



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 10:47 AM UTC

PDB ID : 4HEA / pdb_00004hea
Title : Crystal structure of the entire respiratory complex I from *Thermus thermophilus*
Authors : Baradaran, R.; Berrisford, J.M.; Minhas, G.S.; Sazanov, L.A.
Deposited on : 2012-10-03
Resolution : 3.30 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

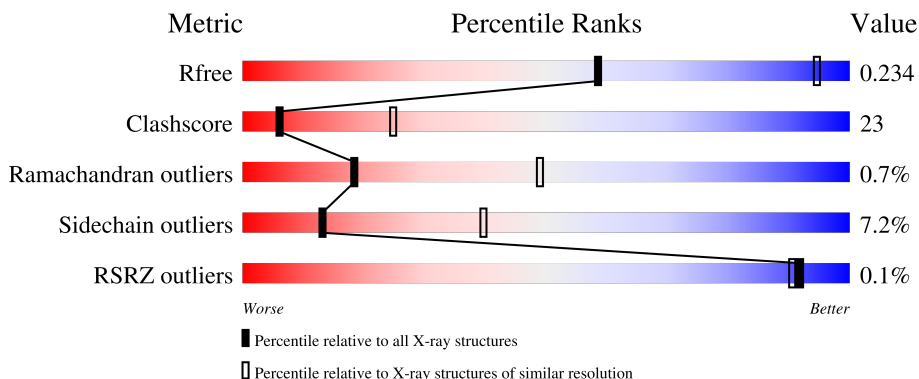
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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




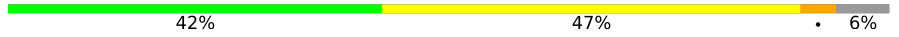



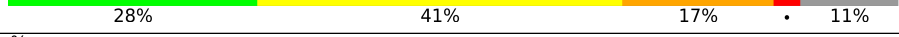
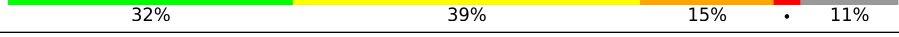

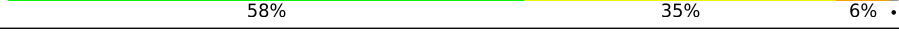

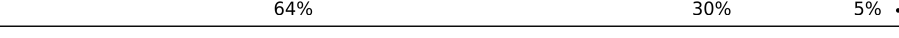
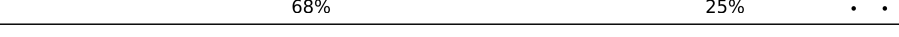

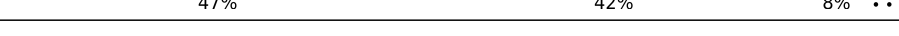


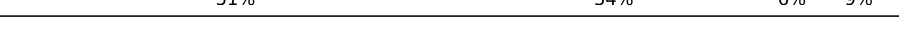

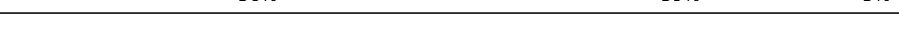






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	59% (green), 37% (yellow), 4% (orange), 2% (red), 0% (grey)
1	B	438	61% (green), 35% (yellow), 4% (orange), 0% (red), 0% (grey)
2	2	181	51% (green), 41% (yellow), 6% (orange), 2% (red), 0% (grey)
2	C	181	49% (green), 45% (yellow), 5% (orange), 1% (red), 0% (grey)
3	3	783	54% (green), 38% (yellow), 5% (orange), 3% (red), 0% (grey)



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Mol	Chain	Length	Quality of chain
3	D	783	 53% 39% 5% .
4	4	409	 42% 47% . 6%
4	E	409	 45% 44% . 6%
5	5	207	 47% 41% 7% 5%
5	F	207	 50% 38% 7% 5%
6	6	181	 28% 41% 17% . 11%
6	G	181	 % 32% 39% 15% . 11%
7	9	182	 57% 35% 7% .
7	O	182	 58% 35% 6% .
8	7	129	 65% 28% 5% ..
8	I	129	 64% 30% 5% .
9	W	131	 68% 25% . .
9	X	131	 68% 24% 5% ..
10	A	119	 47% 42% 8% ..
10	P	119	 47% 44% 8% .
11	J	176	 48% 37% 6% 9%
11	R	176	 51% 34% 6% 9%
12	K	95	 46% 47% 6%
12	S	95	 56% 39% 5%
13	L	606	 59% 35% . .
13	T	606	 62% 33% . .
14	M	469	 49% 44% 5% .
14	U	469	 49% 45% 5%
15	N	427	 62% 35% .
15	V	427	 63% 35% .

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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	6	201	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	B	501	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	201	-	-	X	-
17	SF4	O	202	-	-	X	-
19	FES	D	804	-	-	X	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 73998 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
			Total	C	N	O	S			
1	1	437	3417	2180	595	624	18	0	0	0
1	B	437	3417	2180	595	624	18	0	0	0

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

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

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

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

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

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

- 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	161	Total	C	N	O	S	0	0	0
			1245	787	227	218	13			
6	G	161	Total	C	N	O	S	0	0	0
			1245	787	227	218	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 Putative uncharacterized protein TTHA1528.

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
			Total	C	N	O	S			
10	P	117	910	624	138	144	4	0	0	0

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

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

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

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

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

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

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

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

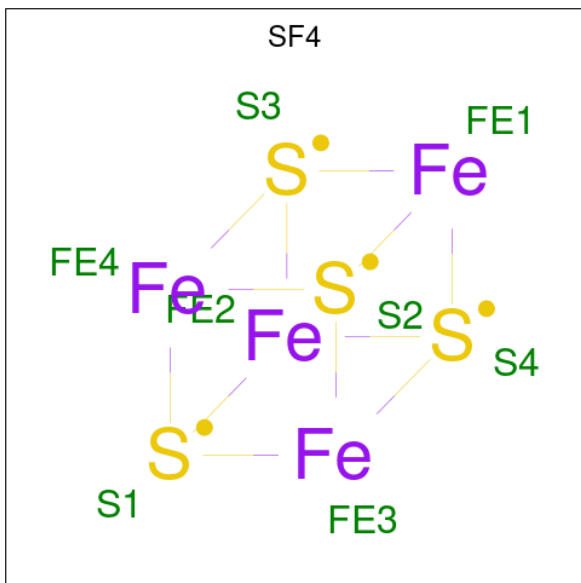
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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

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

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

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



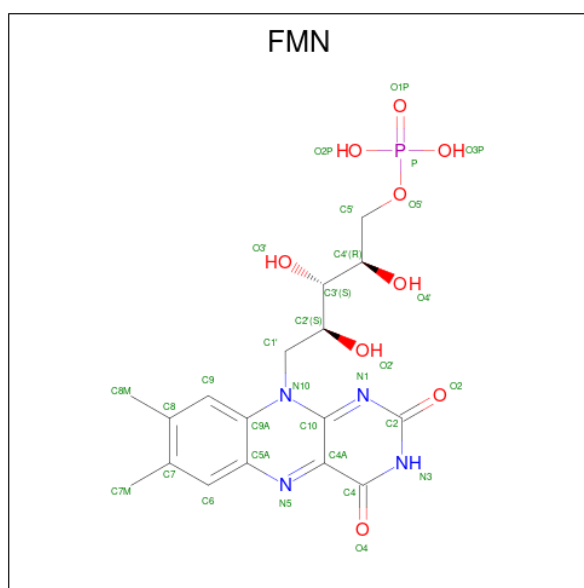
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	Fe S			
17	1	1	Total 8	Fe 4	S 4	0	0
17	3	1	Total 8	Fe 4	S 4	0	0
17	3	1	Total 8	Fe 4	S 4	0	0
17	3	1	Total 8	Fe 4	S 4	0	0
17	6	1	Total 8	Fe 4	S 4	0	0
17	9	1	Total 8	Fe 4	S 4	0	0
17	9	1	Total 8	Fe 4	S 4	0	0
17	B	1	Total 8	Fe 4	S 4	0	0
17	D	1	Total 8	Fe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

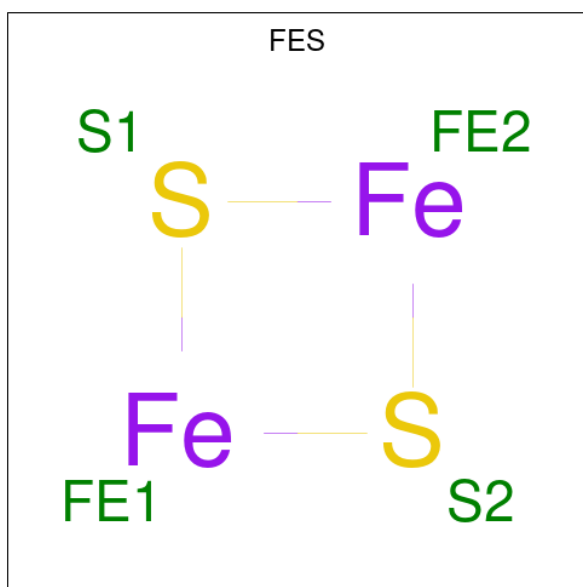
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	G	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 18 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



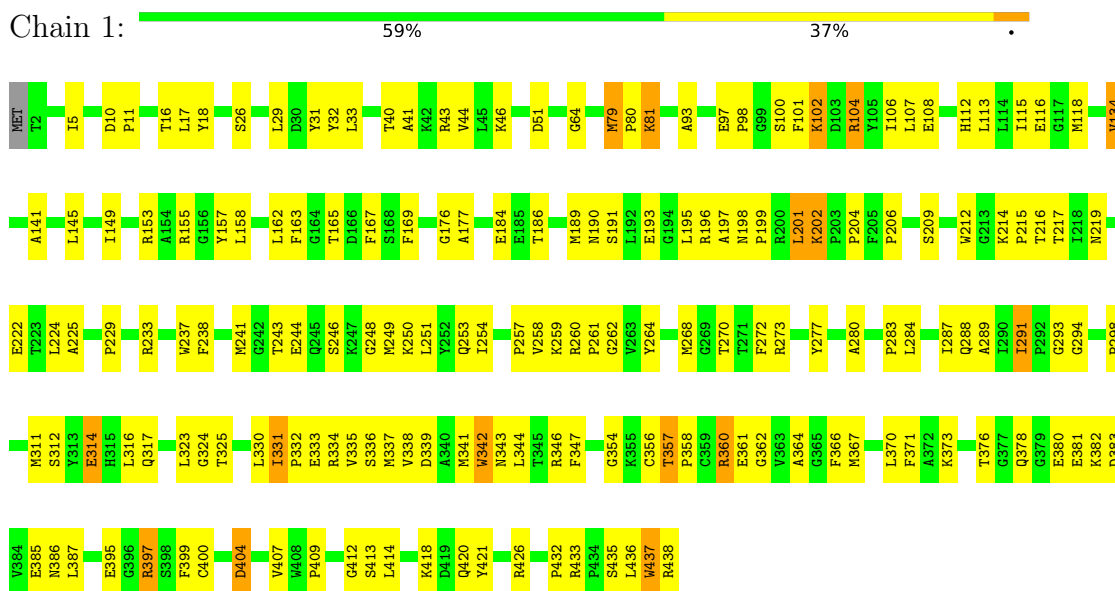


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	2	1	Total	Fe	S	0	0
			4	2	2		
19	3	1	Total	Fe	S	0	0
			4	2	2		
19	C	1	Total	Fe	S	0	0
			4	2	2		
19	D	1	Total	Fe	S	0	0
			4	2	2		

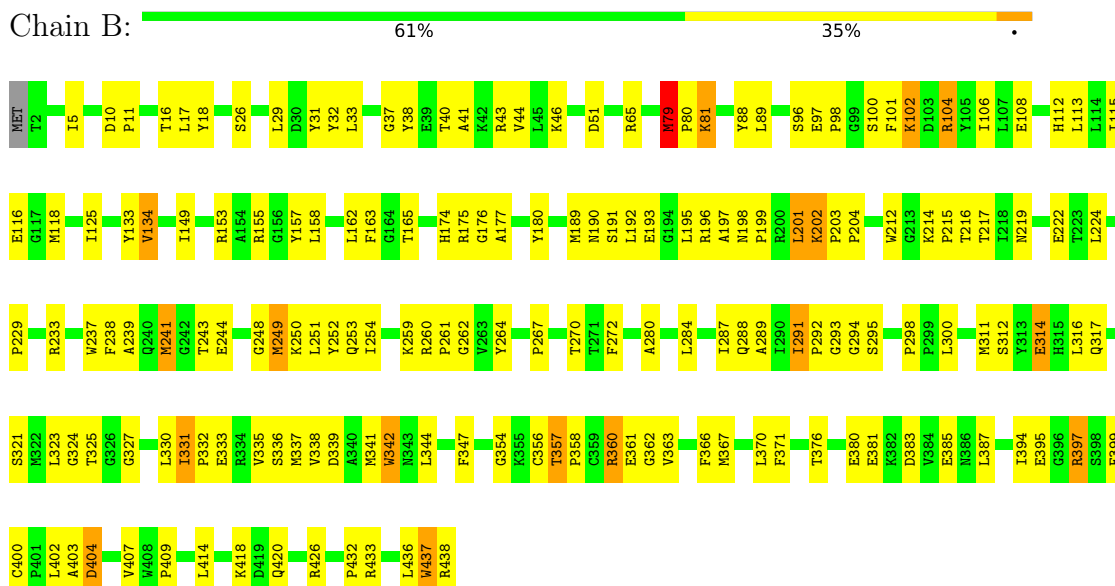
3 Residue-property plots

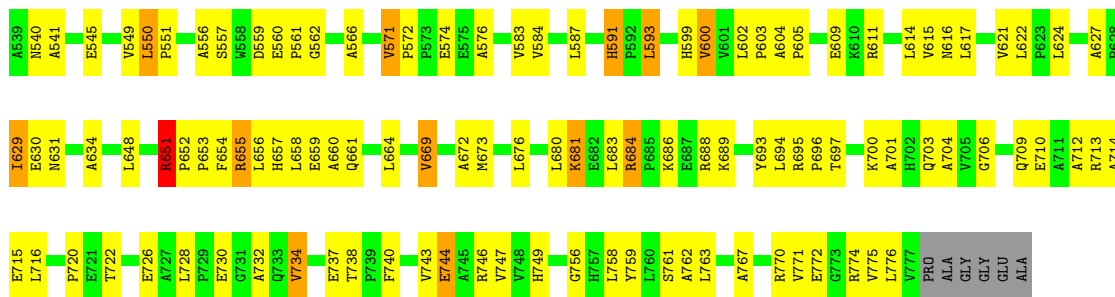
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

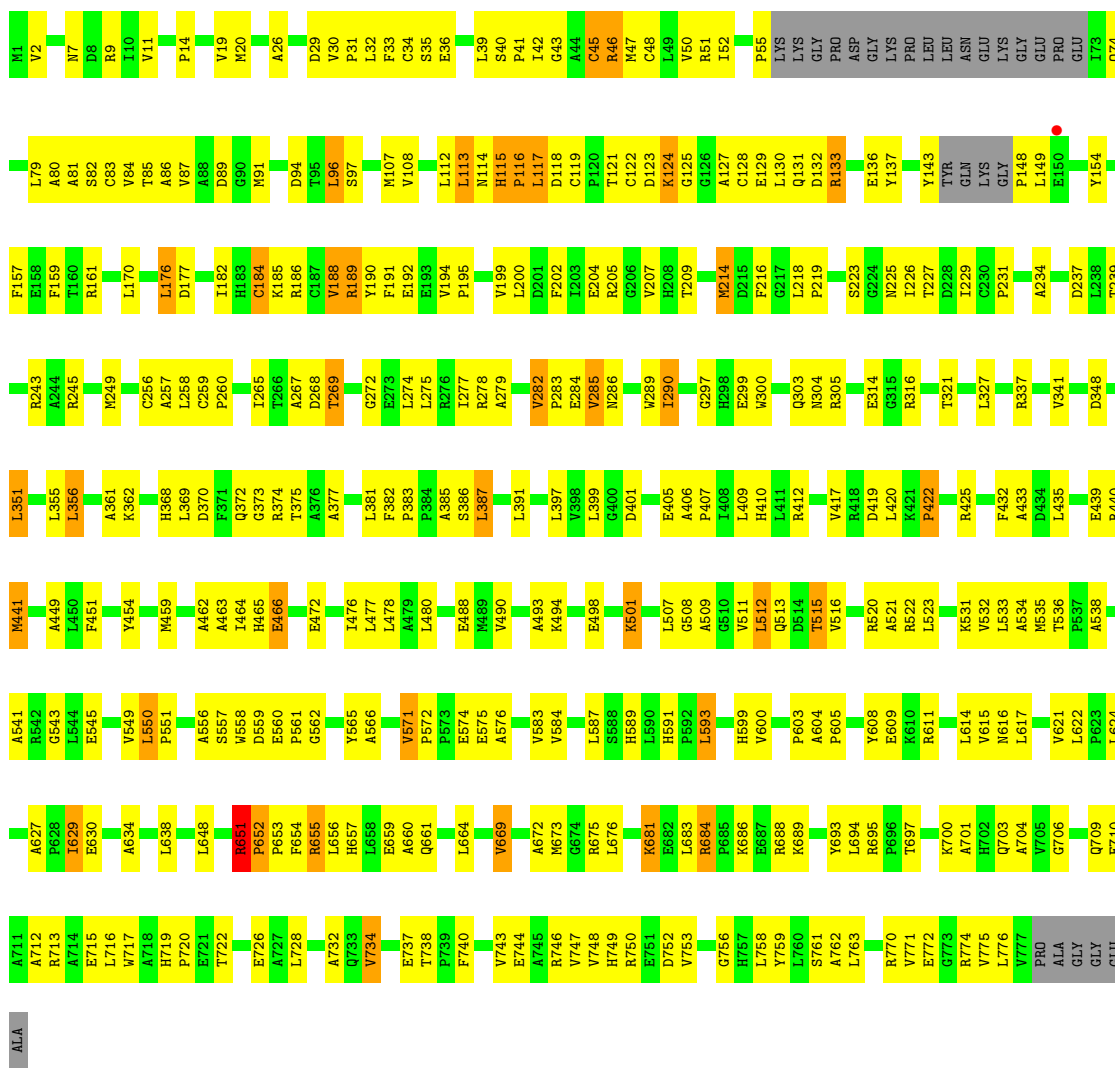


- Molecule 1: NADH-quinone oxidoreductase subunit 1



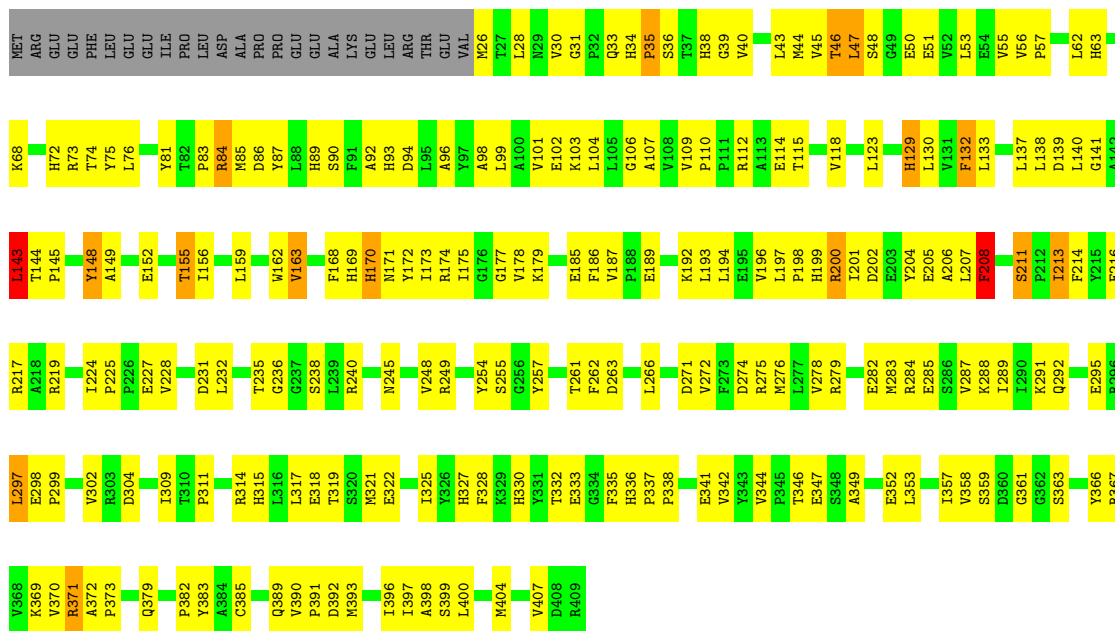


• Molecule 3: NADH-quinone oxidoreductase subunit 3

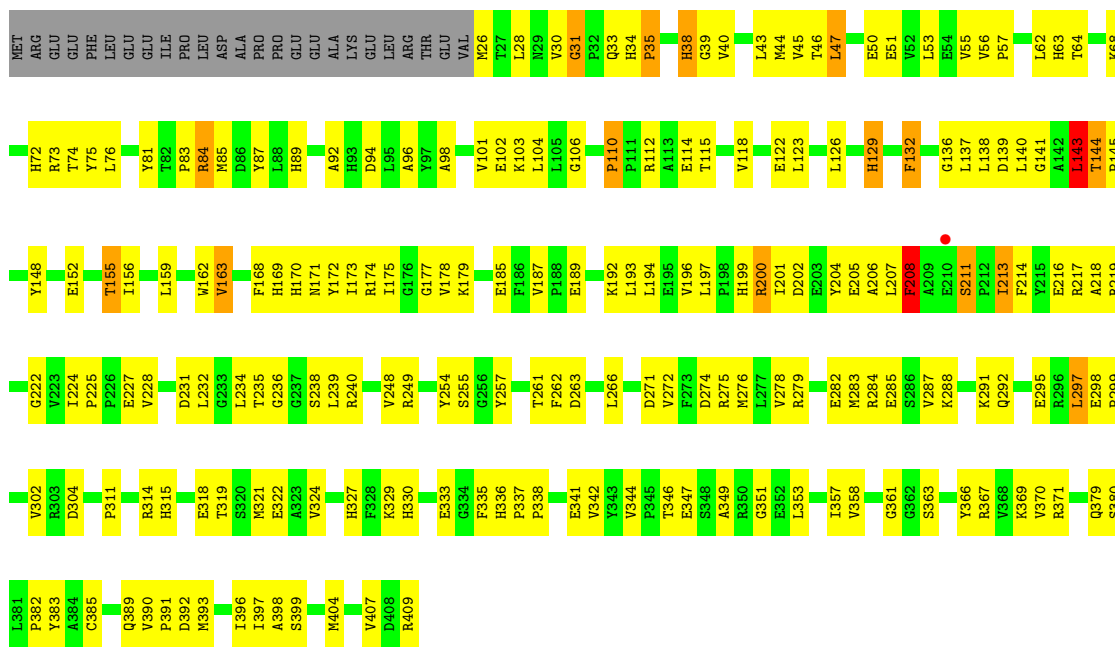


• Molecule 4: NADH-quinone oxidoreductase subunit 4

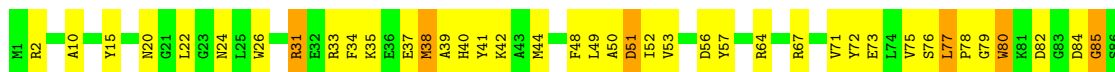


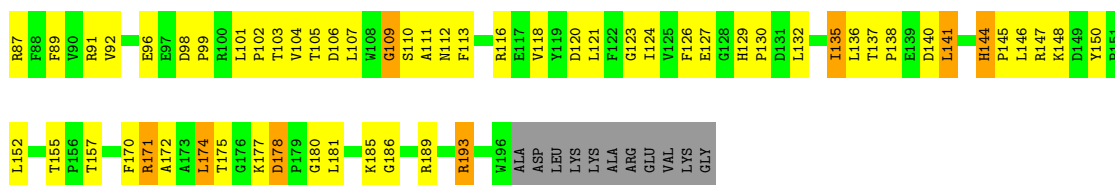


• Molecule 4: NADH-quinone oxidoreductase subunit 4



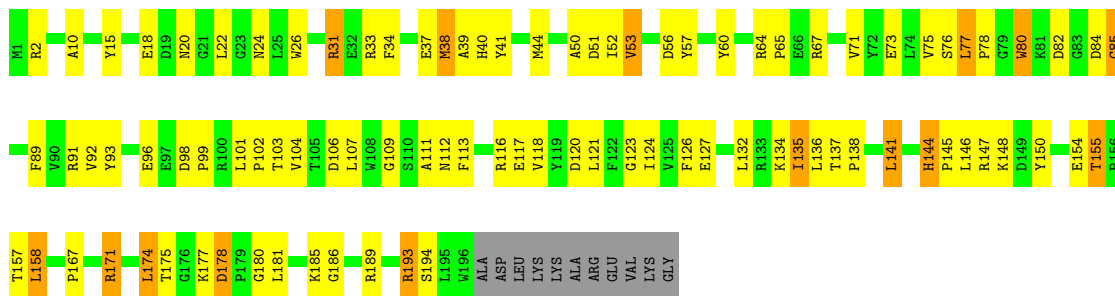
• Molecule 5: NADH-quinone oxidoreductase subunit 5





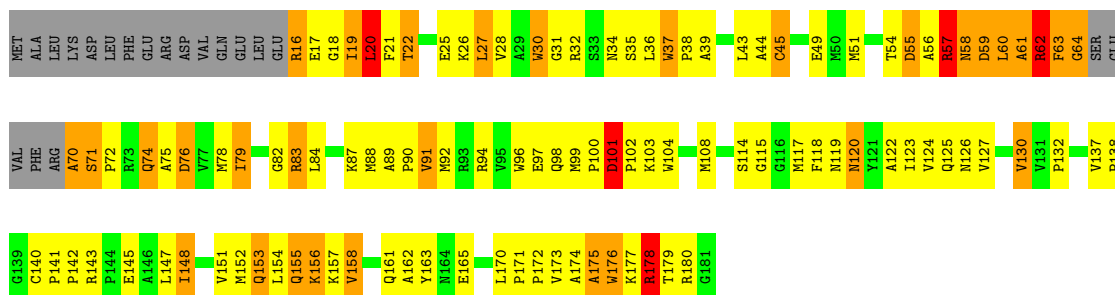
- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F: 50% 38% 7% 5%



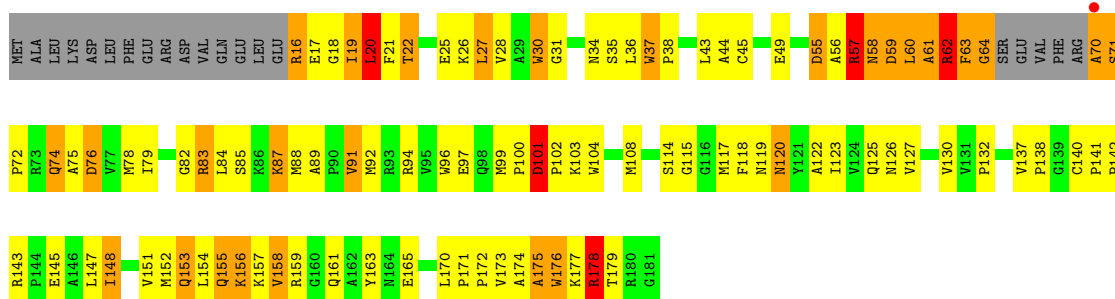
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6: 28% 41% 17% 11%



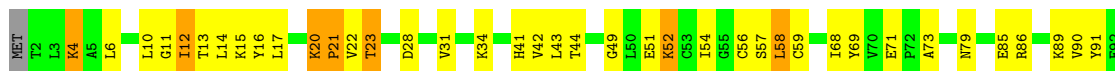
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G: 32% 39% 15% 11%

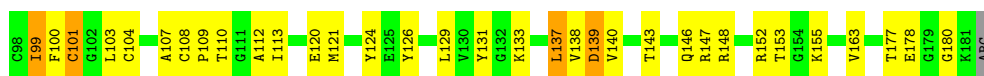


- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9: 57% 35% 7%



• Molecule 7: NADH-quinone oxidoreductase subunit 9



• Molecule 8: NADH-quinone oxidoreductase subunit 15



• Molecule 8: NADH-quinone oxidoreductase subunit 15

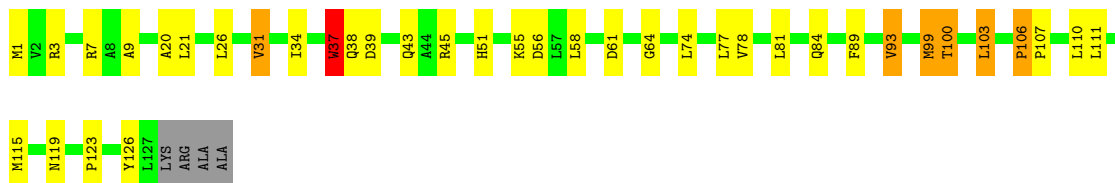


• Molecule 9: Putative uncharacterized protein TTHA1528



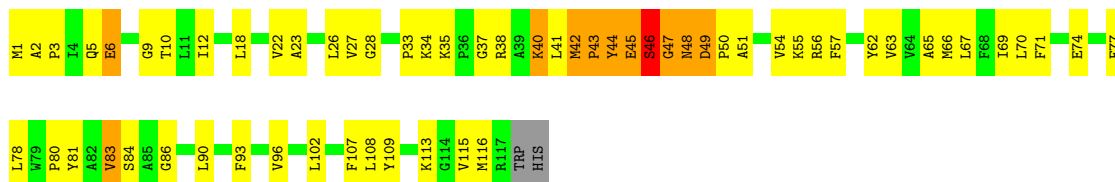
• Molecule 9: Putative uncharacterized protein TTHA1528





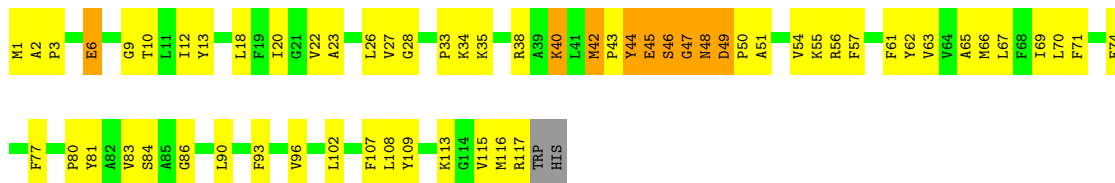
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A: 47% 42% 8% ..



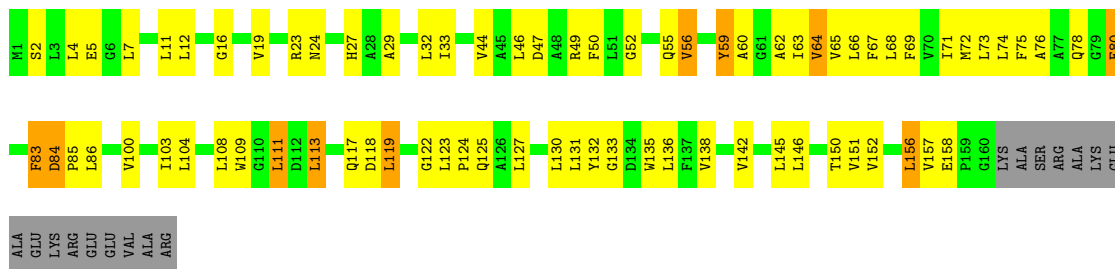
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P: 47% 44% 8% .



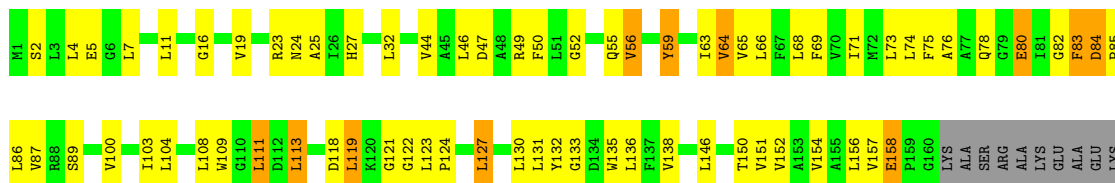
- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J: 48% 37% 6% 9%

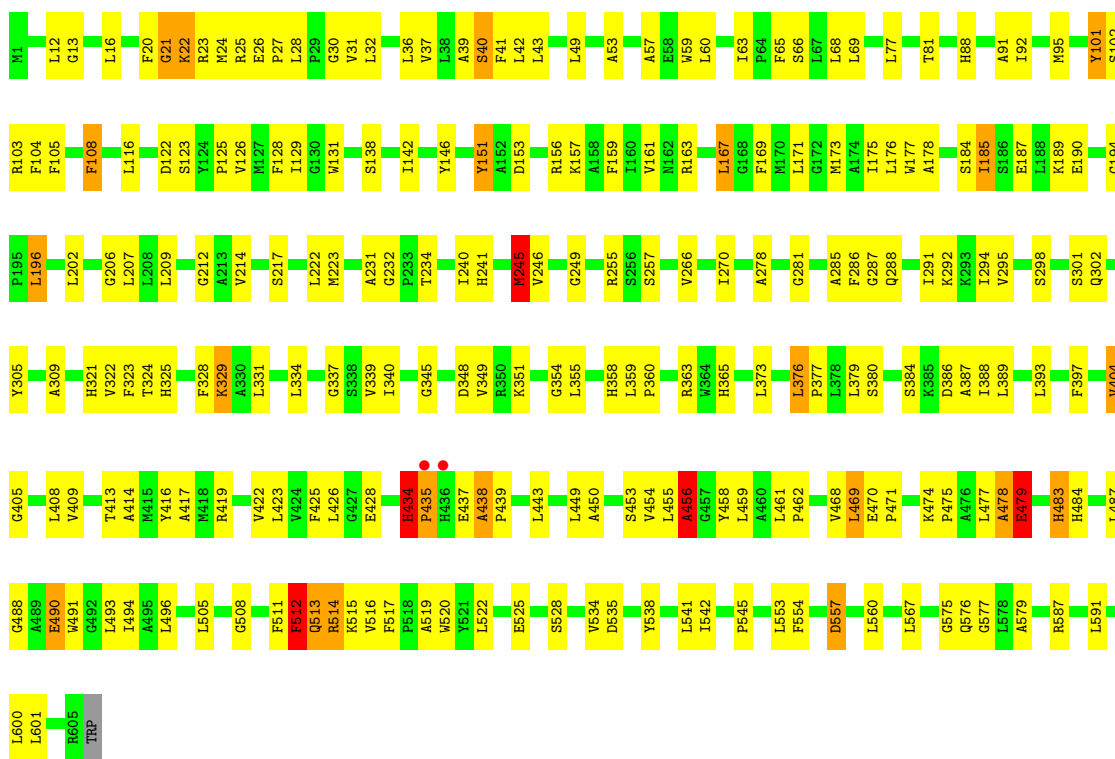


- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R: 51% 34% 6% 9%

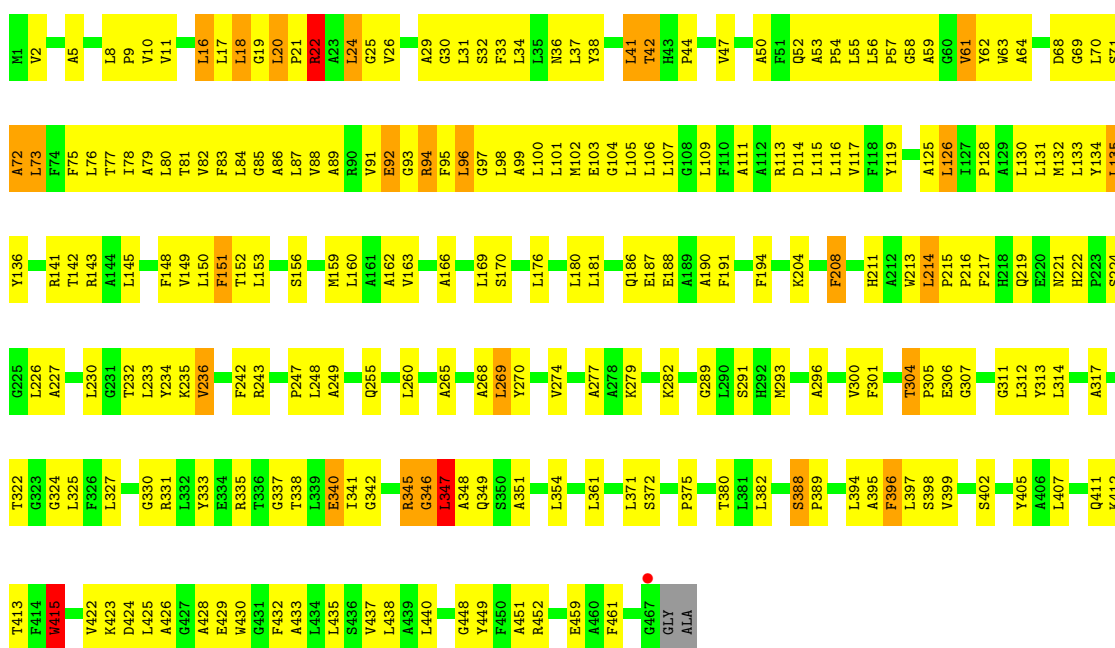


Chain T:  62% 33%



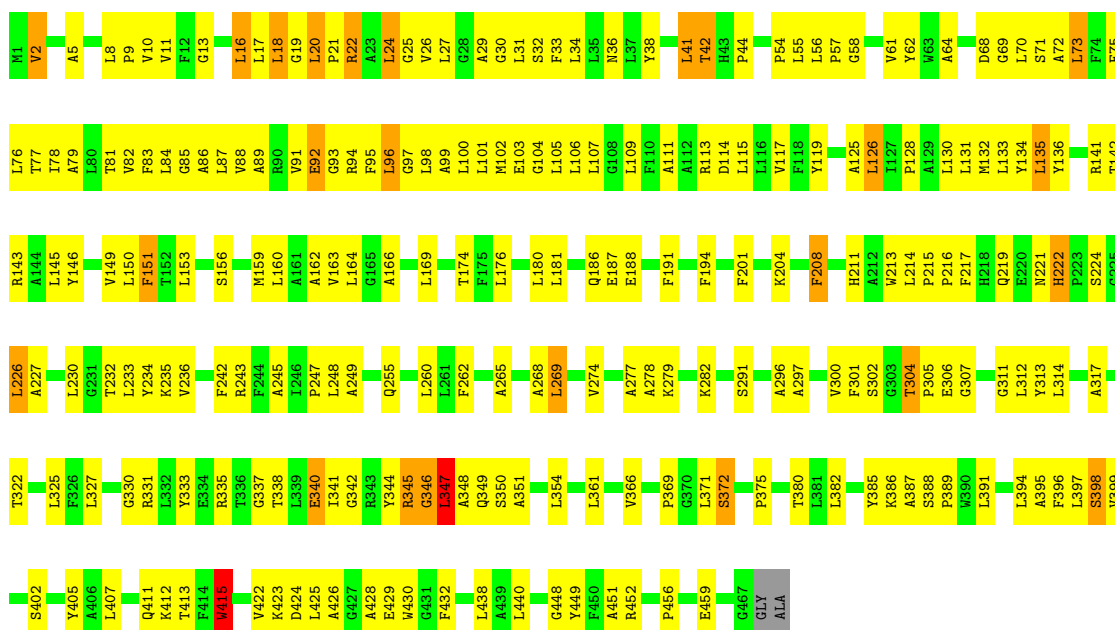
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain M:  49% 44% 5%



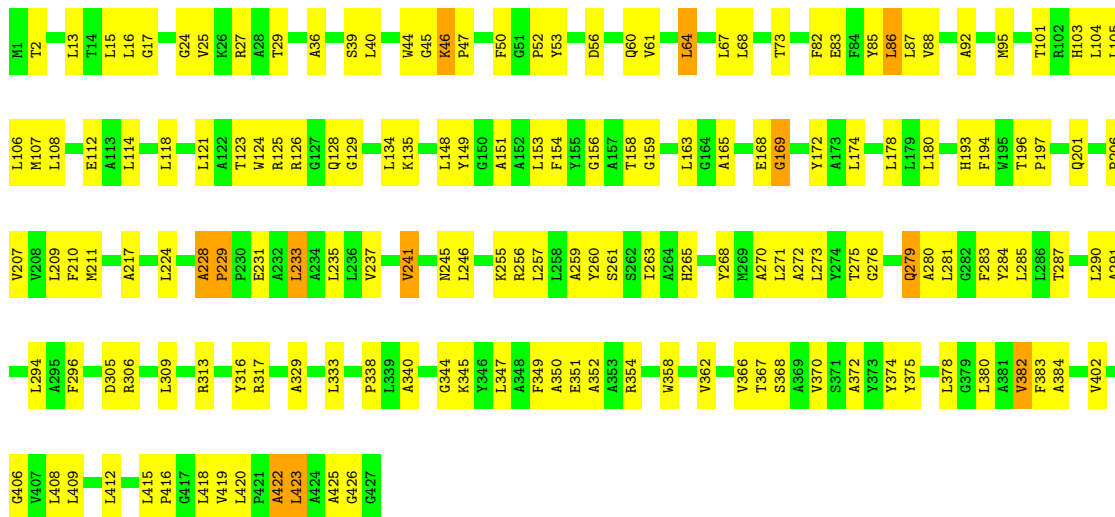
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U:  49% 45% 5%



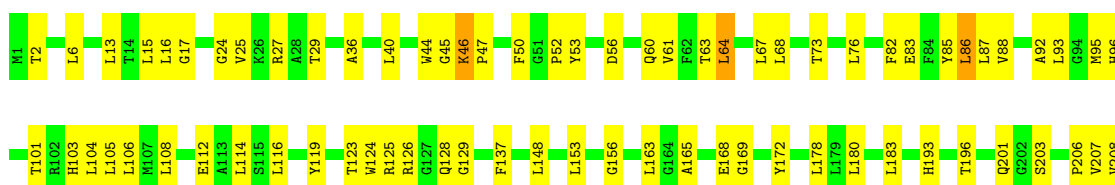
• Molecule 15: NADH-quinone oxidoreductase subunit 14

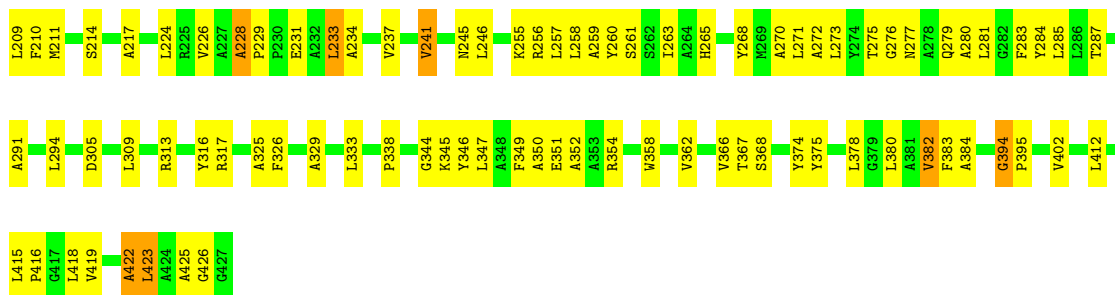
Chain N:  62% 35% 3%



• Molecule 15: NADH-quinone oxidoreductase subunit 14

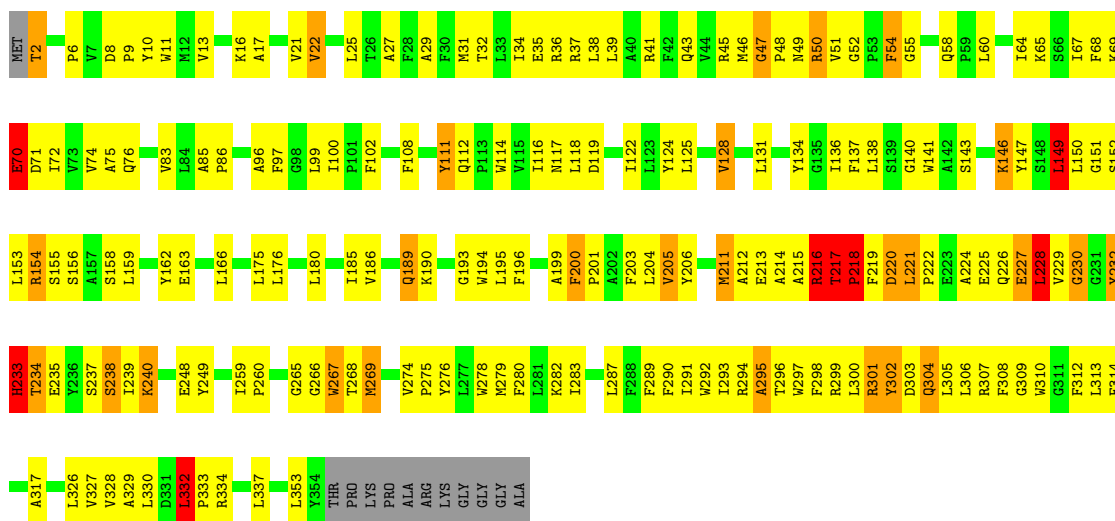
Chain V:  63% 35% 2%





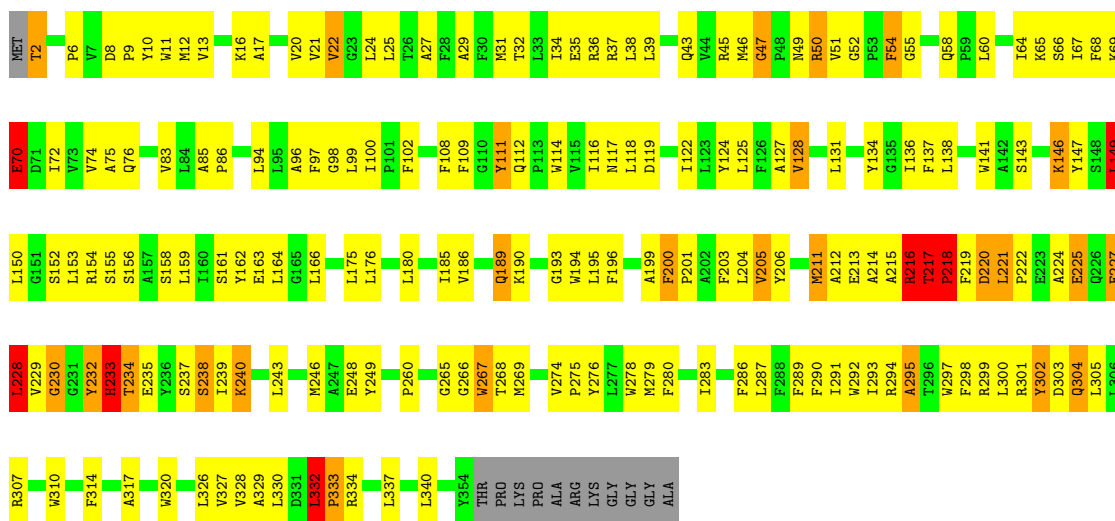
- Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H: 45% 42% 7%



- Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q: 45% 42% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.28Å 340.89Å 263.30Å 90.00° 100.57° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 40.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (40.00-3.30) 93.7 (40.00-3.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.32Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1041)	Depositor
R, R_{free}	0.202 , 0.239 0.202 , 0.234	Depositor DCC
R_{free} test set	2417 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtrriage
Anisotropy	0.003	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 16.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	0.377 for h,-k,-h-l	Xtrriage
Reported twinning fraction	0.470 for -h,-k,h+1	Depositor
Outliers	0 of 233384 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	73998	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FES, FMN, 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	0.45	0/3506	0.98	7/4745 (0.1%)
1	B	0.44	0/3506	0.97	8/4745 (0.2%)
2	2	0.51	0/1439	1.05	8/1953 (0.4%)
2	C	0.50	0/1439	1.03	7/1953 (0.4%)
3	3	0.59	0/6035	1.17	51/8185 (0.6%)
3	D	0.57	0/6035	1.15	45/8185 (0.5%)
4	4	0.54	0/3150	1.14	24/4284 (0.6%)
4	E	0.52	0/3150	1.11	25/4284 (0.6%)
5	5	0.48	0/1656	1.10	7/2246 (0.3%)
5	F	0.45	0/1656	1.07	10/2246 (0.4%)
6	6	0.76	1/1273 (0.1%)	1.46	24/1723 (1.4%)
6	G	0.77	1/1273 (0.1%)	1.45	23/1723 (1.3%)
7	9	0.64	0/1423	1.19	12/1933 (0.6%)
7	O	0.59	0/1423	1.15	7/1933 (0.4%)
8	7	0.50	0/1059	1.00	3/1429 (0.2%)
8	I	0.43	0/1059	0.96	1/1429 (0.1%)
9	W	0.52	0/985	1.10	7/1335 (0.5%)
9	X	0.52	0/985	1.10	10/1335 (0.7%)
10	A	0.53	0/940	1.14	10/1280 (0.8%)
10	P	0.52	0/940	1.12	6/1280 (0.5%)
11	J	0.50	0/1206	0.97	2/1649 (0.1%)
11	R	0.54	0/1206	0.97	2/1649 (0.1%)
12	K	0.51	0/710	0.96	0/962
12	S	0.50	0/710	0.95	0/962
13	L	0.47	0/4741	1.05	25/6460 (0.4%)
13	T	0.46	0/4741	1.04	23/6460 (0.4%)
14	M	0.52	0/3591	1.08	21/4896 (0.4%)
14	U	0.54	0/3591	1.07	22/4896 (0.4%)
15	N	0.48	1/3238 (0.0%)	1.05	13/4434 (0.3%)
15	V	0.47	0/3238	1.02	14/4434 (0.3%)
16	H	0.63	1/2935 (0.0%)	1.16	21/4014 (0.5%)
16	Q	0.63	1/2935 (0.0%)	1.16	18/4014 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.53	5/75774 (0.0%)	1.10	456/103056 (0.4%)

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
6	6	0	5
6	G	0	5
7	9	0	3
7	O	0	3
12	K	0	1
12	S	0	1
13	L	0	4
13	T	0	4
14	M	0	1
14	U	0	1
15	N	0	2
15	V	0	2
16	H	0	6
16	Q	0	6
All	All	0	44

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	149	LEU	CA-C	-6.12	1.45	1.52
6	G	63	PHE	CA-C	-5.87	1.45	1.52
15	N	229	PRO	CA-C	5.78	1.55	1.51
6	6	63	PHE	CA-C	-5.16	1.46	1.52
16	H	149	LEU	CA-C	-5.06	1.46	1.52

The worst 5 of 456 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	228	ALA	CA-C-N	14.85	130.50	119.66
15	N	228	ALA	C-N-CA	14.85	130.50	119.66
6	6	59	ASP	N-CA-C	-14.55	98.03	114.62
6	G	59	ASP	N-CA-C	-14.53	98.06	114.62
15	V	228	ALA	CA-C-N	13.95	129.84	119.66

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	6	175	ALA	Peptide
6	6	20	LEU	Peptide
6	6	56	ALA	Peptide
6	6	57	ARG	Peptide
6	6	70	ALA	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	150	0
1	B	3417	0	3388	136	0
2	2	1406	0	1373	83	0
2	C	1406	0	1373	80	0
3	3	5895	0	5930	242	0
3	D	5895	0	5930	246	0
4	4	3067	0	3049	200	0
4	E	3067	0	3049	186	0
5	5	1607	0	1574	106	0
5	F	1607	0	1574	89	0
6	6	1245	0	1255	162	0
6	G	1245	0	1255	149	0
7	9	1388	0	1383	67	0
7	O	1388	0	1383	61	0
8	7	1031	0	1029	41	0
8	I	1031	0	1029	43	0
9	W	967	0	1010	30	0
9	X	967	0	1010	27	0
10	A	910	0	939	80	0
10	P	910	0	939	82	0
11	J	1183	0	1286	72	0
11	R	1183	0	1286	64	0
12	K	703	0	747	50	0
12	S	703	0	747	38	0
13	L	4604	0	4734	173	0
13	T	4604	0	4734	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	3489	0	3606	201	0
14	U	3489	0	3606	186	0
15	N	3154	0	3343	118	0
15	V	3154	0	3343	111	0
16	H	2838	0	2903	214	0
16	Q	2838	0	2903	206	0
17	1	8	0	0	1	0
17	3	24	0	0	0	0
17	6	8	0	0	2	0
17	9	16	0	0	6	0
17	B	8	0	0	2	0
17	D	24	0	0	0	0
17	G	8	0	0	2	0
17	O	16	0	0	7	0
18	1	31	0	19	4	0
18	B	31	0	19	3	0
19	2	4	0	0	1	0
19	3	4	0	0	1	0
19	C	4	0	0	1	0
19	D	4	0	0	2	0
All	All	73998	0	75136	3370	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 23.

The worst 5 of 3370 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)
6:6:57:ARG:CD	6:6:60:LEU:HD11	1.35	1.55
6:G:57:ARG:CD	6:G:60:LEU:HD11	1.43	1.49
6:6:57:ARG:HD2	6:6:60:LEU:CD1	1.46	1.46
6:G:57:ARG:HD2	6:G:60:LEU:CD1	1.52	1.40
6:6:57:ARG:CD	6:6:60:LEU:CD1	2.05	1.20

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	405 (93%)	28 (6%)	2 (0%)	24	55
1	B	435/438 (99%)	406 (93%)	27 (6%)	2 (0%)	24	55
2	2	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	21	52
2	C	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	21	52
3	3	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	48	75
3	D	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	48	75
4	4	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	24	55
4	E	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	24	55
5	5	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
5	F	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
6	6	157/181 (87%)	140 (89%)	15 (10%)	2 (1%)	9	35
6	G	157/181 (87%)	141 (90%)	14 (9%)	2 (1%)	9	35
7	9	178/182 (98%)	166 (93%)	11 (6%)	1 (1%)	21	52
7	O	178/182 (98%)	167 (94%)	10 (6%)	1 (1%)	21	52
8	7	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
8	I	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
9	W	125/131 (95%)	121 (97%)	3 (2%)	1 (1%)	16	45
9	X	125/131 (95%)	121 (97%)	3 (2%)	1 (1%)	16	45
10	A	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	4	23
10	P	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	4	23
11	J	158/176 (90%)	143 (90%)	14 (9%)	1 (1%)	21	52
11	R	158/176 (90%)	142 (90%)	15 (10%)	1 (1%)	21	52
12	K	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	39
12	S	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	39
13	L	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	T	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	16	45
14	M	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	14	43
14	U	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	14	43
15	N	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	24	55
15	V	425/427 (100%)	396 (93%)	27 (6%)	2 (0%)	24	55
16	H	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	4	23
16	Q	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	4	23
All	All	9464/9796 (97%)	8730 (92%)	664 (7%)	70 (1%)	18	49

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	5	ILE
6	6	61	ALA
7	9	23	THR
10	A	43	PRO
13	L	434	HIS

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%)	338 (95%)	17 (5%)	23	52
1	B	355/356 (100%)	337 (95%)	18 (5%)	21	50
2	2	150/152 (99%)	137 (91%)	13 (9%)	9	32
2	C	150/152 (99%)	136 (91%)	14 (9%)	8	30
3	3	609/628 (97%)	559 (92%)	50 (8%)	10	35
3	D	609/628 (97%)	560 (92%)	49 (8%)	11	36
4	4	332/355 (94%)	313 (94%)	19 (6%)	18	47
4	E	332/355 (94%)	313 (94%)	19 (6%)	18	47
5	5	167/175 (95%)	157 (94%)	10 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	167/175 (95%)	157 (94%)	10 (6%)	17	46
6	6	130/149 (87%)	108 (83%)	22 (17%)	2	10
6	G	130/149 (87%)	108 (83%)	22 (17%)	2	10
7	9	148/150 (99%)	138 (93%)	10 (7%)	14	42
7	O	148/150 (99%)	138 (93%)	10 (7%)	14	42
8	7	104/106 (98%)	98 (94%)	6 (6%)	18	47
8	I	104/106 (98%)	98 (94%)	6 (6%)	18	47
9	W	99/101 (98%)	93 (94%)	6 (6%)	17	45
9	X	99/101 (98%)	92 (93%)	7 (7%)	13	40
10	A	90/92 (98%)	83 (92%)	7 (8%)	11	36
10	P	90/92 (98%)	84 (93%)	6 (7%)	15	42
11	J	118/130 (91%)	100 (85%)	18 (15%)	3	13
11	R	118/130 (91%)	100 (85%)	18 (15%)	3	13
12	K	71/71 (100%)	63 (89%)	8 (11%)	5	21
12	S	71/71 (100%)	64 (90%)	7 (10%)	7	27
13	L	453/454 (100%)	430 (95%)	23 (5%)	21	50
13	T	453/454 (100%)	429 (95%)	24 (5%)	20	49
14	M	332/332 (100%)	305 (92%)	27 (8%)	11	36
14	U	332/332 (100%)	306 (92%)	26 (8%)	11	36
15	N	302/302 (100%)	292 (97%)	10 (3%)	33	59
15	V	302/302 (100%)	292 (97%)	10 (3%)	33	59
16	H	293/300 (98%)	268 (92%)	25 (8%)	10	33
16	Q	293/300 (98%)	268 (92%)	25 (8%)	10	33
All	All	7506/7706 (97%)	6964 (93%)	542 (7%)	13	40

5 of 542 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	T	185	ILE
13	T	516	VAL
13	T	176	LEU
16	Q	50	ARG
13	L	245	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	616	ASN
12	S	81	HIS
3	D	709	GLN
6	G	153	GLN
16	Q	183	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
17	SF4	6	201	6	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
18	FMN	1	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.45	11 (22%)
17	SF4	3	801	3	0,12,12	-	-	-		
17	SF4	D	801	3	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	FES	2	201	2	0,4,4	-	-	-		
17	SF4	G	201	6	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
18	FMN	B	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.37	9 (18%)
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	D	802	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
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
19	FES	3	804	3	-	-	0/1/1/1
18	FMN	B	502	-	-	9/18/18/18	0/3/3/3
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	502	FMN	C4A-N5	3.36	1.38	1.30
18	1	502	FMN	C4A-N5	3.31	1.37	1.30
18	B	502	FMN	C10-N1	2.74	1.38	1.33
18	1	502	FMN	C10-N1	2.65	1.38	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	502	FMN	C4-N3-C2	-3.56	119.32	125.64
18	B	502	FMN	C4-N3-C2	-3.53	119.37	125.64
18	1	502	FMN	C5A-C9A-N10	3.08	120.75	117.97
18	1	502	FMN	C4A-C10-N1	-2.77	117.80	124.59
18	B	502	FMN	C5A-C9A-N10	2.74	120.44	117.97

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

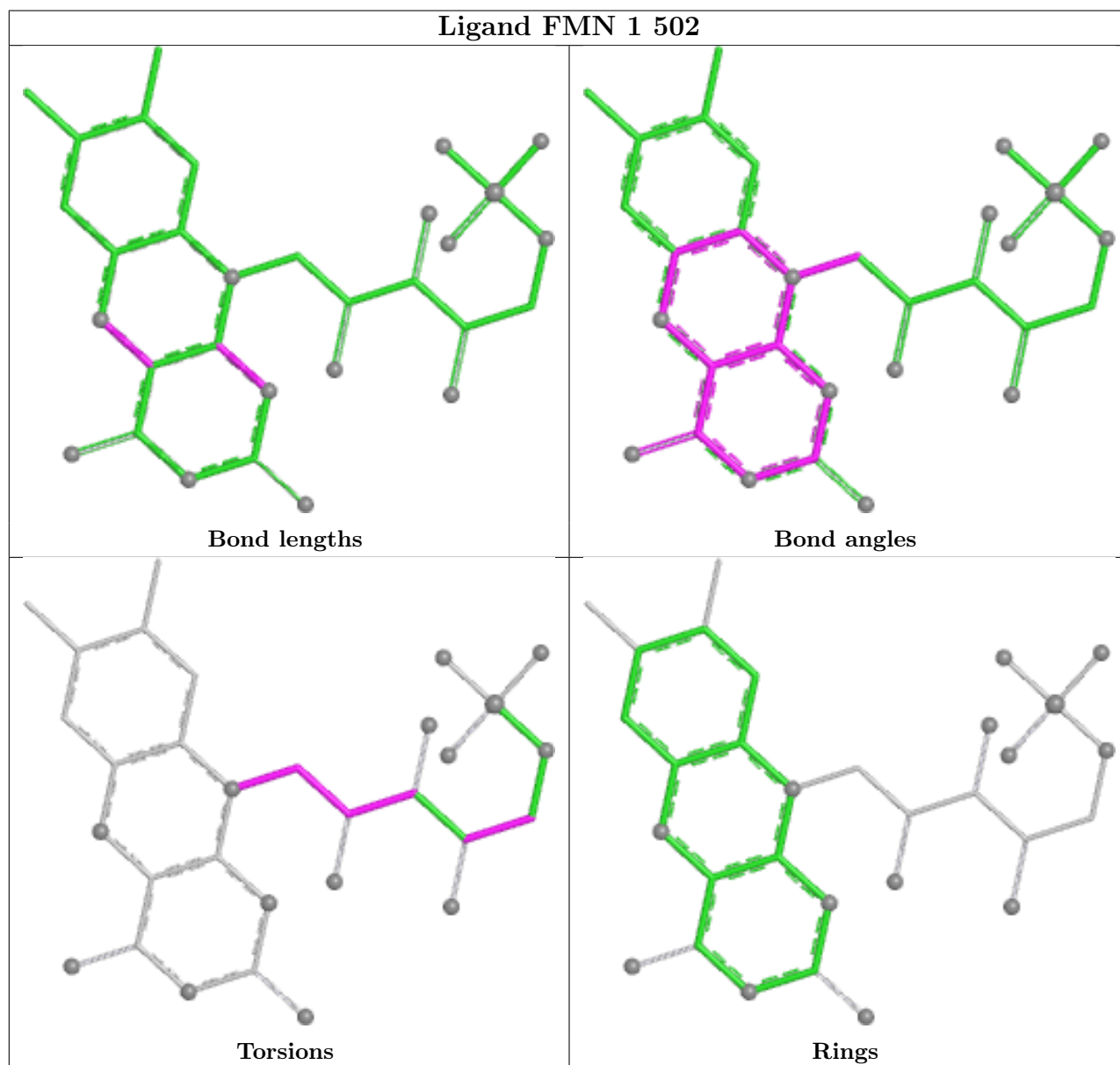
Mol	Chain	Res	Type	Atoms
18	1	502	FMN	C2'-C1'-N10-C10
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	N10-C1'-C2'-C3'
18	1	502	FMN	C1'-C2'-C3'-O3'
18	1	502	FMN	C1'-C2'-C3'-C4'

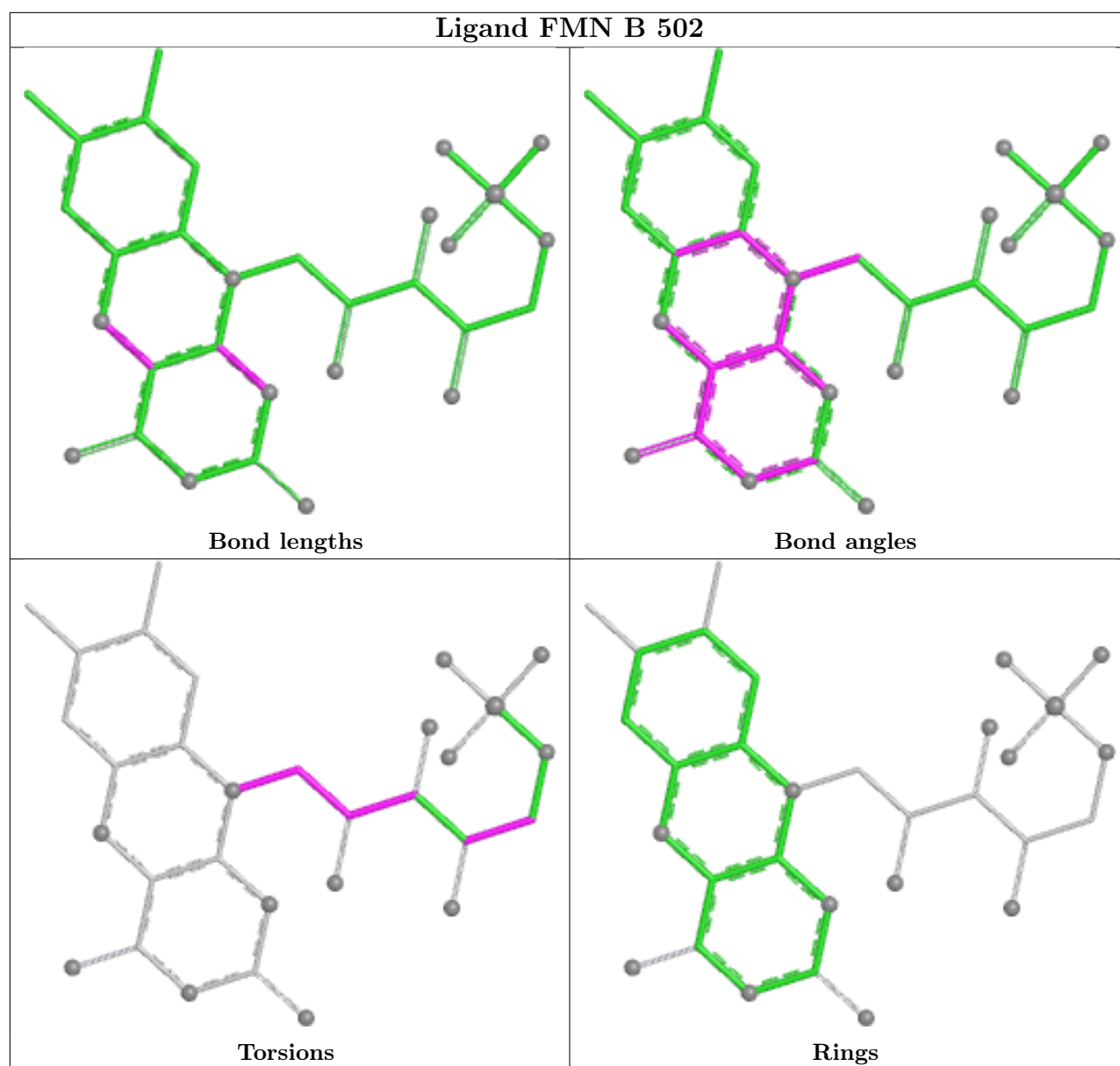
There are no ring outliers.

14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	6	201	SF4	2	0
17	9	202	SF4	4	0
18	1	502	FMN	4	0
17	B	501	SF4	2	0
17	O	201	SF4	2	0
19	2	201	FES	1	0
17	G	201	SF4	2	0
19	D	804	FES	2	0
19	3	804	FES	1	0
18	B	502	FMN	3	0
17	1	501	SF4	1	0
17	9	201	SF4	2	0
19	C	201	FES	1	0
17	O	202	SF4	5	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](#)

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%)	-1.50	0 100 100	22, 85, 158, 280	0
1	B	437/438 (99%)	-1.46	0 100 100	20, 89, 156, 270	0
2	2	178/181 (98%)	-1.48	0 100 100	17, 73, 132, 165	0
2	C	178/181 (98%)	-1.49	0 100 100	18, 76, 134, 188	0
3	3	756/783 (96%)	-1.62	0 100 100	4, 39, 102, 257	0
3	D	756/783 (96%)	-1.57	1 (0%) 92 90	5, 41, 105, 245	0
4	4	384/409 (93%)	-1.50	0 100 100	6, 63, 135, 222	0
4	E	384/409 (93%)	-1.48	1 (0%) 90 82	15, 64, 140, 218	0
5	5	196/207 (94%)	-1.54	0 100 100	9, 62, 134, 204	0
5	F	196/207 (94%)	-1.59	0 100 100	7, 67, 138, 180	0
6	6	161/181 (88%)	-1.60	0 100 100	11, 38, 131, 255	0
6	G	161/181 (88%)	-1.49	1 (0%) 85 73	11, 44, 133, 256	0
7	9	180/182 (98%)	-1.59	0 100 100	9, 41, 105, 178	0
7	O	180/182 (98%)	-1.50	0 100 100	9, 47, 120, 191	0
8	7	127/129 (98%)	-1.61	0 100 100	14, 61, 121, 150	0
8	I	127/129 (98%)	-1.48	0 100 100	16, 70, 123, 150	0
9	W	127/131 (96%)	-1.51	0 100 100	15, 84, 155, 290	0
9	X	127/131 (96%)	-1.31	0 100 100	10, 82, 164, 294	0
10	A	117/119 (98%)	-1.44	0 100 100	12, 70, 190, 274	0
10	P	117/119 (98%)	-1.38	0 100 100	21, 74, 190, 299	0
11	J	160/176 (90%)	-1.48	0 100 100	17, 61, 131, 173	0
11	R	160/176 (90%)	-1.54	0 100 100	17, 61, 125, 170	0
12	K	95/95 (100%)	-1.41	0 100 100	15, 60, 129, 170	0
12	S	95/95 (100%)	-1.57	0 100 100	15, 54, 121, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	L	605/606 (99%)	-1.35	0 100 100	24, 90, 181, 382	0
13	T	605/606 (99%)	-1.41	2 (0%) 90 82	23, 92, 181, 381	0
14	M	467/469 (99%)	-1.34	1 (0%) 91 86	21, 74, 142, 186	0
14	U	467/469 (99%)	-1.43	0 100 100	23, 75, 145, 195	0
15	N	427/427 (100%)	-1.45	0 100 100	23, 68, 122, 203	0
15	V	427/427 (100%)	-1.44	0 100 100	21, 61, 128, 211	0
16	H	353/365 (96%)	-1.43	0 100 100	17, 76, 138, 220	0
16	Q	353/365 (96%)	-1.44	0 100 100	21, 76, 144, 222	0
All	All	9540/9796 (97%)	-1.48	6 (0%) 92 90	4, 68, 145, 382	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	T	435	PRO	4.0
3	D	150	GLU	3.3
6	G	70	ALA	2.8
14	M	467	GLY	2.6
4	E	210	GLU	2.1

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	B	502	31/31	0.99	0.05	176,200,223,231	0
17	SF4	3	801	8/8	1.00	0.01	14,14,14,14	0

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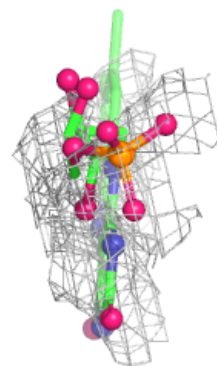
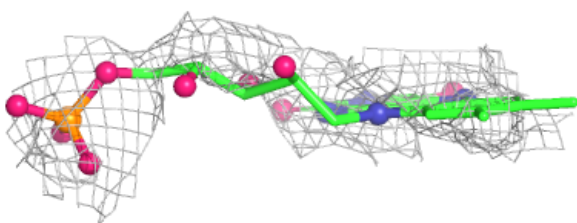
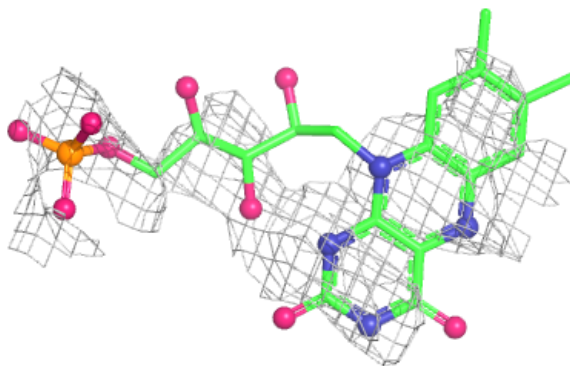
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	SF4	3	802	8/8	1.00	0.01	21,21,21,21	0
17	SF4	3	803	8/8	1.00	0.01	5,5,5,5	0
17	SF4	6	201	8/8	1.00	0.01	22,22,22,22	0
17	SF4	9	201	8/8	1.00	0.01	8,8,8,8	0
17	SF4	9	202	8/8	1.00	0.01	10,10,10,10	0
17	SF4	B	501	8/8	1.00	0.02	46,46,46,46	0
17	SF4	D	801	8/8	1.00	0.01	8,8,8,8	0
17	SF4	D	802	8/8	1.00	0.01	7,7,7,7	0
17	SF4	D	803	8/8	1.00	0.01	27,27,27,27	0
17	SF4	G	201	8/8	1.00	0.02	32,32,32,32	0
17	SF4	O	201	8/8	1.00	0.01	8,8,8,8	0
17	SF4	O	202	8/8	1.00	0.01	16,16,16,16	0
18	FMN	1	502	31/31	1.00	0.03	0,37,61,71	0
17	SF4	1	501	8/8	1.00	0.02	36,36,36,36	0
19	FES	2	201	4/4	1.00	0.01	37,37,37,37	0
19	FES	3	804	4/4	1.00	0.01	21,21,21,21	0
19	FES	C	201	4/4	1.00	0.02	74,74,74,74	0
19	FES	D	804	4/4	1.00	0.01	20,20,20,20	0

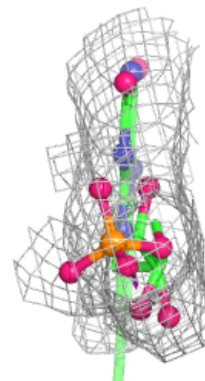
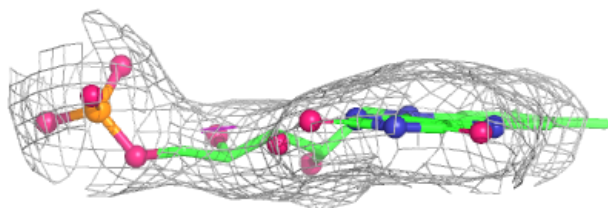
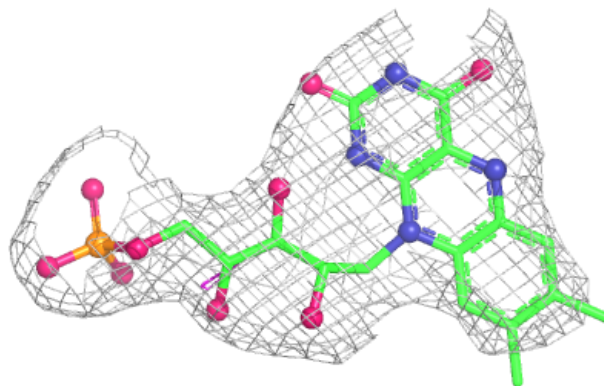
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN 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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.