



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 05:30 PM EDT

PDB ID : 6Q8X  
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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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	:	<b>FAILED</b>
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

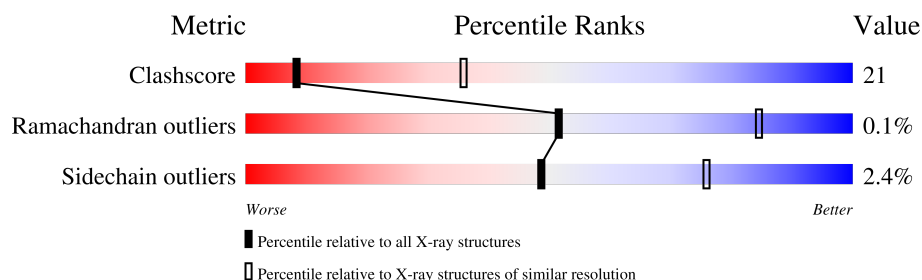
# 1 Overall quality at a glance

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))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)











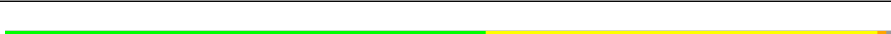



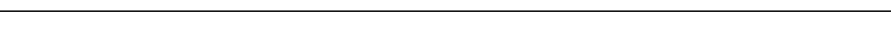
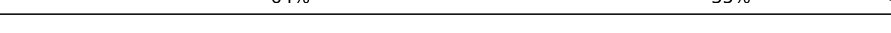








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	57% 42% .
1	B	438	48% 50% .
2	2	181	65% 31% ..
2	C	181	57% 39% ..
3	3	783	59% 37% ..
3	D	783	57% 39% ..
4	4	409	49% 44% . 6%
4	E	409	44% 49% . 6%

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Mol	Chain	Length	Quality of chain
5	5	207	 54% 39% 5%
5	F	207	 50% 43% 5%
6	6	181	 43% 45% 8%
6	G	181	 44% 43% 5% 8%
7	9	182	 60% 38% .
7	O	182	 51% 48% .
8	7	129	 59% 38% . .
8	I	129	 60% 36% . .
9	W	131	 65% 32% .
9	X	131	 68% 29% .
10	A	119	 54% 44% . .
10	P	119	 55% 39% . .
11	J	176	 56% 34% . 9%
11	R	176	 57% 32% . 9%
12	K	95	 64% 35% .
12	S	95	 67% 32% .
13	L	606	 60% 39% .
13	T	606	 61% 38% .
14	M	469	 60% 39% .
14	U	469	 59% 39% .
15	N	427	 64% 35%
15	V	427	 62% 38% .
16	H	365	 52% 42% . .
16	Q	365	 48% 46% . .

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	3	803	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	201	-	-	X	-
19	FES	2	201	-	-	X	-

## 2 Entry composition

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			

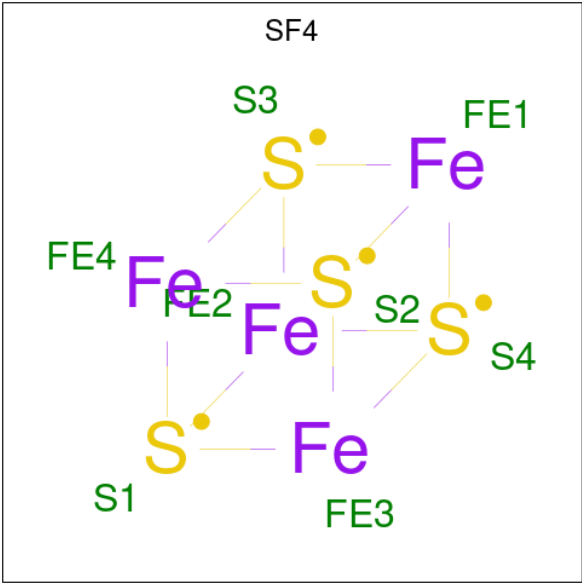
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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 (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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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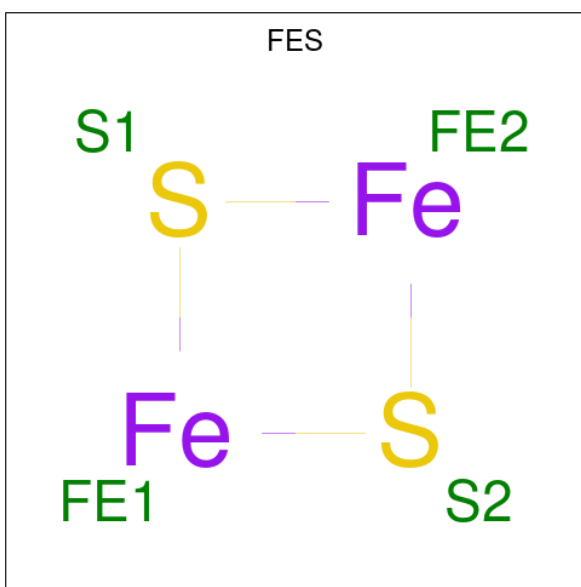


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	D	1	Total 8	Fe 4	S 4	0	0
17	D	1	Total 8	Fe 4	S 4	0	0
17	G	1	Total 8	Fe 4	S 4	0	0
17	O	1	Total 8	Fe 4	S 4	0	0
17	O	1	Total 8	Fe 4	S 4	0	0

- 
- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5) attached to a ribitol chain. The ribitol chain is a five-carbon chain with hydroxyl groups at C2, C3, and C4. The C1 of the ribitol chain is attached to the N10 of the isoalloxazine ring. The C5 of the ribitol chain is attached to a phosphate group (O1P, O2P, O3P, O4P, O5P). The ribitol chain is shown with stereochemistry: C2(S), C3(S), and C4(R). The isoalloxazine ring system is shown with stereochemistry: N1(S), N5(S), C2(S), C3(S), C4(S), C5(S), C6(S), C7(S), C8(S), C9(S), C10(S), C11(S), C12(S), C13(S), C14(S), C15(S), C16(S), C17(S), C18(S), C19(S), C20(S), C21(S), C22(S), C23(S), C24(S), C25(S), C26(S), C27(S), C28(S), C29(S), C30(S), C31(S), C32(S), C33(S), C34(S), C35(S), C36(S), C37(S), C38(S), C39(S), C40(S), C41(S), C42(S), C43(S), C44(S), C45(S), C46(S), C47(S), C48(S), C49(S), C50(S), C51(S), C52(S), C53(S), C54(S), C55(S), C56(S), C57(S), C58(S), C59(S), C60(S), C61(S), C62(S), C63(S), C64(S), C65(S), C66(S), C67(S), C68(S), C69(S), C70(S), C71(S), C72(S), C73(S), C74(S), C75(S), C76(S), C77(S), C78(S), C79(S), C80(S), C81(S), C82(S), C83(S), C84(S), C85(S), C86(S), C87(S), C88(S), C89(S), C90(S), C91(S), C92(S), C93(S), C94(S), C95(S), C96(S), C97(S), C98(S), C99(S), C100(S), C101(S), C102(S), C103(S), C104(S), C105(S), C106(S), C107(S), C108(S), C109(S), C110(S), C111(S), C112(S), C113(S), C114(S), C115(S), 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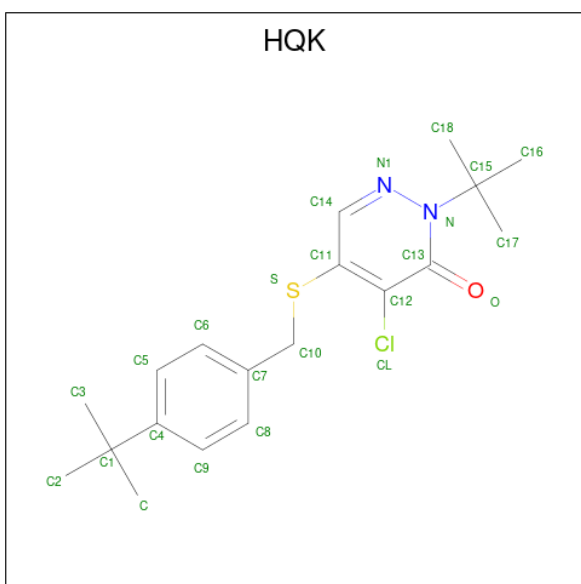
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total 31	C 17	N 4	O 9	P 1	0	0
18	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- 



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

- Molecule 20 is Pyridaben (three-letter code: HQK) (formula: C<sub>19</sub>H<sub>25</sub>ClN<sub>2</sub>OS) (labeled as "Ligand of Interest" by depositor).



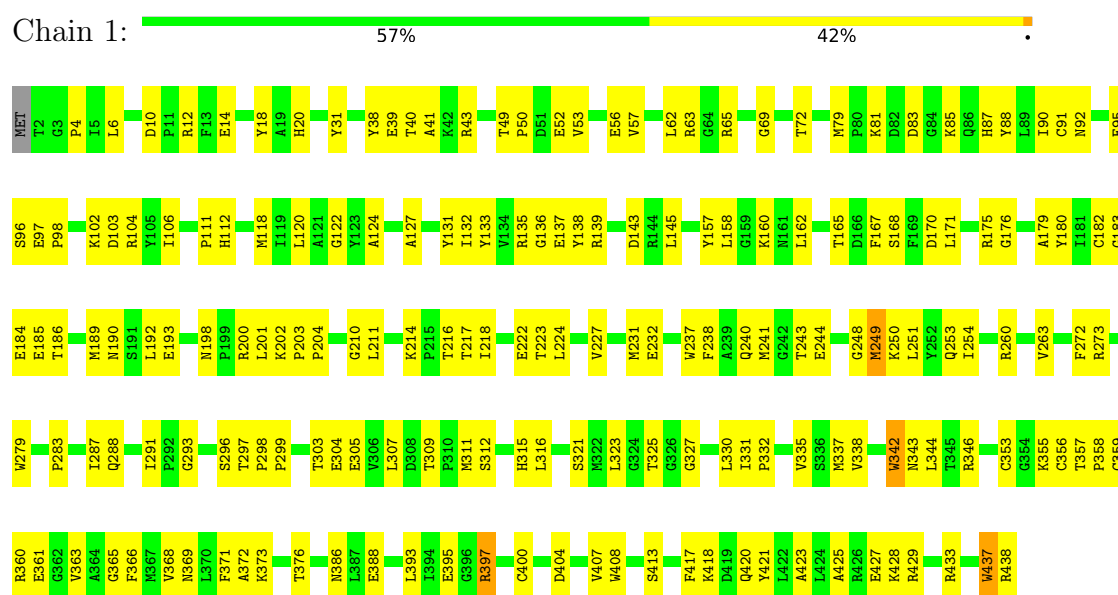
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
20	4	1	Total 24	C 19	Cl 1	N 2	O 1	S 1	0	0
20	E	1	Total 24	C 19	Cl 1	N 2	O 1	S 1	0	0

### 3 Residue-property plots

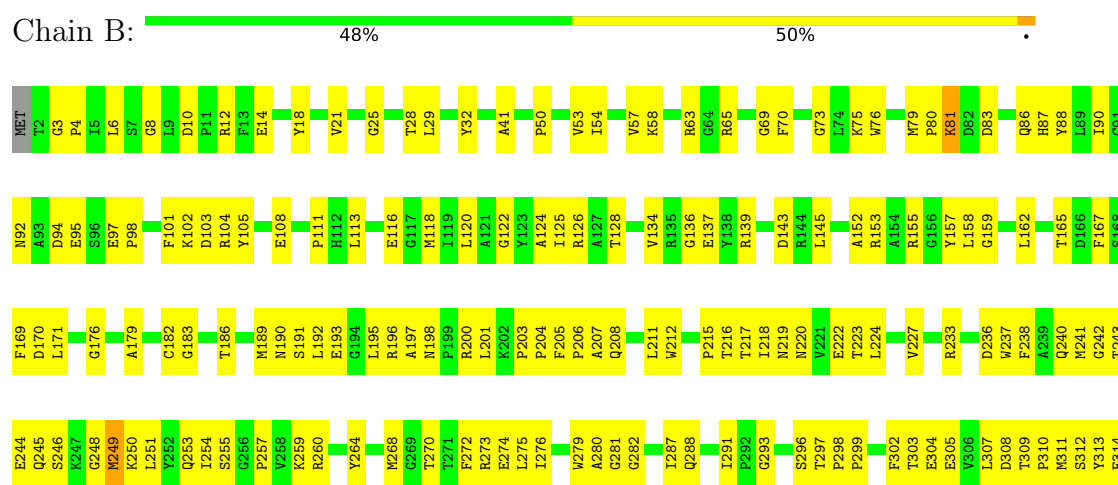
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

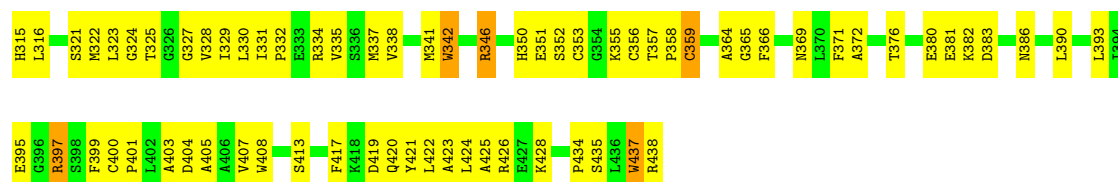
Note EDS failed to run properly.

#### • Molecule 1: NADH-quinone oxidoreductase subunit 1



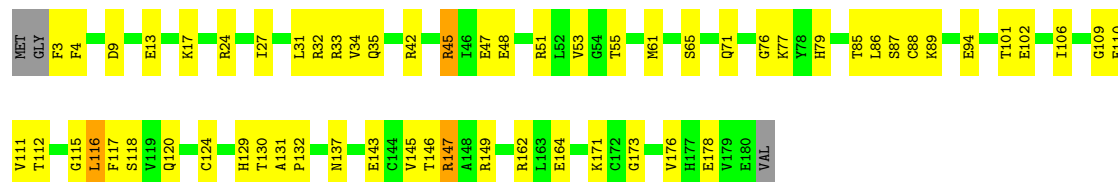
#### • Molecule 1: NADH-quinone oxidoreductase subunit 1





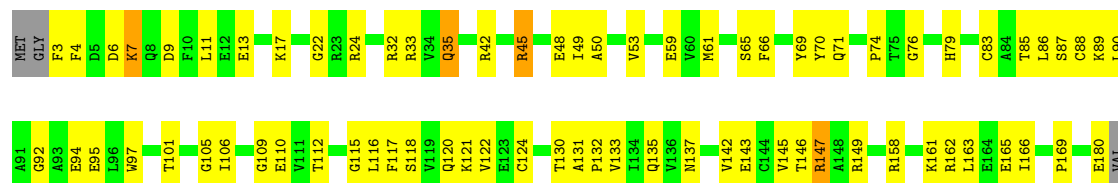
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 65% 31% ..



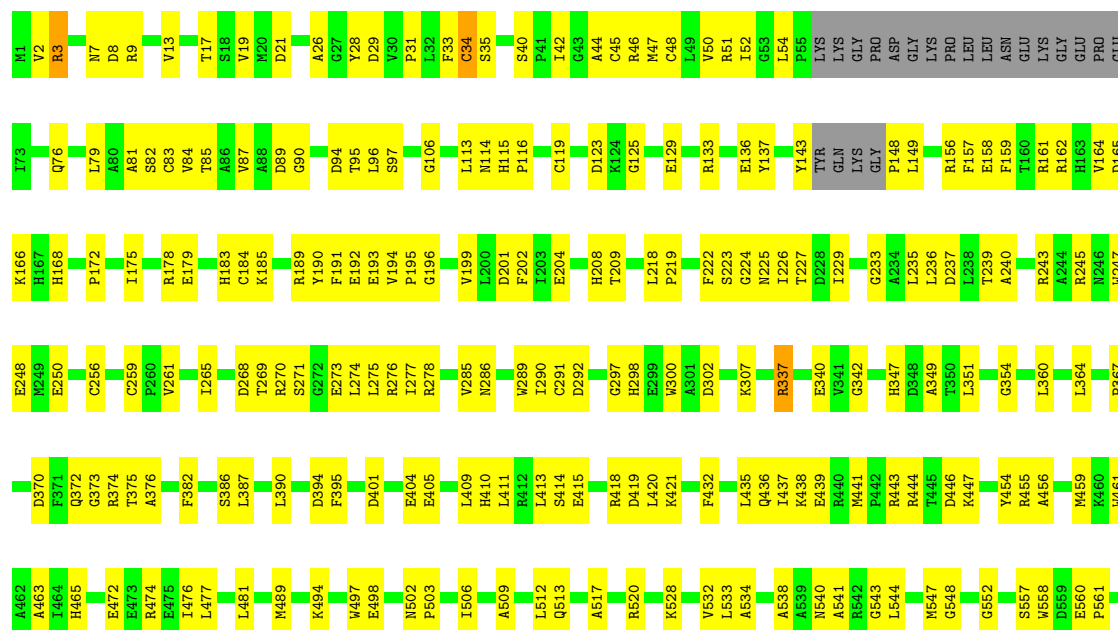
• Molecule 2: NADH-quinone oxidoreductase subunit 2

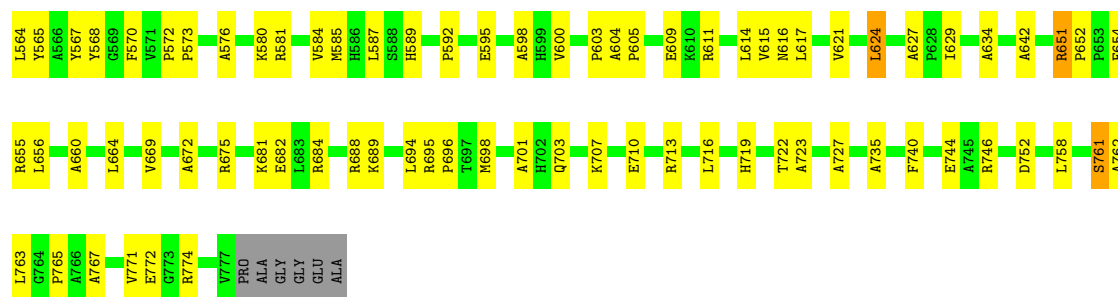
Chain C: 57% 39% ..



• Molecule 3: NADH-quinone oxidoreductase subunit 3

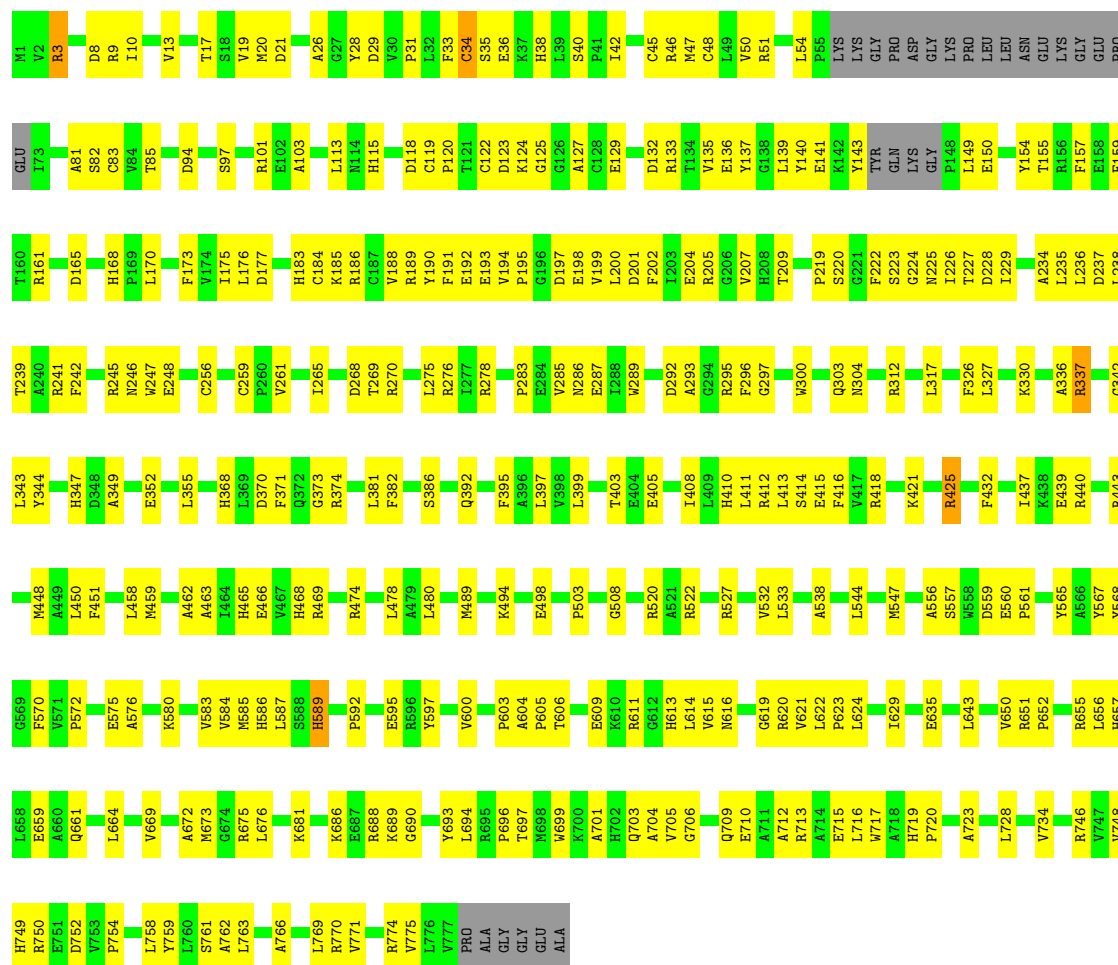
Chain 3: 59% 37% ..





• Molecule 3: NADH-quinone oxidoreductase subunit 3

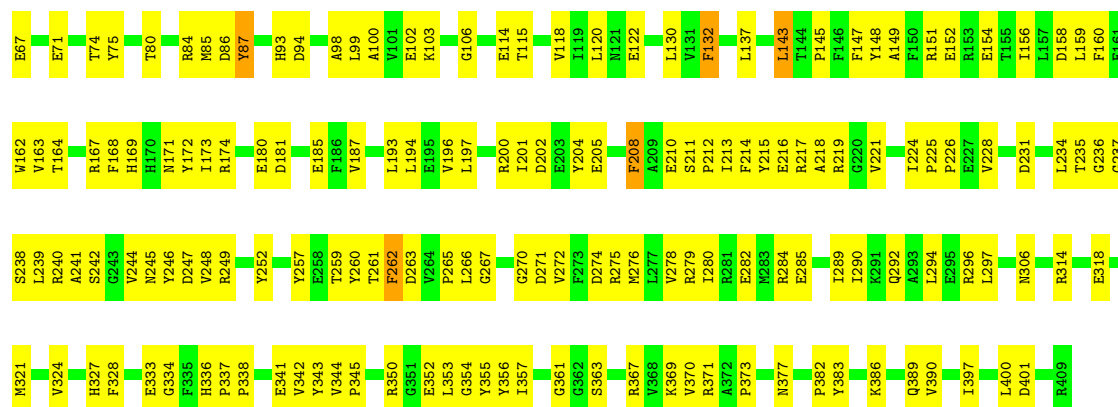
Chain D: 57% 39%



• Molecule 4: NADH-quinone oxidoreductase subunit 4

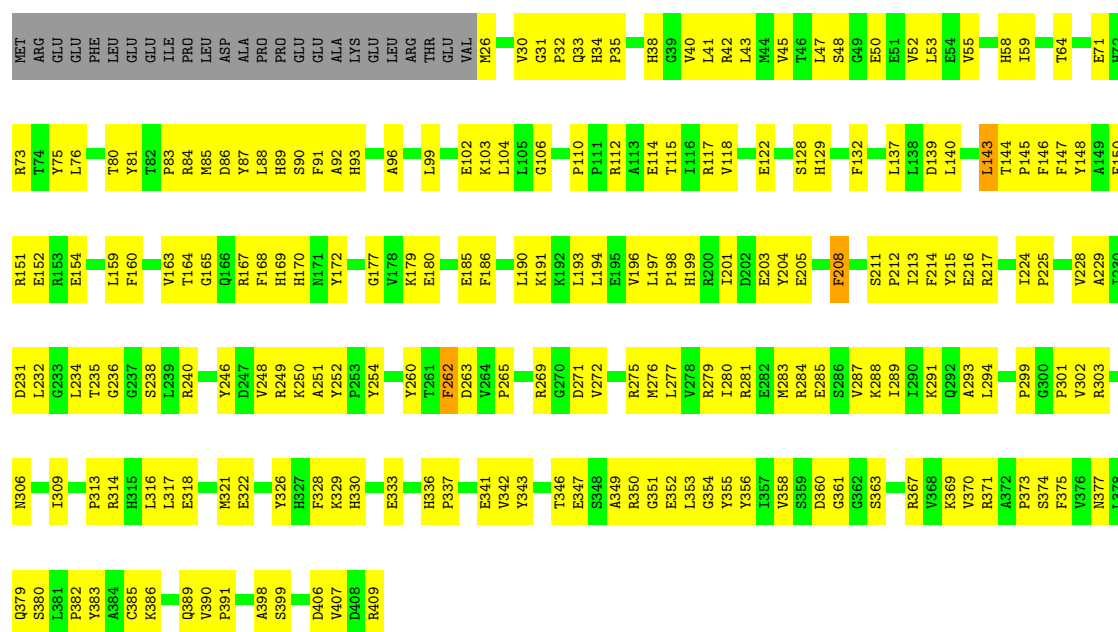
Chain 4: 49% 44% 6%





• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E: 44% 49% 6%



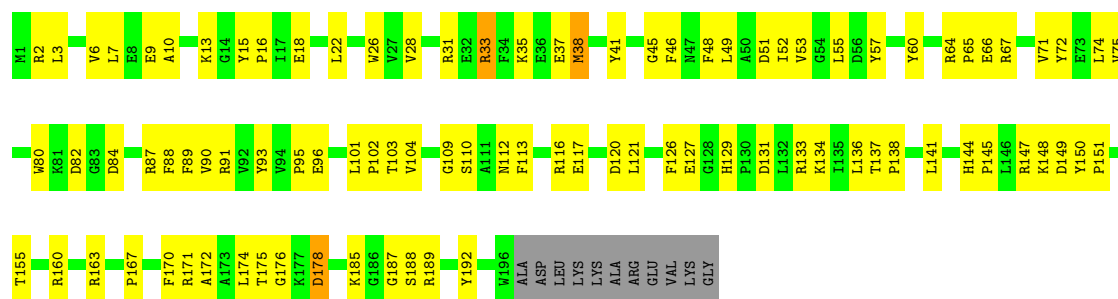
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5: 54% 39% 5%



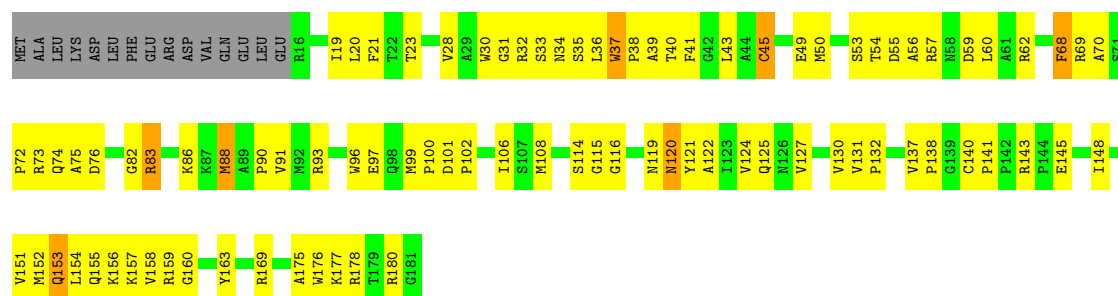
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F:  50% 43% 5%



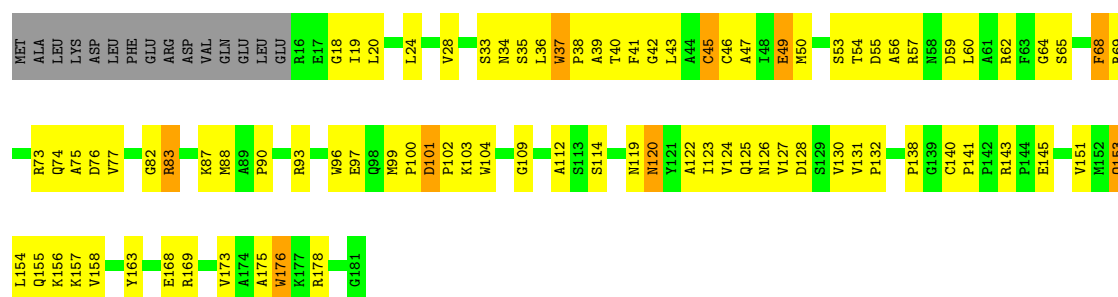
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6:  43% 45% 8%



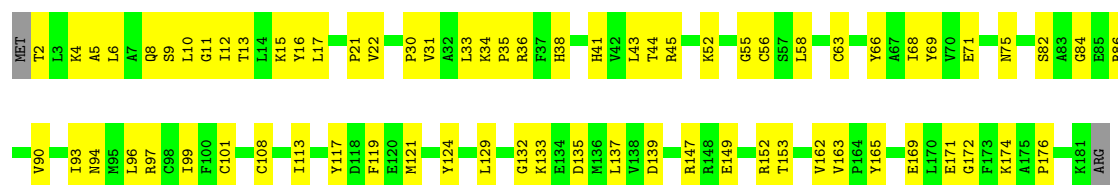
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G:  44% 43% 5% 8%



• Molecule 7: NADH-quinone oxidoreductase subunit 9

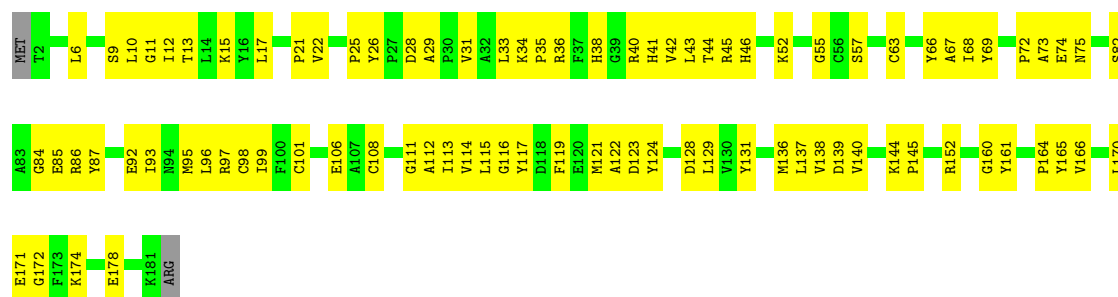
Chain 9:  60% 38% 2%



• Molecule 7: NADH-quinone oxidoreductase subunit 9

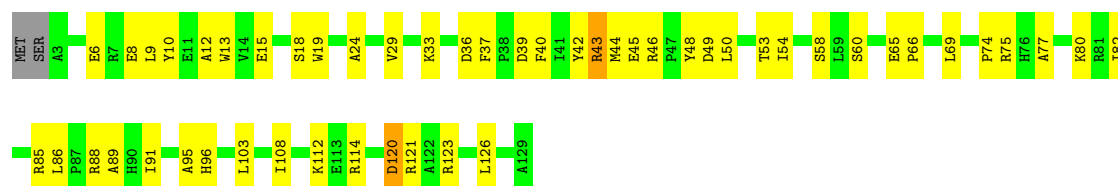


Chain O:  51% 48%



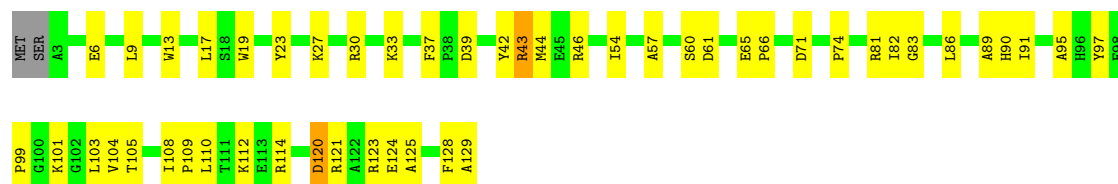
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:  59% 38%



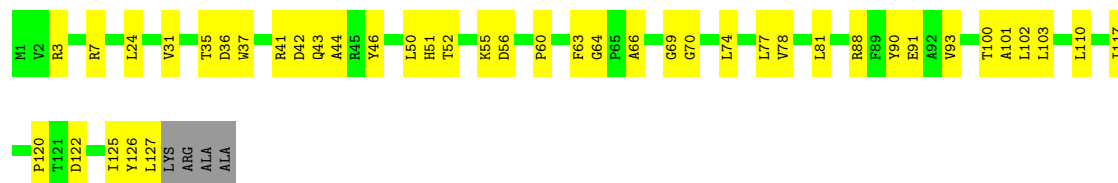
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:  60% 36%



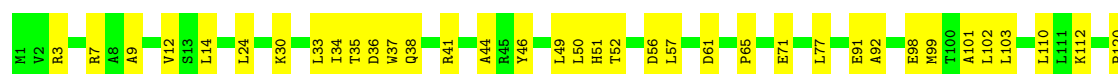
• Molecule 9: Uncharacterized protein

Chain W:  65% 32%



• Molecule 9: Uncharacterized protein

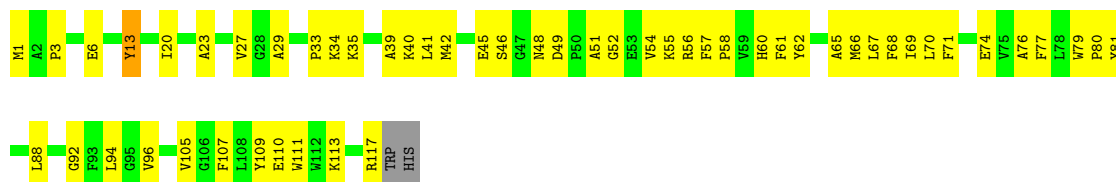
Chain X:  68% 29%





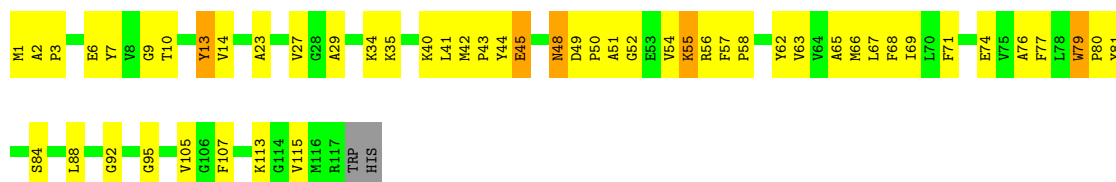
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A: 54% 44% ..



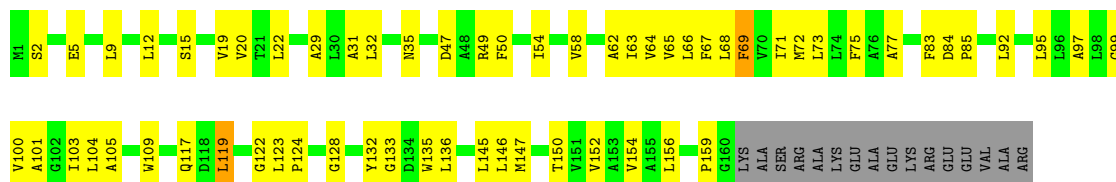
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P: 55% 39% ..



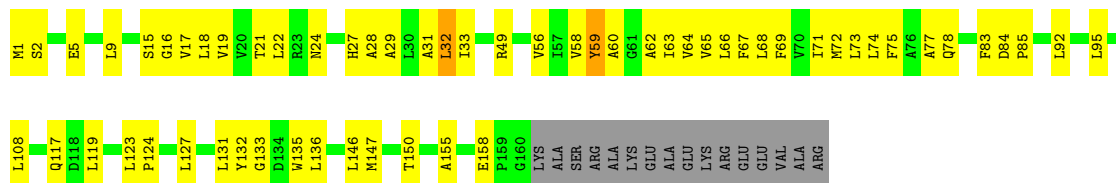
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J: 56% 34% 9%



• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R: 57% 32% 9%



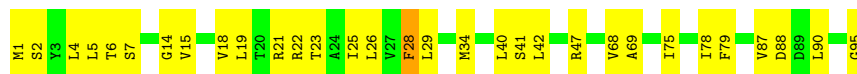
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K: 64% 35%



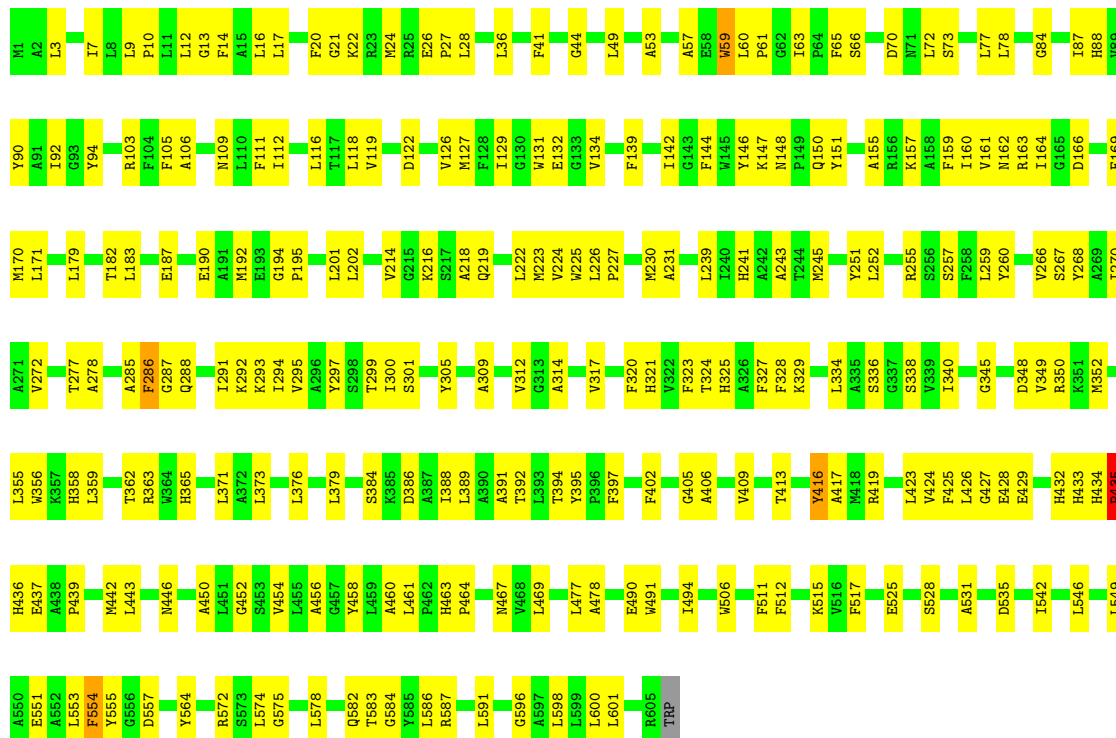
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:  67% 32%



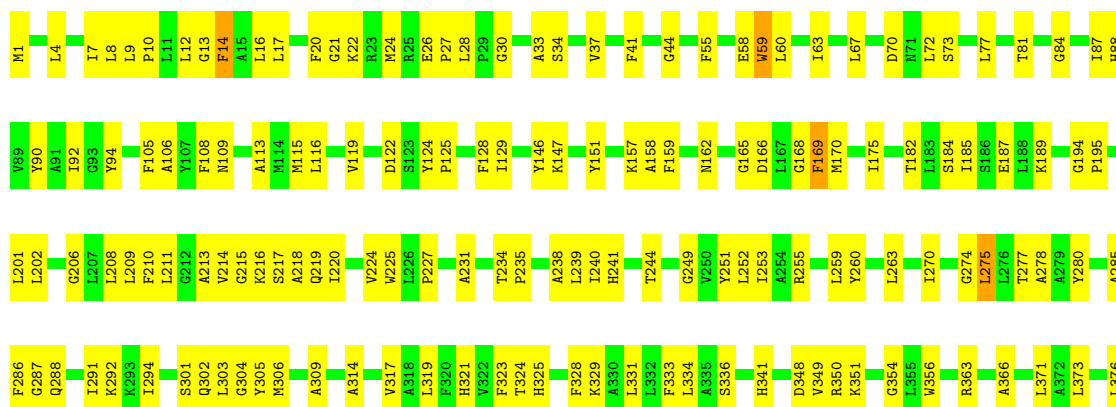
• Molecule 13: NADH-quinone oxidoreductase subunit 12

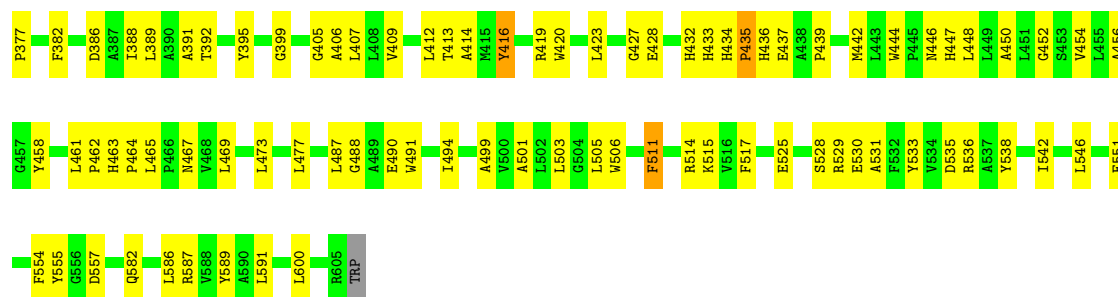
Chain L:  60% 39%



• Molecule 13: NADH-quinone oxidoreductase subunit 12

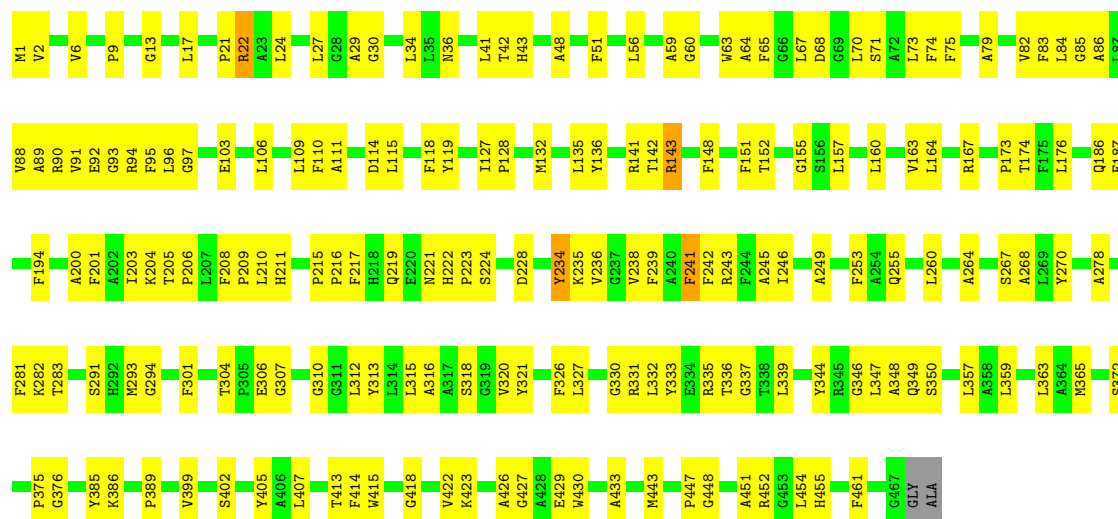
Chain T:  61% 38%





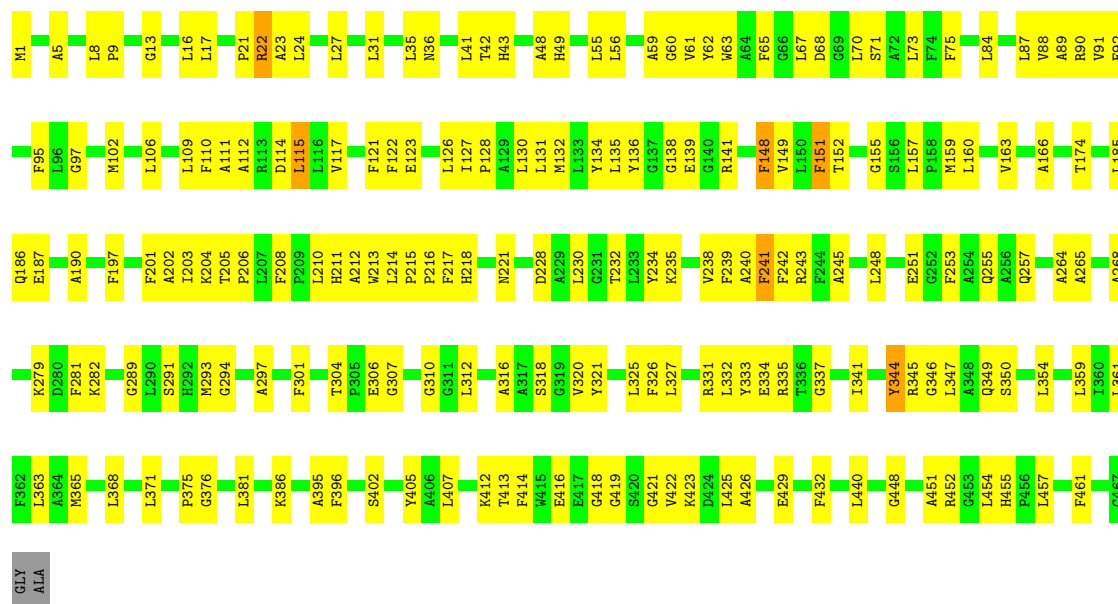
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain M: 60% 39%

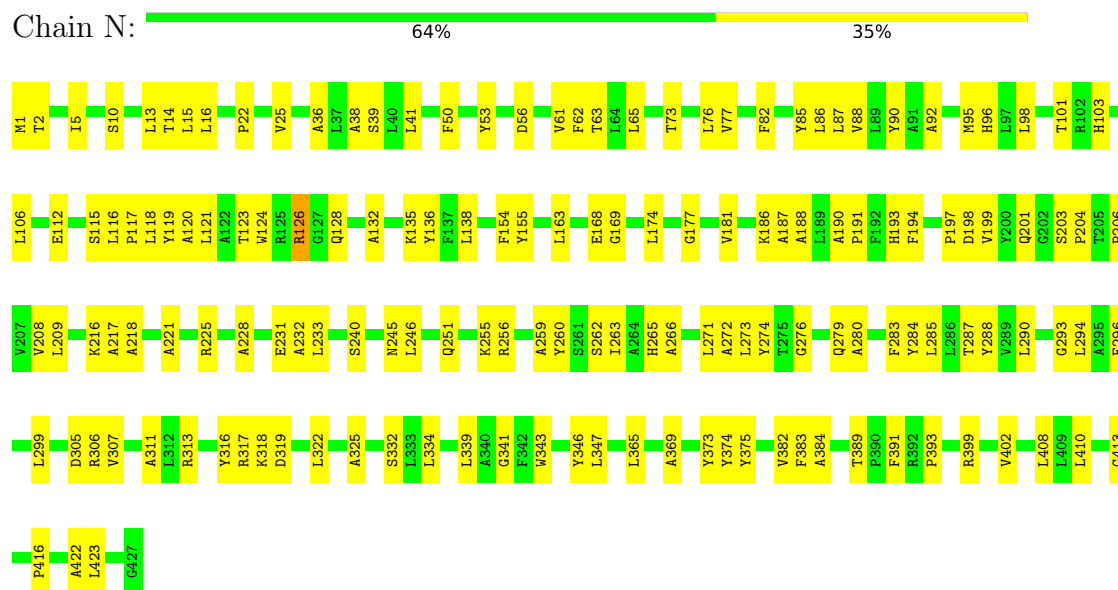


• Molecule 14: NADH-quinone oxidoreductase subunit 13

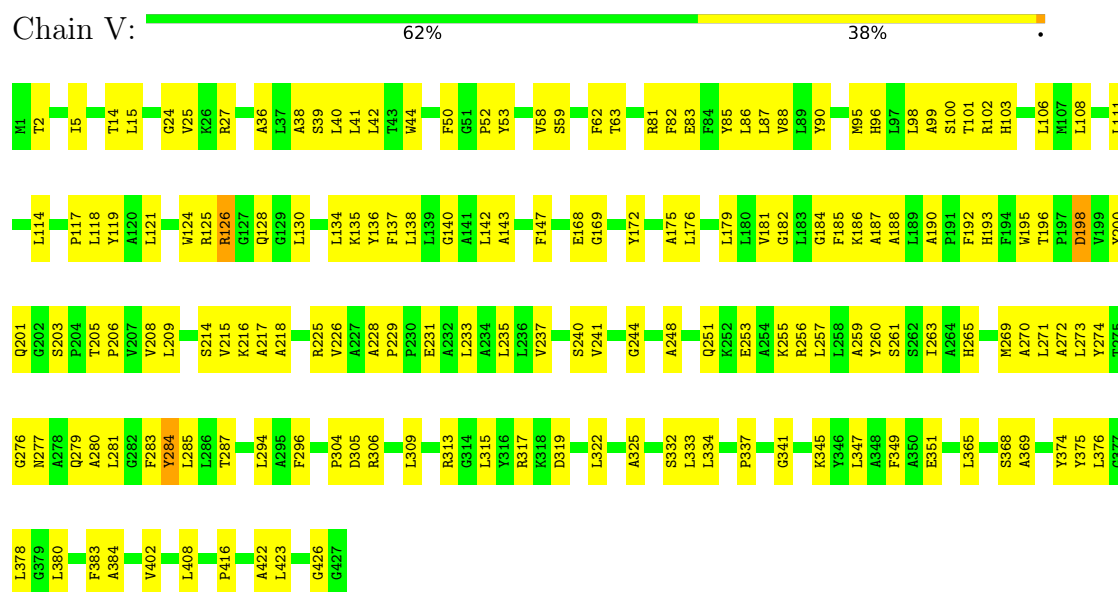
Chain U: 59% 39%



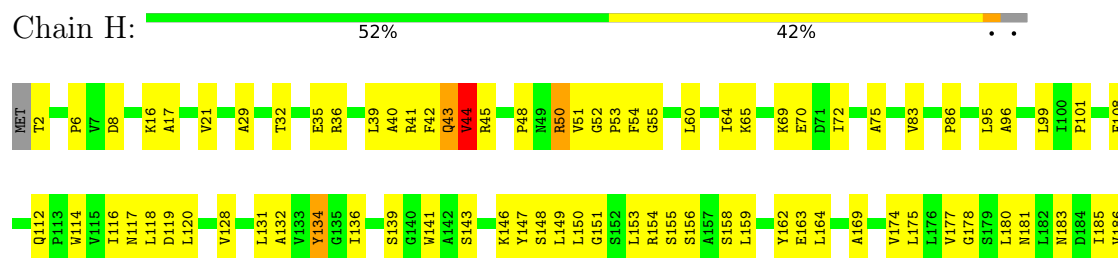
• Molecule 15: NADH-quinone oxidoreductase subunit 14

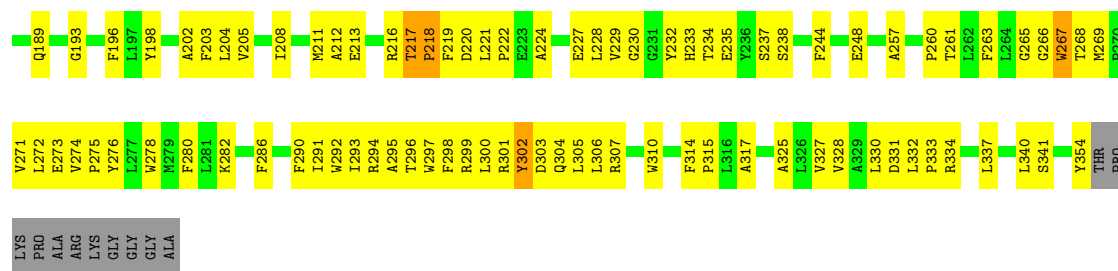


• Molecule 15: NADH-quinone oxidoreductase subunit 14



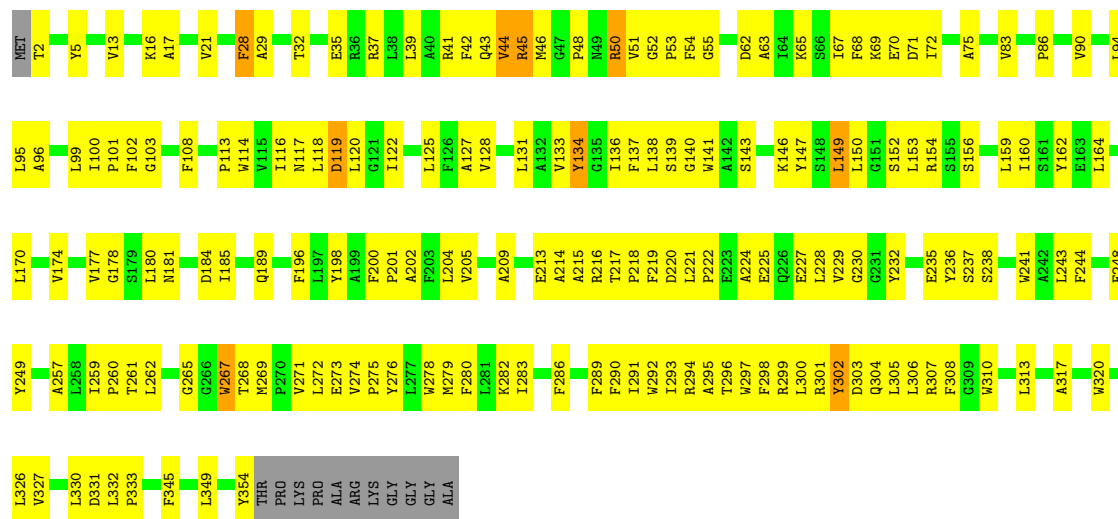
• Molecule 16: NADH-quinone oxidoreductase subunit 8





● Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q: 48% 46%



## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	95.19Å 338.64Å 263.23Å 90.00° 100.41° 90.00°	Depositor
Resolution (Å)	58.41 – 3.51	Depositor
% Data completeness (in resolution range)	81.6 (58.41-3.51)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.13rc1_2961: ???)	Depositor
R, $R_{free}$	0.215 , 0.232	Depositor
Wilson B-factor (Å <sup>2</sup> )	97.6	Xtriage
Anisotropy	0.010	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	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
Total number of atoms	74134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SF4, FES, HQK, FMN

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	0.28	0/3506	0.48	0/4745
1	B	0.29	0/3506	0.48	0/4745
2	2	0.29	0/1439	0.49	0/1953
2	C	0.28	0/1439	0.47	0/1953
3	3	0.31	1/6035 (0.0%)	0.51	0/8185
3	D	0.30	0/6035	0.51	1/8185 (0.0%)
4	4	0.31	0/3150	0.50	0/4284
4	E	0.29	0/3150	0.47	0/4284
5	5	0.30	0/1656	0.51	0/2246
5	F	0.30	0/1656	0.50	0/2246
6	6	0.32	0/1319	0.53	0/1786
6	G	0.31	0/1319	0.52	1/1786 (0.1%)
7	9	0.33	0/1423	0.52	0/1933
7	O	0.33	0/1423	0.52	0/1933
8	7	0.28	0/1059	0.49	0/1429
8	I	0.28	0/1059	0.50	0/1429
9	W	0.30	0/985	0.51	0/1335
9	X	0.30	0/985	0.49	0/1335
10	A	0.30	0/940	0.51	0/1280
10	P	0.29	0/940	0.50	0/1280
11	J	0.26	0/1206	0.47	0/1649
11	R	0.28	0/1206	0.46	0/1649
12	K	0.28	0/710	0.46	0/962
12	S	0.27	0/710	0.45	0/962
13	L	0.28	0/4741	0.46	0/6460
13	T	0.27	0/4741	0.45	0/6460
14	M	0.28	0/3591	0.47	0/4896
14	U	0.28	0/3591	0.47	0/4896
15	N	0.28	0/3238	0.45	0/4434
15	V	0.29	0/3238	0.45	0/4434
16	H	0.30	0/2935	0.53	0/4014
16	Q	0.31	0/2935	0.52	0/4014



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.29	1/75866 (0.0%)	0.49	2/103182 (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)
3	3	624	LEU	C-N	-5.75	1.20	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	169	ARG	C-N-CA	-6.07	106.53	121.70
3	D	650	VAL	C-N-CA	-5.36	108.30	121.70

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 ⓘ

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	138	0
1	B	3417	0	3388	204	0
2	2	1406	0	1373	60	0
2	C	1406	0	1373	67	0
3	3	5895	0	5931	219	0
3	D	5895	0	5930	251	0
4	4	3067	0	3049	179	0
4	E	3067	0	3049	204	0
5	5	1607	0	1574	81	0
5	F	1607	0	1574	95	0
6	6	1289	0	1298	86	0
6	G	1289	0	1299	94	0
7	9	1388	0	1383	75	0
7	O	1388	0	1383	78	0
8	7	1031	0	1029	49	0
8	I	1031	0	1029	47	0
9	W	967	0	1010	27	0
9	X	967	0	1010	26	0
10	A	910	0	939	61	0
10	P	910	0	939	61	0
11	J	1183	0	1286	64	0
11	R	1183	0	1286	60	0
12	K	703	0	747	37	0
12	S	703	0	747	28	0
13	L	4604	0	4734	193	0
13	T	4604	0	4734	180	0
14	M	3489	0	3606	141	0
14	U	3489	0	3606	158	0
15	N	3154	0	3343	120	0
15	V	3154	0	3343	126	0
16	H	2838	0	2903	185	0
16	Q	2838	0	2903	194	0
17	1	8	0	0	0	0
17	3	24	0	0	4	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	2	0
18	B	31	0	19	8	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	3128	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 21.

The worst 5 of 3128 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:N	1.98	1.30
16:H:267:TRP:CD1	16:H:268:THR:N	2.03	1.25
7:9:10:LEU:HD12	16:H:296:THR:HG21	1.28	1.09
16:H:146:LYS:HA	16:H:149:LEU:HB2	1.46	0.98
4:E:110:PRO:HB3	4:E:301:PRO:HG2	1.48	0.96

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	<b>100</b> <b>100</b>

*Continued on next page...*

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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%)	25	64
6	G	164/181 (91%)	151 (92%)	12 (7%)	1 (1%)	25	64
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%)	47	81
13	T	603/606 (100%)	566 (94%)	36 (6%)	1 (0%)	47	81
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%)	11	46
16	Q	351/365 (96%)	304 (87%)	42 (12%)	5 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9478/9796 (97%)	8849 (93%)	615 (6%)	14 (0%)	51 84

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 ⓘ

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 70
1	B	355/356 (100%)	344 (97%)	11 (3%)	40 70
2	2	150/152 (99%)	145 (97%)	5 (3%)	38 68
2	C	150/152 (99%)	144 (96%)	6 (4%)	31 64
3	3	609/628 (97%)	598 (98%)	11 (2%)	59 81
3	D	609/628 (97%)	597 (98%)	12 (2%)	55 79
4	4	332/355 (94%)	327 (98%)	5 (2%)	65 84
4	E	332/355 (94%)	329 (99%)	3 (1%)	78 90
5	5	167/175 (95%)	163 (98%)	4 (2%)	49 76
5	F	167/175 (95%)	163 (98%)	4 (2%)	49 76
6	6	135/149 (91%)	124 (92%)	11 (8%)	11 41
6	G	135/149 (91%)	124 (92%)	11 (8%)	11 41
7	9	148/150 (99%)	147 (99%)	1 (1%)	84 93
7	O	148/150 (99%)	147 (99%)	1 (1%)	84 93
8	7	104/106 (98%)	102 (98%)	2 (2%)	57 80
8	I	104/106 (98%)	102 (98%)	2 (2%)	57 80

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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	78
10	P	90/92 (98%)	86 (96%)	4 (4%)	28	62
11	J	118/130 (91%)	115 (98%)	3 (2%)	47	75
11	R	118/130 (91%)	115 (98%)	3 (2%)	47	75
12	K	71/71 (100%)	70 (99%)	1 (1%)	67	85
12	S	71/71 (100%)	70 (99%)	1 (1%)	67	85
13	L	453/454 (100%)	444 (98%)	9 (2%)	55	79
13	T	453/454 (100%)	442 (98%)	11 (2%)	49	76
14	M	332/332 (100%)	322 (97%)	10 (3%)	41	71
14	U	332/332 (100%)	323 (97%)	9 (3%)	44	73
15	N	302/302 (100%)	298 (99%)	4 (1%)	69	86
15	V	302/302 (100%)	296 (98%)	6 (2%)	55	79
16	H	293/300 (98%)	284 (97%)	9 (3%)	40	70
16	Q	293/300 (98%)	283 (97%)	10 (3%)	37	68
All	All	7516/7706 (98%)	7332 (98%)	184 (2%)	49	76

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	655	ARG
10	P	79	TRP
4	E	208	PHE
6	G	88	MET
13	T	108	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
13	T	341	HIS
13	T	436	HIS
16	Q	43	GLN
13	L	582	GLN
13	L	544	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	$\# Z  > 2$
17	SF4	9	202	7	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
18	FMN	1	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.28	9 (18%)
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	6	201	6	0,12,12	-	-	-		
17	SF4	D	801	3	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	G	201	6	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	HQK	4	501	-	24,25,25	0.23	0	30,38,38	0.33	0
19	FES	2	201	2	0,4,4	-	-	-		
20	HQK	E	501	-	24,25,25	0.22	0	30,38,38	0.32	0
17	SF4	D	803	3	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.16	2 (6%)	48,50,50	1.41	10 (20%)

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
17	SF4	9	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	1	501	1	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
17	SF4	3	802	3	-	-	0/6/5/5
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	G	201	6	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	3	801	3	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
20	HQK	E	501	-	-	0/16/17/17	0/2/2/2
20	HQK	4	501	-	-	0/16/17/17	0/2/2/2
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	D	803	3	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3

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(°)	Ideal(°)
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'

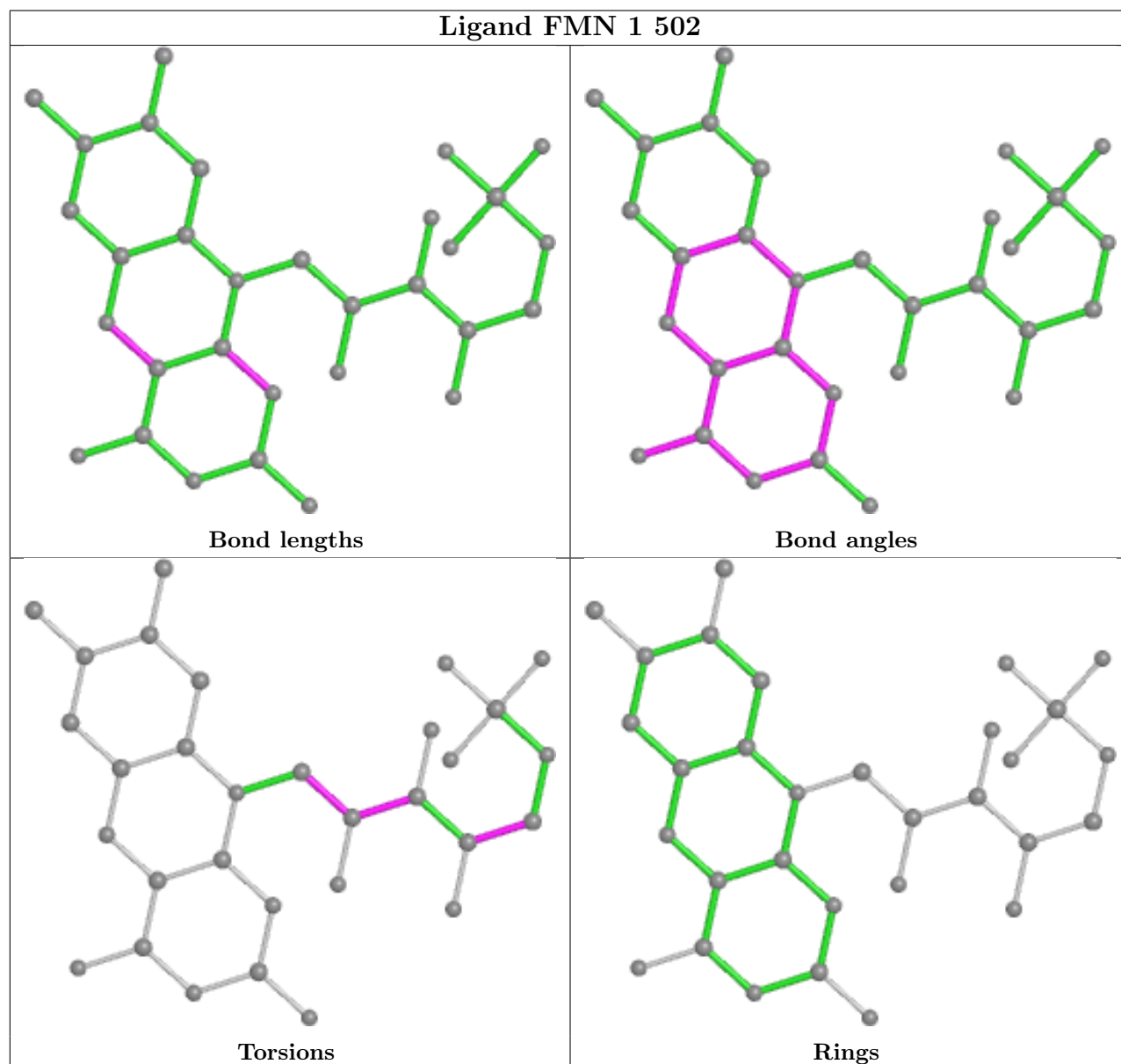
There are no ring outliers.

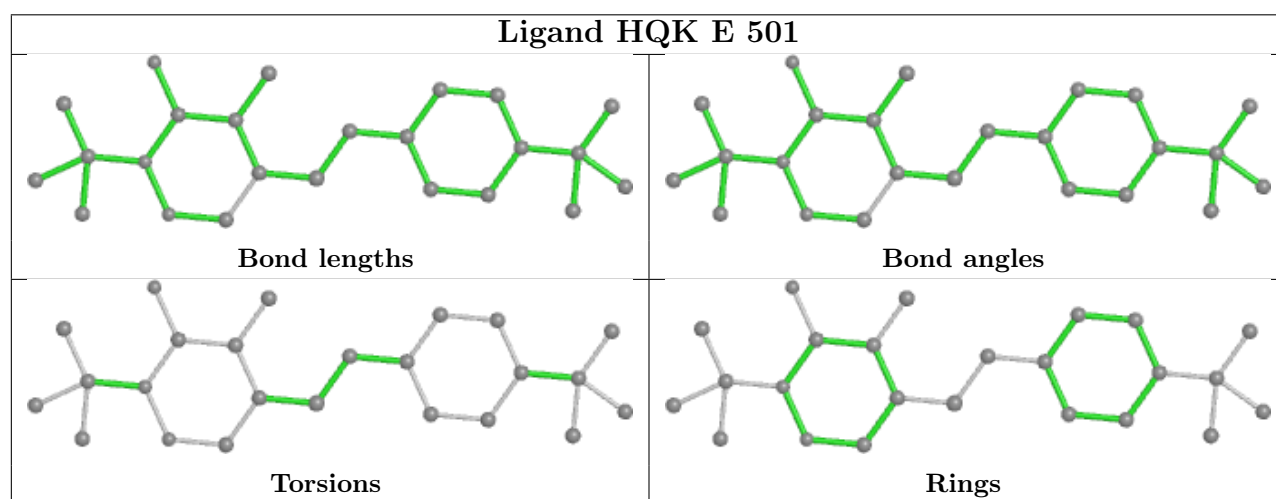
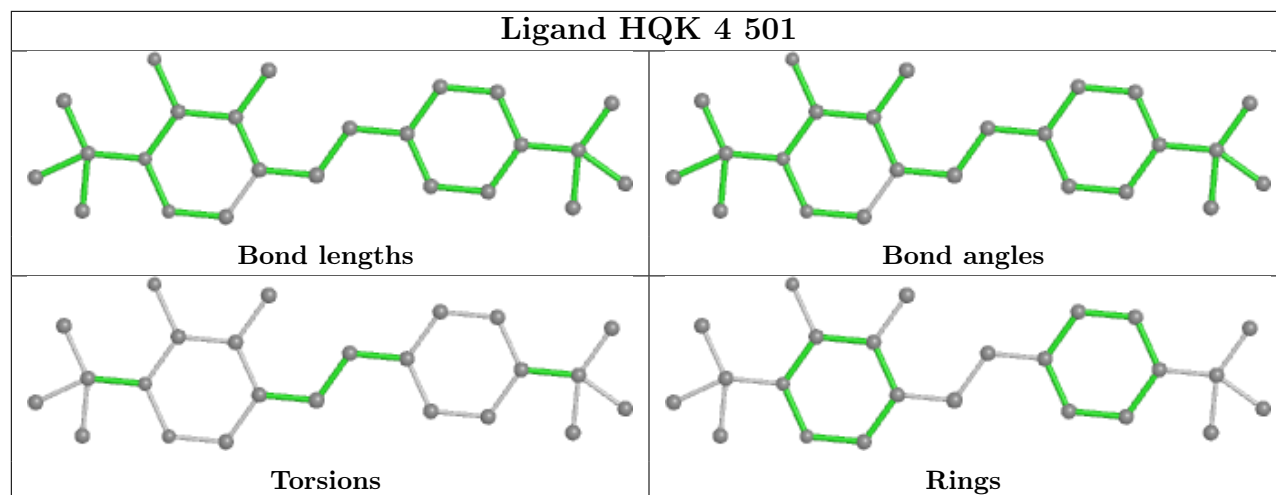
16 monomers are involved in 36 short contacts:

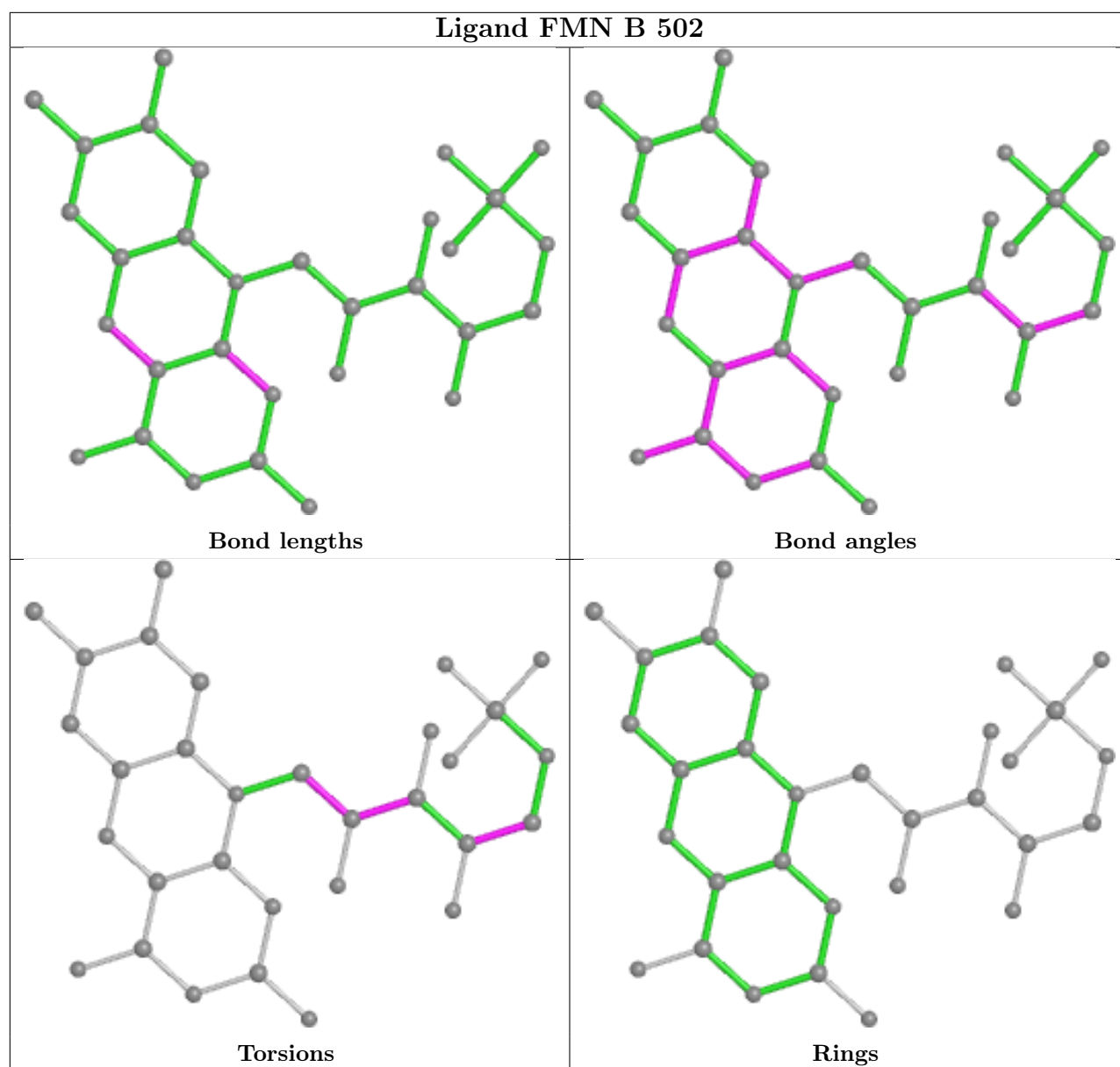
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	9	202	SF4	2	0
17	9	201	SF4	2	0
19	D	804	FES	1	0
18	1	502	FMN	2	0
17	3	803	SF4	3	0
17	6	201	SF4	1	0
17	D	801	SF4	1	0
17	O	201	SF4	2	0
17	O	202	SF4	1	0
17	G	201	SF4	3	0
17	3	801	SF4	1	0
20	4	501	HQK	4	0
19	2	201	FES	2	0
20	E	501	HQK	2	0
17	D	803	SF4	1	0
18	B	502	FMN	8	0

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







## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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