wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2026 – 06:41 pm BST

PDB ID	:	6Q8X / pdb_00006q8x
Title	:	Respiratory complex I from Thermus thermophilus with bound Pyridaben.
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2018-12-16
Resolution	:	3.51 Å(reported)

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

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

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

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

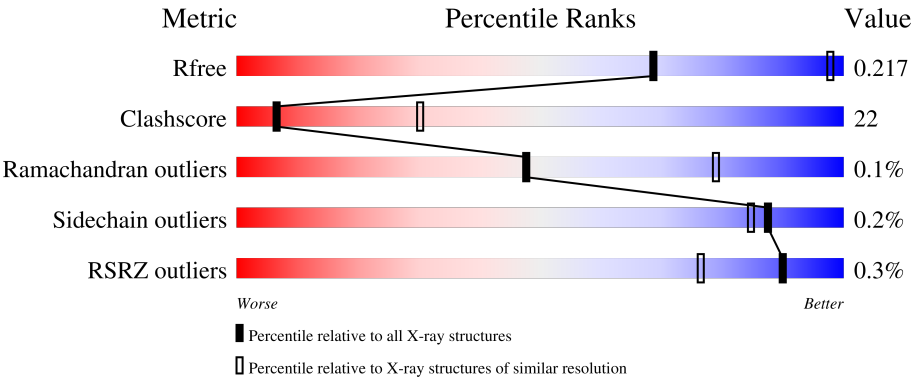
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	438	% 58% 42%
1	B	438	49% 50%
2	2	181	66% 33% .
2	C	181	57% 41% .
3	3	783	59% 38% .

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Mol	Chain	Length	Quality of chain
3	D	783	57% 39%
4	4	409	48% 46% 6%
4	E	409	44% 50% 6%
5	5	207	54% 41% 5%
5	F	207	49% 45% 5%
6	6	181	44% 48% 8%
6	G	181	43% 48% 8%
7	9	182	59% 40%
7	O	182	51% 48%
8	7	129	60% 39%
8	I	129	60% 38%
9	W	131	63% 34%
9	X	131	66% 31%
10	A	119	55% 44%
10	P	119	54% 43%
11	J	176	57% 34% 9%
11	R	176	57% 34% 9%
12	K	95	64% 36%
12	S	95	67% 33%
13	L	606	59% 40%
13	T	606	60% 39%
14	M	469	61% 38%
14	U	469	59% 41%
15	N	427	64% 36%
15	V	427	61% 39%

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Mol	Chain	Length	Quality of chain
16	H	365	
16	Q	365	

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
17	SF4	3	803	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	201	-	-	X	-
18	FMN	B	502	-	-	X	-
19	FES	2	201	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 74134 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			

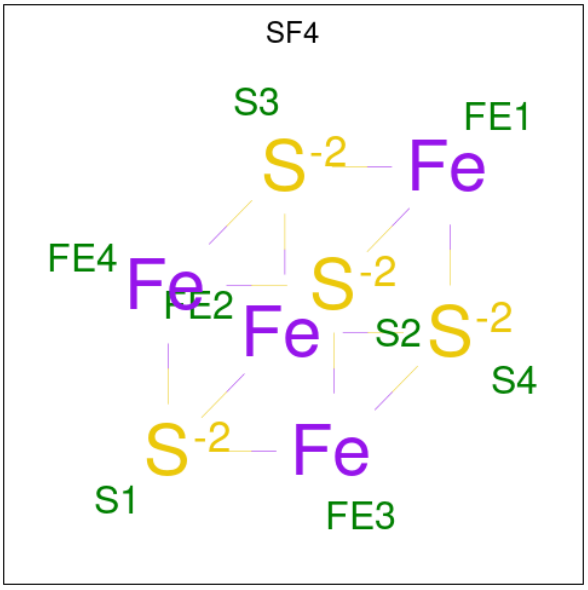
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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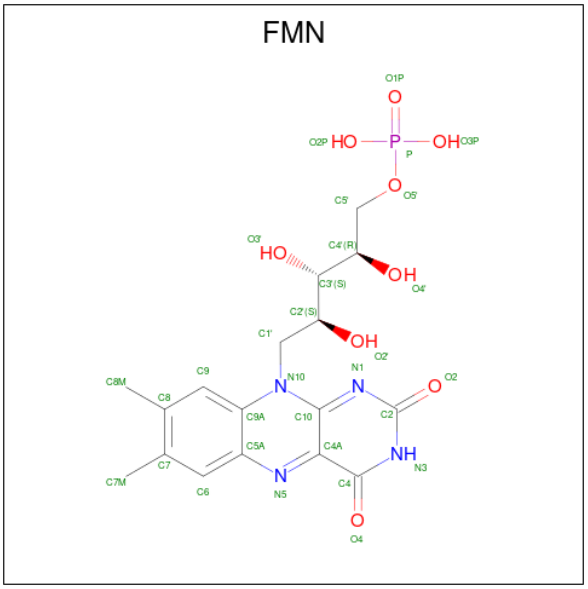
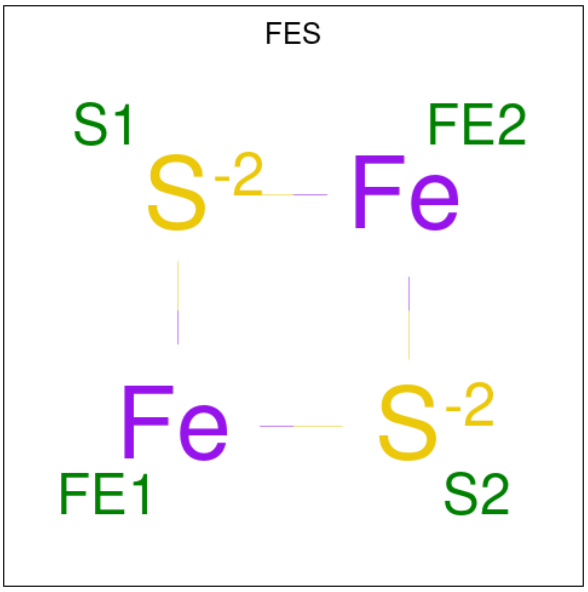
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total Fe S 8 4 4	0	0
17	D	1	Total Fe S 8 4 4	0	0
17	G	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0

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



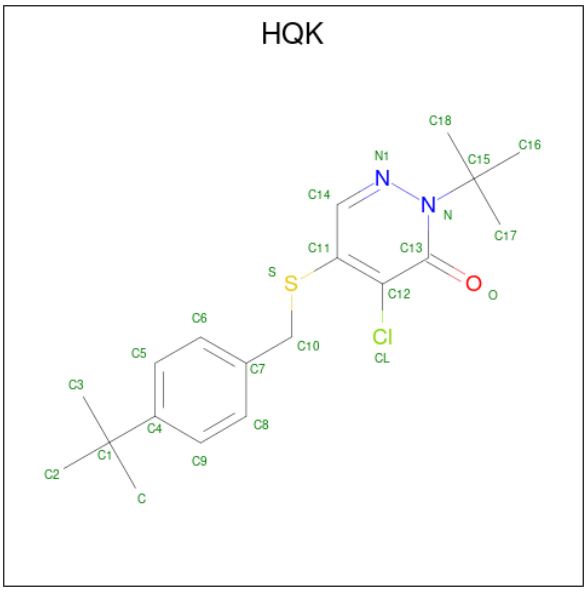
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	1	1	Total C N O P 31 17 4 9 1	0	0
18	B	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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 Pyridaben (CCD ID: HQK) (formula: $C_{19}H_{25}ClN_2OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
20	4	1	Total	C	Cl	N	O	S	0	0
			24	19	1	2	1	1		
20	E	1	Total	C	Cl	N	O	S	0	0
			24	19	1	2	1	1		

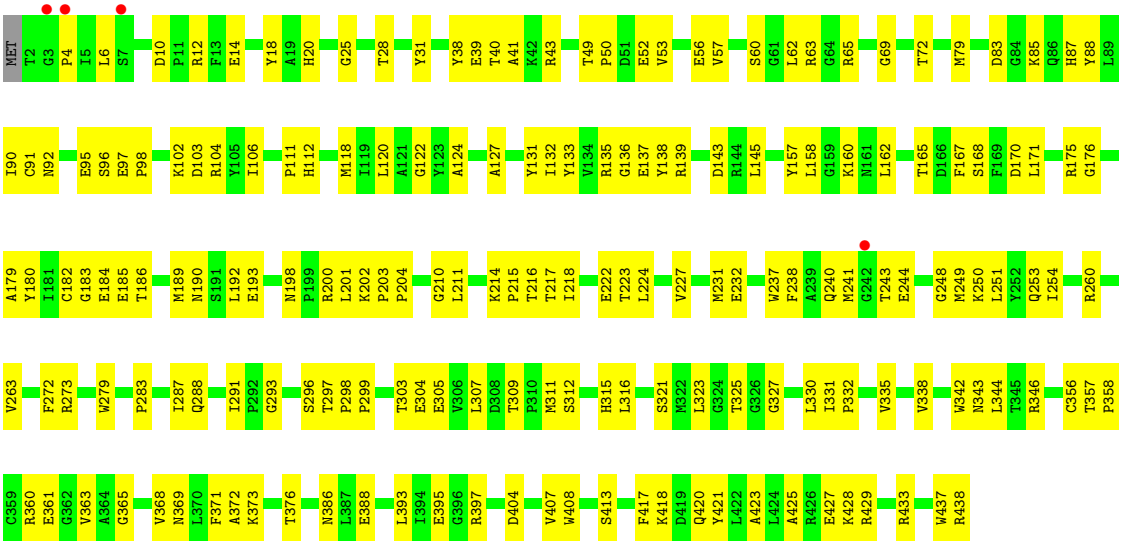
3 Residue-property plots (i)

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 subunit 1

Chain 1:

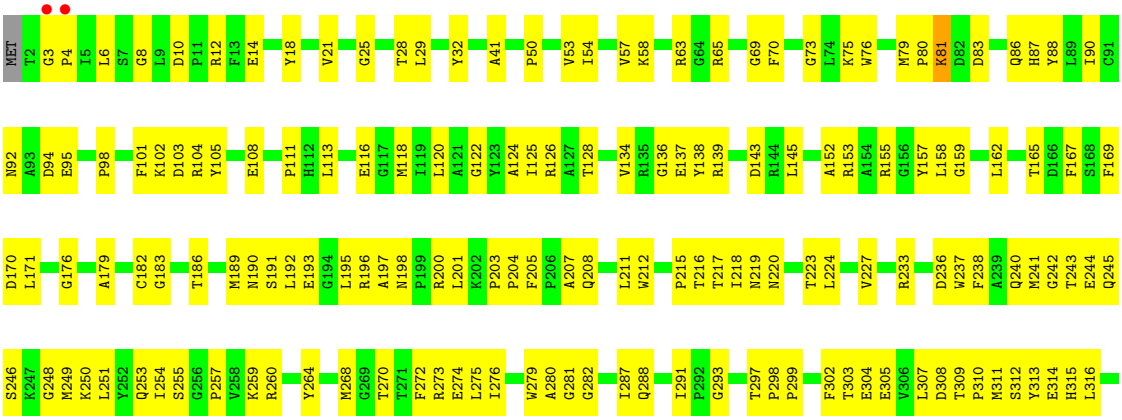


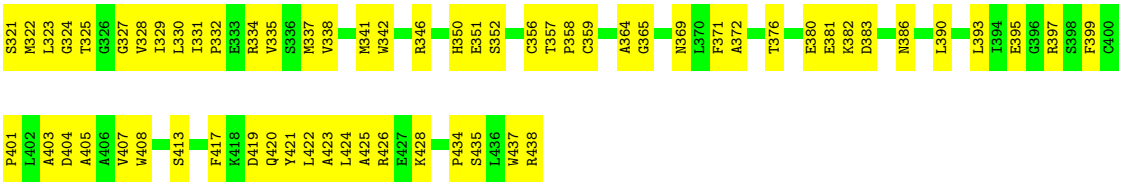


• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain B:



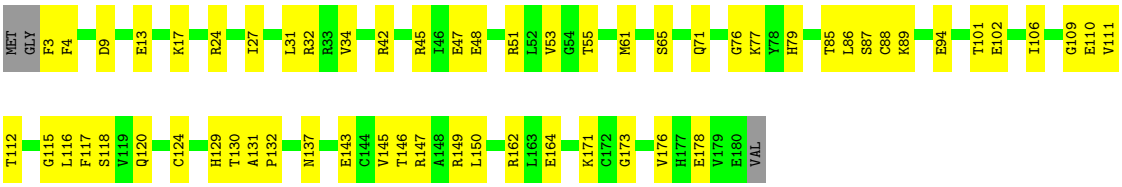




• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:





• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain C:

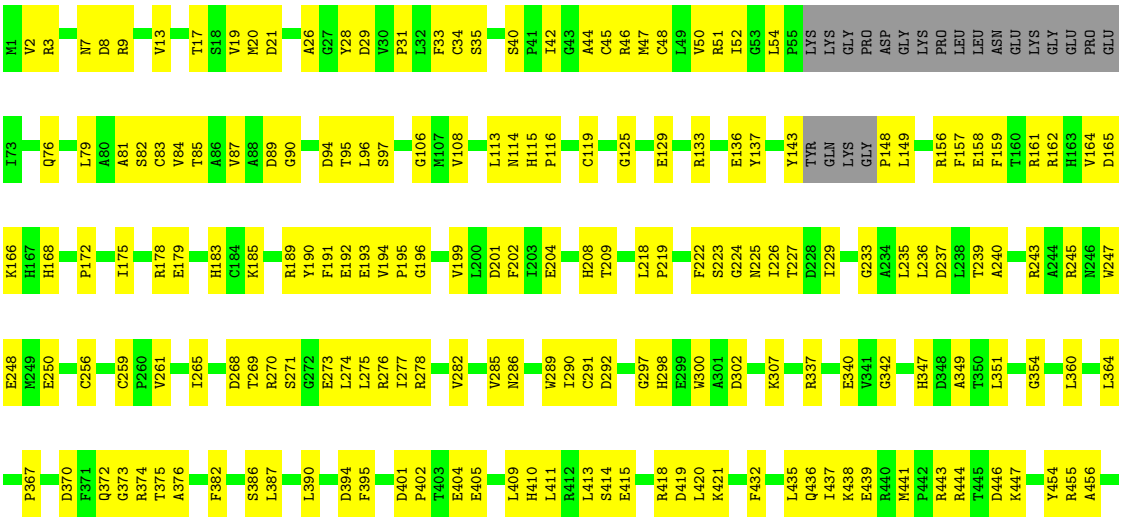




• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3:



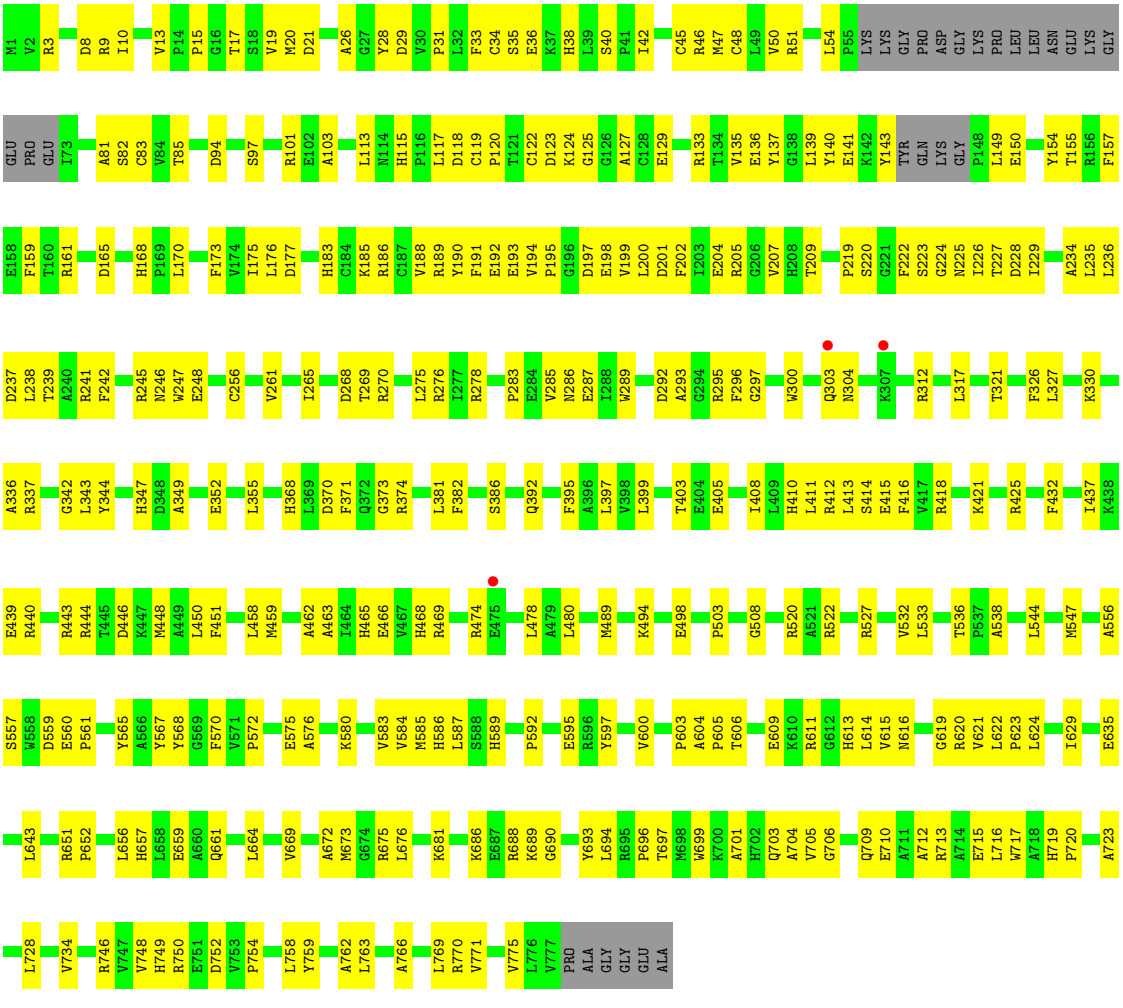




• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D:

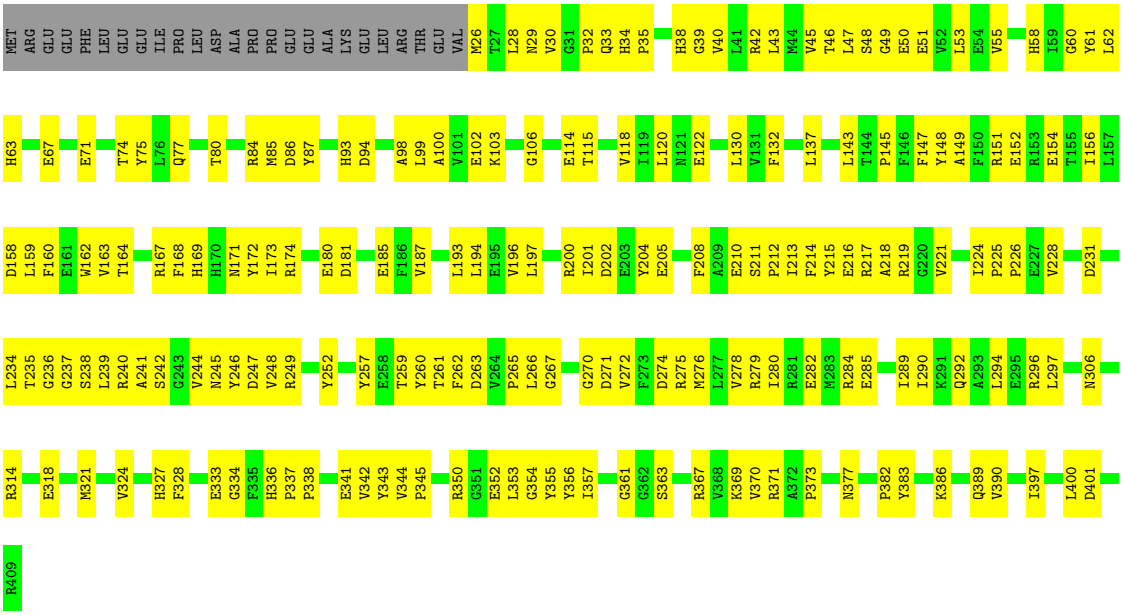




• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4:

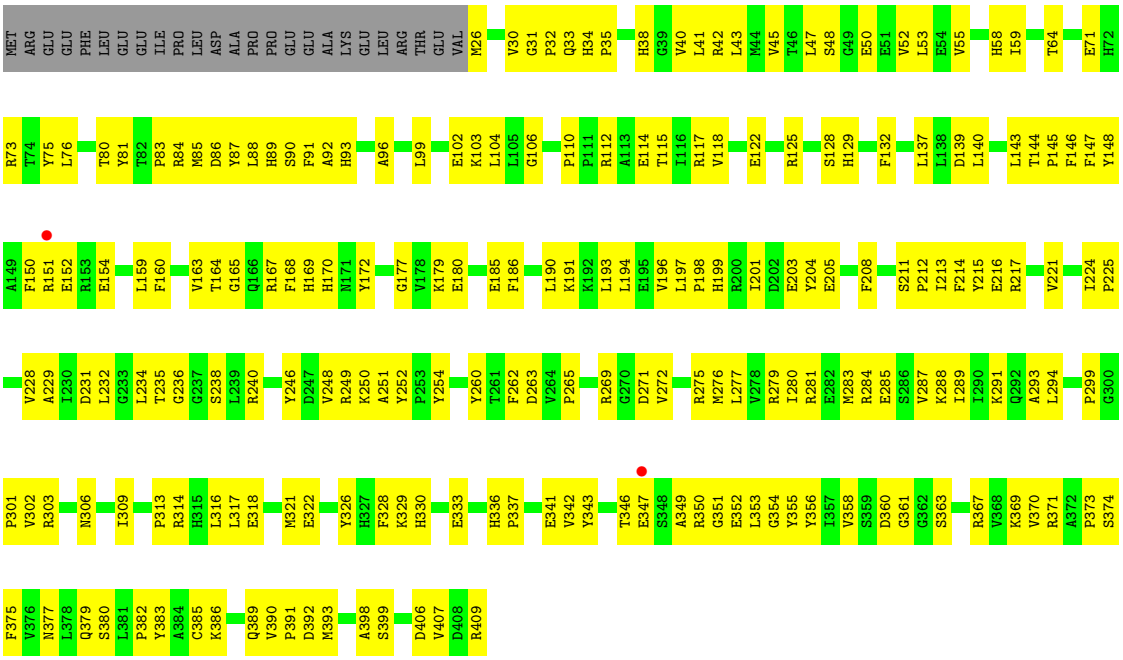




• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E:

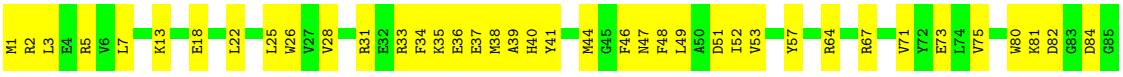


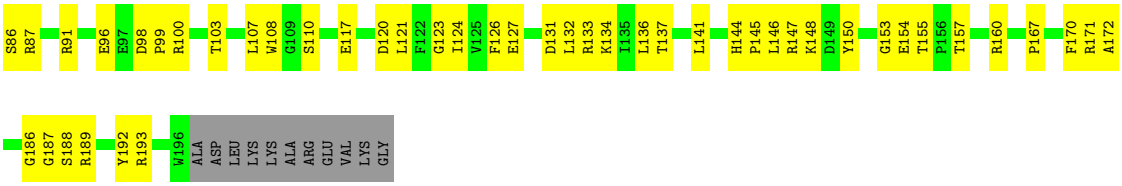


• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5:



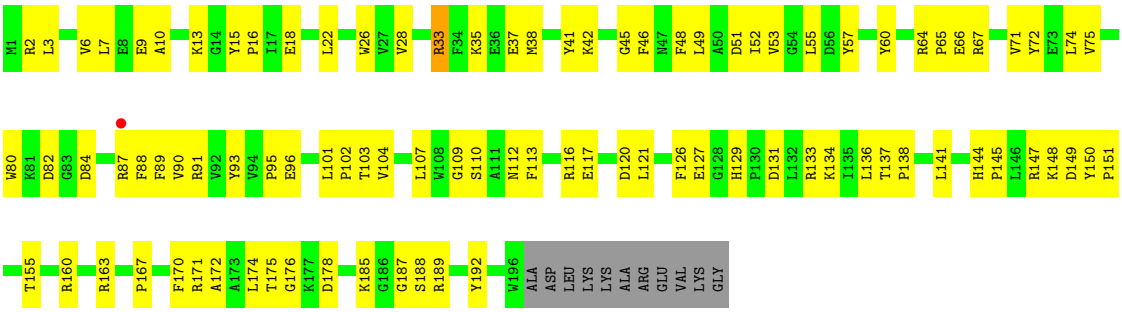




• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F:

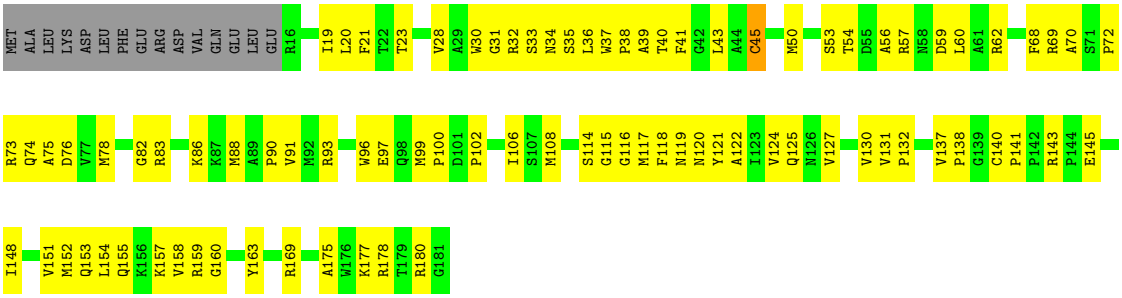




• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6:

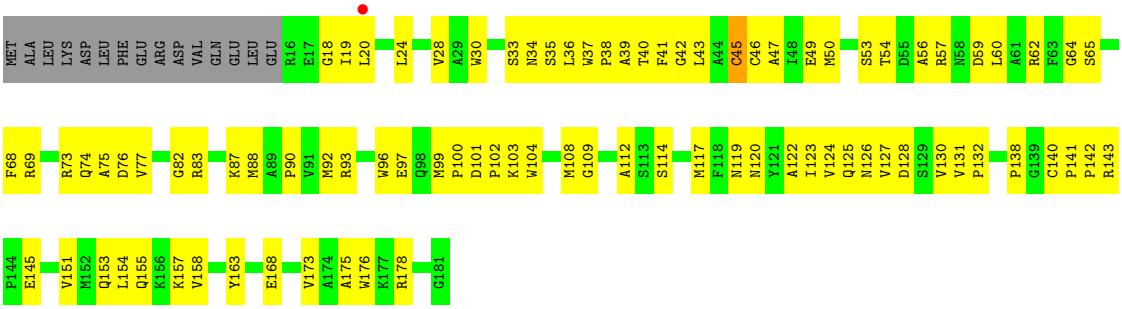




• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G:

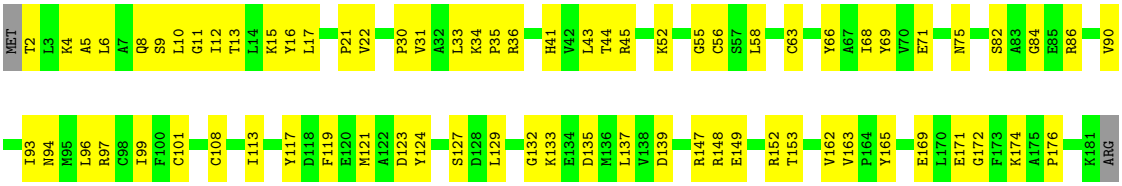




• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:

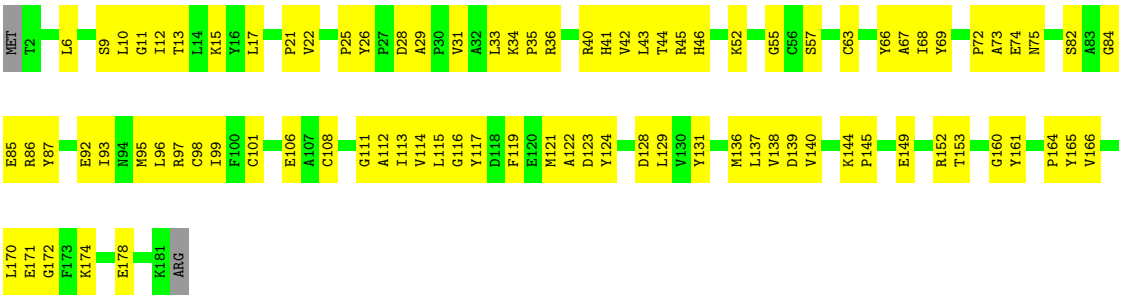




- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:

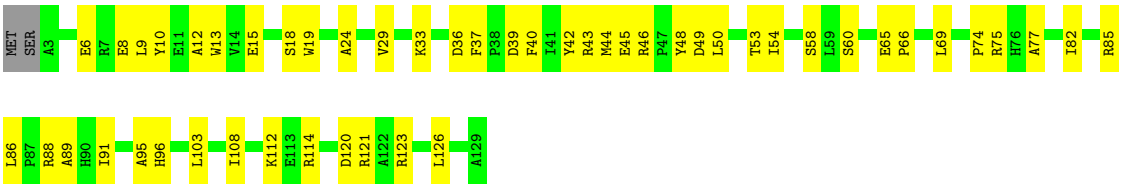




- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:

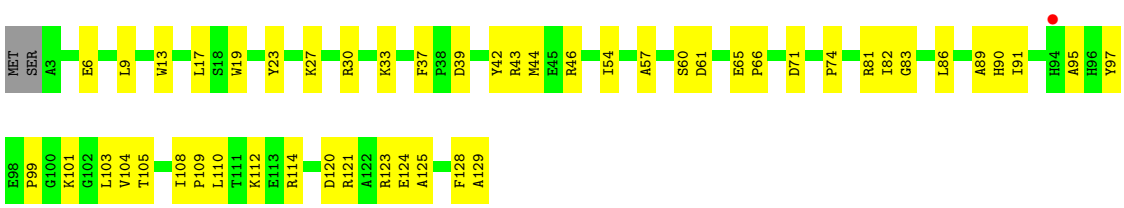




- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:

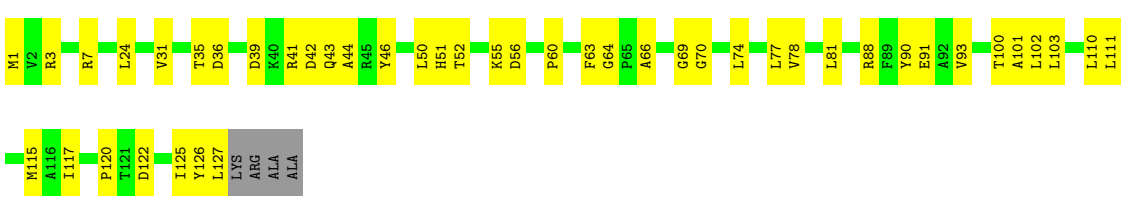




- Molecule 9: Uncharacterized protein

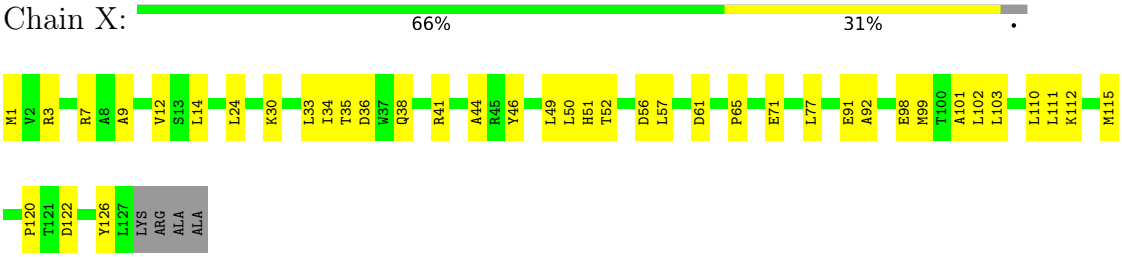
Chain W:





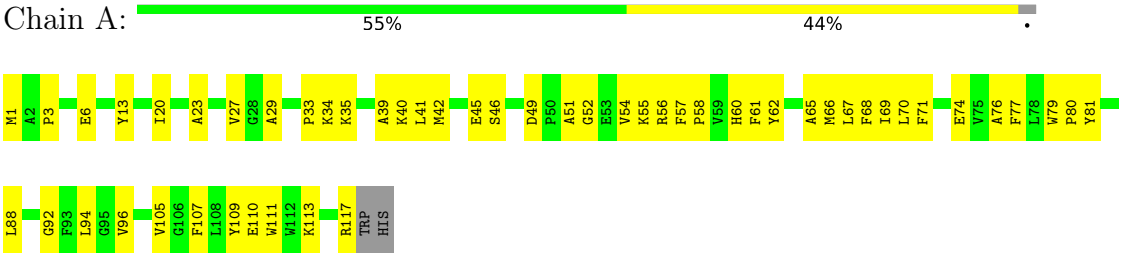
• Molecule 9: Uncharacterized protein

Chain X:



• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:



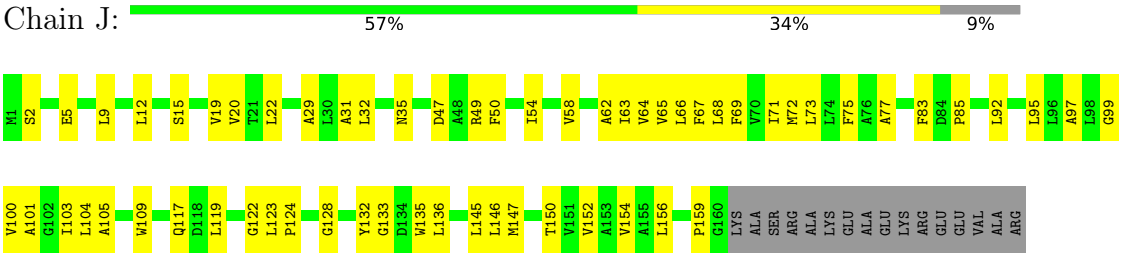
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



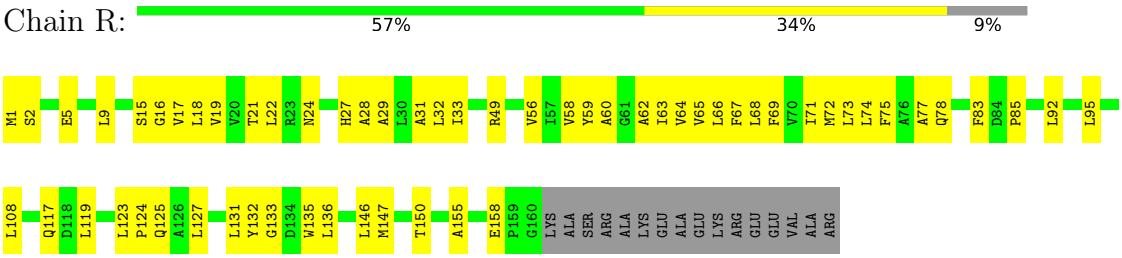
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



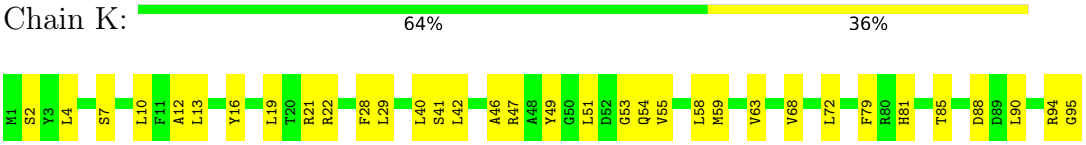
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



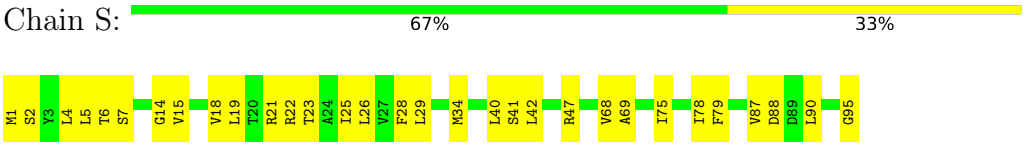
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



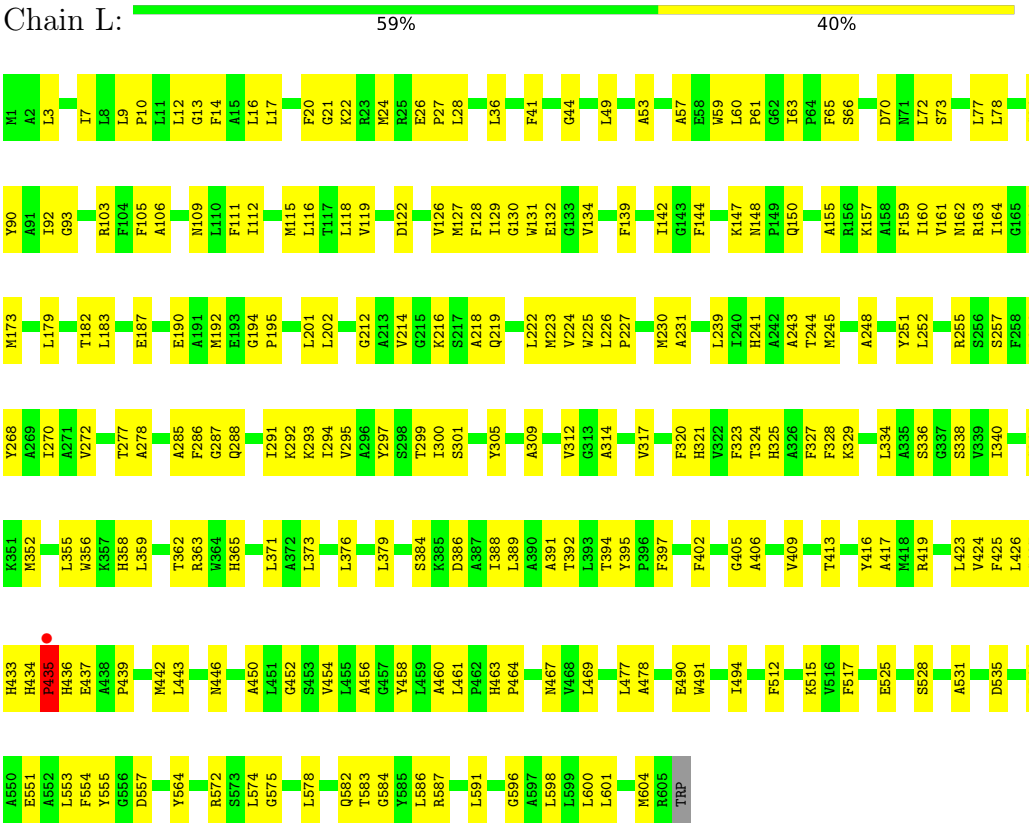
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



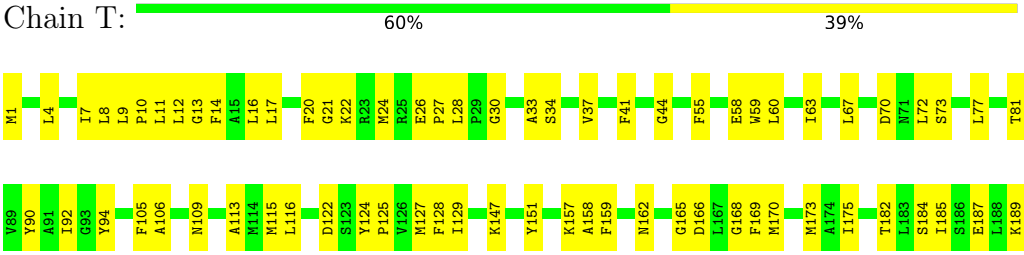
• Molecule 13: NADH-quinone oxidoreductase subunit 12

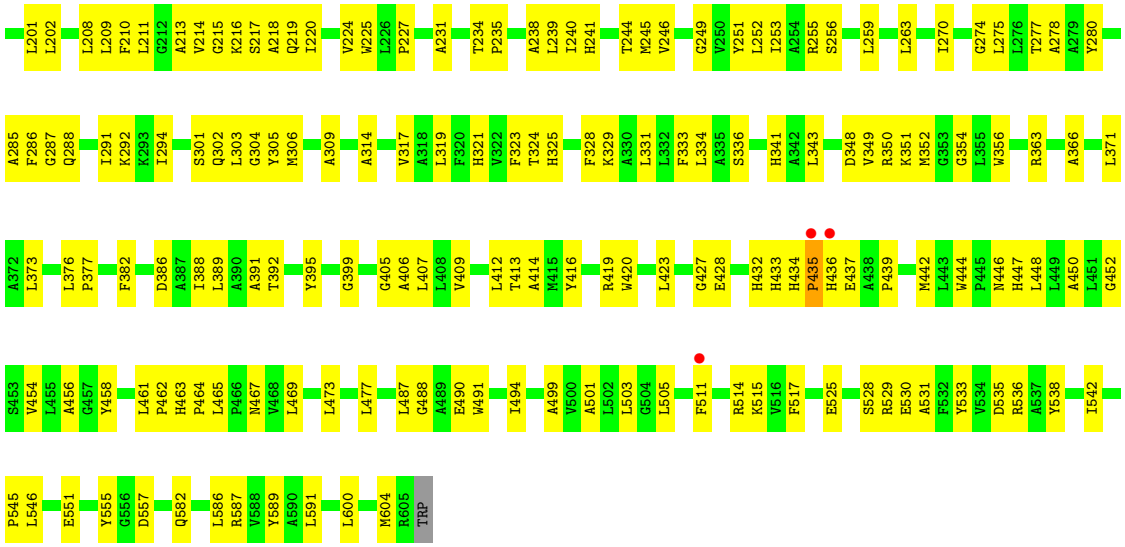
Chain L:



• Molecule 13: NADH-quinone oxidoreductase subunit 12

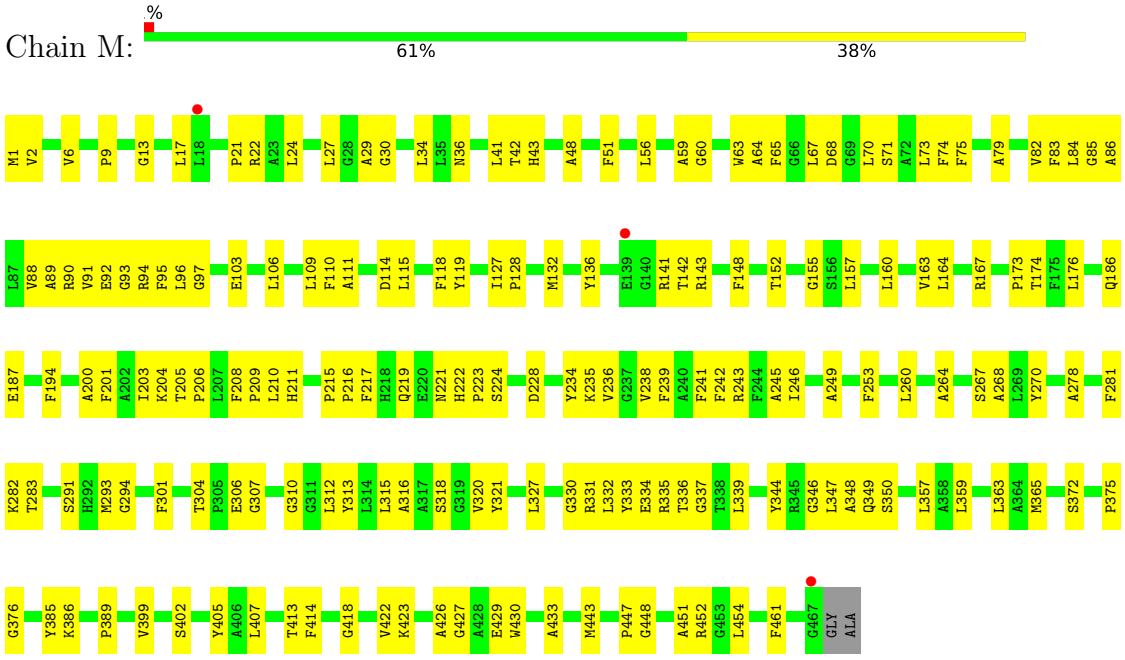
Chain T:





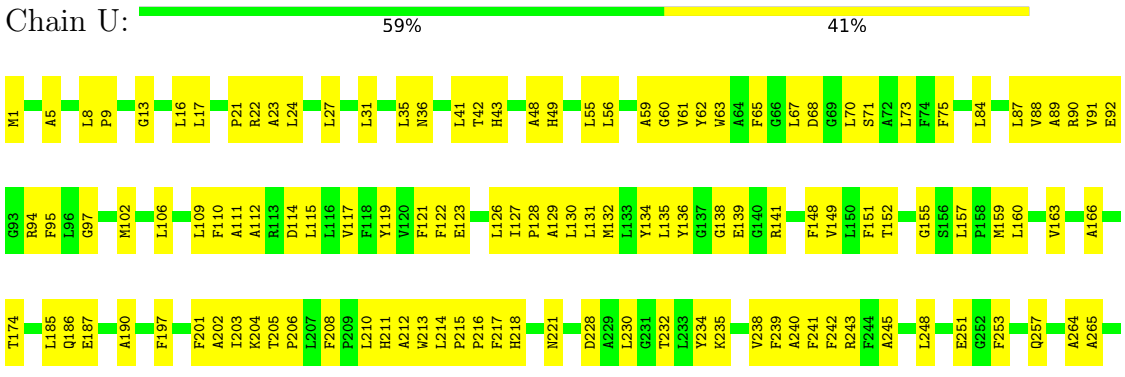
• Molecule 14: NADH-quinone oxidoreductase subunit 13

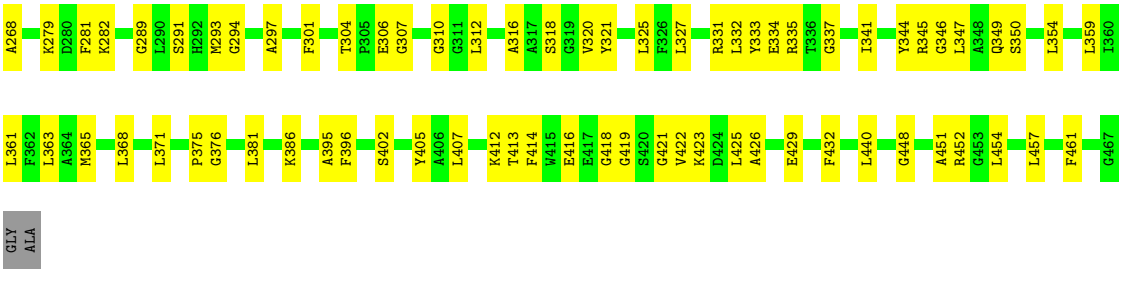
Chain M:



• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U:

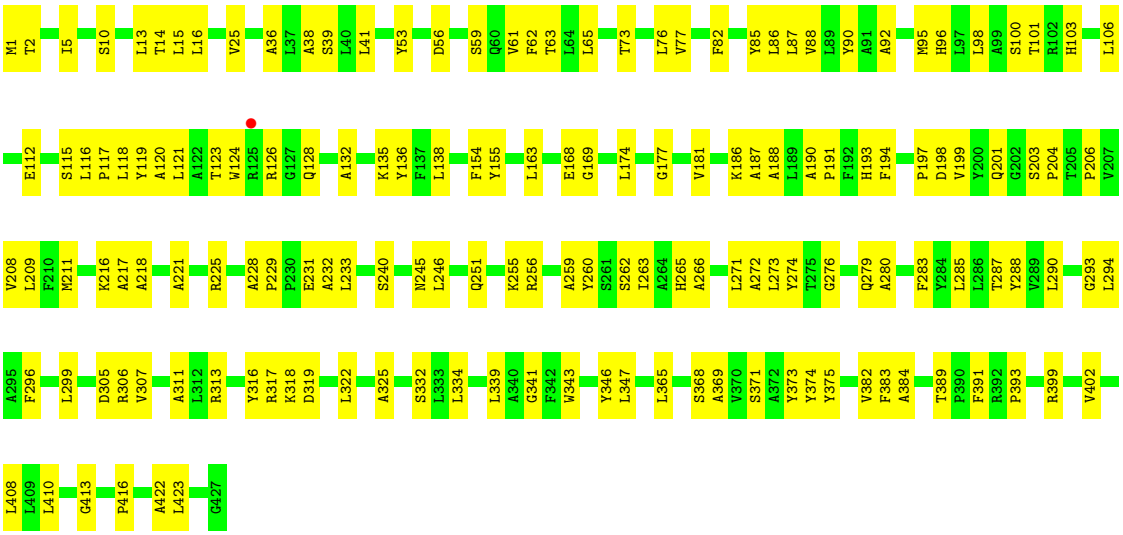




• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N:

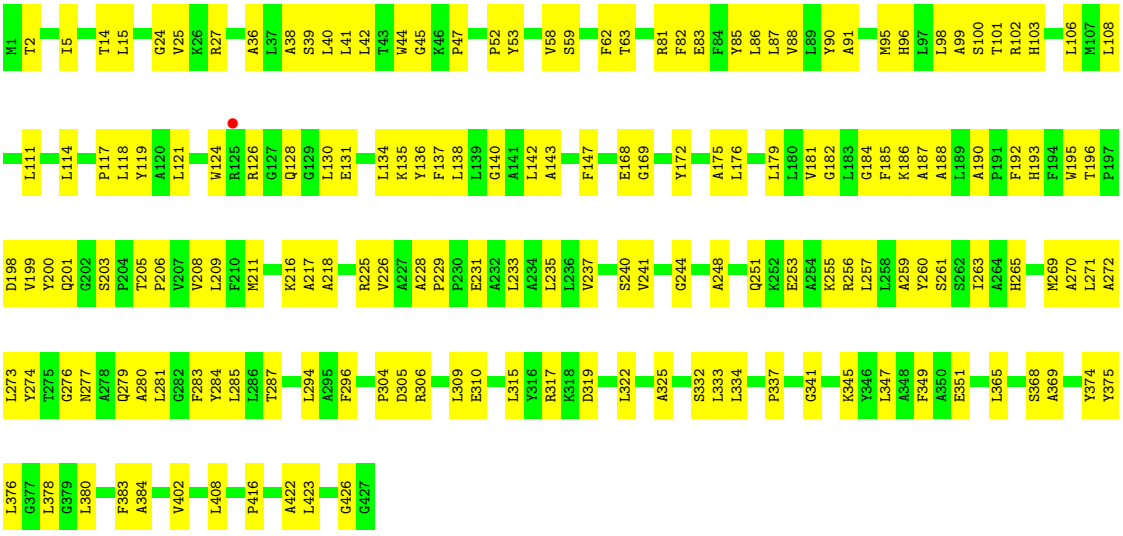




• Molecule 15: NADH-quinone oxidoreductase subunit 14

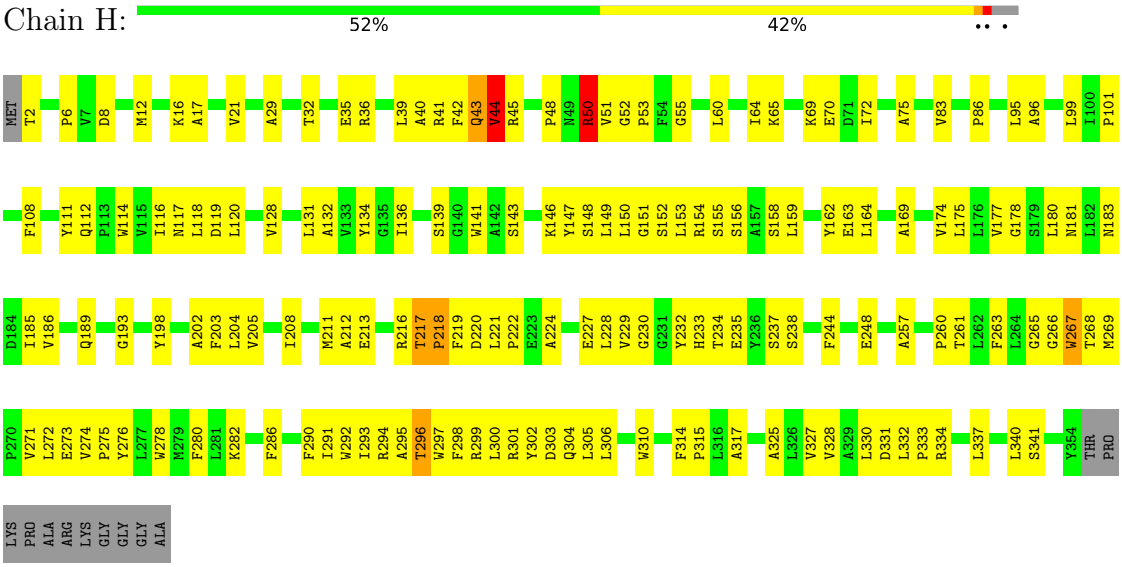
Chain V:





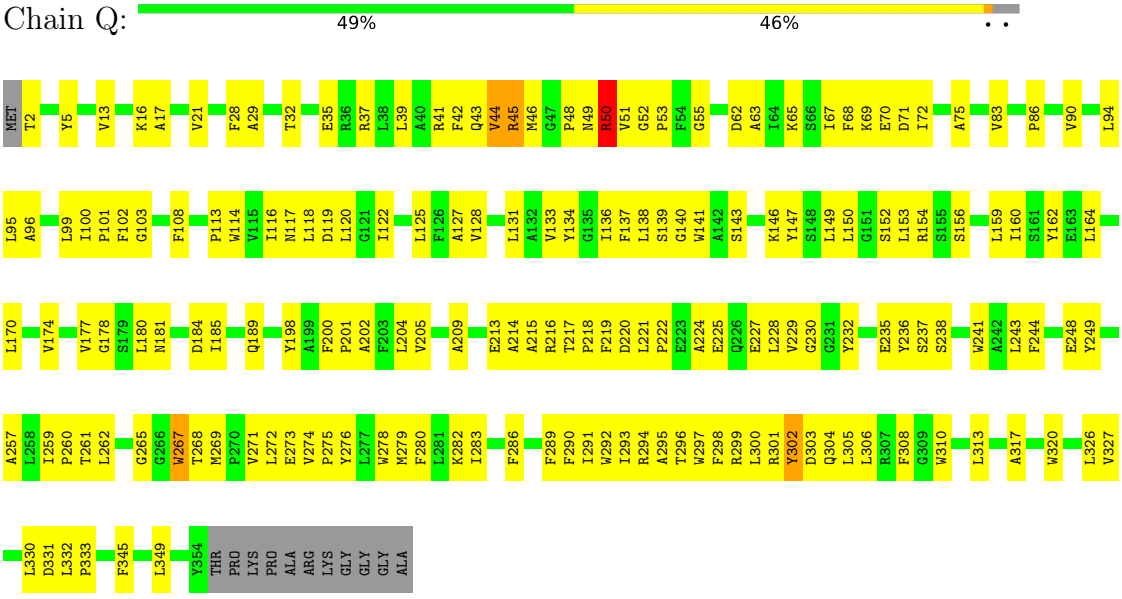
• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H:



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.19Å 338.64Å 263.23Å 90.00° 100.41° 90.00°	Depositor
Resolution (Å)	58.41 – 3.51 58.41 – 3.51	Depositor EDS
% Data completeness (in resolution range)	81.6 (58.41-3.51) 81.7 (58.41-3.51)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.13rc1_2961: ???)	Depositor
R, R_{free}	0.215 , 0.232 0.216 , 0.217	Depositor DCC
R_{free} test set	1691 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 22.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.348 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 166363 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	74134	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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, HQK, FES, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.18	0/3506	0.43	0/4745
1	B	0.18	0/3506	0.43	0/4745
2	2	0.18	0/1439	0.45	0/1953
2	C	0.22	1/1439 (0.1%)	0.44	0/1953
3	3	0.22	0/6035	0.47	0/8185
3	D	0.21	0/6035	0.46	0/8185
4	4	0.22	0/3150	0.46	0/4284
4	E	0.20	0/3150	0.45	0/4284
5	5	0.20	0/1656	0.47	0/2246
5	F	0.19	0/1656	0.45	0/2246
6	6	0.24	0/1319	0.54	0/1786
6	G	0.23	0/1319	0.54	0/1786
7	9	0.21	0/1423	0.45	0/1933
7	O	0.21	0/1423	0.47	0/1933
8	7	0.18	0/1059	0.46	0/1429
8	I	0.19	0/1059	0.48	0/1429
9	W	0.21	0/985	0.46	0/1335
9	X	0.18	0/985	0.42	0/1335
10	A	0.20	0/940	0.50	0/1280
10	P	0.19	0/940	0.47	0/1280
11	J	0.18	0/1206	0.43	0/1649
11	R	0.22	0/1206	0.43	0/1649
12	K	0.20	0/710	0.43	0/962
12	S	0.18	0/710	0.42	0/962
13	L	0.18	0/4741	0.42	0/6460
13	T	0.17	0/4741	0.43	0/6460
14	M	0.18	0/3591	0.42	0/4896
14	U	0.18	0/3591	0.42	0/4896
15	N	0.18	0/3238	0.41	0/4434
15	V	0.18	0/3238	0.40	0/4434
16	H	0.22	0/2935	0.56	2/4014 (0.0%)
16	Q	0.22	0/2935	0.56	4/4014 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.20	1/75866 (0.0%)	0.46	6/103182 (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
7	O	0	1
10	P	0	1
13	L	0	1
13	T	0	1
16	H	0	1
16	Q	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	19	PRO	CA-C	5.40	1.54	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	49	ASN	CA-C-N	6.11	133.20	121.54
16	Q	49	ASN	C-N-CA	6.11	133.20	121.54
16	Q	50	ARG	CA-C-N	5.35	131.60	121.97
16	Q	50	ARG	C-N-CA	5.35	131.60	121.97
16	H	50	ARG	CA-C-N	5.04	131.04	121.97

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	21	PRO	Peptide
16	H	217	THR	Peptide
13	L	435	PRO	Peptide
7	O	21	PRO	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	3388	144	0
1	B	3417	0	3388	208	0
2	2	1406	0	1373	61	0
2	C	1406	0	1373	68	0
3	3	5895	0	5931	225	0
3	D	5895	0	5930	256	0
4	4	3067	0	3049	188	0
4	E	3067	0	3049	217	0
5	5	1607	0	1574	85	0
5	F	1607	0	1574	99	0
6	6	1289	0	1298	89	0
6	G	1289	0	1299	100	0
7	9	1388	0	1383	76	0
7	O	1388	0	1383	80	0
8	7	1031	0	1029	50	0
8	I	1031	0	1029	48	0
9	W	967	0	1010	30	0
9	X	967	0	1010	28	0
10	A	910	0	939	62	0
10	P	910	0	939	62	0
11	J	1183	0	1286	63	0
11	R	1183	0	1286	60	0
12	K	703	0	747	37	0
12	S	703	0	747	29	0
13	L	4604	0	4734	202	0
13	T	4604	0	4734	193	0
14	M	3489	0	3606	143	0
14	U	3489	0	3606	162	0
15	N	3154	0	3343	124	0
15	V	3154	0	3343	129	0
16	H	2838	0	2903	191	0
16	Q	2838	0	2903	199	0
17	1	8	0	0	0	0
17	3	24	0	0	3	0
17	6	8	0	0	1	0
17	9	16	0	0	4	0
17	B	8	0	0	0	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	3	0
17	O	16	0	0	3	0
18	1	31	0	19	3	0
18	B	31	0	19	9	0
19	2	4	0	0	2	0
19	3	4	0	0	0	0
19	C	4	0	0	0	0
19	D	4	0	0	1	0
20	4	24	0	0	4	0
20	E	24	0	0	2	0
All	All	74134	0	75224	3238	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 22.

The worst 5 of 3238 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)
16:Q:267:TRP:CD1	16:Q:268:THR:H	1.21	1.58
16:H:267:TRP:CD1	16:H:268:THR:H	1.41	1.37
16:H:267:TRP:CG	16:H:268:THR:H	1.43	1.34
16:Q:267:TRP:CD1	16:Q:268:THR:N	1.98	1.30
16:Q:267:TRP:CG	16:Q:268:THR:H	1.43	1.28

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%)	411 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	435/438 (99%)	410 (94%)	25 (6%)	0	100	100
2	2	176/181 (97%)	170 (97%)	6 (3%)	0	100	100
2	C	176/181 (97%)	168 (96%)	8 (4%)	0	100	100
3	3	750/783 (96%)	699 (93%)	51 (7%)	0	100	100
3	D	750/783 (96%)	699 (93%)	51 (7%)	0	100	100
4	4	382/409 (93%)	362 (95%)	20 (5%)	0	100	100
4	E	382/409 (93%)	359 (94%)	23 (6%)	0	100	100
5	5	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
5	F	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
6	6	164/181 (91%)	149 (91%)	14 (8%)	1 (1%)	21	54
6	G	164/181 (91%)	151 (92%)	12 (7%)	1 (1%)	21	54
7	9	178/182 (98%)	168 (94%)	10 (6%)	0	100	100
7	O	178/182 (98%)	168 (94%)	10 (6%)	0	100	100
8	7	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
8	I	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
9	W	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
9	X	125/131 (95%)	119 (95%)	6 (5%)	0	100	100
10	A	115/119 (97%)	105 (91%)	10 (9%)	0	100	100
10	P	115/119 (97%)	104 (90%)	11 (10%)	0	100	100
11	J	158/176 (90%)	145 (92%)	13 (8%)	0	100	100
11	R	158/176 (90%)	144 (91%)	14 (9%)	0	100	100
12	K	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
12	S	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
13	L	603/606 (100%)	567 (94%)	35 (6%)	1 (0%)	43	74
13	T	603/606 (100%)	566 (94%)	36 (6%)	1 (0%)	43	74
14	M	465/469 (99%)	440 (95%)	25 (5%)	0	100	100
14	U	465/469 (99%)	439 (94%)	26 (6%)	0	100	100
15	N	425/427 (100%)	403 (95%)	22 (5%)	0	100	100
15	V	425/427 (100%)	403 (95%)	22 (5%)	0	100	100
16	H	351/365 (96%)	297 (85%)	49 (14%)	5 (1%)	9	38
16	Q	351/365 (96%)	304 (87%)	42 (12%)	5 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9478/9796 (97%)	8849 (93%)	615 (6%)	14 (0%)	48 79

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL
16	Q	51	VAL
16	H	44	VAL
16	Q	44	VAL
16	H	50	ARG

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%)	355 (100%)	0	100 100
1	B	355/356 (100%)	354 (100%)	1 (0%)	86 83
2	2	150/152 (99%)	149 (99%)	1 (1%)	76 78
2	C	150/152 (99%)	150 (100%)	0	100 100
3	3	609/628 (97%)	608 (100%)	1 (0%)	87 85
3	D	609/628 (97%)	607 (100%)	2 (0%)	86 83
4	4	332/355 (94%)	332 (100%)	0	100 100
4	E	332/355 (94%)	332 (100%)	0	100 100
5	5	167/175 (95%)	167 (100%)	0	100 100
5	F	167/175 (95%)	166 (99%)	1 (1%)	78 79
6	6	135/149 (91%)	135 (100%)	0	100 100
6	G	135/149 (91%)	135 (100%)	0	100 100
7	9	148/150 (99%)	148 (100%)	0	100 100
7	O	148/150 (99%)	148 (100%)	0	100 100
8	7	104/106 (98%)	104 (100%)	0	100 100
8	I	104/106 (98%)	104 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	W	99/101 (98%)	99 (100%)	0	100 100
9	X	99/101 (98%)	99 (100%)	0	100 100
10	A	90/92 (98%)	90 (100%)	0	100 100
10	P	90/92 (98%)	89 (99%)	1 (1%)	65 74
11	J	118/130 (91%)	118 (100%)	0	100 100
11	R	118/130 (91%)	118 (100%)	0	100 100
12	K	71/71 (100%)	71 (100%)	0	100 100
12	S	71/71 (100%)	71 (100%)	0	100 100
13	L	453/454 (100%)	453 (100%)	0	100 100
13	T	453/454 (100%)	453 (100%)	0	100 100
14	M	332/332 (100%)	332 (100%)	0	100 100
14	U	332/332 (100%)	332 (100%)	0	100 100
15	N	302/302 (100%)	302 (100%)	0	100 100
15	V	302/302 (100%)	302 (100%)	0	100 100
16	H	293/300 (98%)	289 (99%)	4 (1%)	59 71
16	Q	293/300 (98%)	291 (99%)	2 (1%)	76 78
All	All	7516/7706 (98%)	7503 (100%)	13 (0%)	87 85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	141	GLU
3	D	321	THR
16	Q	302	TYR
10	P	55	LYS
16	Q	267	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	246	ASN
11	R	117	GLN
3	D	709	GLN
6	G	98	GLN
13	T	341	HIS

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 oligosaccharides 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	$\#\|Z\| > 2$
19	FES	3	804	3	0,4,4	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
20	HQK	4	501	-	24,25,25	0.23	0	30,38,38	0.33	0
17	SF4	G	201	6	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.16	2 (6%)	48,50,50	1.41	10 (20%)
19	FES	D	804	3	0,4,4	-	-	-		
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		
18	FMN	1	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.28	9 (18%)
20	HQK	E	501	-	24,25,25	0.22	0	30,38,38	0.32	0
17	SF4	D	802	3	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		
17	SF4	D	801	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	SF4	D	803	3	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
17	SF4	6	201	6	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
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
20	HQK	4	501	-	-	0/16/17/17	0/2/2/2
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	G	201	6	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
20	HQK	E	501	-	-	0/16/17/17	0/2/2/2
17	SF4	D	802	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4A-N5	3.94	1.38	1.30
18	B	502	FMN	C4A-N5	3.72	1.38	1.30
18	B	502	FMN	C10-N1	2.76	1.38	1.33
18	1	502	FMN	C10-N1	2.58	1.38	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	502	FMN	C4-N3-C2	-3.28	119.58	125.64
18	1	502	FMN	C4-N3-C2	-3.21	119.70	125.64
18	B	502	FMN	O4-C4-C4A	-3.02	118.58	126.60
18	B	502	FMN	C5'-C4'-C3'	-3.02	106.36	112.20
18	B	502	FMN	C4A-C4-N3	2.88	120.52	113.19

There are no chirality outliers.

5 of 16 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	O4'-C4'-C5'-O5'

There are no ring outliers.

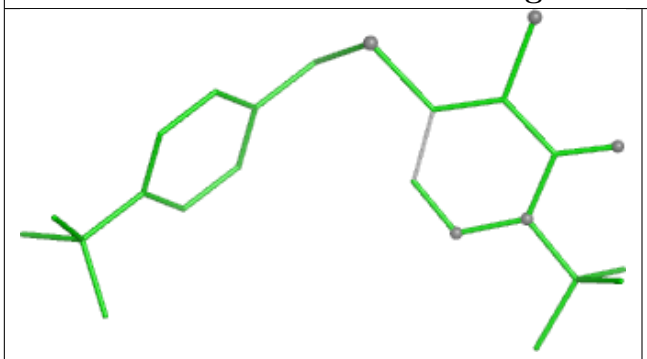
16 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	O	201	SF4	2	0
20	4	501	HQK	4	0
17	G	201	SF4	3	0
18	B	502	FMN	9	0
19	D	804	FES	1	0
17	O	202	SF4	1	0
17	3	803	SF4	2	0
17	9	202	SF4	2	0
19	2	201	FES	2	0
18	1	502	FMN	3	0
20	E	501	HQK	2	0
17	D	801	SF4	1	0
17	D	803	SF4	1	0
17	9	201	SF4	2	0
17	3	801	SF4	1	0
17	6	201	SF4	1	0

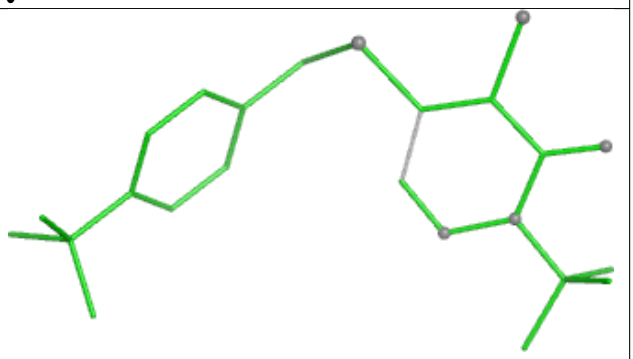
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

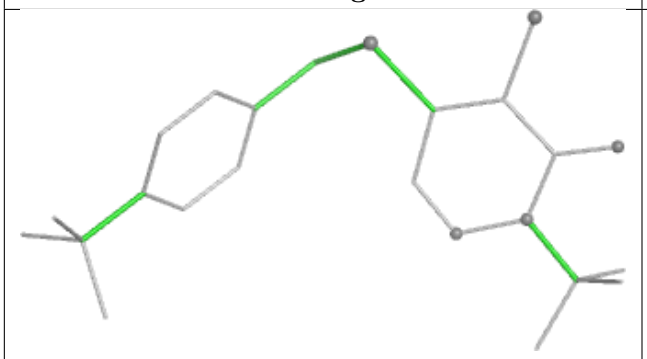
Ligand HQK 4 501



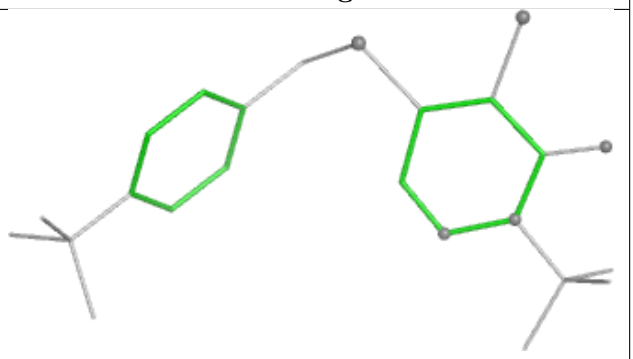
Bond lengths



Bond angles

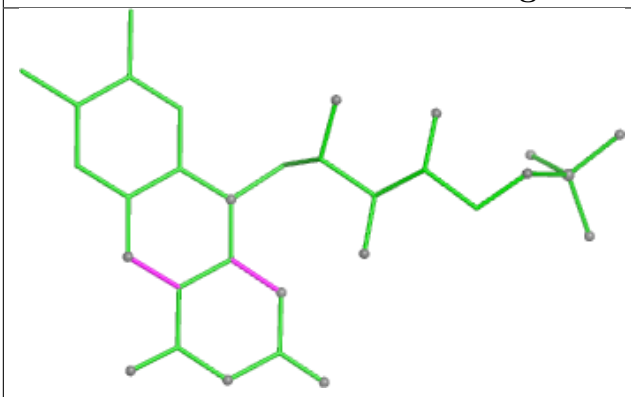


Torsions

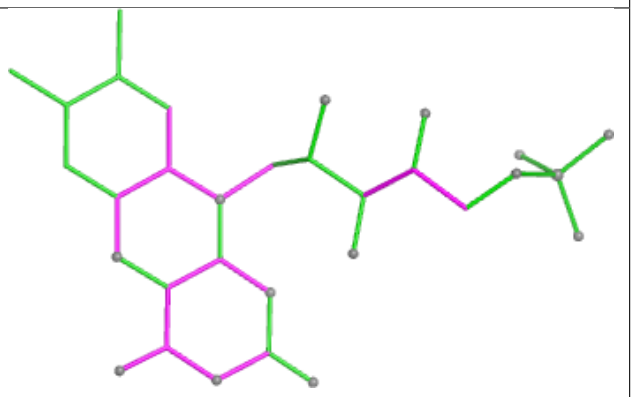


Rings

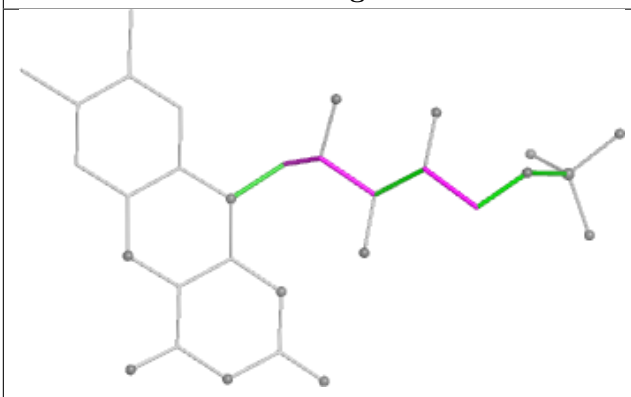
Ligand FMN B 502



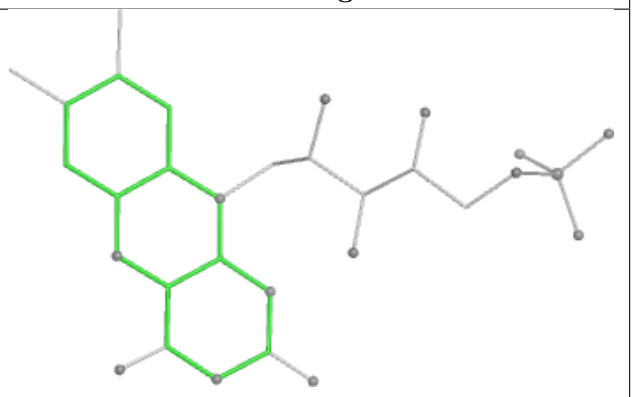
Bond lengths



Bond angles

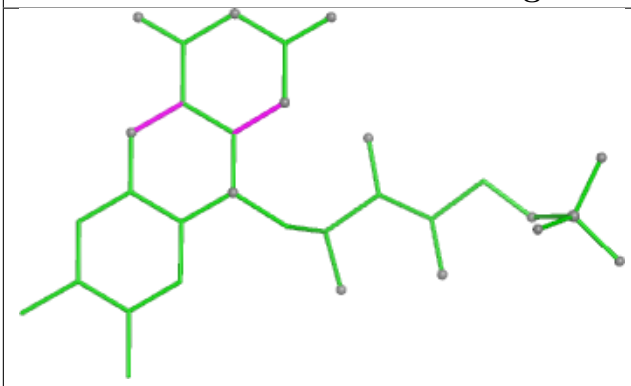


Torsions

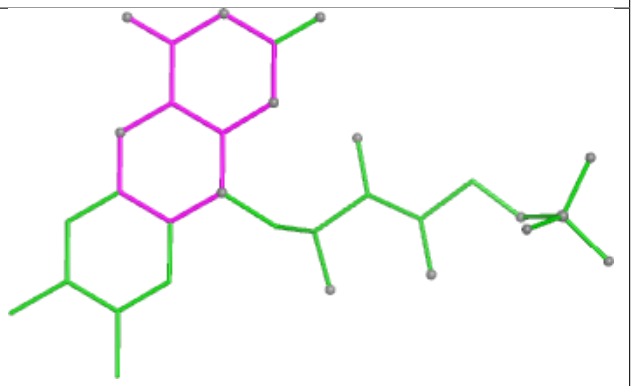


Rings

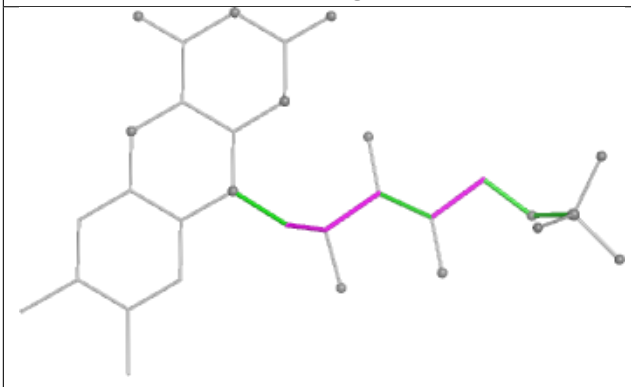
Ligand FMN 1 502



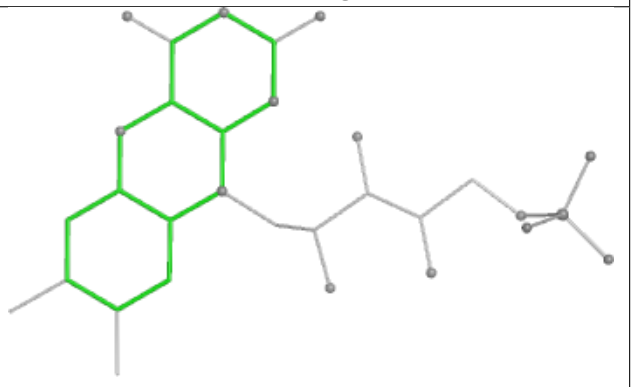
Bond lengths



Bond angles

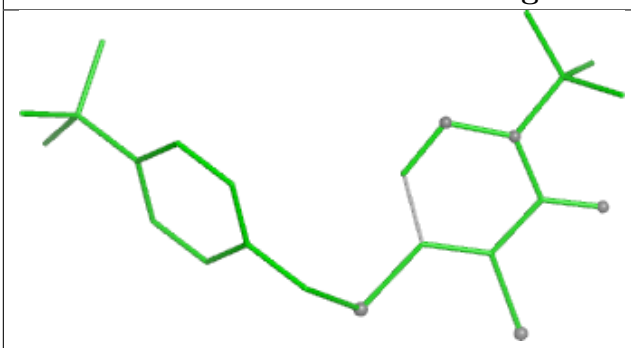


Torsions

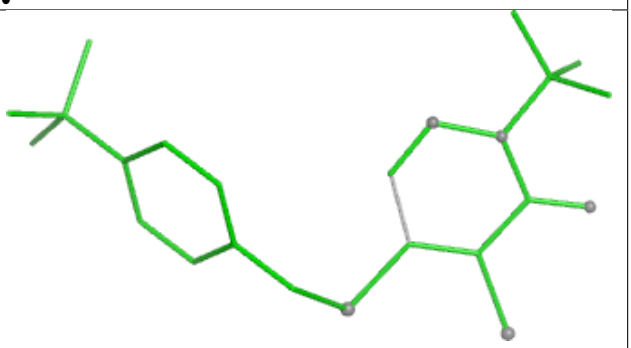


Rings

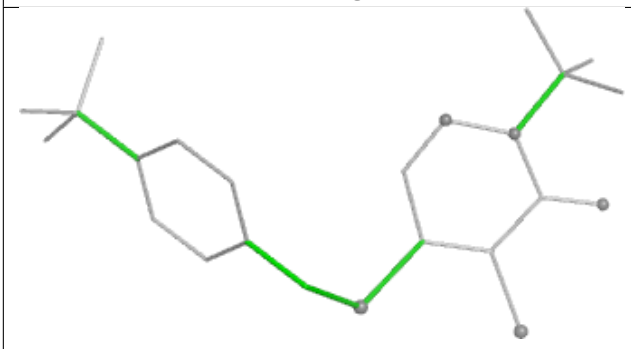
Ligand HQK E 501



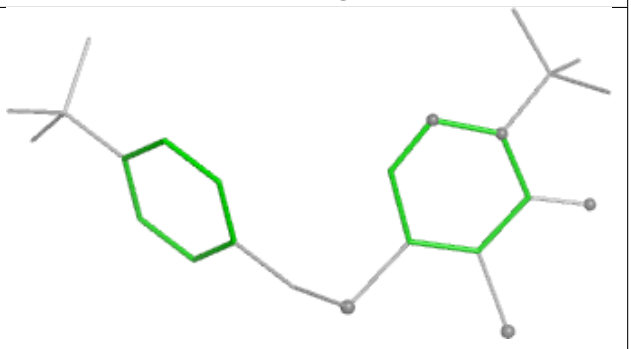
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	437/438 (99%)	-1.05	4 (0%) 81 58	33, 106, 150, 240	0
1	B	437/438 (99%)	-0.89	2 (0%) 87 68	83, 144, 204, 240	0
2	2	178/181 (98%)	-1.21	0 100 100	50, 96, 129, 150	0
2	C	178/181 (98%)	-1.14	0 100 100	35, 107, 174, 186	0
3	3	756/783 (96%)	-1.26	1 (0%) 92 86	23, 61, 107, 205	0
3	D	756/783 (96%)	-1.09	3 (0%) 88 72	24, 78, 119, 241	0
4	4	384/409 (93%)	-1.12	0 100 100	29, 74, 122, 161	0
4	E	384/409 (93%)	-0.99	2 (0%) 87 68	56, 115, 166, 204	0
5	5	196/207 (94%)	-1.26	0 100 100	35, 69, 136, 175	0
5	F	196/207 (94%)	-1.17	1 (0%) 87 68	52, 97, 132, 143	0
6	6	166/181 (91%)	-1.08	0 100 100	42, 61, 134, 193	0
6	G	166/181 (91%)	-0.89	1 (0%) 85 65	43, 83, 173, 200	0
7	9	180/182 (98%)	-1.20	0 100 100	22, 61, 106, 129	0
7	O	180/182 (98%)	-1.11	0 100 100	38, 78, 132, 186	0
8	7	127/129 (98%)	-1.22	0 100 100	50, 83, 137, 156	0
8	I	127/129 (98%)	-1.03	1 (0%) 82 60	55, 98, 133, 164	0
9	W	127/131 (96%)	-1.38	0 100 100	21, 52, 90, 142	0
9	X	127/131 (96%)	-1.17	0 100 100	70, 106, 154, 189	0
10	A	117/119 (98%)	-1.11	0 100 100	46, 85, 193, 221	0
10	P	117/119 (98%)	-0.93	0 100 100	32, 109, 175, 203	0
11	J	160/176 (90%)	-1.28	0 100 100	41, 79, 146, 170	0
11	R	160/176 (90%)	-1.11	0 100 100	31, 110, 141, 161	0
12	K	95/95 (100%)	-1.25	0 100 100	52, 82, 147, 176	0
12	S	95/95 (100%)	-1.33	0 100 100	65, 97, 117, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	L	605/606 (99%)	-1.07	1 (0%) 91 82	38, 108, 161, 296	0
13	T	605/606 (99%)	-1.07	3 (0%) 87 68	70, 115, 171, 290	0
14	M	467/469 (99%)	-1.14	3 (0%) 85 65	51, 96, 141, 174	0
14	U	467/469 (99%)	-1.12	0 100 100	65, 108, 144, 186	0
15	N	427/427 (100%)	-1.12	1 (0%) 91 82	54, 100, 153, 224	0
15	V	427/427 (100%)	-1.14	1 (0%) 91 82	48, 86, 132, 193	0
16	H	353/365 (96%)	-1.06	0 100 100	47, 97, 132, 158	0
16	Q	353/365 (96%)	-1.11	0 100 100	46, 96, 137, 218	0
All	All	9550/9796 (97%)	-1.11	24 (0%) 90 76	21, 95, 155, 296	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	T	435	PRO	7.0
13	T	436	HIS	5.0
6	G	20	LEU	3.4
1	1	4	PRO	3.1
14	M	139	GLU	3.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
18	FMN	1	502	31/31	0.99	0.04	69,100,112,116	0
18	FMN	B	502	31/31	0.99	0.05	121,139,149,152	0

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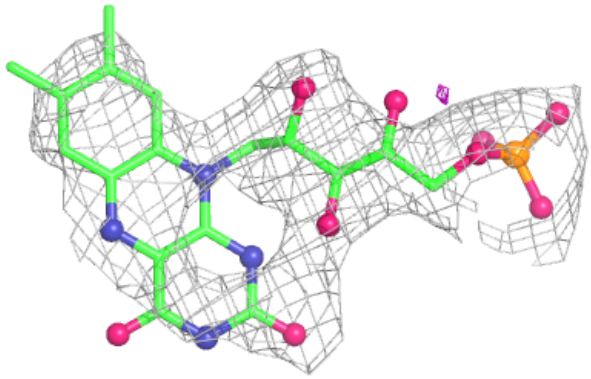
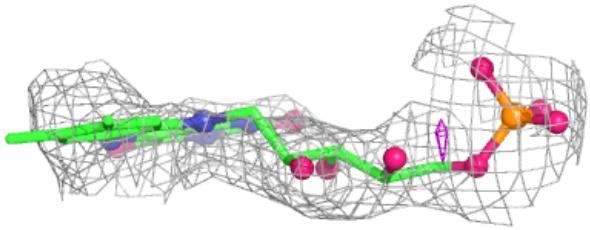
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	HQK	4	501	24/24	0.99	0.07	82,90,101,104	0
20	HQK	E	501	24/24	0.99	0.05	65,85,132,135	0
17	SF4	6	201	8/8	1.00	0.01	51,51,51,51	0
17	SF4	9	201	8/8	1.00	0.03	37,37,37,37	0
17	SF4	9	202	8/8	1.00	0.03	39,39,39,39	0
17	SF4	B	501	8/8	1.00	0.01	69,69,69,69	0
17	SF4	D	801	8/8	1.00	0.02	47,47,47,47	0
17	SF4	D	802	8/8	1.00	0.02	54,54,54,54	0
17	SF4	D	803	8/8	1.00	0.02	38,38,38,38	0
17	SF4	G	201	8/8	1.00	0.03	55,55,55,55	0
17	SF4	O	201	8/8	1.00	0.02	41,41,41,41	0
17	SF4	O	202	8/8	1.00	0.04	42,42,42,42	0
17	SF4	1	501	8/8	1.00	0.01	66,66,66,66	0
17	SF4	3	801	8/8	1.00	0.02	43,43,43,43	0
19	FES	2	201	4/4	1.00	0.01	67,67,67,67	0
19	FES	3	804	4/4	1.00	0.01	51,51,51,51	0
19	FES	C	201	4/4	1.00	0.02	70,70,70,70	0
19	FES	D	804	4/4	1.00	0.01	54,54,54,54	0
17	SF4	3	802	8/8	1.00	0.01	51,51,51,51	0
17	SF4	3	803	8/8	1.00	0.01	35,35,35,35	0

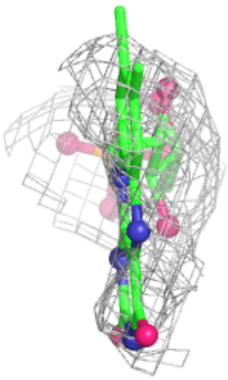
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN 1 502:

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

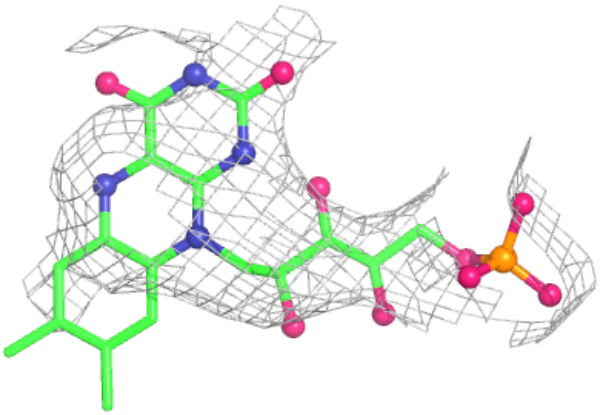


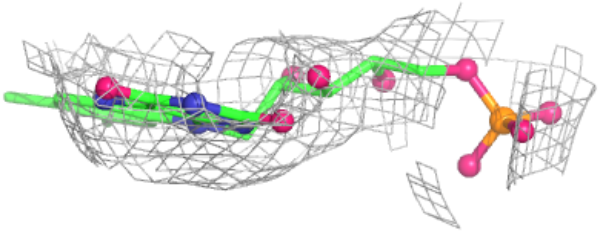


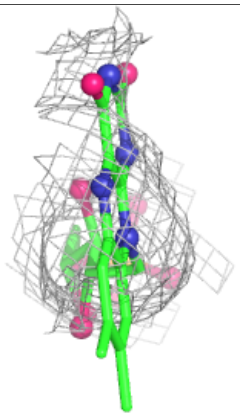


Electron density around FMN B 502:

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

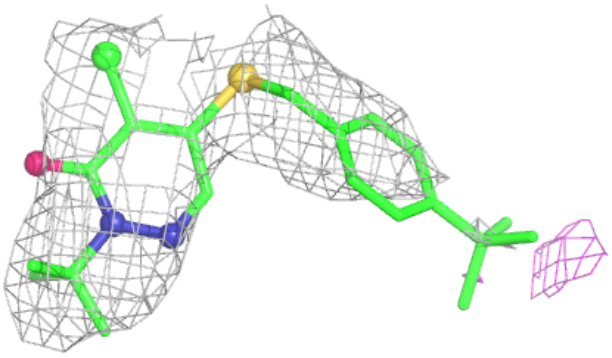


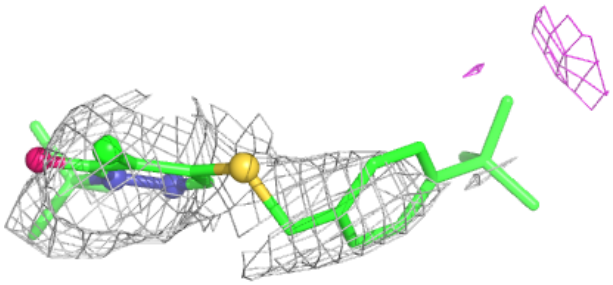


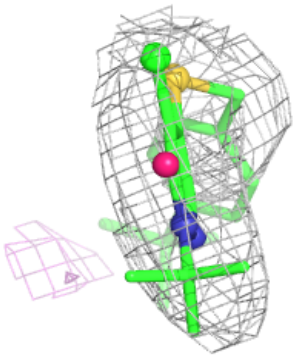


Electron density around HQK 4 501:

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

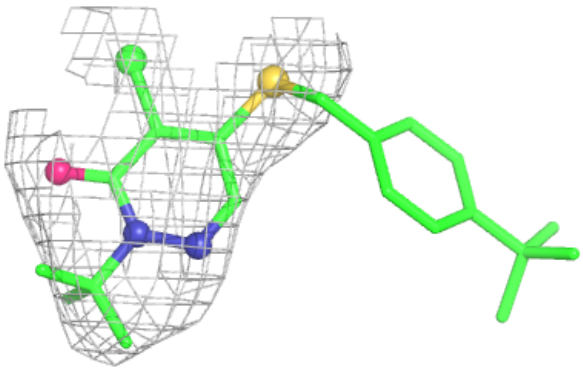


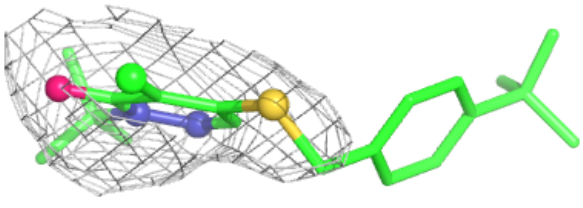


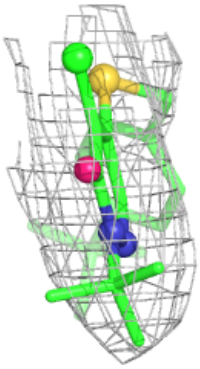


Electron density around HQK E 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.