wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 07:33 AM EDT

PDB ID	:	3M9S
Title	:	Crystal structure of respiratory complex I from Thermus thermophilus
Authors	:	Efremov, R.G.; Baradaran, R.; Sazanov, L.A.
Deposited on	:	2010-03-22
Resolution	:	4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

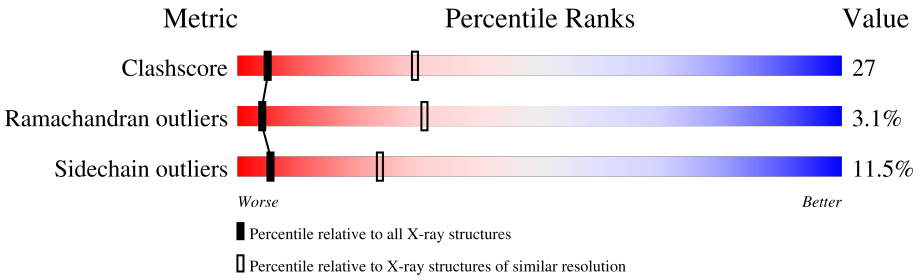
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.50 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	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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%

Mol	Chain	Length	Quality of chain
1	1	438	50% 42% 8%
1	A	438	50% 42% 8%
2	2	181	58% 29% 11% ••
2	B	181	58% 29% 11% ••
3	3	783	45% 44% 7% •
3	C	783	45% 44% 7% •
4	4	409	44% 40% 9% 8%
4	D	409	44% 40% 9% 8%

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Mol	Chain	Length	Quality of chain
5	5	207	40% 49% 6% 5%
5	E	207	40% 49% 6% 5%
6	6	181	35% 37% 8% 20%
6	F	181	35% 37% 8% 20%
7	9	182	47% 32% 5% 15%
7	G	182	47% 32% 5% 15%
8	7	129	63% 30% 5%
8	J	129	63% 30% 5%
9	L	469	94% 6%
9	O	469	94% 6%
10	M	392	95%
10	P	392	95%
11	N	379	96%
11	Q	379	96%
12	R	274	97%
12	S	274	97%
13	H	181	97%
13	T	181	97%

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
14	SF4	1	439	-	-	X	-
14	SF4	3	784	-	-	X	-
14	SF4	3	786	-	-	X	-
14	SF4	6	182	-	-	X	-
14	SF4	A	439	-	-	X	-
14	SF4	C	784	-	-	X	-
14	SF4	C	786	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	SF4	F	182	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 47664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	C	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	D	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	F	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			

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

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			

- 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	J	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
9	L	469	Total	C	N	0	0	0
			1407	938	469			
9	O	469	Total	C	N	0	0	0
			1407	938	469			

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
10	M	391	Total	C	N	0	0	0
			1173	782	391			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
10	P	391	Total 1173	C 782	N 391	0	0	0

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
11	N	378	Total 1134	C 756	N 378	0	0	0
11	Q	378	Total 1134	C 756	N 378	0	0	0

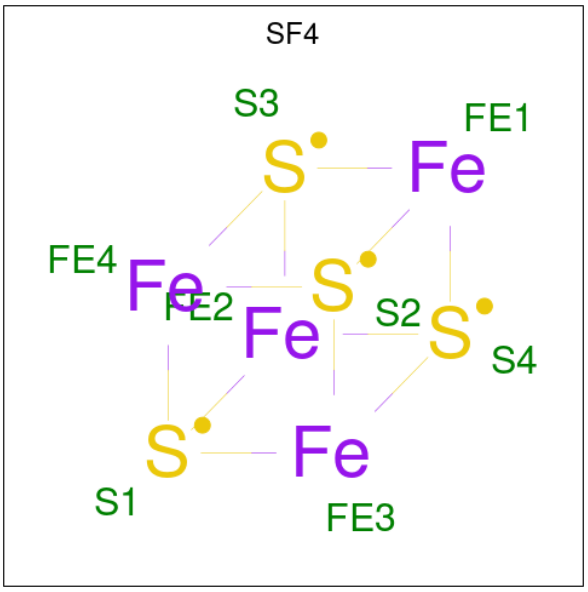
- Molecule 12 is a protein called NADH-quinone oxidoreductase subunits 7, 10 and 11.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
12	R	274	Total 822	C 548	N 274	0	0	0
12	S	274	Total 822	C 548	N 274	0	0	0

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 8.

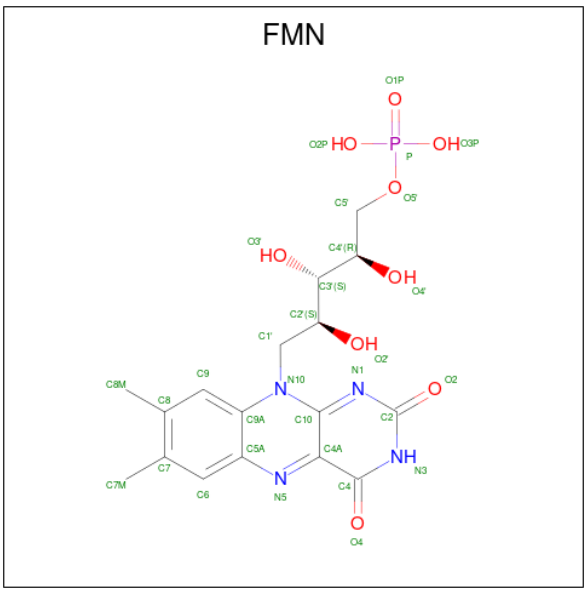
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	H	181	Total 543	C 362	N 181	0	0	0
13	T	181	Total 543	C 362	N 181	0	0	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



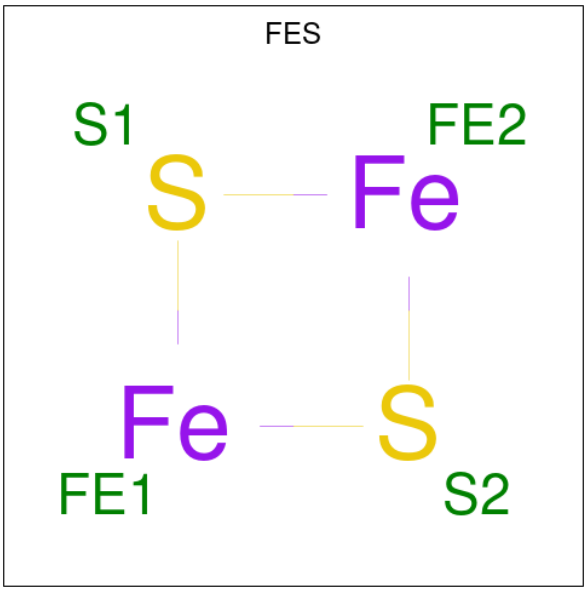
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	1	1	Total Fe S 8 4 4	0	0
14	3	1	Total Fe S 8 4 4	0	0
14	3	1	Total Fe S 8 4 4	0	0
14	3	1	Total Fe S 8 4 4	0	0
14	6	1	Total Fe S 8 4 4	0	0
14	9	1	Total Fe S 8 4 4	0	0
14	9	1	Total Fe S 8 4 4	0	0
14	A	1	Total Fe S 8 4 4	0	0
14	C	1	Total Fe S 8 4 4	0	0
14	C	1	Total Fe S 8 4 4	0	0
14	C	1	Total Fe S 8 4 4	0	0
14	F	1	Total Fe S 8 4 4	0	0
14	G	1	Total Fe S 8 4 4	0	0
14	G	1	Total Fe S 8 4 4	0	0

- Molecule 15 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
15	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	2	1	Total	Fe	S		0	0
			4	2	2			

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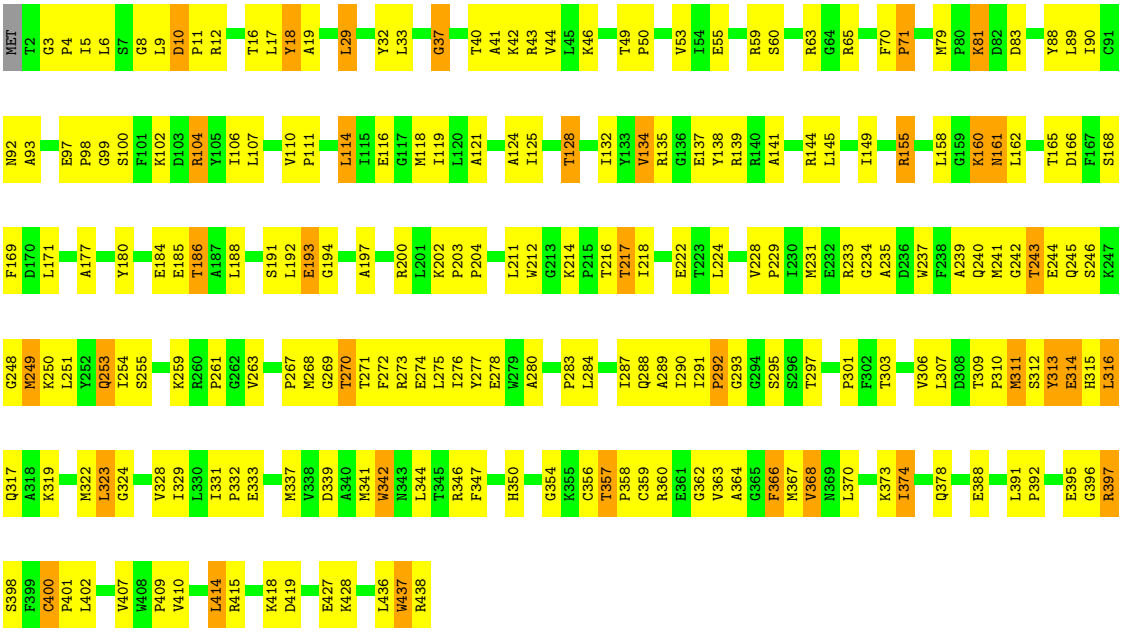
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	3	1	Total	Fe	S	0	0
			4	2	2		
16	B	1	Total	Fe	S	0	0
			4	2	2		
16	C	1	Total	Fe	S	0	0
			4	2	2		

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.

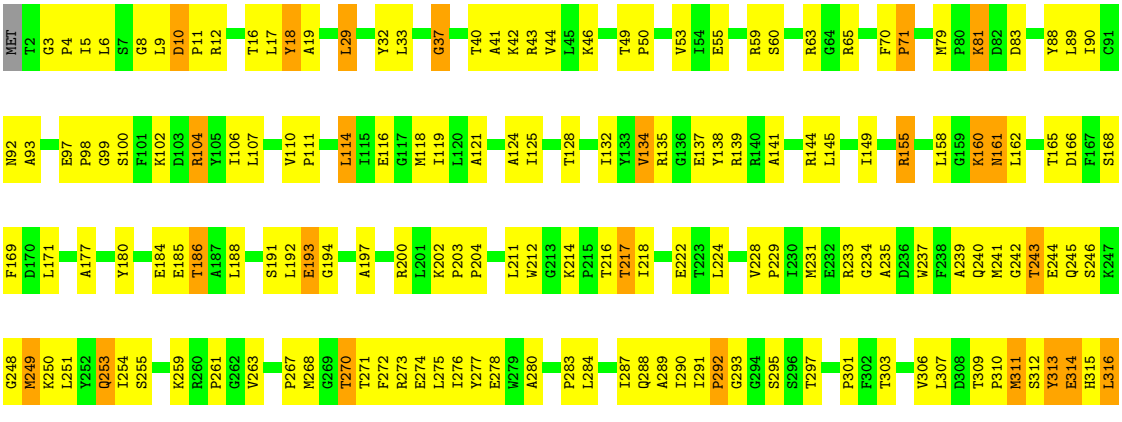
- Molecule 1: NADH-quinone oxidoreductase subunit 1

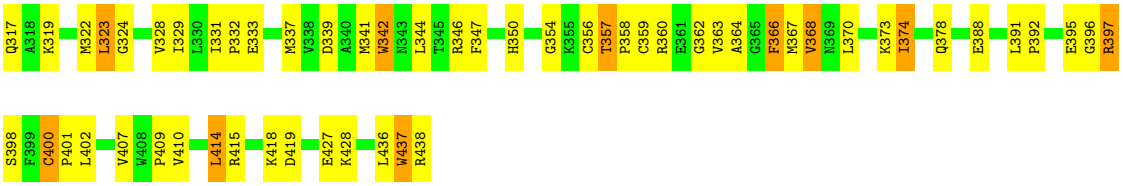
Chain 1:



- Molecule 1: NADH-quinone oxidoreductase subunit 1

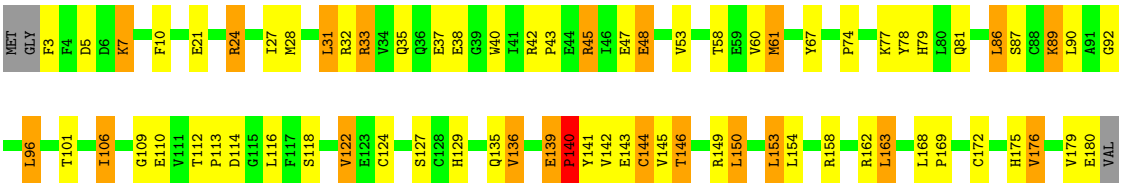
Chain A:





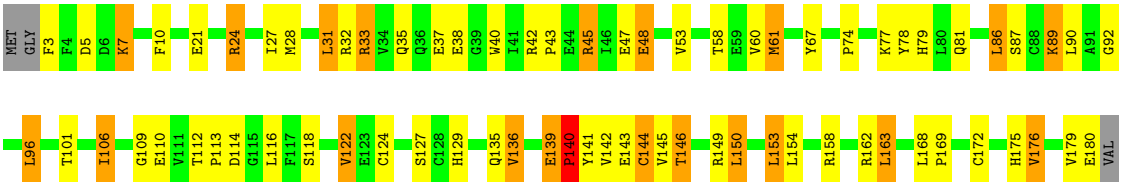
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:



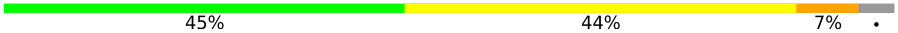
• Molecule 2: NADH-quinone oxidoreductase subunit 2

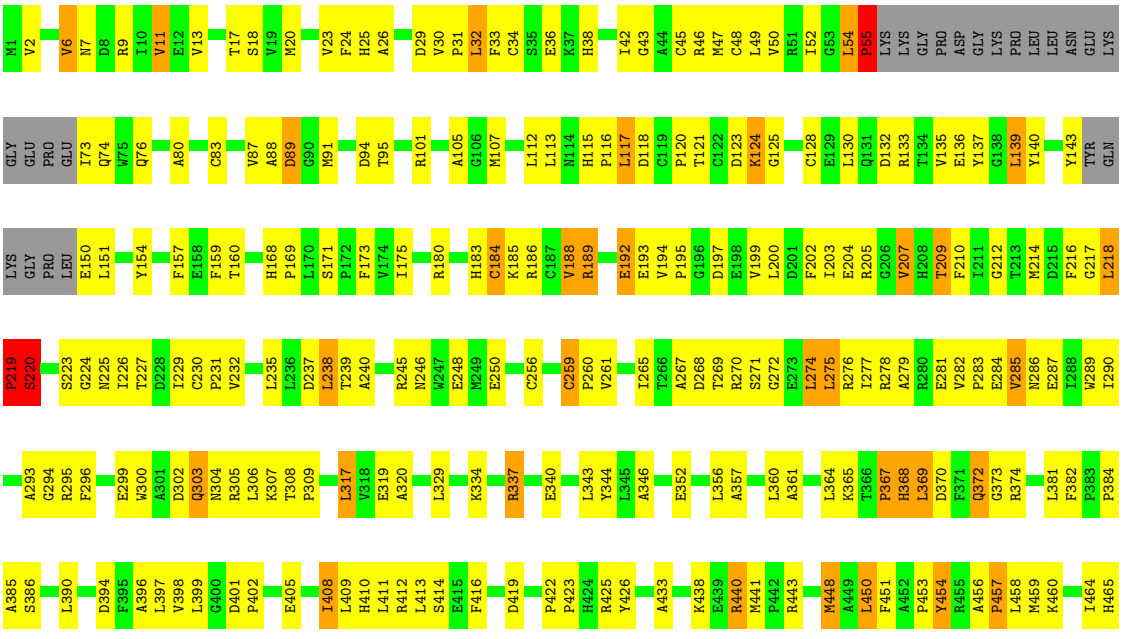
Chain B:

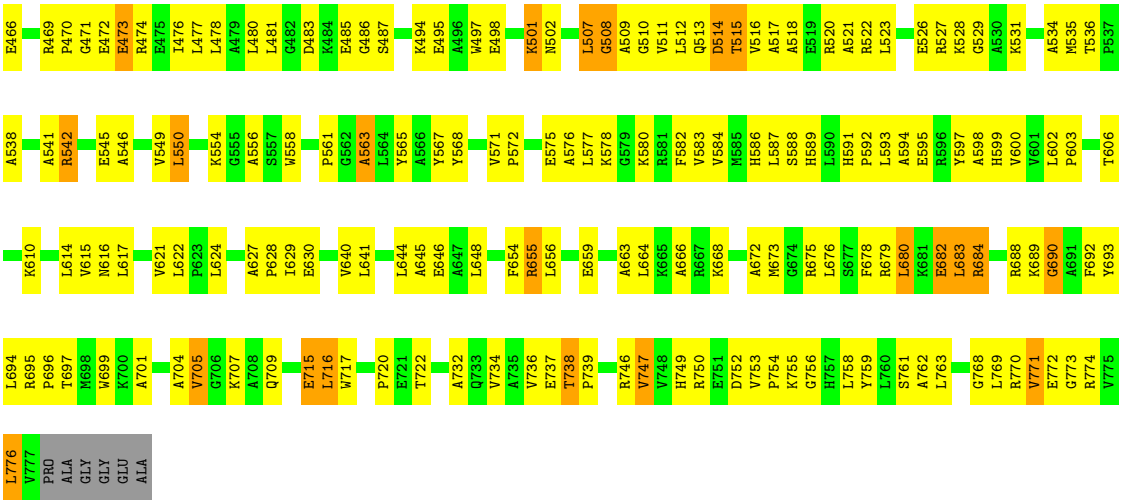


• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3:

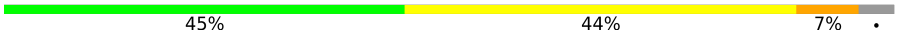


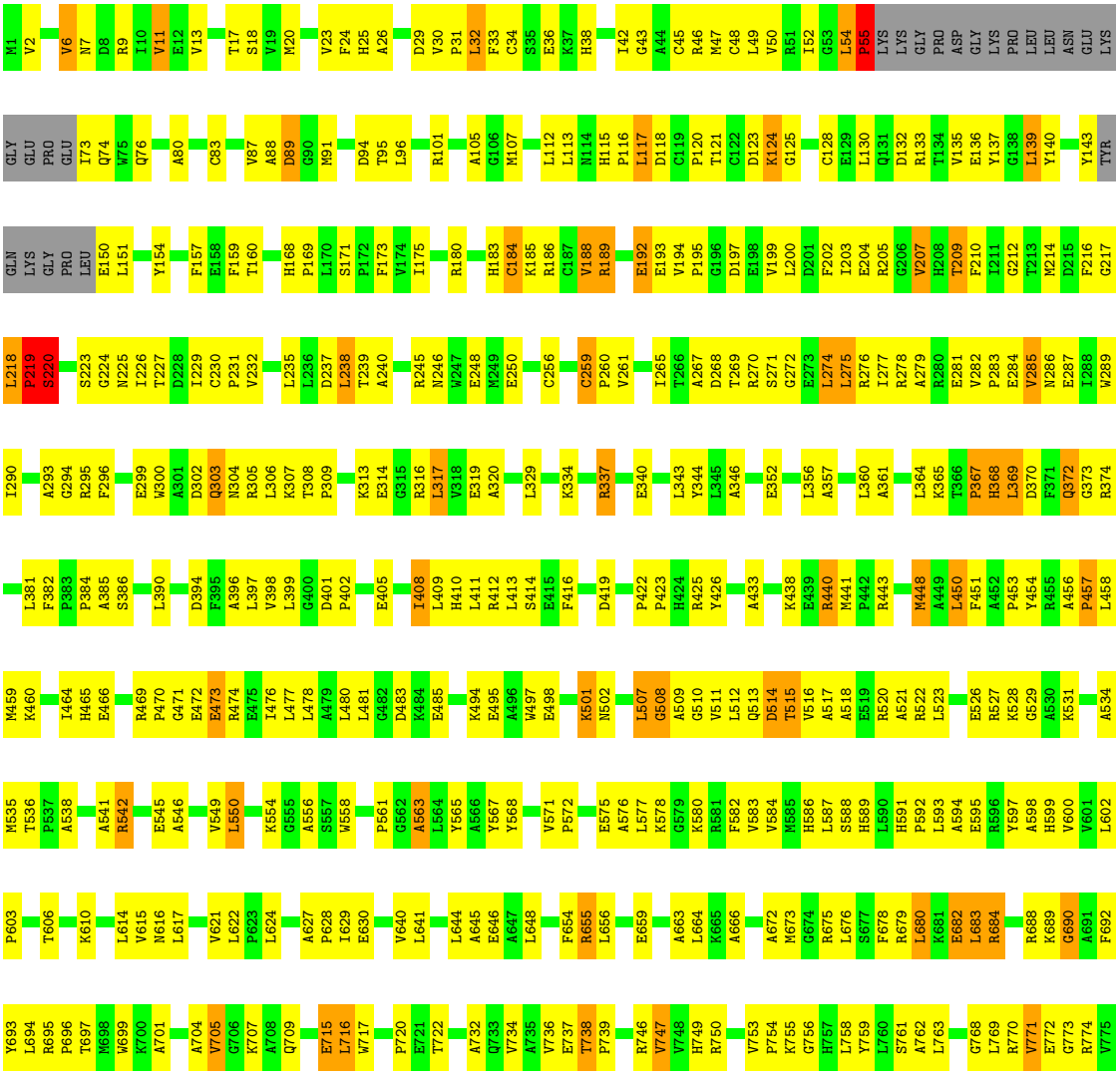




• Molecule 3: NADH-quinone oxidoreductase subunit 3

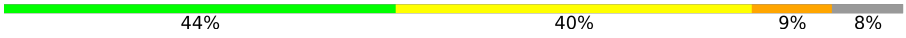
Chain C:

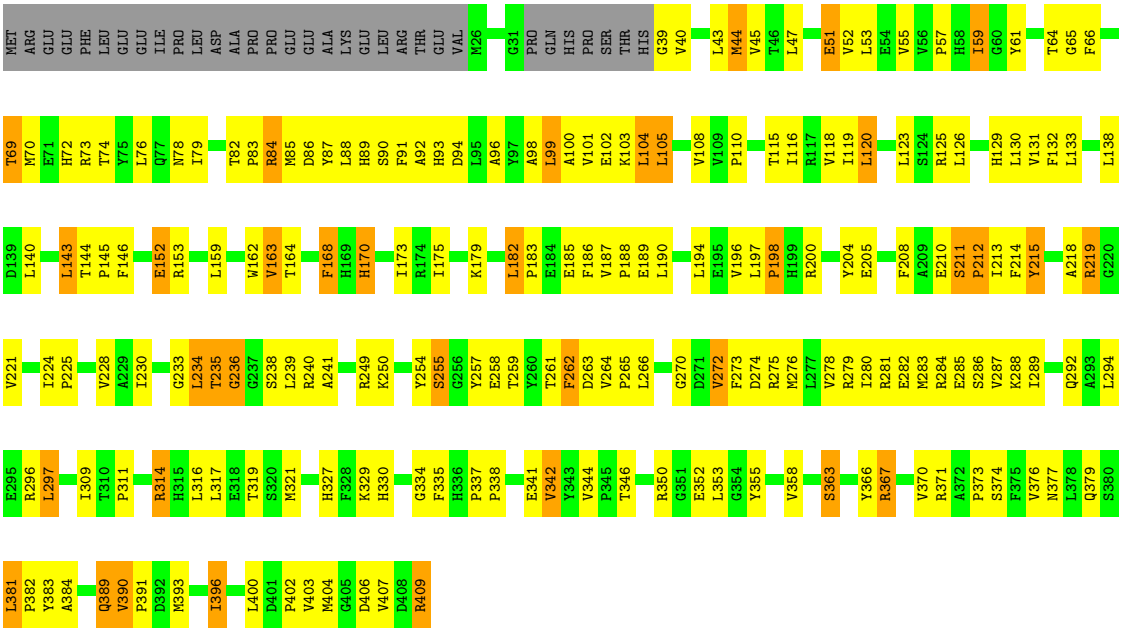




• Molecule 4: NADH-quinone oxidoreductase subunit 4

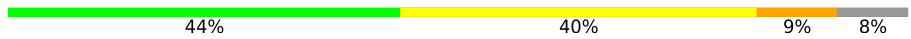
Chain 4:

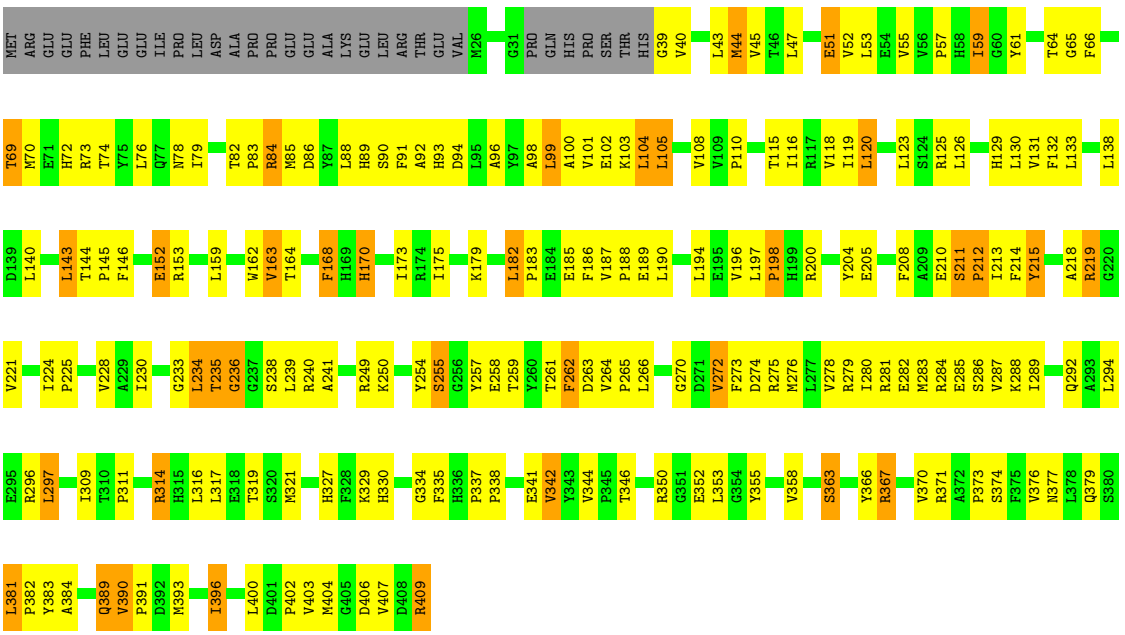




• Molecule 4: NADH-quinone oxidoreductase subunit 4

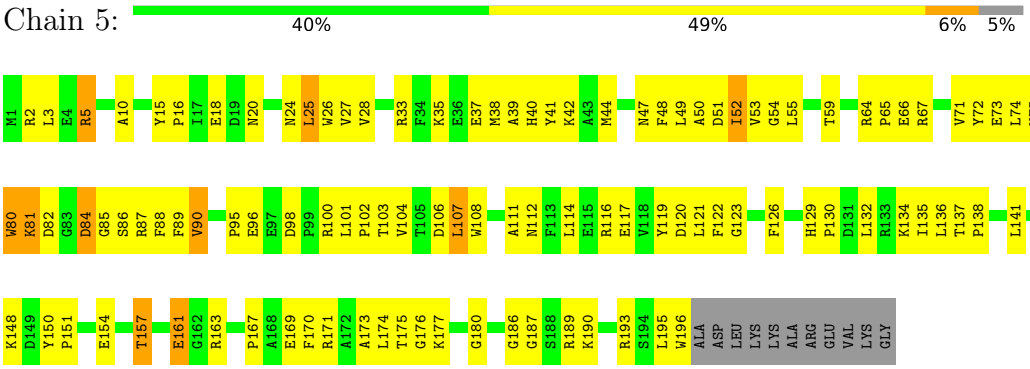
Chain D:





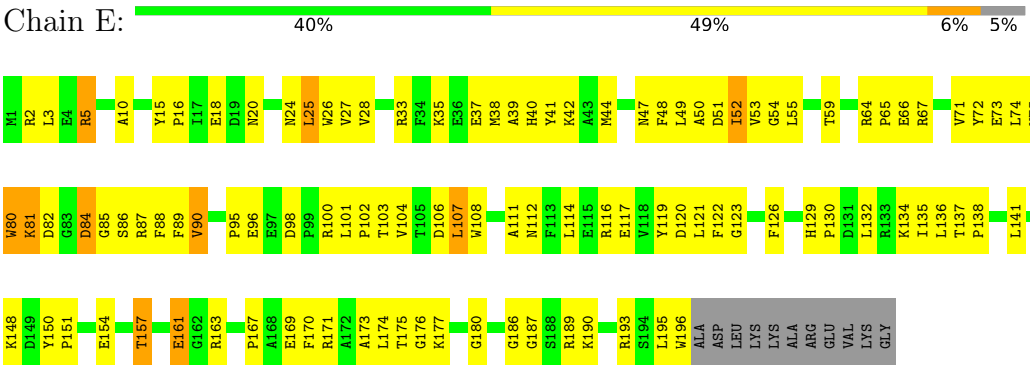
• Molecule 5: NADH-quinone oxidoreductase subunit C

Chain 5:



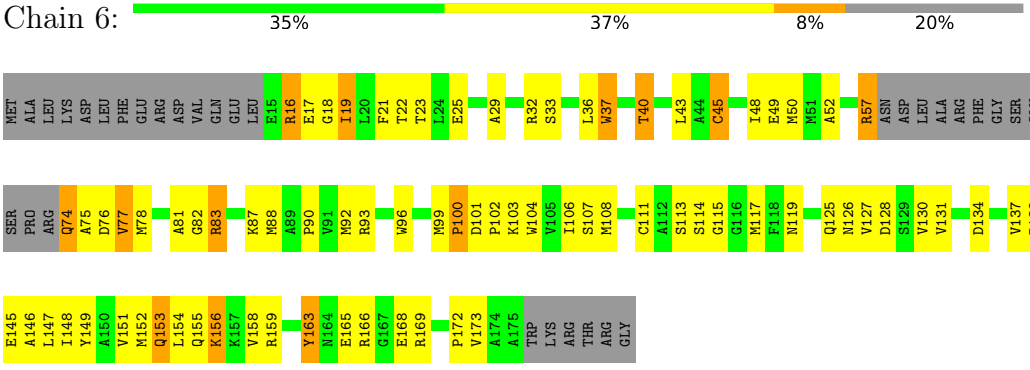
• Molecule 5: NADH-quinone oxidoreductase subunit C

Chain E:



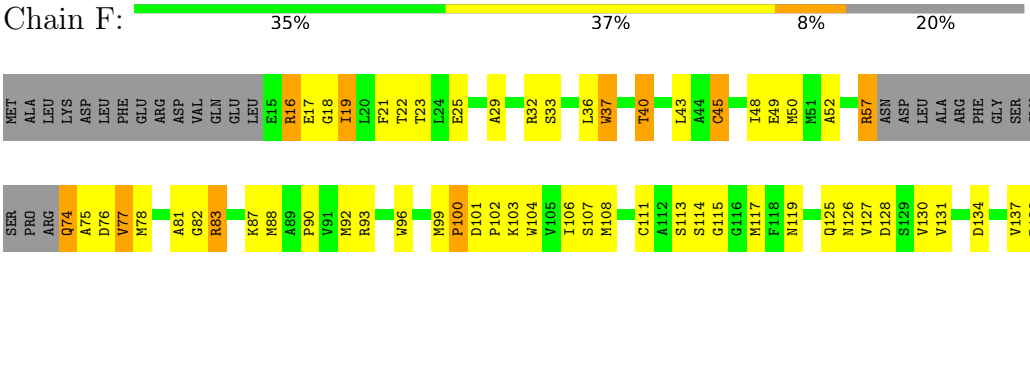
• Molecule 6: NADH-quinone oxidoreductase subunit B

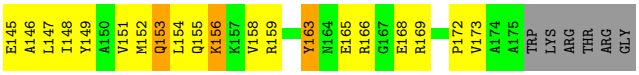
Chain 6:



• Molecule 6: NADH-quinone oxidoreductase subunit B

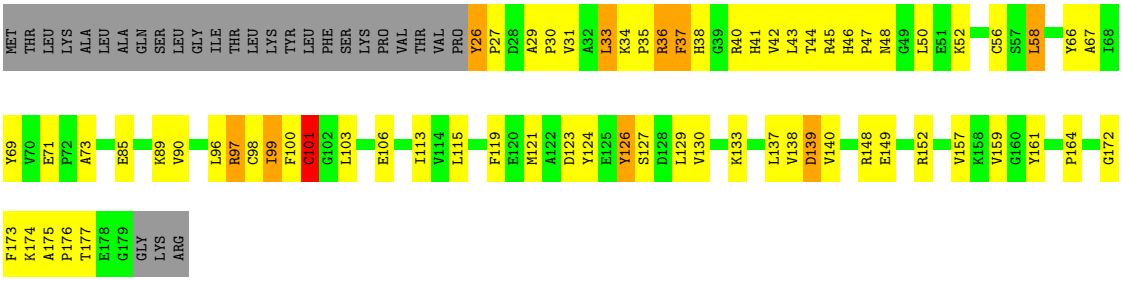
Chain F:





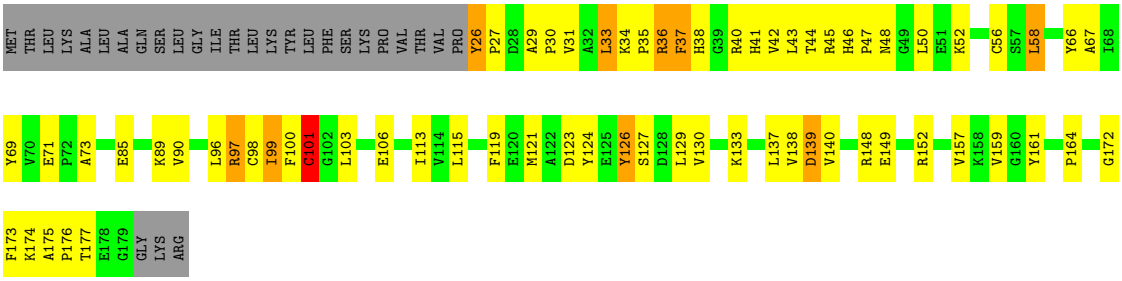
• Molecule 7: NADH-quinone oxidoreductase subunit I

Chain 9:



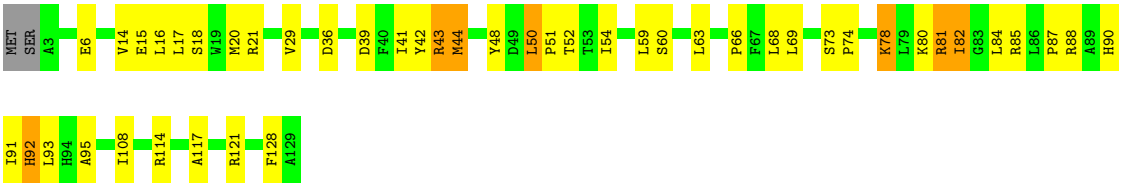
• Molecule 7: NADH-quinone oxidoreductase subunit I

Chain G:



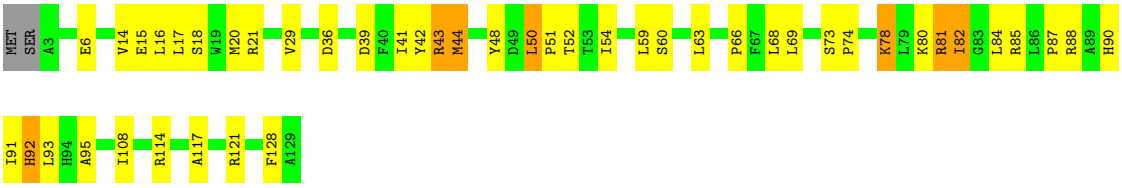
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:



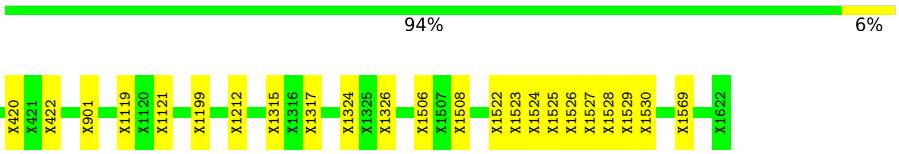
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain J:



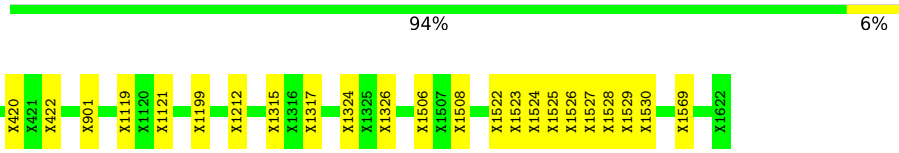
• Molecule 9: NADH-quinone oxidoreductase subunit 12

Chain L:



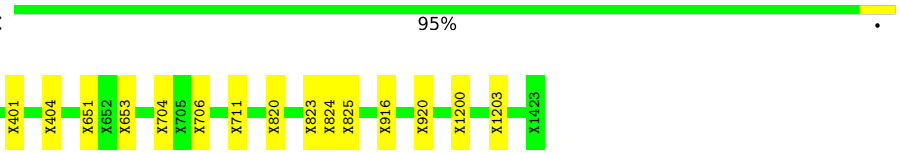
• Molecule 9: NADH-quinone oxidoreductase subunit 12

Chain O:



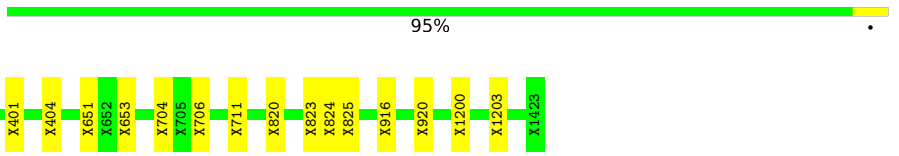
• Molecule 10: NADH-quinone oxidoreductase subunit 13

Chain M:



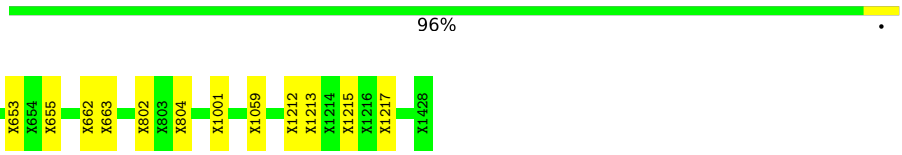
• Molecule 10: NADH-quinone oxidoreductase subunit 13

Chain P:



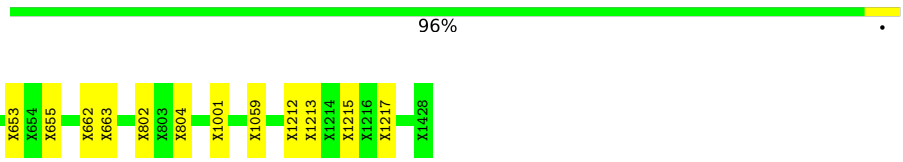
• Molecule 11: NADH-quinone oxidoreductase subunit 14

Chain N:



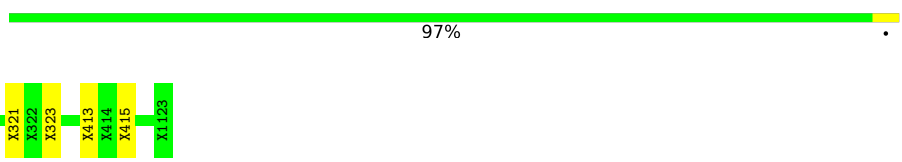
• Molecule 11: NADH-quinone oxidoreductase subunit 14

Chain Q:



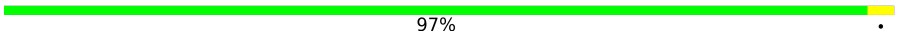
• Molecule 12: NADH-quinone oxidoreductase subunits 7, 10 and 11

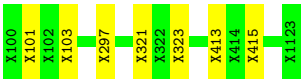
Chain R:



• Molecule 12: NADH-quinone oxidoreductase subunits 7, 10 and 11

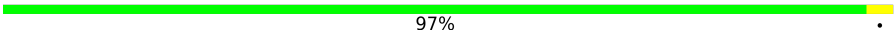
Chain S:

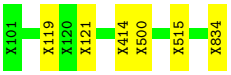




• Molecule 13: NADH-quinone oxidoreductase subunit 8

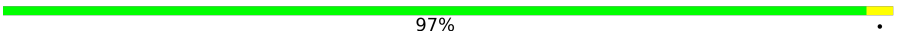
Chain H:

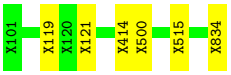




• Molecule 13: NADH-quinone oxidoreductase subunit 8

Chain T:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.39Å 336.09Å 262.24Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	30.00 – 4.50 29.96 – 4.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-4.50) 75.0 (29.96-4.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 4.42Å)	Xtriage
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available) 0.394 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	168.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.309 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	47664	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.48	1/3506 (0.0%)	0.68	1/4745 (0.0%)
1	A	0.48	1/3506 (0.0%)	0.68	1/4745 (0.0%)
2	2	0.49	0/1439	0.66	0/1953
2	B	0.49	0/1439	0.66	0/1953
3	3	0.46	0/6019	0.70	3/8163 (0.0%)
3	C	0.46	0/6019	0.70	3/8163 (0.0%)
4	4	0.43	0/3089	0.64	1/4197 (0.0%)
4	D	0.43	0/3089	0.64	1/4197 (0.0%)
5	5	0.42	0/1656	0.64	0/2246
5	E	0.42	0/1656	0.64	0/2246
6	6	0.47	0/1137	0.68	0/1542
6	F	0.47	0/1137	0.68	0/1542
7	9	0.52	1/1224 (0.1%)	0.65	0/1663
7	G	0.52	1/1224 (0.1%)	0.65	0/1663
8	7	0.45	0/1059	0.61	0/1429
8	J	0.45	0/1059	0.61	0/1429
All	All	0.46	4/38258 (0.0%)	0.67	10/51876 (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
9	L	0	2
9	O	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	356	CYS	CB-SG	-6.06	1.72	1.82
1	A	356	CYS	CB-SG	-6.05	1.72	1.82
7	9	101	CYS	CB-SG	-5.44	1.73	1.81
7	G	101	CYS	CB-SG	-5.43	1.73	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	143	TYR	CA-C-O	-14.73	89.16	120.10
3	C	143	TYR	CA-C-O	-14.72	89.18	120.10
3	C	55	PRO	CB-CA-C	-5.80	97.49	112.00
3	3	55	PRO	CB-CA-C	-5.79	97.53	112.00
4	4	39	GLY	N-CA-C	-5.39	99.61	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	L	1212	UNK	Peptide
9	L	1569	UNK	Peptide
9	O	1212	UNK	Peptide
9	O	1569	UNK	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	207	0
1	A	3417	0	3388	206	0
2	2	1406	0	1373	72	0
2	B	1406	0	1373	73	0
3	3	5880	0	5911	427	7
3	C	5880	0	5911	406	9
4	4	3011	0	3000	211	0
4	D	3011	0	3000	209	0
5	5	1607	0	1574	106	0
5	E	1607	0	1574	106	0
6	6	1113	0	1121	92	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1113	0	1121	113	0
7	9	1193	0	1160	69	0
7	G	1193	0	1160	68	0
8	7	1031	0	1029	41	0
8	J	1031	0	1029	41	0
9	L	1407	0	50	15	0
9	O	1407	0	50	15	0
10	M	1173	0	37	15	0
10	P	1173	0	37	15	0
11	N	1134	0	36	12	0
11	Q	1134	0	36	12	0
12	R	822	0	24	4	0
12	S	822	0	24	4	0
13	H	543	0	20	6	0
13	T	543	0	20	6	0
14	1	8	0	0	2	0
14	3	24	0	0	8	0
14	6	8	0	0	4	0
14	9	16	0	0	0	0
14	A	8	0	0	2	0
14	C	24	0	0	7	0
14	F	8	0	0	4	0
14	G	16	0	0	0	0
15	1	31	0	19	8	0
15	A	31	0	19	8	0
16	2	4	0	0	0	0
16	3	4	0	0	1	0
16	B	4	0	0	0	0
16	C	4	0	0	1	0
All	All	47664	0	37484	2325	9

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 27.

The worst 5 of 2325 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)
11:N:1001:UNK:CA	11:N:1059:UNK:C	1.85	1.51
11:Q:1001:UNK:CA	11:Q:1059:UNK:C	1.85	1.51
3:3:485:GLU:CD	6:F:16:ARG:HG3	1.39	1.43
9:L:1527:UNK:C	9:L:1530:UNK:N	1.88	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:1527:UNK:C	9:O:1530:UNK:N	1.88	1.37

The worst 5 of 9 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)
3:3:319:GLU:OE2	3:C:679:ARG:CZ[1_655]	1.75	0.45
3:3:319:GLU:OE1	3:C:679:ARG:NH1[1_655]	1.84	0.36
6:6:16:ARG:CG	3:C:485:GLU:OE1[1_655]	1.91	0.29
6:6:16:ARG:CD	3:C:485:GLU:O[1_655]	1.99	0.21
3:3:319:GLU:CD	3:C:679:ARG:CZ[1_655]	2.07	0.13

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%)	362 (83%)	58 (13%)	15 (3%)	3	29
1	A	435/438 (99%)	362 (83%)	58 (13%)	15 (3%)	3	29
2	2	176/181 (97%)	156 (89%)	16 (9%)	4 (2%)	6	37
2	B	176/181 (97%)	156 (89%)	16 (9%)	4 (2%)	6	37
3	3	748/783 (96%)	634 (85%)	91 (12%)	23 (3%)	4	31
3	C	748/783 (96%)	634 (85%)	91 (12%)	23 (3%)	4	31
4	4	373/409 (91%)	322 (86%)	37 (10%)	14 (4%)	3	27
4	D	373/409 (91%)	321 (86%)	38 (10%)	14 (4%)	3	27
5	5	194/207 (94%)	165 (85%)	23 (12%)	6 (3%)	4	31
5	E	194/207 (94%)	165 (85%)	23 (12%)	6 (3%)	4	31
6	6	141/181 (78%)	114 (81%)	22 (16%)	5 (4%)	3	29
6	F	141/181 (78%)	114 (81%)	22 (16%)	5 (4%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	9	152/182 (84%)	131 (86%)	17 (11%)	4 (3%)	5 35
7	G	152/182 (84%)	131 (86%)	17 (11%)	4 (3%)	5 35
8	7	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	19 60
8	J	125/129 (97%)	112 (90%)	12 (10%)	1 (1%)	19 60
All	All	4688/5020 (93%)	3991 (85%)	553 (12%)	144 (3%)	4 31

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
1	1	81	LYS
2	2	86	LEU
2	2	136	VAL
2	2	140	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	355/356 (100%)	318 (90%)	37 (10%)	7 27
1	A	355/356 (100%)	319 (90%)	36 (10%)	7 27
2	2	150/152 (99%)	123 (82%)	27 (18%)	1 11
2	B	150/152 (99%)	123 (82%)	27 (18%)	1 11
3	3	607/628 (97%)	537 (88%)	70 (12%)	5 23
3	C	607/628 (97%)	537 (88%)	70 (12%)	5 23
4	4	325/355 (92%)	291 (90%)	34 (10%)	7 26
4	D	325/355 (92%)	292 (90%)	33 (10%)	7 27
5	5	167/175 (95%)	151 (90%)	16 (10%)	8 29
5	E	167/175 (95%)	151 (90%)	16 (10%)	8 29
6	6	118/149 (79%)	104 (88%)	14 (12%)	5 23
6	F	118/149 (79%)	104 (88%)	14 (12%)	5 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	9	126/150 (84%)	111 (88%)	15 (12%)	5 23
7	G	126/150 (84%)	111 (88%)	15 (12%)	5 23
8	7	104/106 (98%)	91 (88%)	13 (12%)	4 21
8	J	104/106 (98%)	91 (88%)	13 (12%)	4 21
All	All	3904/4142 (94%)	3454 (88%)	450 (12%)	5 23

5 of 450 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	VAL
8	J	54	ILE
2	B	163	LEU
8	J	39	ASP
5	E	90	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	38	HIS
3	C	368	HIS
8	J	92	HIS
3	C	246	ASN
3	C	702	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	FMN	A	440	-	33,33,33	1.34	3 (9%)	48,50,50	1.63	15 (31%)
14	SF4	C	786	3	0,12,12	-	-	-		
14	SF4	9	184	7	0,12,12	-	-	-		
14	SF4	1	439	1	0,12,12	-	-	-		
14	SF4	3	786	3	0,12,12	-	-	-		
15	FMN	1	440	-	33,33,33	1.34	3 (9%)	48,50,50	1.63	15 (31%)
14	SF4	C	785	3	0,12,12	-	-	-		
16	FES	2	182	2	0,4,4	-	-	-		
14	SF4	G	183	7	0,12,12	-	-	-		
14	SF4	A	439	1	0,12,12	-	-	-		
16	FES	B	182	2	0,4,4	-	-	-		
14	SF4	F	182	6	0,12,12	-	-	-		
16	FES	3	787	3	0,4,4	-	-	-		
14	SF4	3	784	3	0,12,12	-	-	-		
14	SF4	6	182	6	0,12,12	-	-	-		
16	FES	C	787	3	0,4,4	-	-	-		
14	SF4	G	184	7	0,12,12	-	-	-		
14	SF4	C	784	3	0,12,12	-	-	-		
14	SF4	9	183	7	0,12,12	-	-	-		
14	SF4	3	785	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FMN	A	440	-	-	9/18/18/18	0/3/3/3
14	SF4	C	786	3	-	-	0/6/5/5
14	SF4	9	184	7	-	-	0/6/5/5
14	SF4	1	439	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	3	786	3	-	-	0/6/5/5
15	FMN	1	440	-	-	9/18/18/18	0/3/3/3
14	SF4	C	785	3	-	-	0/6/5/5
16	FES	2	182	2	-	-	0/1/1/1
14	SF4	G	183	7	-	-	0/6/5/5
14	SF4	A	439	1	-	-	0/6/5/5
16	FES	B	182	2	-	-	0/1/1/1
14	SF4	F	182	6	-	-	0/6/5/5
16	FES	3	787	3	-	-	0/1/1/1
14	SF4	3	784	3	-	-	0/6/5/5
14	SF4	6	182	6	-	-	0/6/5/5
16	FES	C	787	3	-	-	0/1/1/1
14	SF4	G	184	7	-	-	0/6/5/5
14	SF4	C	784	3	-	-	0/6/5/5
14	SF4	9	183	7	-	-	0/6/5/5
14	SF4	3	785	3	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	440	FMN	C4A-N5	3.95	1.38	1.30
15	A	440	FMN	C4A-N5	3.91	1.38	1.30
15	A	440	FMN	C9A-N10	-3.15	1.35	1.41
15	1	440	FMN	C9A-N10	-3.11	1.35	1.41
15	1	440	FMN	C4A-C10	-2.13	1.37	1.44

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	440	FMN	P-O5'-C5'	3.15	126.97	118.30
15	A	440	FMN	P-O5'-C5'	3.14	126.95	118.30
15	A	440	FMN	C4-N3-C2	-2.88	120.32	125.64
15	1	440	FMN	C4-N3-C2	-2.86	120.36	125.64
15	1	440	FMN	O4'-C4'-C3'	-2.82	102.23	109.10

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	1	440	FMN	N10-C1'-C2'-O2'
15	1	440	FMN	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
15	1	440	FMN	C3'-C4'-C5'-O5'
15	1	440	FMN	O4'-C4'-C5'-O5'
15	A	440	FMN	N10-C1'-C2'-O2'

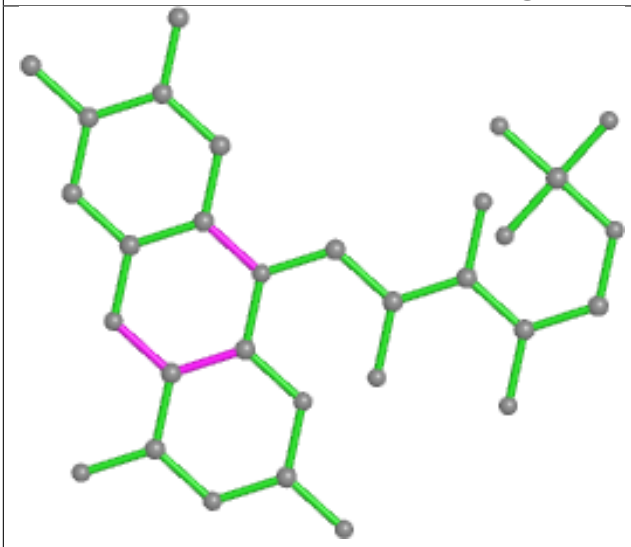
There are no ring outliers.

14 monomers are involved in 45 short contacts:

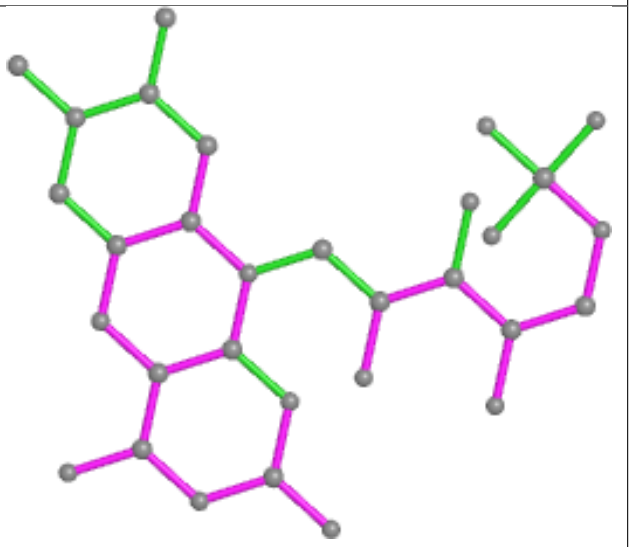
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	440	FMN	8	0
14	C	786	SF4	3	0
14	1	439	SF4	2	0
14	3	786	SF4	4	0
15	1	440	FMN	8	0
14	C	785	SF4	1	0
14	A	439	SF4	2	0
14	F	182	SF4	4	0
16	3	787	FES	1	0
14	3	784	SF4	3	0
14	6	182	SF4	4	0
16	C	787	FES	1	0
14	C	784	SF4	3	0
14	3	785	SF4	1	0

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.

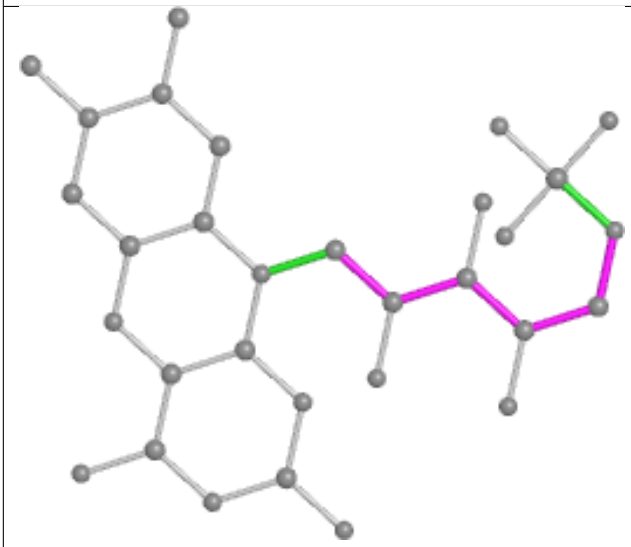
Ligand FMN A 440



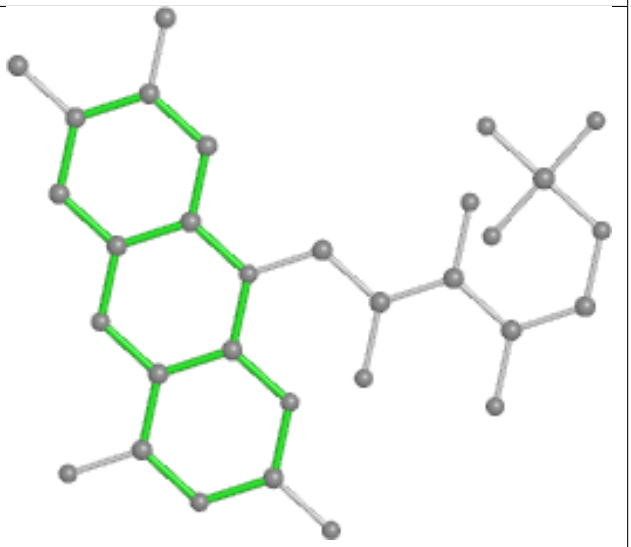
Bond lengths



Bond angles

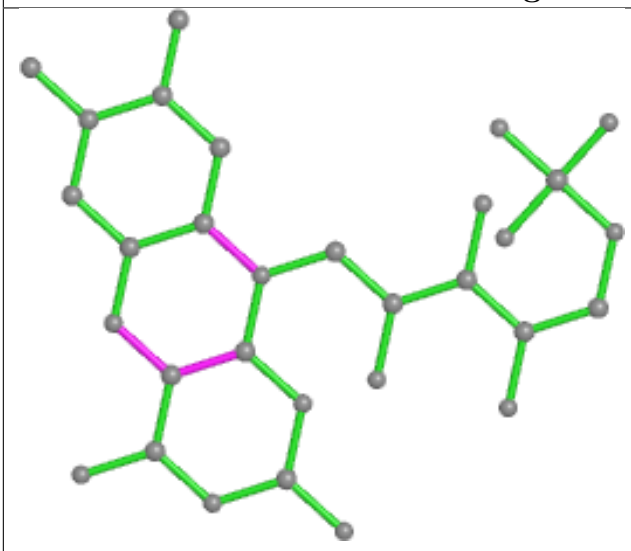


Torsions

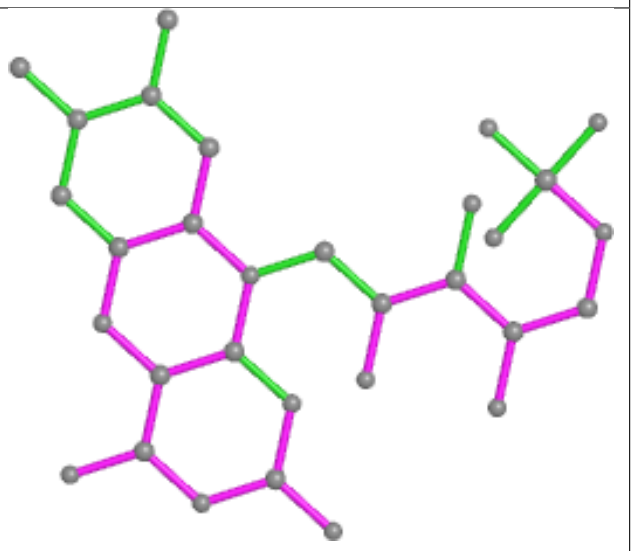


Rings

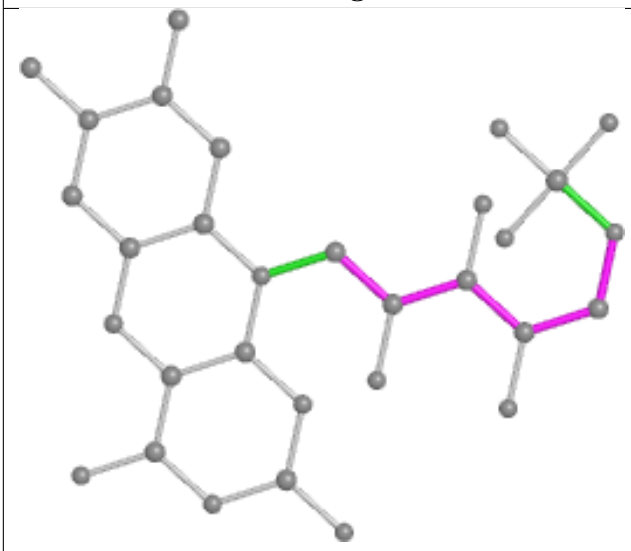
Ligand FMN 1 440



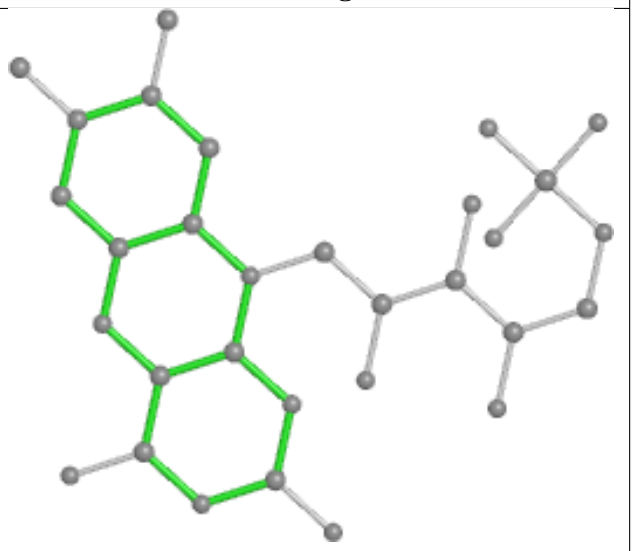
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	L	20
9	O	20
10	M	16

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
10	P	16
11	N	16
11	Q	16
12	R	10
12	S	10
13	H	8
13	T	8

The worst 5 of 140 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	428:UNK	C	495:UNK	N	56.90
1	O	428:UNK	C	495:UNK	N	56.90
1	M	1024:UNK	C	1050:UNK	N	55.04
1	P	1024:UNK	C	1050:UNK	N	55.04
1	N	366:UNK	C	395:UNK	N	50.88

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

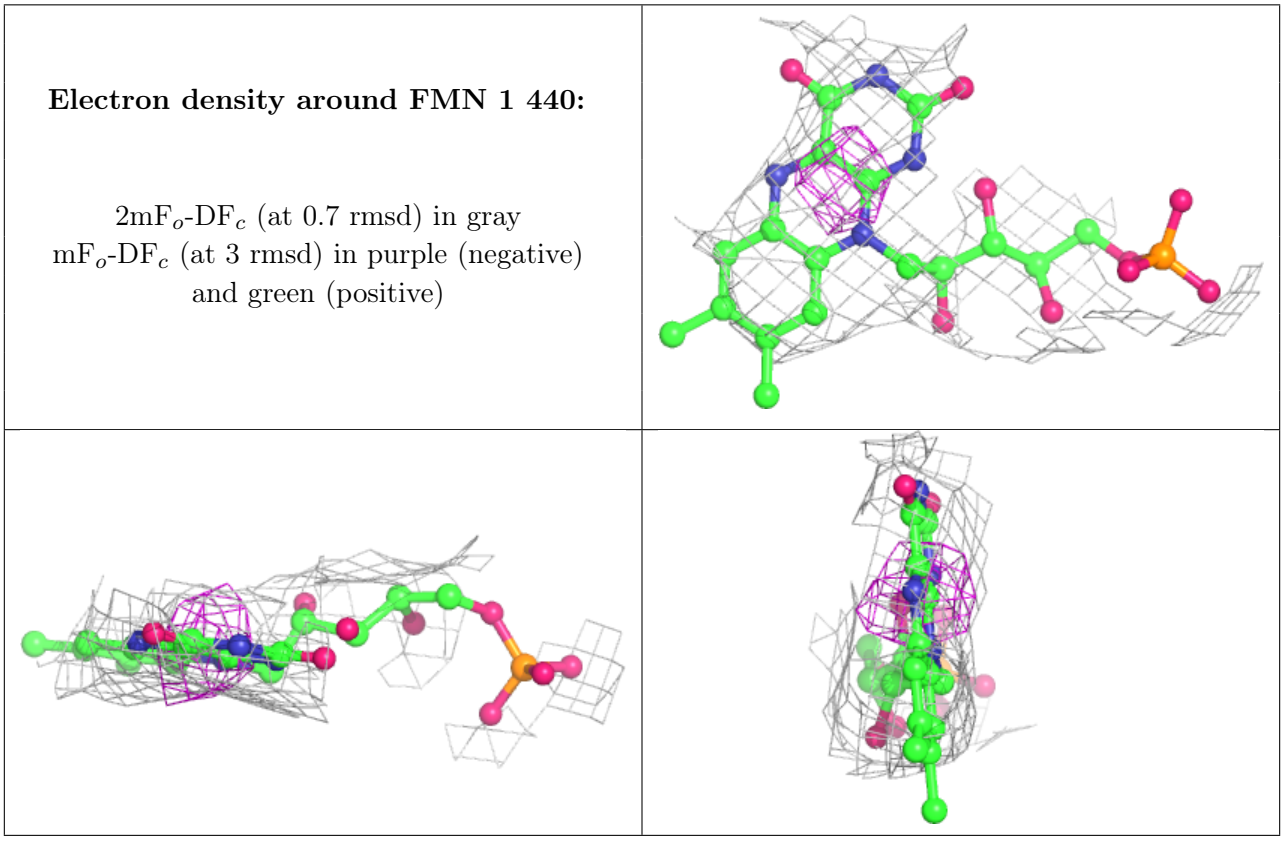
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

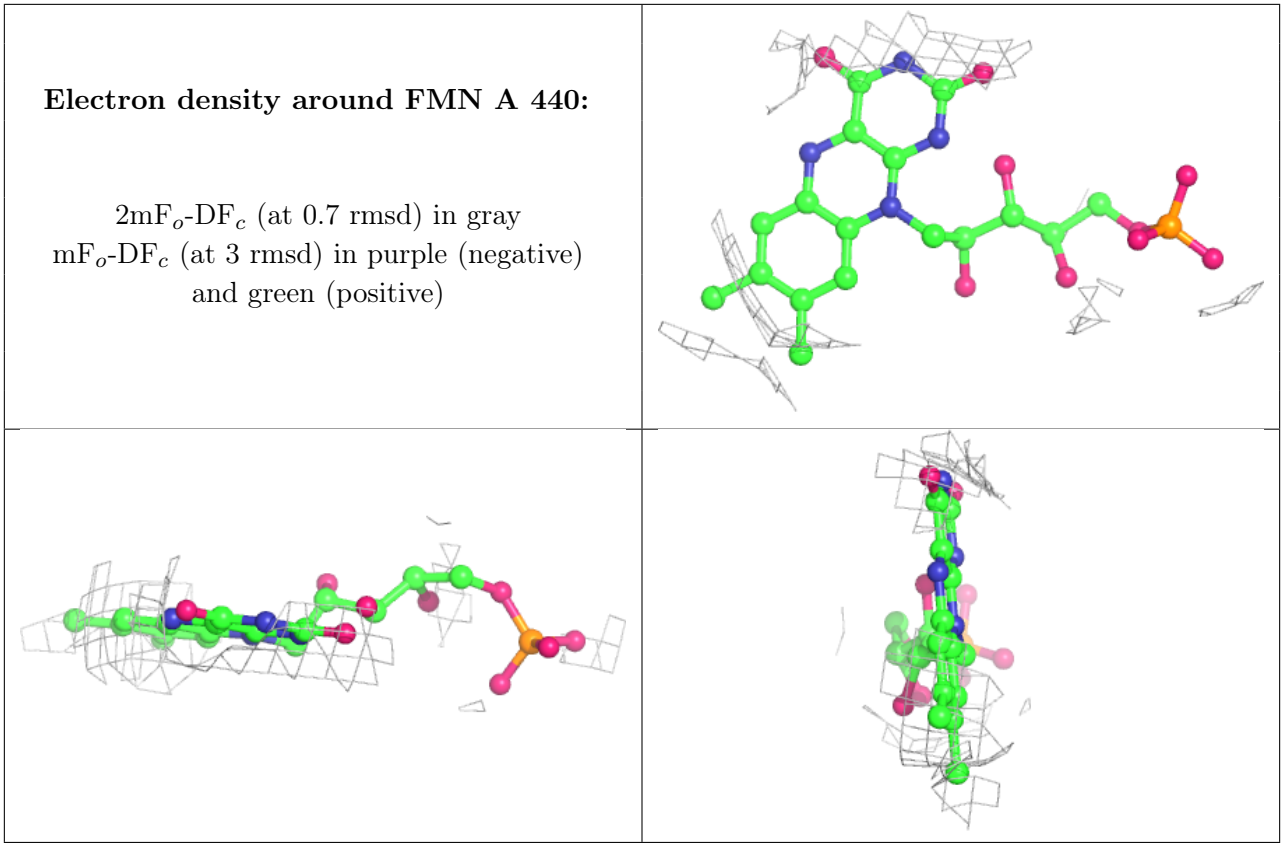
Electron density around FMN 1 440:

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



Electron density around FMN A 440:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.