wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 05:15 PM EDT

PDB ID	:	6Q8W
Title	:	Respiratory complex I from Thermus thermophilus with bound Aureothin.
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2018-12-16
Resolution	:	3.40 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 (1)) were used in the production of this report:

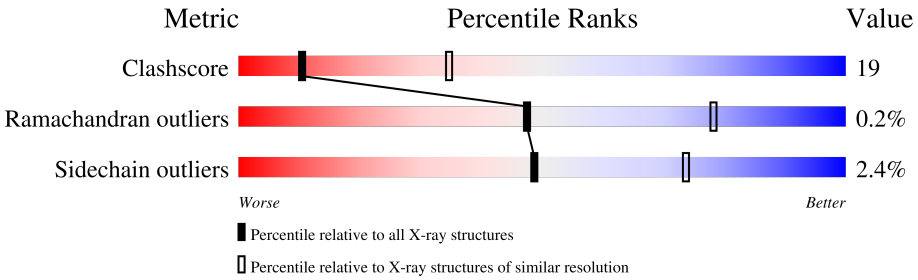
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	64% 34% ·
1	B	438	57% 41% ·
2	2	181	66% 30% · ·
2	C	181	62% 34% · ·
3	3	783	59% 37% · ·
3	D	783	62% 34% · ·
4	4	409	51% 43% 6%
4	E	409	50% 42% · 6%

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Mol	Chain	Length	Quality of chain
5	5	207	57% 36% • 5%
5	F	207	60% 33% • 5%
6	6	181	35% 54% • 8%
6	G	181	44% 45% • 8%
7	9	182	61% 37% ••
7	O	182	60% 38% •••
8	7	129	71% 27% ••
8	I	129	70% 28% ••
9	W	131	68% 28% ••
9	X	131	76% 20% ••
10	A	119	51% 45% ••
10	P	119	55% 40% ••
11	J	176	53% 37% • 9%
11	R	176	55% 35% • 9%
12	K	95	64% 34% •
12	S	95	69% 29% •
13	L	606	66% 33% •
13	T	606	66% 33% •
14	M	469	65% 34% •
14	U	469	64% 35% •
15	N	427	67% 32% •
15	V	427	69% 30%
16	H	365	50% 43% ••
16	Q	365	50% 43% •••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	1	501	-	-	X	-
17	SF4	B	501	-	-	X	-
19	FES	3	804	-	-	X	-
19	FES	C	201	-	-	X	-
19	FES	D	804	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 74144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-quinone oxidoreductase subunit 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called Uncharacterized protein.

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

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

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

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

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

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

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

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

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

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

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

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

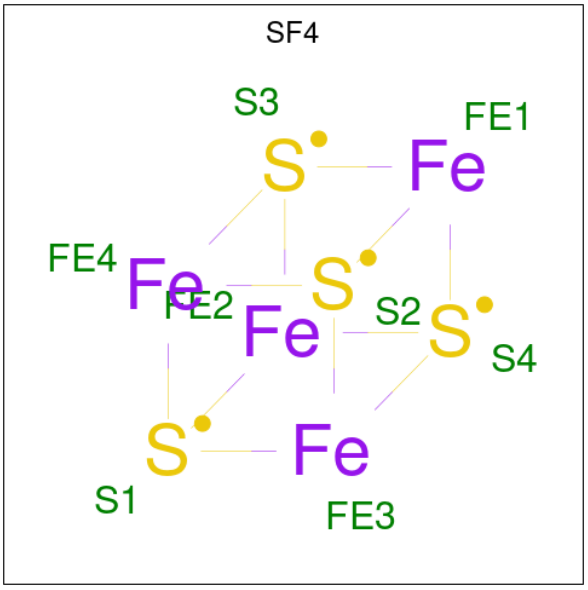
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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

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

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

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



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

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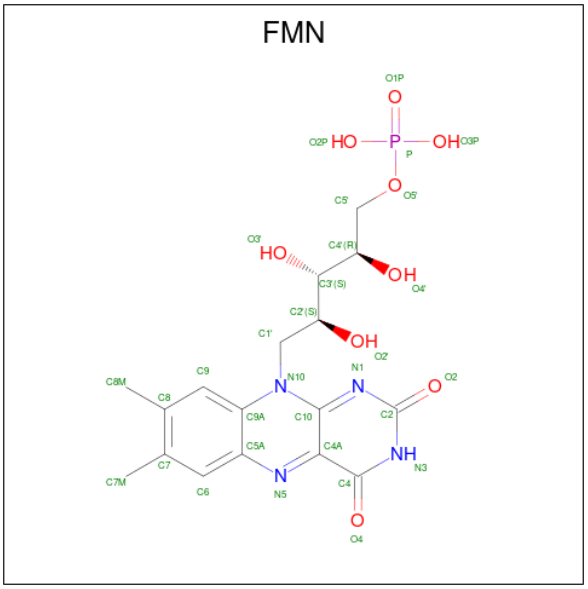
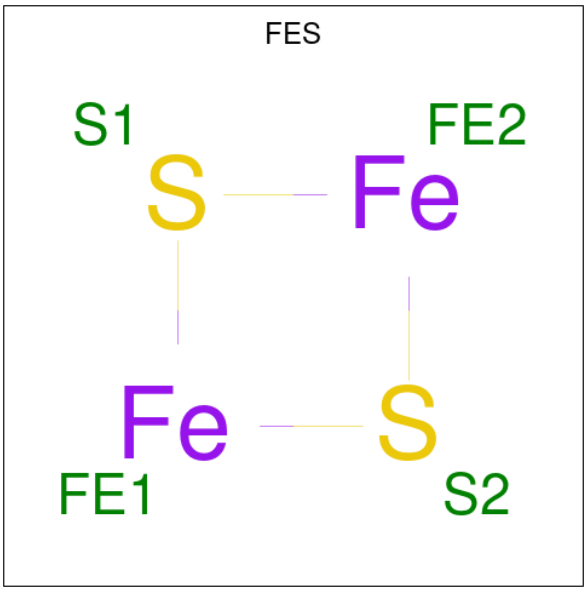
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total Fe S 8 4 4	0	0
17	D	1	Total Fe S 8 4 4	0	0
17	G	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0

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



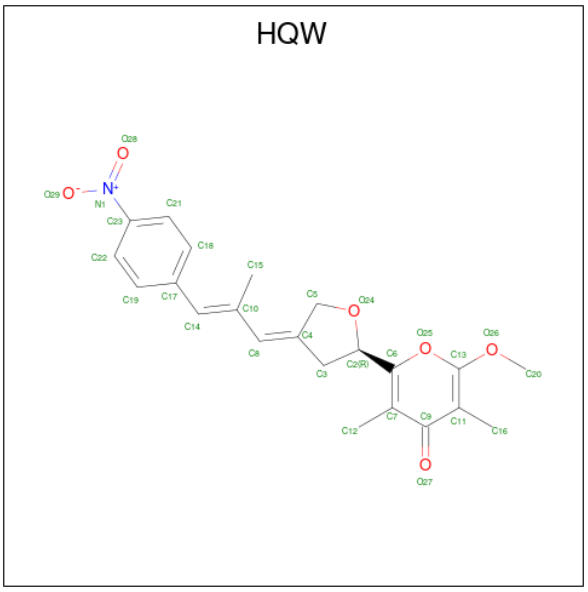
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	1	1	Total C N O P 31 17 4 9 1	0	0
18	B	1	Total C N O P 31 17 4 9 1	0	0

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



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

- Molecule 20 is Aureothin (three-letter code: HQW) (formula: $C_{22}H_{23}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	4	1	Total	C	N	O	0	0
			29	22	1	6		
20	E	1	Total	C	N	O	0	0
			29	22	1	6		

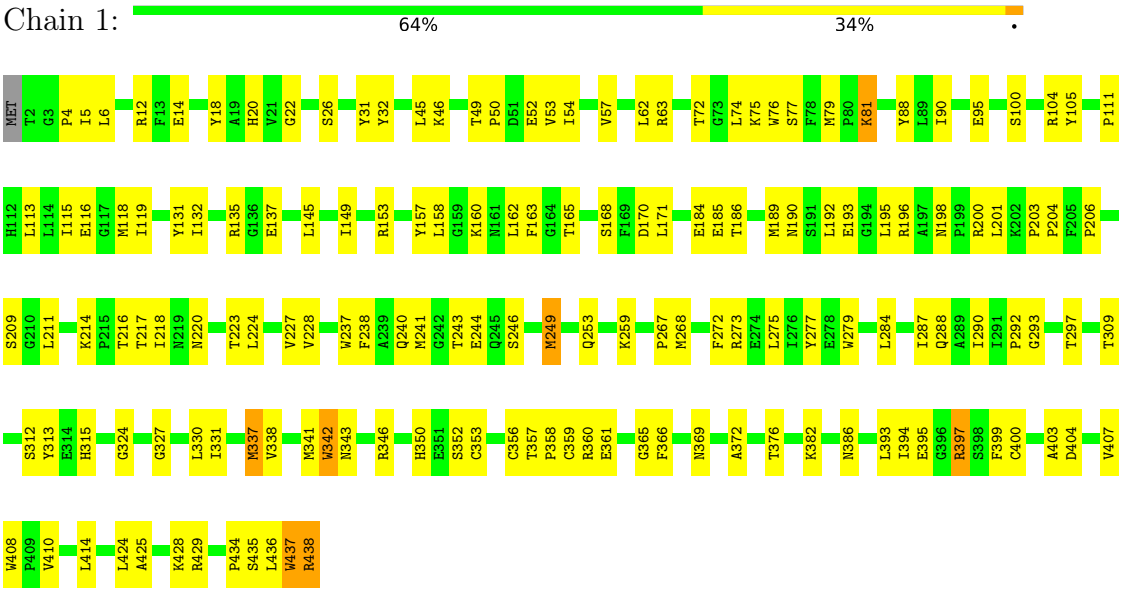
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

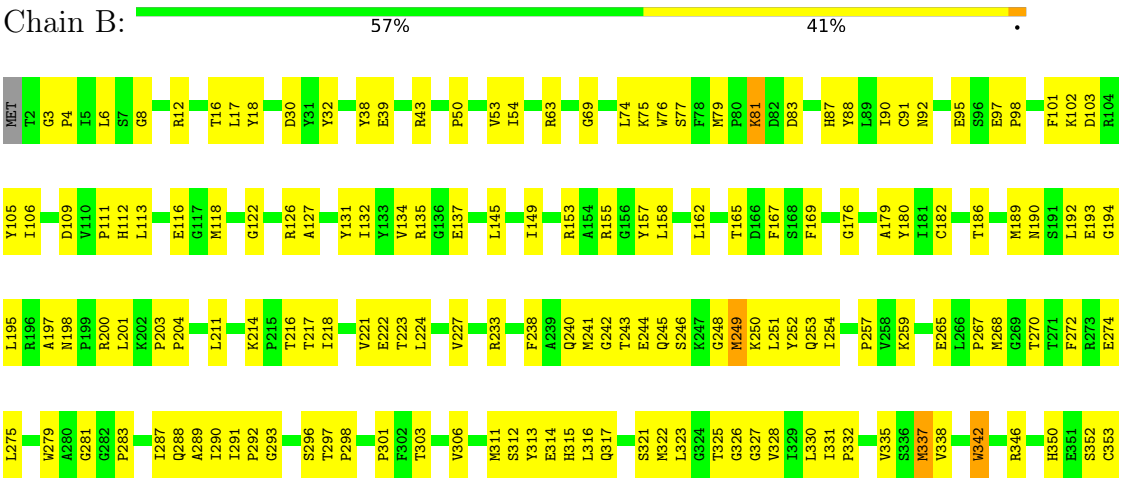
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain 1:



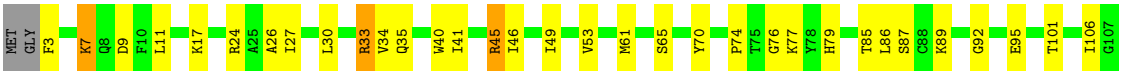
• Molecule 1: NADH-quinone oxidoreductase subunit 1

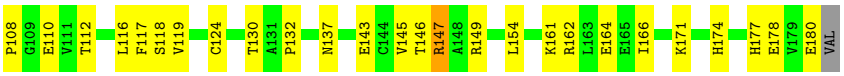
Chain B:



• Molecule 2: NADH-quinone oxidoreductase subunit 2

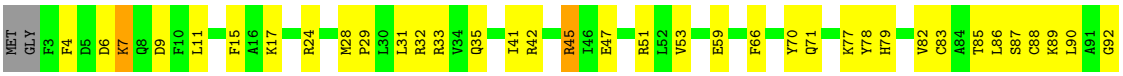
Chain 2:

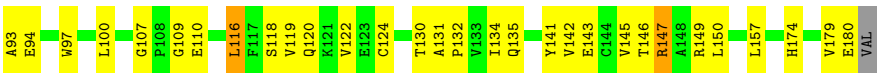




• Molecule 2: NADH-quinone oxidoreductase subunit 2

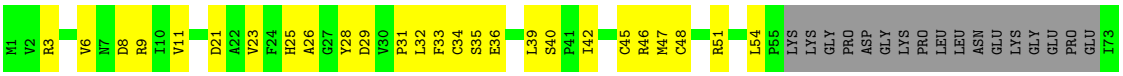
Chain C:

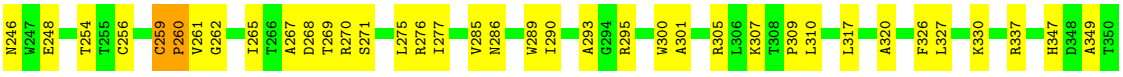


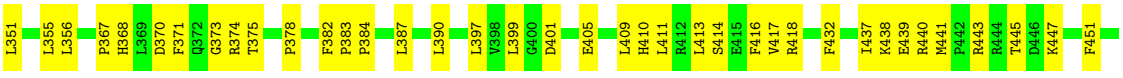


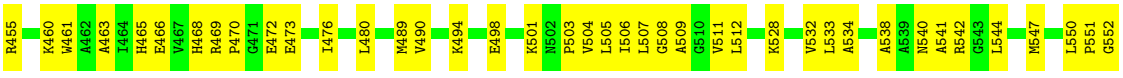
• Molecule 3: NADH-quinone oxidoreductase subunit 3

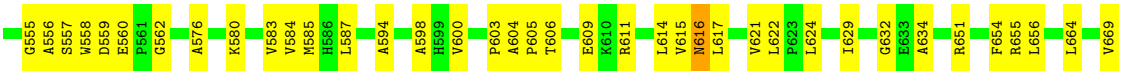
Chain 3:

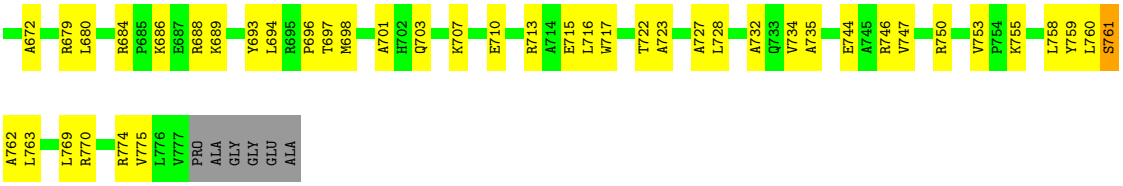






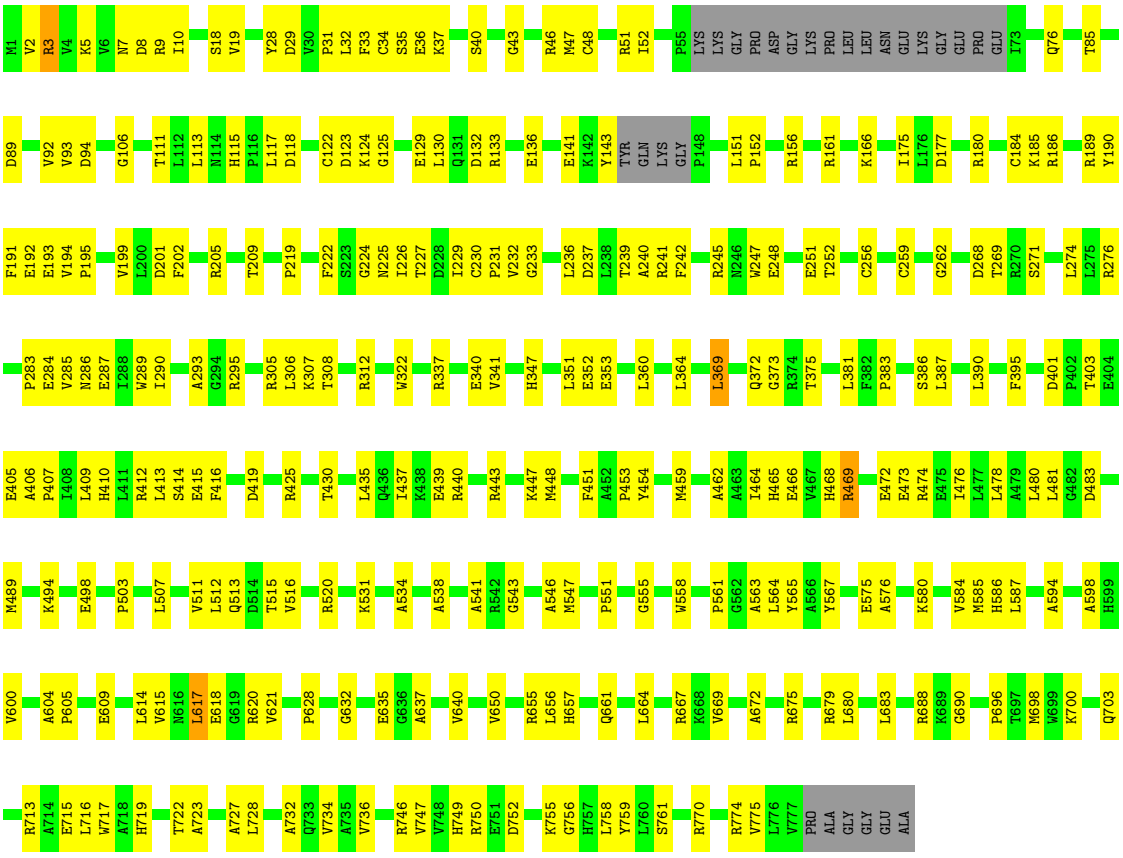






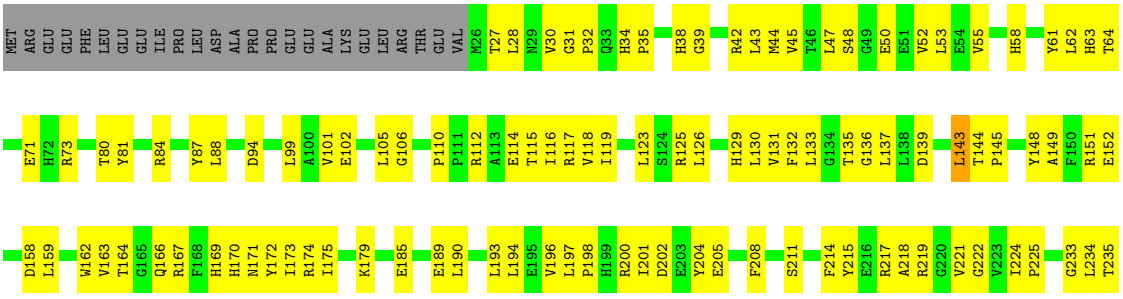
• Molecule 3: NADH-quinone oxidoreductase subunit 3

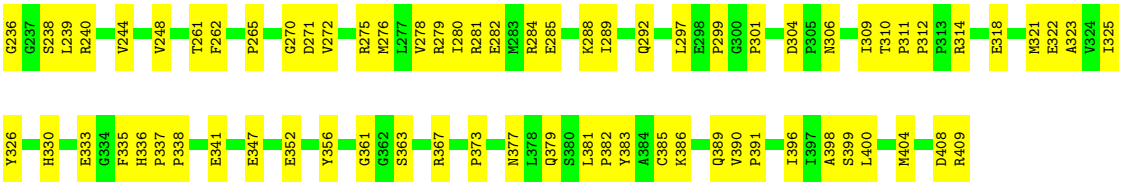
Chain D:



• Molecule 4: NADH-quinone oxidoreductase subunit 4

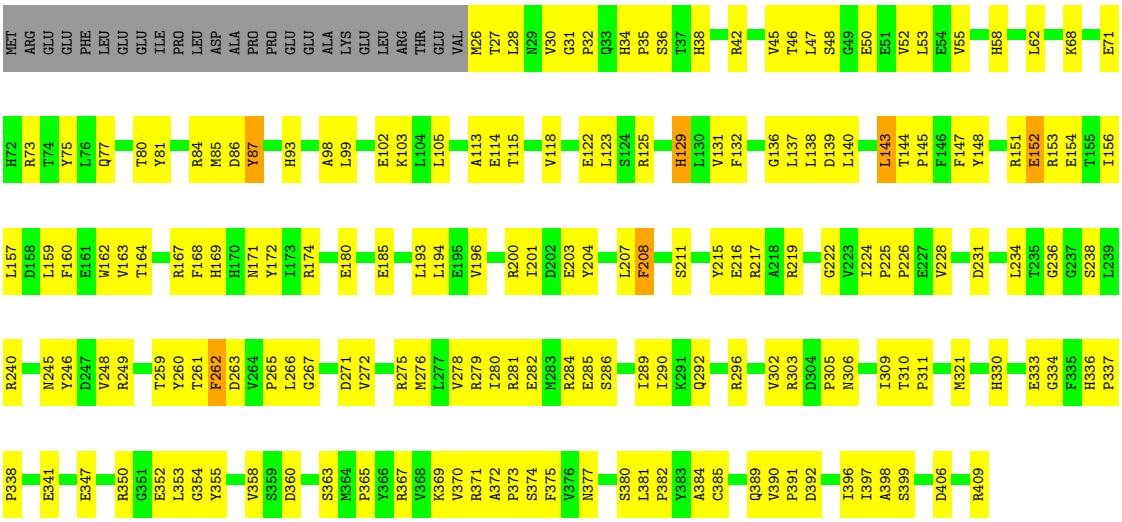
Chain 4:





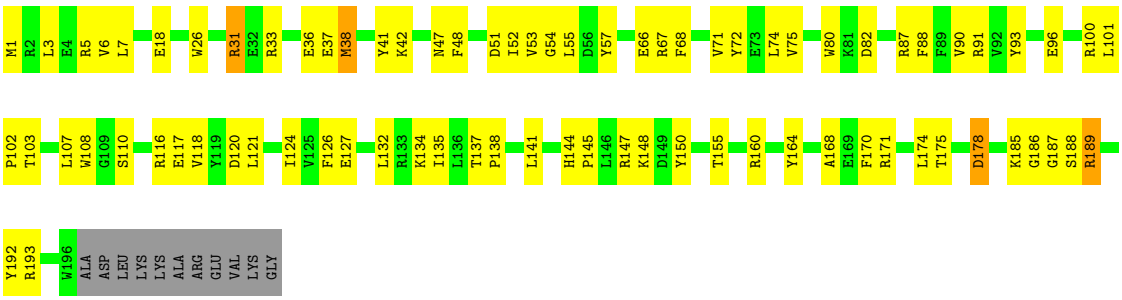
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E:



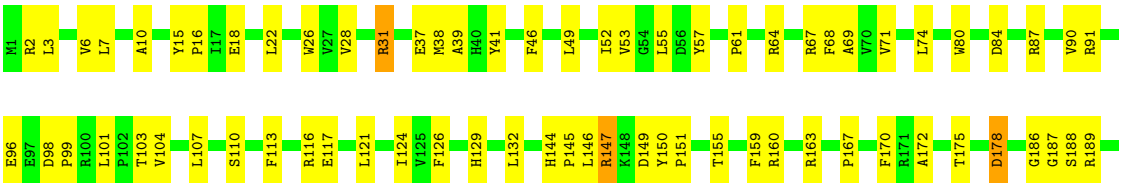
• Molecule 5: NADH-quinone oxidoreductase subunit 5

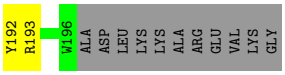
Chain 5:



• Molecule 5: NADH-quinone oxidoreductase subunit 5

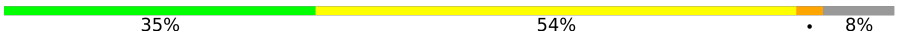
Chain F:

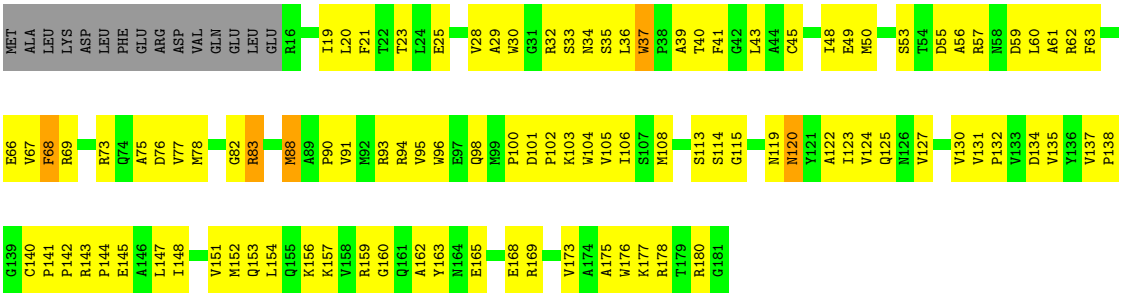




• Molecule 6: NADH-quinone oxidoreductase subunit 6

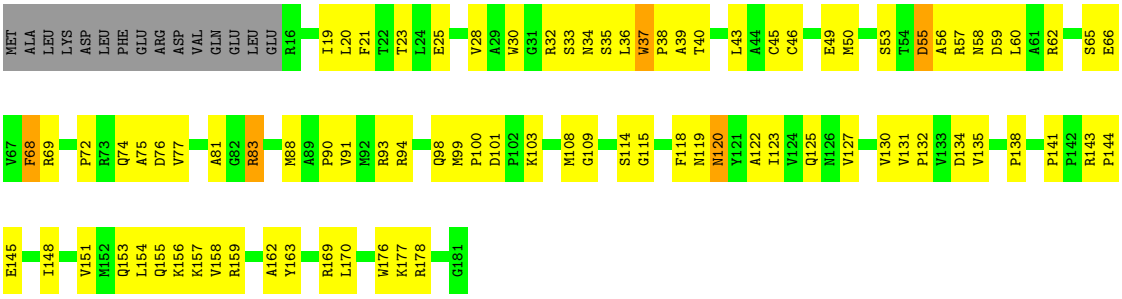
Chain 6:





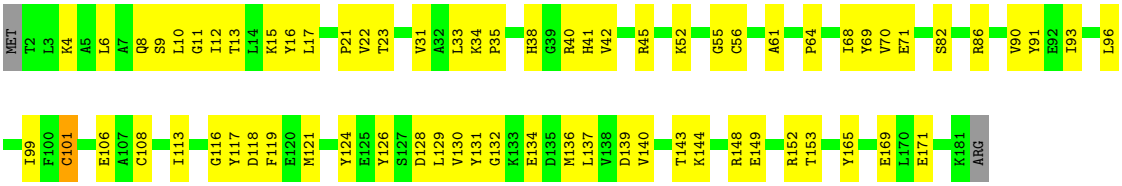
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G:



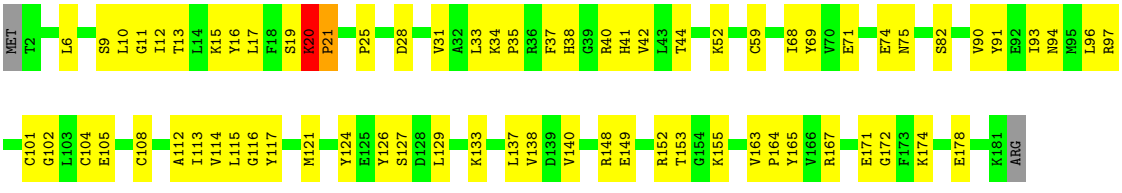
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:



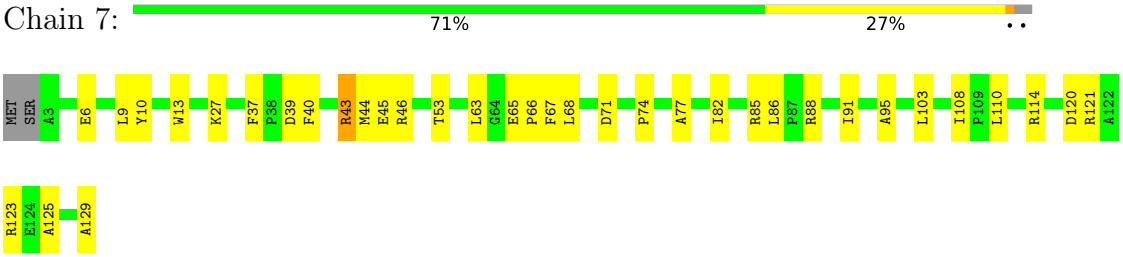
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:



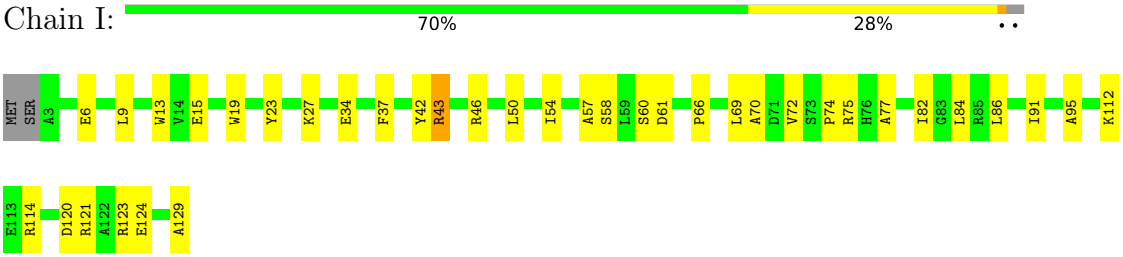
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:



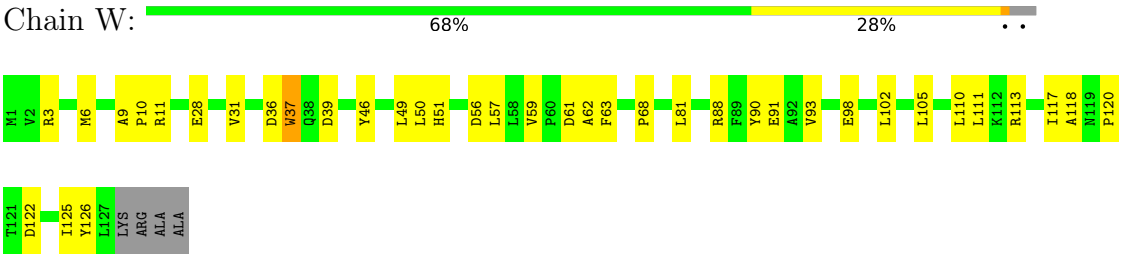
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:



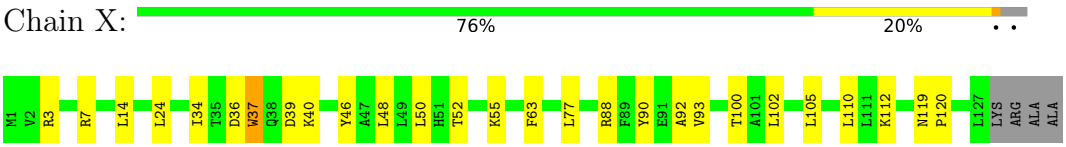
• Molecule 9: Uncharacterized protein

Chain W:



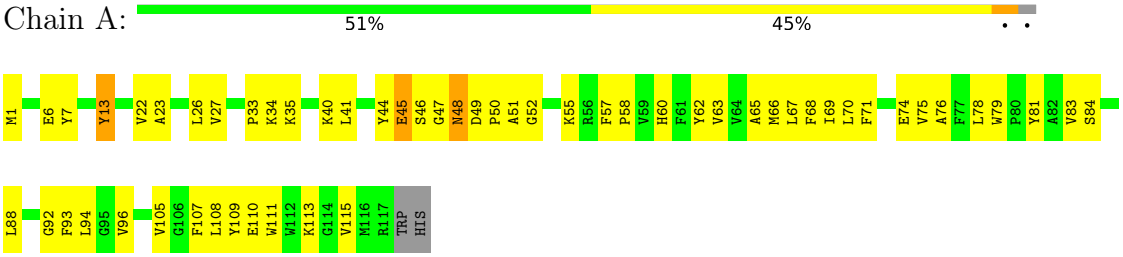
• Molecule 9: Uncharacterized protein

Chain X:



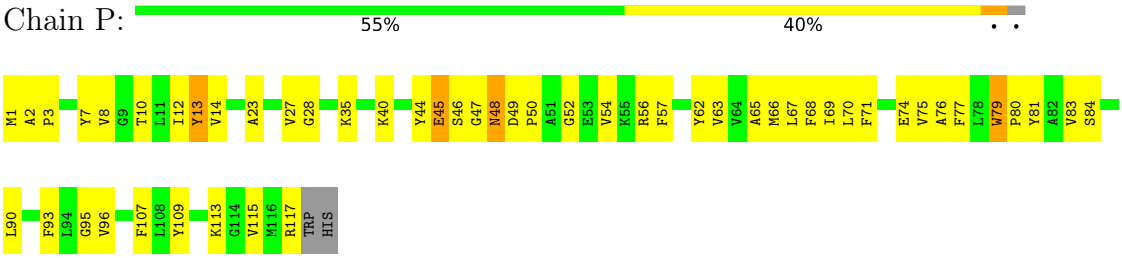
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:



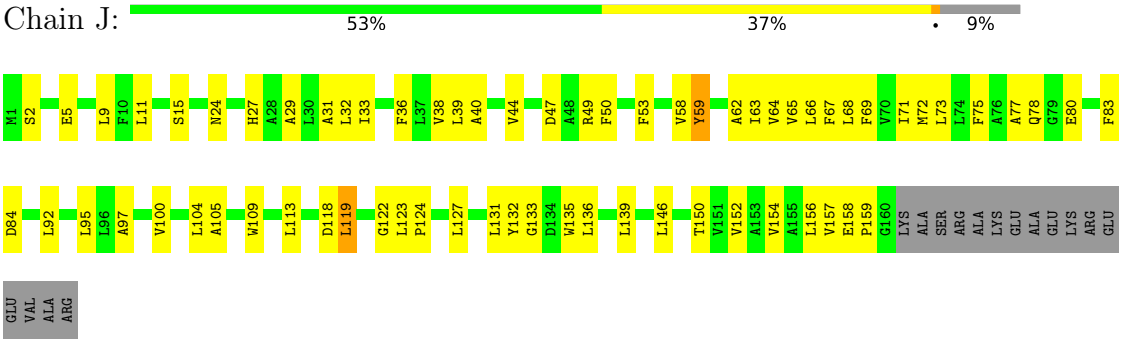
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



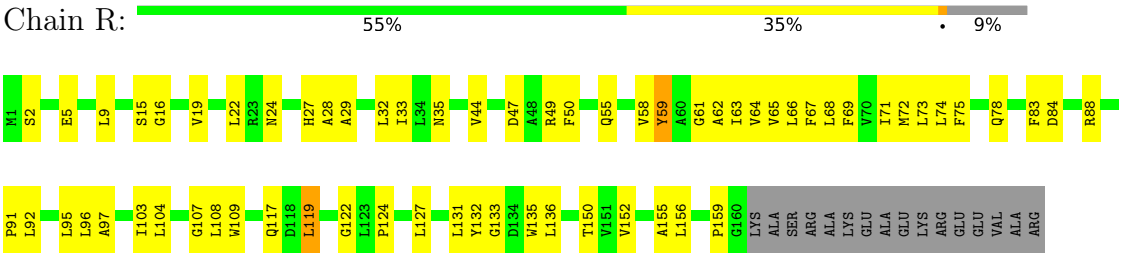
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



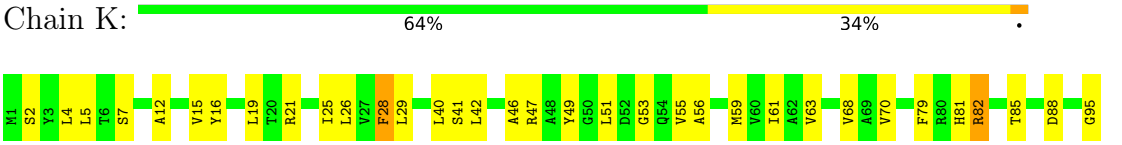
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



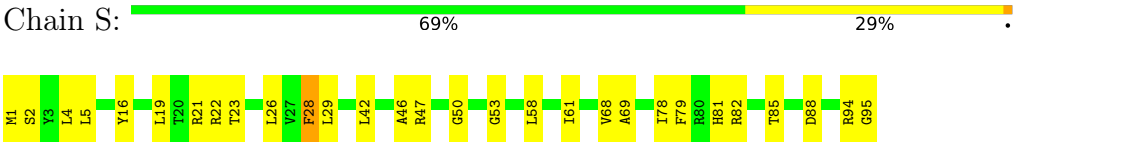
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



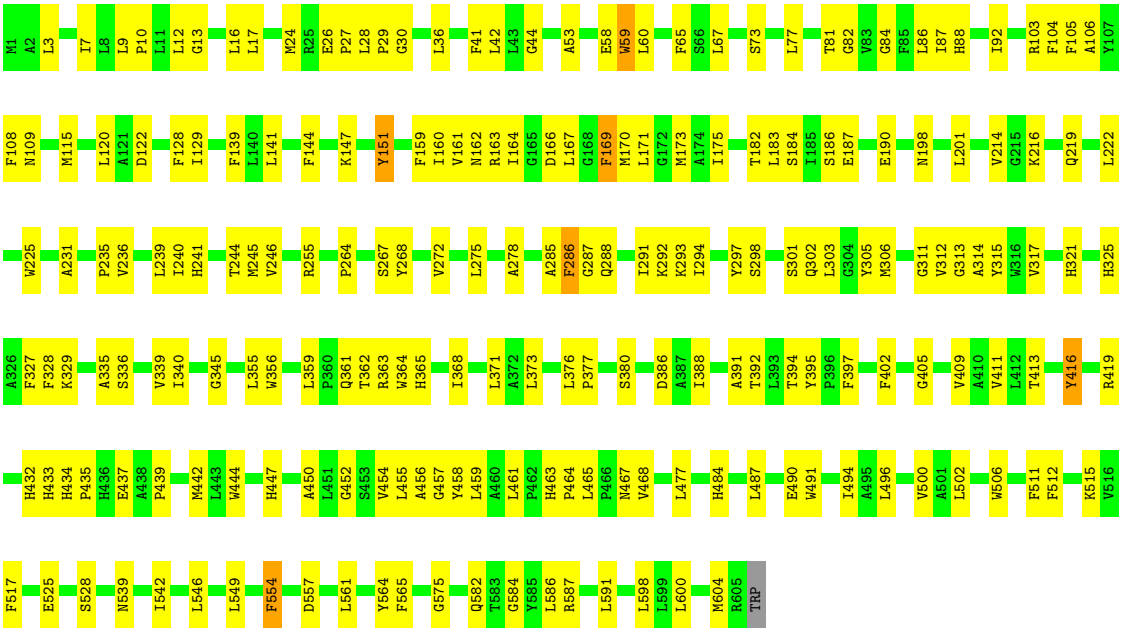
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



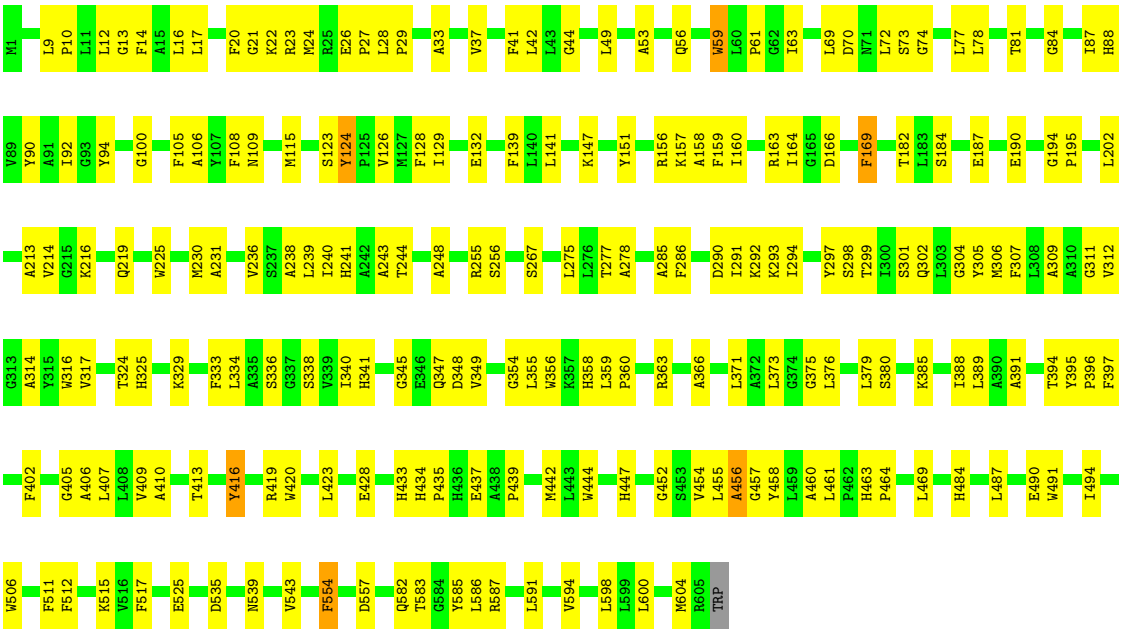
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:



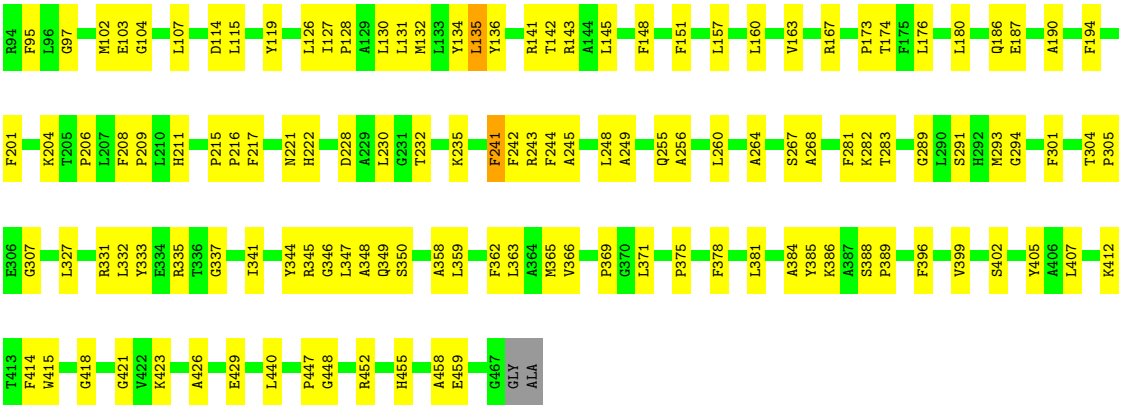
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain T:



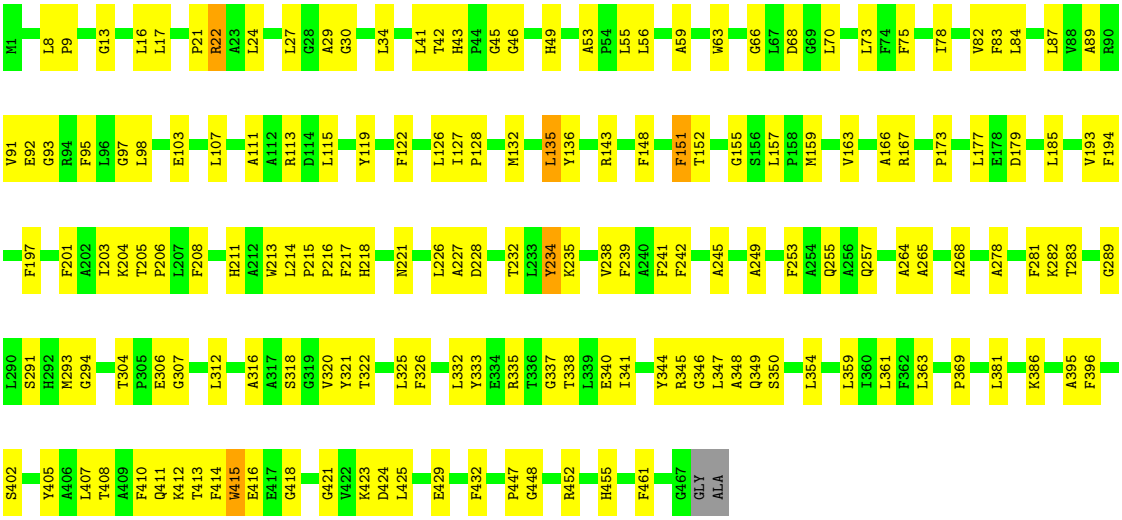
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain M:



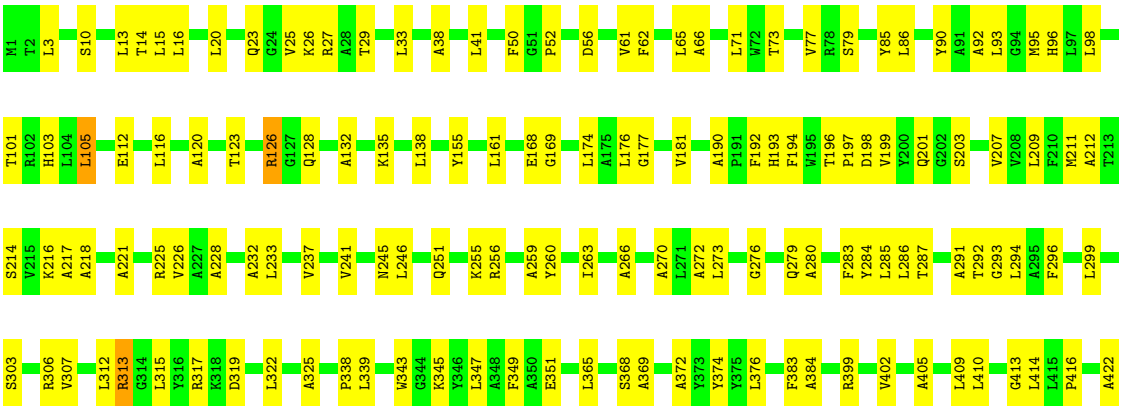
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U:



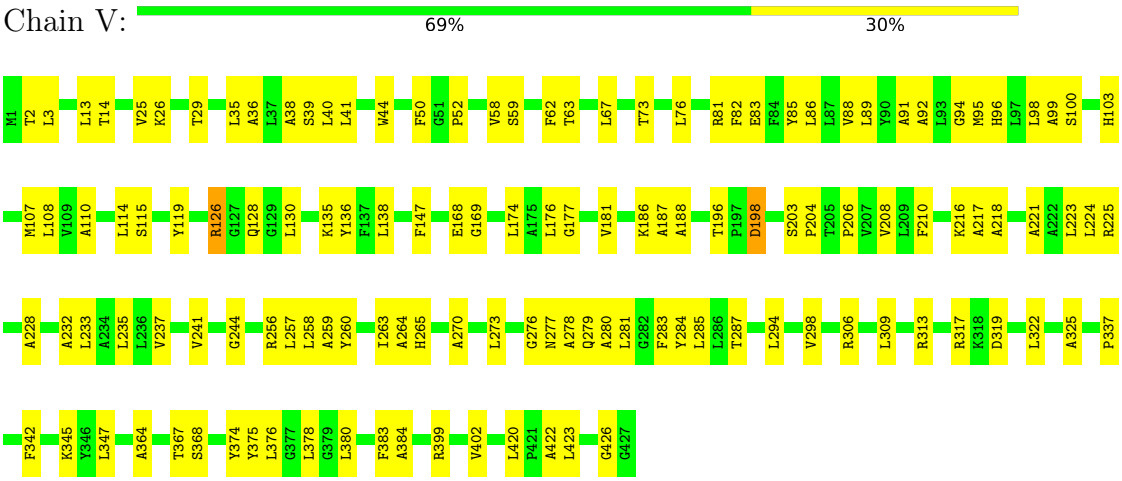
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N:



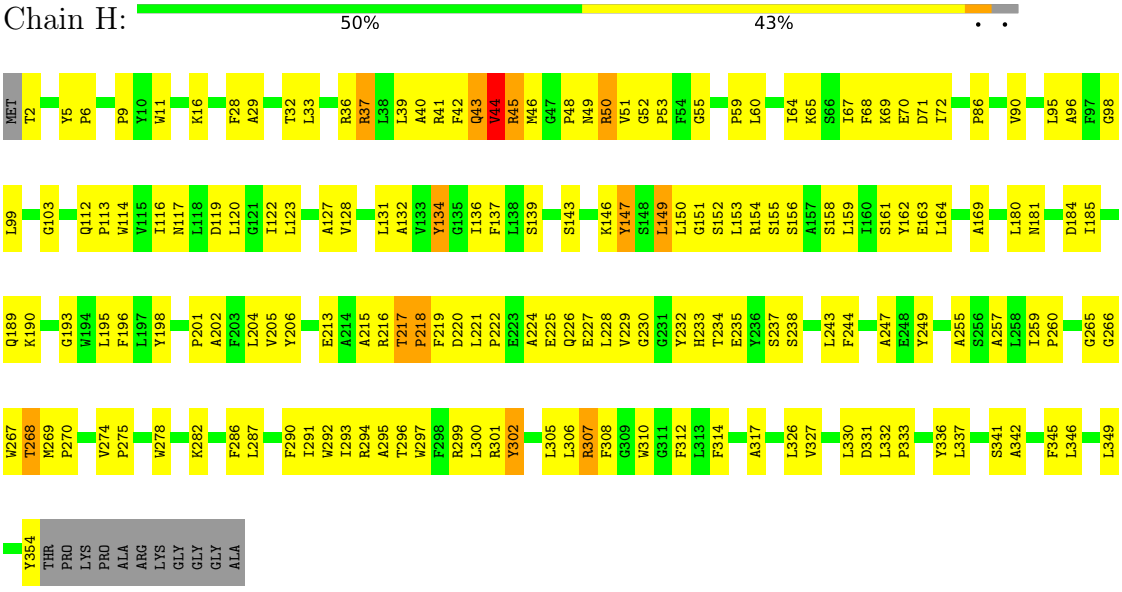
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V:



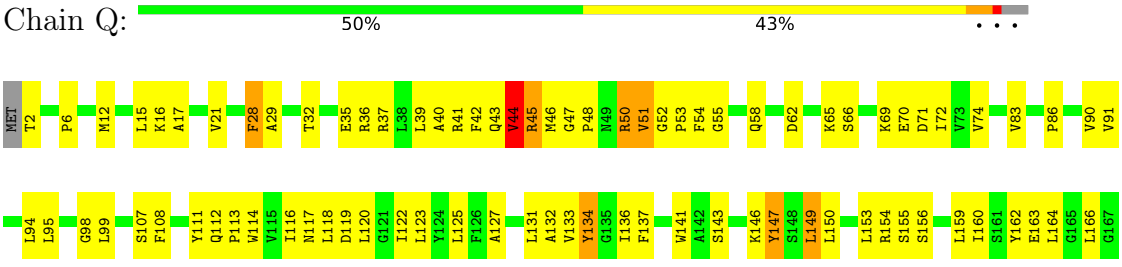
• Molecule 16: NADH-quinone oxidoreductase subunit 8

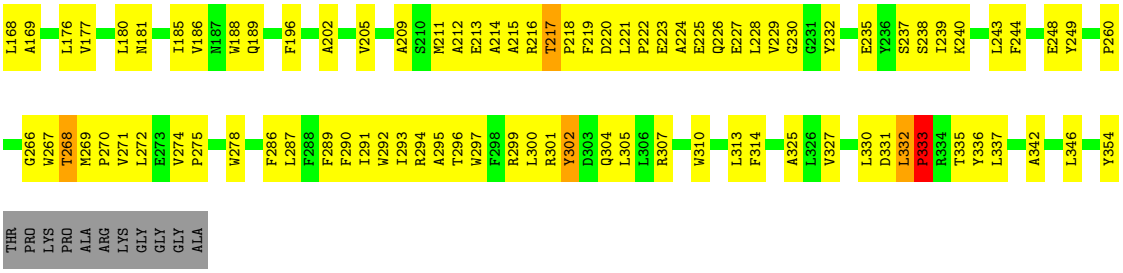
Chain H:



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:




L168 A169 L176 V177 L180 N181 I185 V186 N187 W188 Q189 F196 A202 V205 A209 S210 M211 A212 E213 A214 A215 R216 T217 P218 F219 D220 L221 P222 E223 A224 E225 Q226 E227 L228 V229 G230 G231 Y232 E235 Y236 S237 S238 I239 K240 L243 F244 E248 Y249 P260
G266 W267 T268 M269 P270 V271 L272 E273 V274 P275 W278 F286 L287 F288 F289 F290 I291 W292 I293 R294 A295 T296 W297 F298 R299 L300 R301 Y302 D303 Q304 L305 L306 R307 W310 L313 F314 A325 L326 V327 L330 D331 L332 P333 R334 T335 Y336 L337 A342 L346 Y354
THR PRO LYS PRO ALA ARG LYS GLY GLY GLY ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.98Å 340.50Å 264.27Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	49.71 – 3.40	Depositor
% Data completeness (in resolution range)	84.1 (49.71-3.40)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.40Å)	Xtriage
Refinement program	PHENIX (dev_3026: ???)	Depositor
R, R_{free}	0.213 , 0.234	Depositor
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.027	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.379 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 191608 reflections	Xtriage
Total number of atoms	74144	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3506	0.54	0/4745
1	B	0.29	0/3506	0.49	0/4745
2	2	0.33	0/1439	0.50	0/1953
2	C	0.29	0/1439	0.47	0/1953
3	3	0.43	0/6035	0.66	0/8185
3	D	0.41	0/6035	0.62	1/8185 (0.0%)
4	4	0.39	0/3150	0.60	1/4284 (0.0%)
4	E	0.32	0/3150	0.52	0/4284
5	5	0.40	0/1656	0.60	1/2246 (0.0%)
5	F	0.36	0/1656	0.57	0/2246
6	6	0.46	0/1319	0.66	0/1786
6	G	0.40	0/1319	0.63	1/1786 (0.1%)
7	9	0.51	1/1423 (0.1%)	0.64	0/1933
7	O	0.38	0/1423	0.71	1/1933 (0.1%)
8	7	0.34	0/1059	0.56	1/1429 (0.1%)
8	I	0.31	0/1059	0.53	0/1429
9	W	0.41	0/985	0.68	1/1335 (0.1%)
9	X	0.38	0/985	0.57	0/1335
10	A	0.34	0/940	0.53	0/1280
10	P	0.33	0/940	0.53	0/1280
11	J	0.33	0/1206	0.54	0/1649
11	R	0.29	0/1206	0.49	0/1649
12	K	0.31	0/710	0.51	0/962
12	S	0.30	0/710	0.50	0/962
13	L	0.31	0/4741	0.49	0/6460
13	T	0.28	0/4741	0.46	0/6460
14	M	0.33	0/3591	0.53	0/4896
14	U	0.28	0/3591	0.47	0/4896
15	N	0.34	0/3238	0.50	0/4434
15	V	0.31	0/3238	0.47	0/4434
16	H	0.33	0/2935	0.55	0/4014
16	Q	0.33	0/2935	0.57	1/4014 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.35	1/75866 (0.0%)	0.55	8/103182 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	9	0	1
10	A	0	1
10	P	0	1
13	T	0	2
16	H	0	2
16	Q	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	101	CYS	CB-SG	-5.81	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	20	LYS	C-N-CD	-16.21	84.94	120.60
4	4	133	LEU	CA-CB-CG	6.46	130.16	115.30
6	G	169	ARG	C-N-CA	-6.21	106.17	121.70
5	5	189	ARG	NE-CZ-NH1	5.99	123.29	120.30
16	Q	332	LEU	CA-CB-CG	5.45	127.83	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	21	PRO	Peptide
10	A	45	GLU	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
10	P	45	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3389	122	0
1	B	3417	0	3389	155	0
2	2	1406	0	1373	63	0
2	C	1406	0	1373	58	0
3	3	5895	0	5931	235	0
3	D	5895	0	5930	196	0
4	4	3067	0	3049	166	0
4	E	3067	0	3049	166	0
5	5	1607	0	1574	81	0
5	F	1607	0	1574	65	0
6	6	1289	0	1299	104	0
6	G	1289	0	1298	99	0
7	9	1388	0	1383	70	0
7	O	1388	0	1383	65	0
8	7	1031	0	1029	35	0
8	I	1031	0	1029	30	0
9	W	967	0	1010	32	0
9	X	967	0	1010	20	0
10	A	910	0	939	59	0
10	P	910	0	939	56	0
11	J	1183	0	1286	55	0
11	R	1183	0	1286	61	0
12	K	703	0	747	34	0
12	S	703	0	747	29	0
13	L	4604	0	4734	170	0
13	T	4604	0	4734	169	0
14	M	3489	0	3606	127	0
14	U	3489	0	3606	125	0
15	N	3154	0	3343	109	0
15	V	3154	0	3343	104	0
16	H	2838	0	2903	173	0
16	Q	2838	0	2903	179	0
17	1	8	0	0	2	0
17	3	24	0	0	1	0
17	6	8	0	0	1	0
17	9	16	0	0	2	0
17	B	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	24	0	0	2	0
17	G	8	0	0	1	0
17	O	16	0	0	2	0
18	1	31	0	19	1	0
18	B	31	0	19	2	0
19	2	4	0	0	1	0
19	3	4	0	0	2	0
19	C	4	0	0	2	0
19	D	4	0	0	2	0
20	4	29	0	0	0	0
20	E	29	0	0	0	0
All	All	74144	0	75226	2779	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 19.

The worst 5 of 2779 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)
9:W:102:LEU:O	9:W:110:LEU:HD13	1.16	1.26
3:D:283:PRO:HG3	3:D:425:ARG:HH21	1.00	1.13
7:O:20:LYS:N	7:O:21:PRO:HD3	1.64	1.08
3:D:283:PRO:CG	3:D:425:ARG:HH21	1.68	1.04
6:6:56:ALA:HB1	16:H:44:VAL:CG1	1.87	1.02

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%)	403 (93%)	32 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	435/438 (99%)	399 (92%)	36 (8%)	0	100	100
2	2	176/181 (97%)	170 (97%)	6 (3%)	0	100	100
2	C	176/181 (97%)	169 (96%)	7 (4%)	0	100	100
3	3	750/783 (96%)	702 (94%)	48 (6%)	0	100	100
3	D	750/783 (96%)	700 (93%)	50 (7%)	0	100	100
4	4	382/409 (93%)	361 (94%)	21 (6%)	0	100	100
4	E	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
5	5	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
5	F	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
6	6	164/181 (91%)	144 (88%)	20 (12%)	0	100	100
6	G	164/181 (91%)	148 (90%)	16 (10%)	0	100	100
7	9	178/182 (98%)	166 (93%)	12 (7%)	0	100	100
7	O	178/182 (98%)	172 (97%)	5 (3%)	1 (1%)	25	57
8	7	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
8	I	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
9	W	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
9	X	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
10	A	115/119 (97%)	105 (91%)	10 (9%)	0	100	100
10	P	115/119 (97%)	105 (91%)	10 (9%)	0	100	100
11	J	158/176 (90%)	148 (94%)	10 (6%)	0	100	100
11	R	158/176 (90%)	146 (92%)	12 (8%)	0	100	100
12	K	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
12	S	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
13	L	603/606 (100%)	568 (94%)	34 (6%)	1 (0%)	47	78
13	T	603/606 (100%)	569 (94%)	33 (6%)	1 (0%)	47	78
14	M	465/469 (99%)	438 (94%)	27 (6%)	0	100	100
14	U	465/469 (99%)	437 (94%)	28 (6%)	0	100	100
15	N	425/427 (100%)	400 (94%)	25 (6%)	0	100	100
15	V	425/427 (100%)	402 (95%)	23 (5%)	0	100	100
16	H	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	7	30
16	Q	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9478/9796 (97%)	8826 (93%)	635 (7%)	17 (0%)	47 78

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	45	ARG
16	H	51	VAL
7	O	21	PRO
16	Q	51	VAL
16	H	44	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	355/356 (100%)	344 (97%)	11 (3%)	40 68
1	B	355/356 (100%)	345 (97%)	10 (3%)	43 70
2	2	150/152 (99%)	144 (96%)	6 (4%)	31 60
2	C	150/152 (99%)	144 (96%)	6 (4%)	31 60
3	3	609/628 (97%)	599 (98%)	10 (2%)	62 81
3	D	609/628 (97%)	598 (98%)	11 (2%)	59 79
4	4	332/355 (94%)	328 (99%)	4 (1%)	71 85
4	E	332/355 (94%)	326 (98%)	6 (2%)	59 79
5	5	167/175 (95%)	163 (98%)	4 (2%)	49 74
5	F	167/175 (95%)	164 (98%)	3 (2%)	59 79
6	6	135/149 (91%)	125 (93%)	10 (7%)	13 42
6	G	135/149 (91%)	126 (93%)	9 (7%)	16 46
7	9	148/150 (99%)	147 (99%)	1 (1%)	84 92
7	O	148/150 (99%)	146 (99%)	2 (1%)	67 83
8	7	104/106 (98%)	103 (99%)	1 (1%)	76 88
8	I	104/106 (98%)	103 (99%)	1 (1%)	76 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	W	99/101 (98%)	98 (99%)	1 (1%)	76 88
9	X	99/101 (98%)	98 (99%)	1 (1%)	76 88
10	A	90/92 (98%)	88 (98%)	2 (2%)	52 75
10	P	90/92 (98%)	87 (97%)	3 (3%)	38 66
11	J	118/130 (91%)	114 (97%)	4 (3%)	37 65
11	R	118/130 (91%)	115 (98%)	3 (2%)	47 72
12	K	71/71 (100%)	69 (97%)	2 (3%)	43 70
12	S	71/71 (100%)	69 (97%)	2 (3%)	43 70
13	L	453/454 (100%)	445 (98%)	8 (2%)	59 79
13	T	453/454 (100%)	445 (98%)	8 (2%)	59 79
14	M	332/332 (100%)	324 (98%)	8 (2%)	49 74
14	U	332/332 (100%)	323 (97%)	9 (3%)	44 70
15	N	302/302 (100%)	297 (98%)	5 (2%)	60 80
15	V	302/302 (100%)	297 (98%)	5 (2%)	60 80
16	H	293/300 (98%)	280 (96%)	13 (4%)	28 58
16	Q	293/300 (98%)	282 (96%)	11 (4%)	33 61
All	All	7516/7706 (98%)	7336 (98%)	180 (2%)	49 74

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	761	SER
11	R	84	ASP
4	E	143	LEU
6	G	83	ARG
13	T	169	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	92	ASN
3	D	168	HIS
16	Q	251	HIS
14	U	255	GLN
1	B	219	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	HQW	4	501	-	29,31,31	1.30	4 (13%)	29,44,44	1.49	6 (20%)
18	FMN	1	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.29	9 (18%)
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
20	HQW	E	501	-	29,31,31	1.01	1 (3%)	29,44,44	1.58	6 (20%)
17	SF4	D	801	3	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.31	7 (14%)
17	SF4	6	201	6	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	SF4	G	201	6	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		

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
20	HQW	4	501	-	-	4/13/27/27	0/3/3/3
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
20	HQW	E	501	-	-	4/13/27/27	0/3/3/3
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	6	201	6	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4A-N5	4.23	1.39	1.30
18	B	502	FMN	C4A-N5	3.90	1.38	1.30
20	E	501	HQW	C23-N1	2.87	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	501	HQW	C23-N1	2.72	1.51	1.45
20	4	501	HQW	O25-C13	2.69	1.40	1.35

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	E	501	HQW	C17-C14-C10	-4.13	123.70	130.74
20	E	501	HQW	O24-C5-C4	3.26	109.16	105.58
20	4	501	HQW	C17-C14-C10	-3.06	125.53	130.74
18	1	502	FMN	C4-N3-C2	-2.98	120.14	125.64
18	B	502	FMN	C4-N3-C2	-2.96	120.17	125.64

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

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

There are no ring outliers.

17 monomers are involved in 24 short contacts:

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

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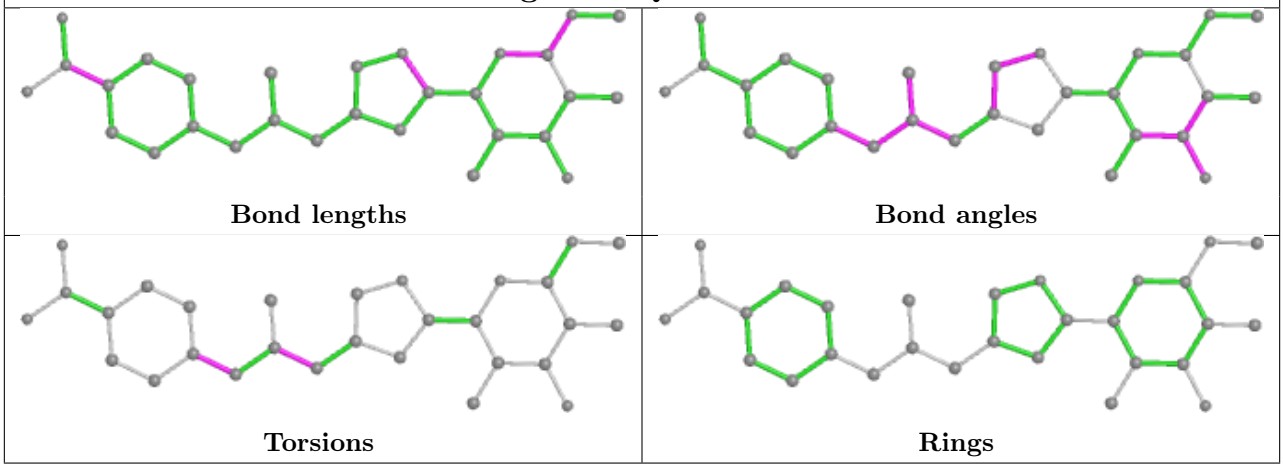
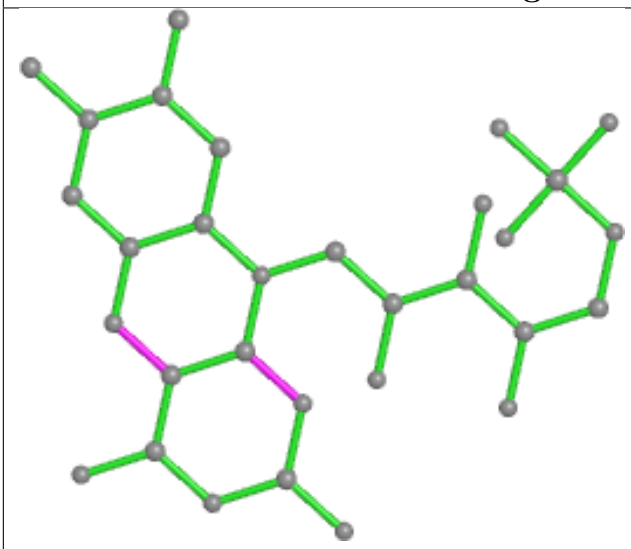
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	501	SF4	2	0
19	C	201	FES	2	0

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.

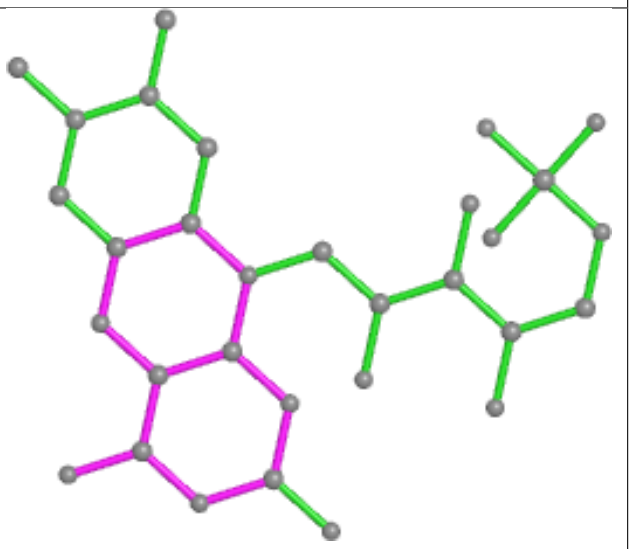
Ligand HQW 4 501



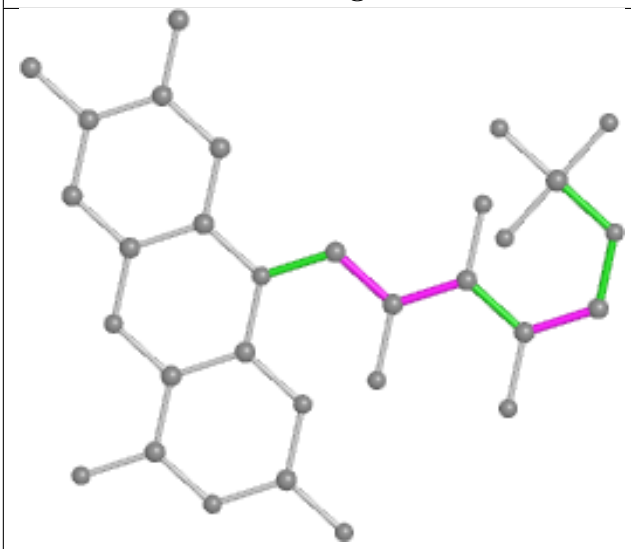
Ligand FMN 1 502



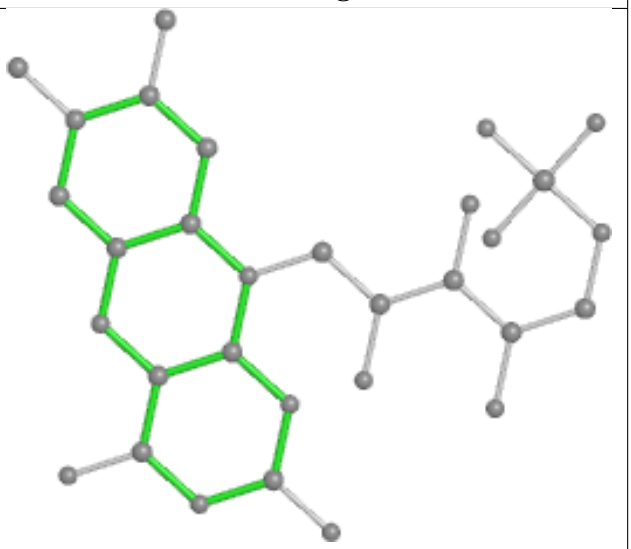
Bond lengths



Bond angles

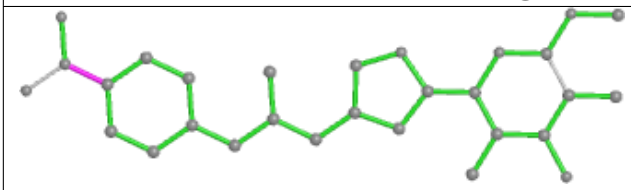


Torsions

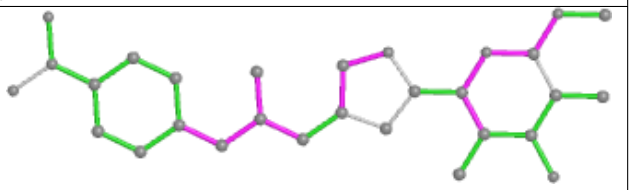


Rings

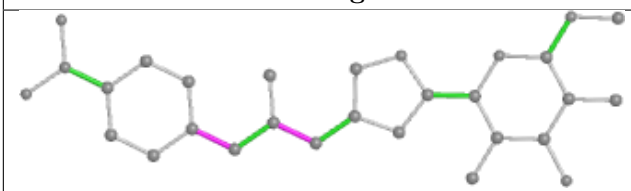
Ligand HQW E 501



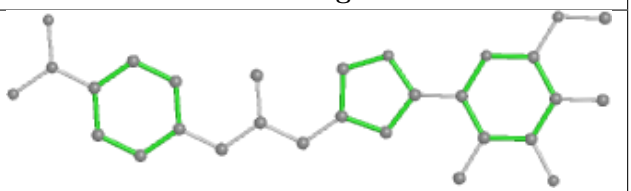
Bond lengths



Bond angles

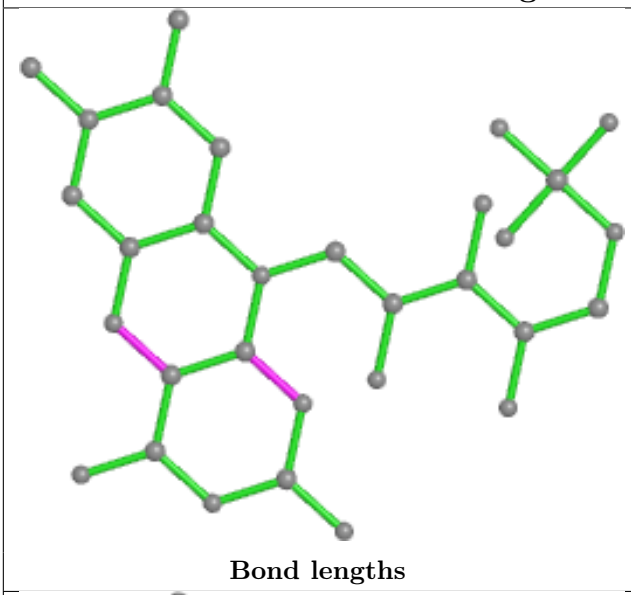


Torsions

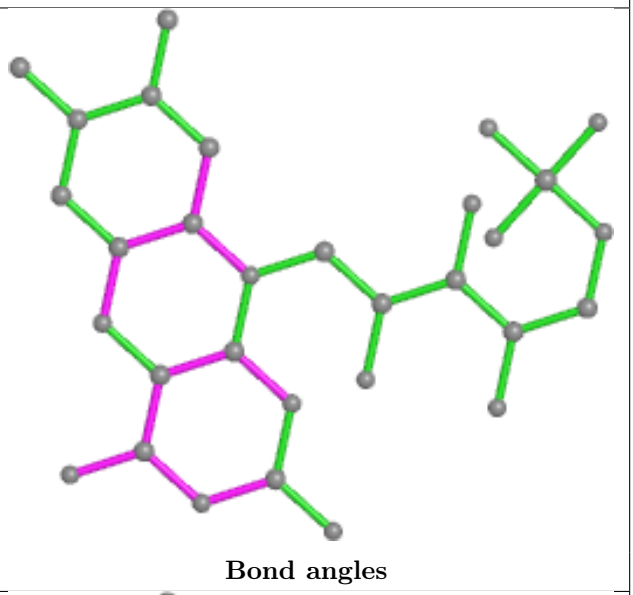


Rings

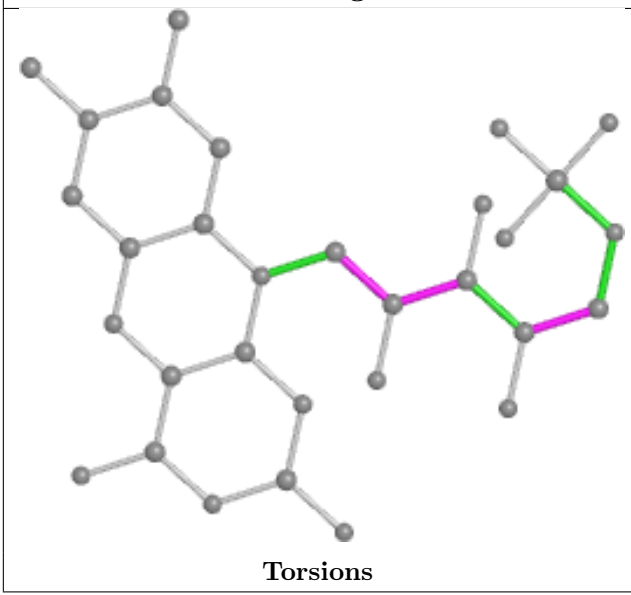
Ligand FMN B 502



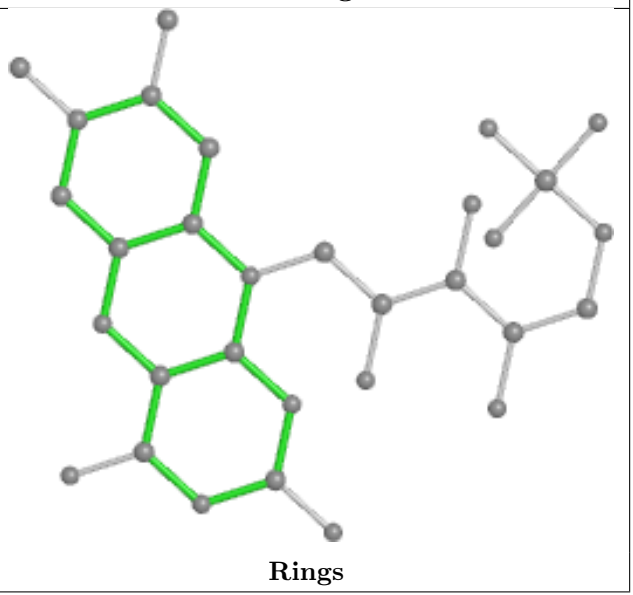
Bond lengths



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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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