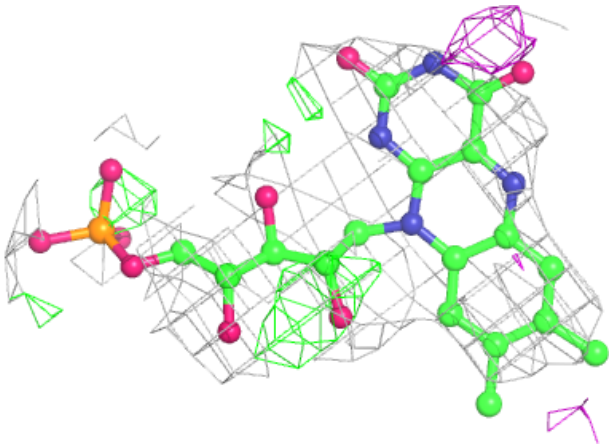
Continued from previous page...

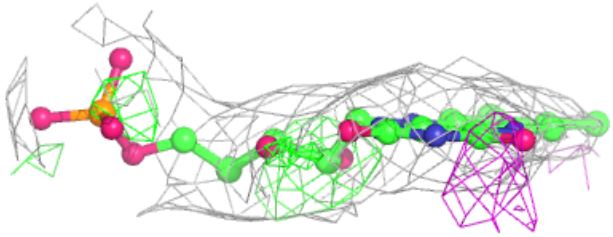
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	FMN	Z	500	31/31	0.91	0.32	99,103,105,106	0
11	FMN	7	500	31/31	0.92	0.28	75,80,83,87	0
9	SF4	Y	183	8/8	0.98	0.19	20,27,29,44	0
9	SF4	X	182	8/8	0.98	0.17	21,42,47,61	0
9	SF4	3	784	8/8	0.99	0.18	1,12,15,16	0
9	SF4	U	784	8/8	0.99	0.17	1,17,19,19	0
10	FES	3	787	4/4	0.99	0.14	1,1,12,15	0
9	SF4	G	183	8/8	0.99	0.18	1,23,24,25	0
9	SF4	3	785	8/8	0.99	0.20	1,17,21,21	0
9	SF4	Y	184	8/8	0.99	0.17	7,20,22,22	0
9	SF4	G	184	8/8	0.99	0.17	1,16,19,21	0
9	SF4	U	786	8/8	0.99	0.19	19,40,45,45	0
9	SF4	C	785	8/8	0.99	0.19	1,16,17,18	0
9	SF4	O	182	8/8	0.99	0.17	4,14,18,18	0
9	SF4	J	439	8/8	0.99	0.19	1,8,14,18	0
9	SF4	C	786	8/8	0.99	0.19	12,31,36,38	0
10	FES	L	787	4/4	0.99	0.14	1,1,9,14	0
10	FES	C	787	4/4	0.99	0.12	1,4,16,18	0
9	SF4	S	439	8/8	0.99	0.19	14,30,33,34	0
9	SF4	P	183	8/8	0.99	0.19	1,25,26,32	0
10	FES	2	182	4/4	0.99	0.13	1,4,19,19	0
10	FES	T	182	4/4	0.99	0.11	2,9,29,30	0
9	SF4	9	183	8/8	0.99	0.18	1,17,18,29	0
9	SF4	A	439	8/8	0.99	0.17	1,17,22,24	0
9	SF4	9	184	8/8	0.99	0.18	1,15,24,25	0
9	SF4	L	785	8/8	0.99	0.20	1,13,15,16	0
9	SF4	F	182	8/8	0.99	0.17	1,16,16,17	0
9	SF4	P	184	8/8	0.99	0.20	3,18,20,20	0
9	SF4	1	439	8/8	0.99	0.18	1,9,17,17	0
9	SF4	C	784	8/8	0.99	0.18	1,10,19,20	0
9	SF4	U	785	8/8	0.99	0.19	9,18,20,21	0
10	FES	U	787	4/4	0.99	0.12	4,5,15,17	0
9	SF4	L	786	8/8	0.99	0.15	17,28,31,35	0
9	SF4	6	182	8/8	0.99	0.18	12,32,33,34	0
9	SF4	3	786	8/8	0.99	0.18	5,31,32,34	0
10	FES	B	182	4/4	1.00	0.13	2,13,32,33	0
10	FES	K	182	4/4	1.00	0.12	2,5,21,23	0
9	SF4	L	784	8/8	1.00	0.18	1,8,15,17	0

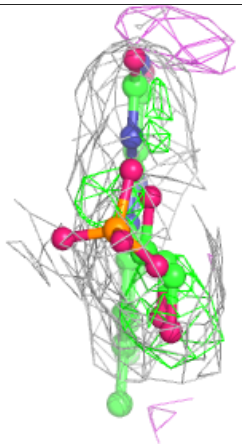
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN H 500:

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

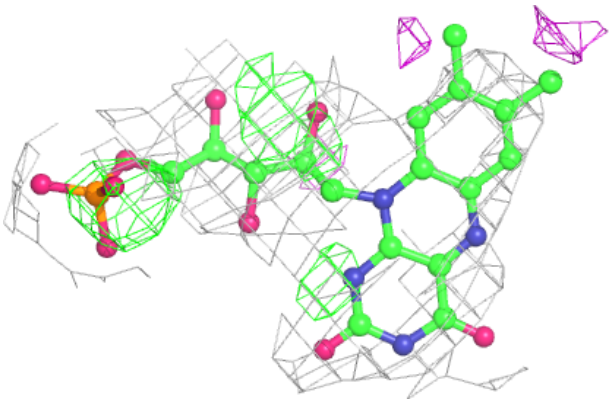


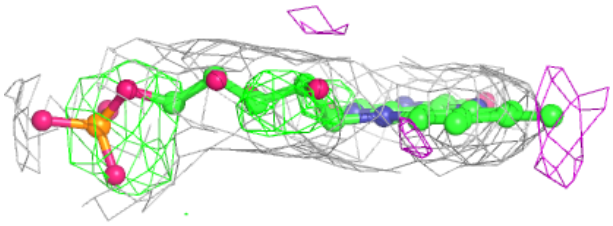


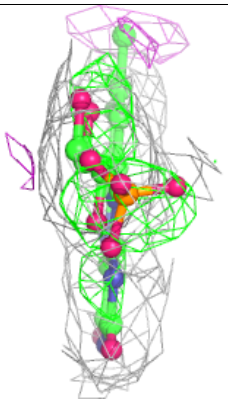


Electron density around FMN Q 500:

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

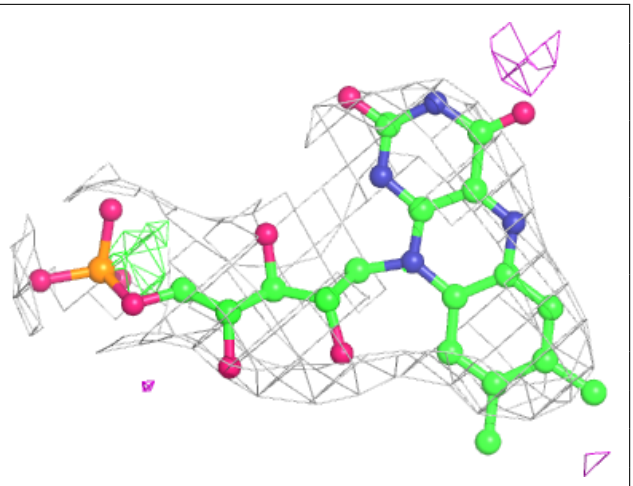


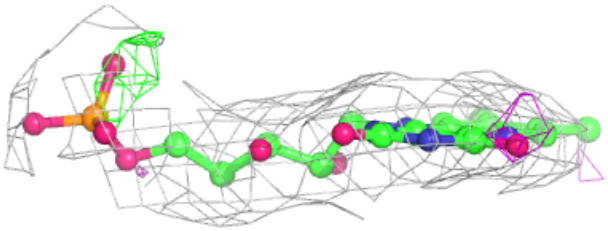


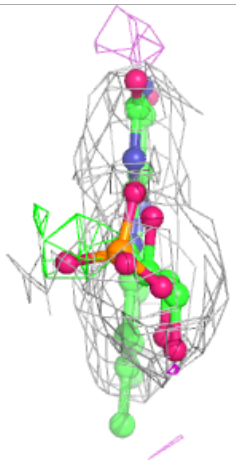


Electron density around FMN Z 500:

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

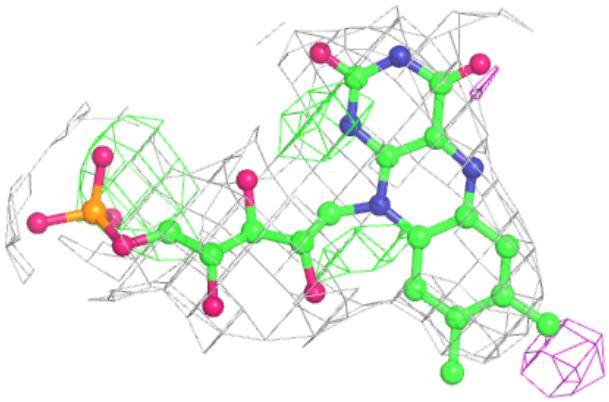


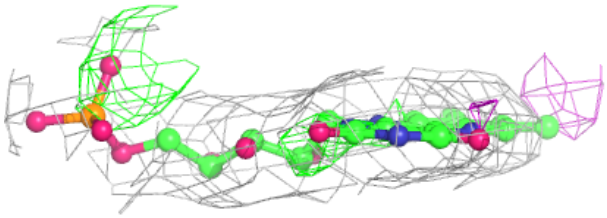


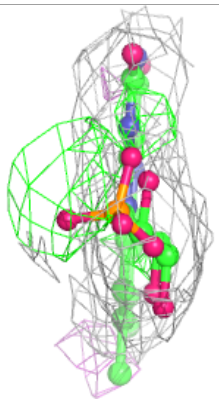


Electron density around FMN 7 500:

$2mF_o$-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

There are no such residues in this entry.