wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 07:31 PM GMT

PDB ID	:	4HEA
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

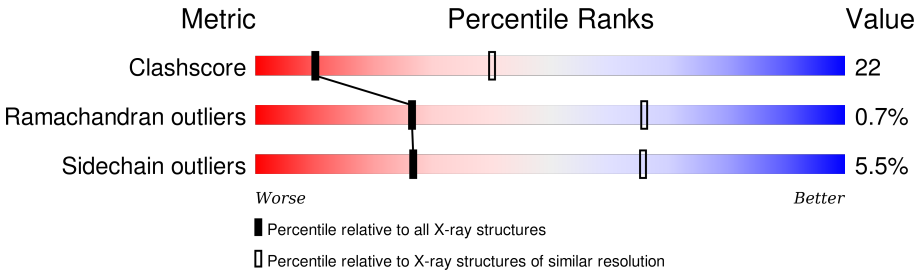
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	60% 37%
1	B	438	62% 36%
2	2	181	52% 43%
2	C	181	51% 44%
3	3	783	57% 37%
3	D	783	56% 38%
4	4	409	46% 45% 6%

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Mol	Chain	Length	Quality of chain
4	E	409	48% 43% • 6%
5	5	207	50% 41% • 5%
5	F	207	51% 40% • 5%
6	6	181	34% 43% 10% • 11%
6	G	181	37% 40% 9% • 11%
7	9	182	60% 35% • •
7	O	182	60% 35% • •
8	7	129	65% 31% • •
8	I	129	64% 33% • •
9	W	131	73% 24% • •
9	X	131	76% 20% • • •
10	A	119	50% 44% • •
10	P	119	50% 43% 5% •
11	J	176	51% 37% • 9%
11	R	176	55% 34% • 9%
12	K	95	49% 44% 6%
12	S	95	58% 37% 5%
13	L	606	63% 33% •
13	T	606	65% 32% •
14	M	469	51% 46% •
14	U	469	52% 45% •
15	N	427	63% 36% •
15	V	427	65% 34% •
16	H	365	47% 43% 5% • •
16	Q	365	46% 44% 5% • •

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

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

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

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

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

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

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

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

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

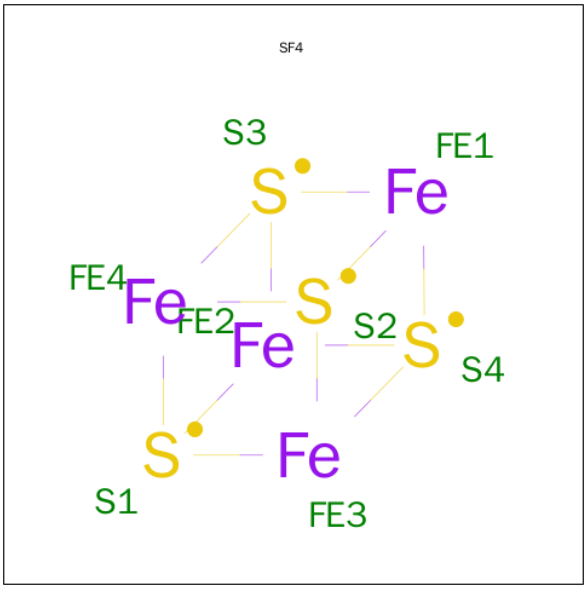
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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

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

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

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



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

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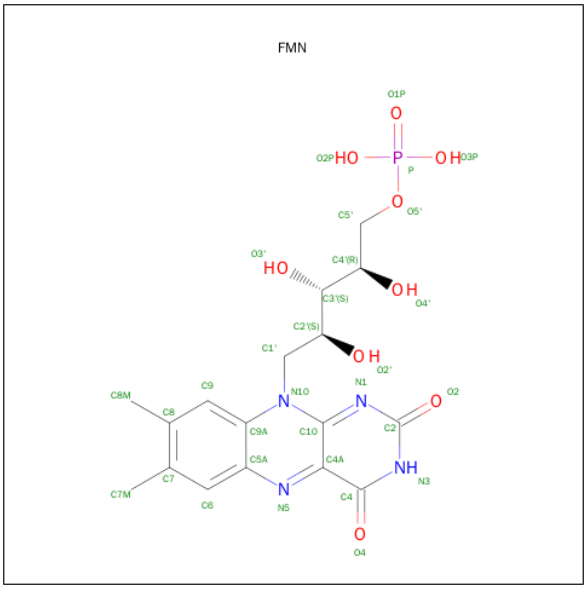
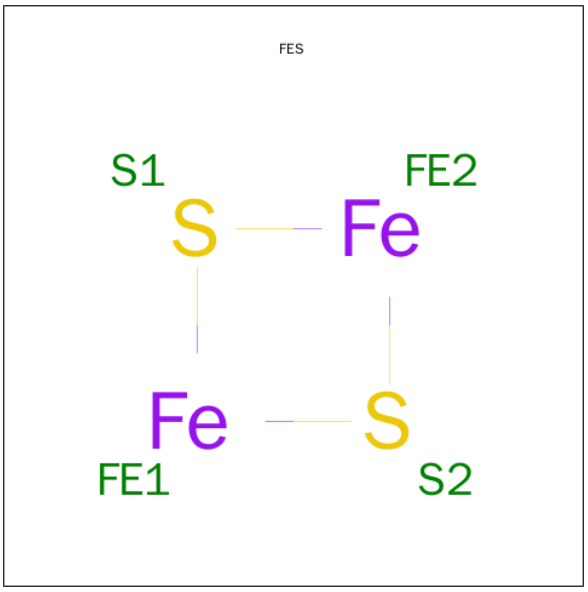
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total Fe S 8 4 4	0	0
17	D	1	Total Fe S 8 4 4	0	0
17	G	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0
17	O	1	Total Fe S 8 4 4	0	0

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



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

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



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

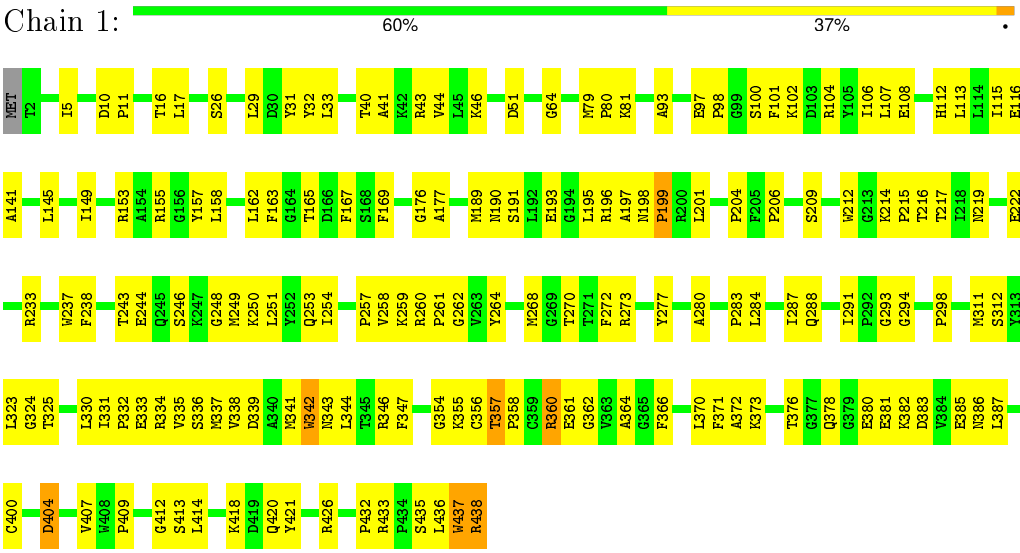
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS failed to run properly.

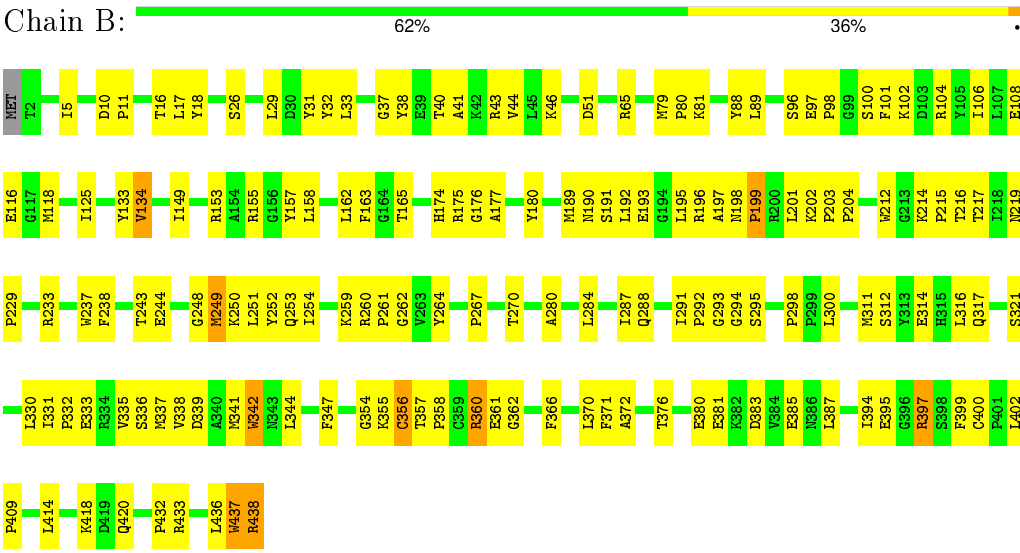
- Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain 1:



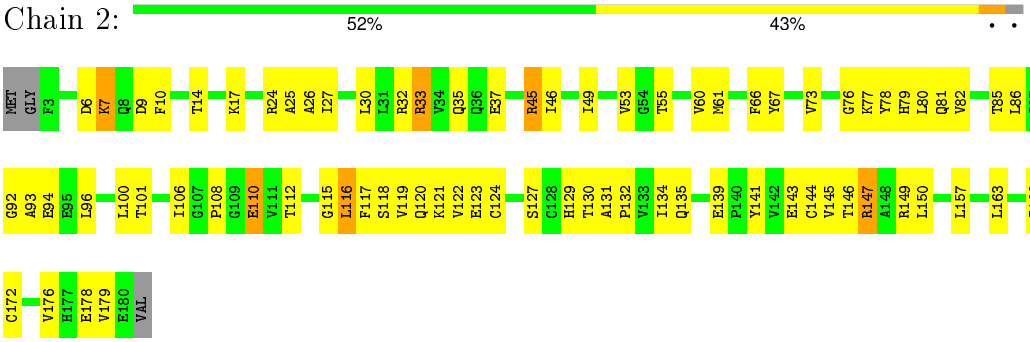
- Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain B:



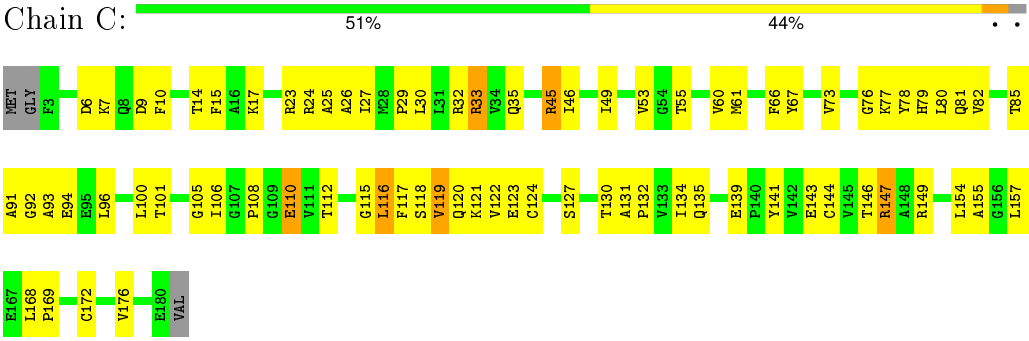
- Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:



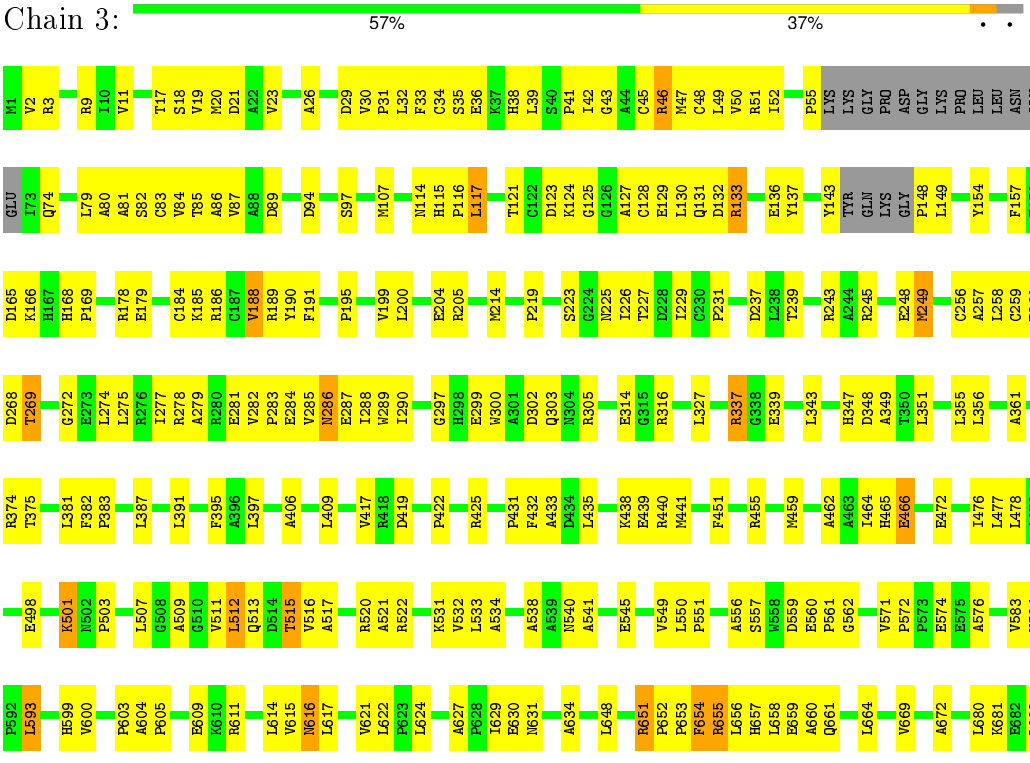
- Molecule 2: NADH-quinone oxidoreductase subunit 2

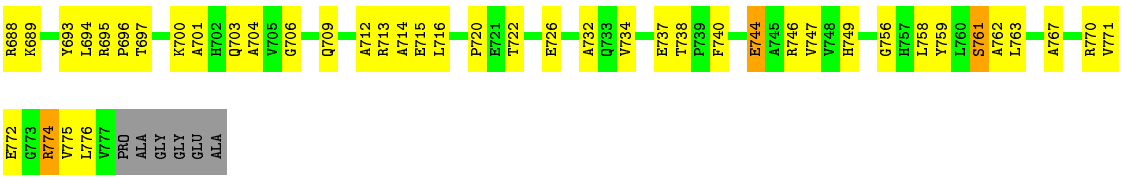
Chain C:



- Molecule 3: NADH-quinone oxidoreductase subunit 3

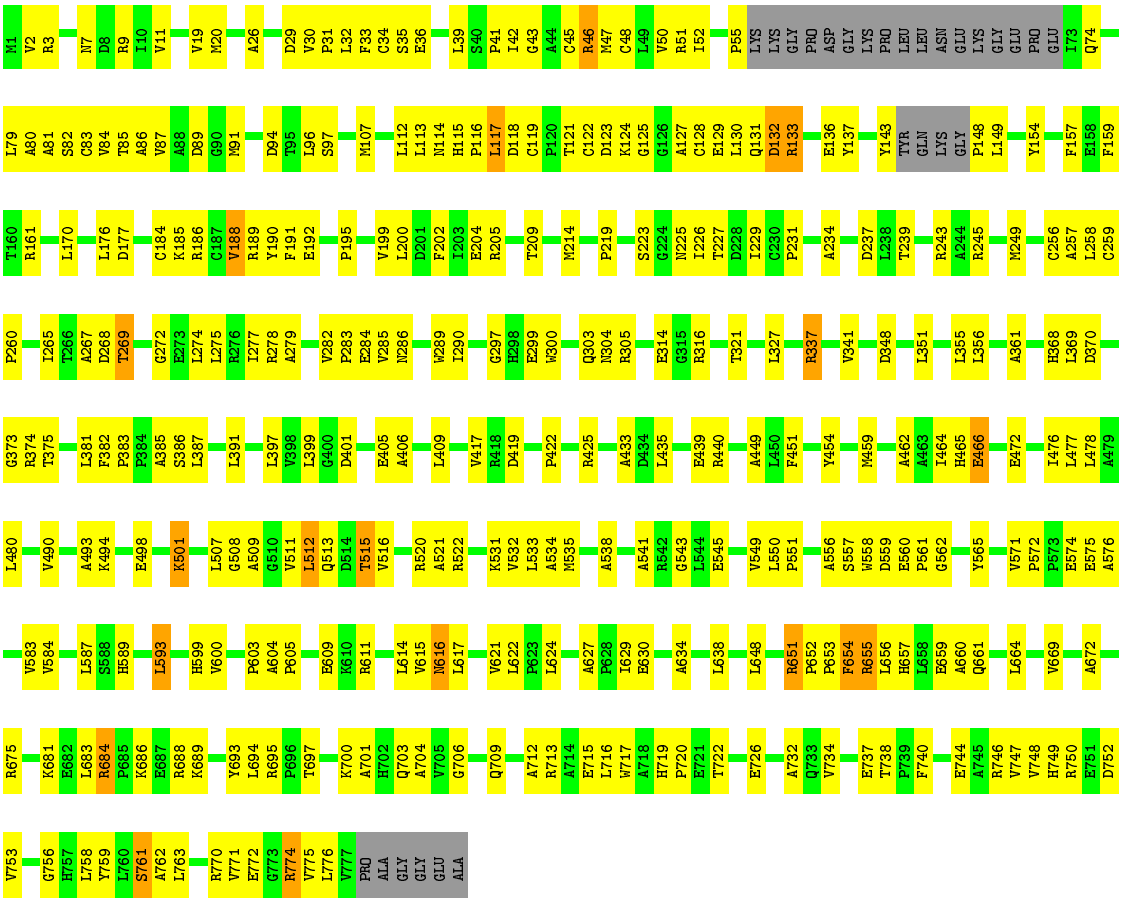
Chain 3:





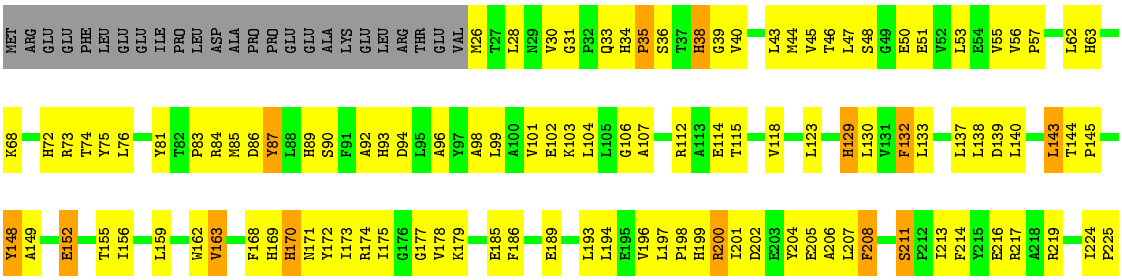
• Molecule 3: NADH-quinone oxidoreductase subunit 3

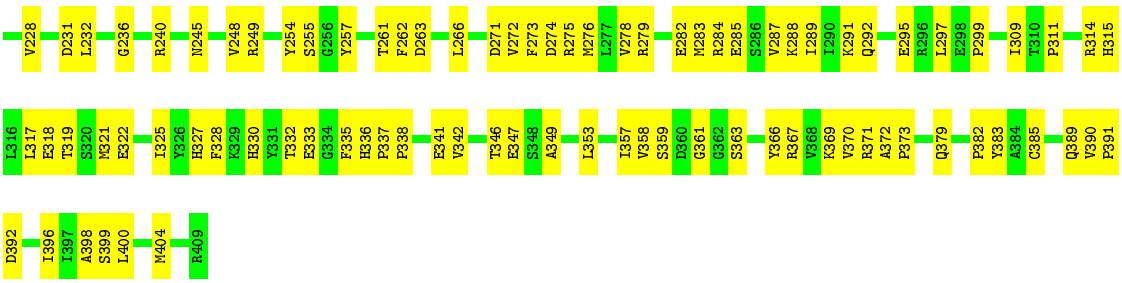
Chain D:



• Molecule 4: NADH-quinone oxidoreductase subunit 4

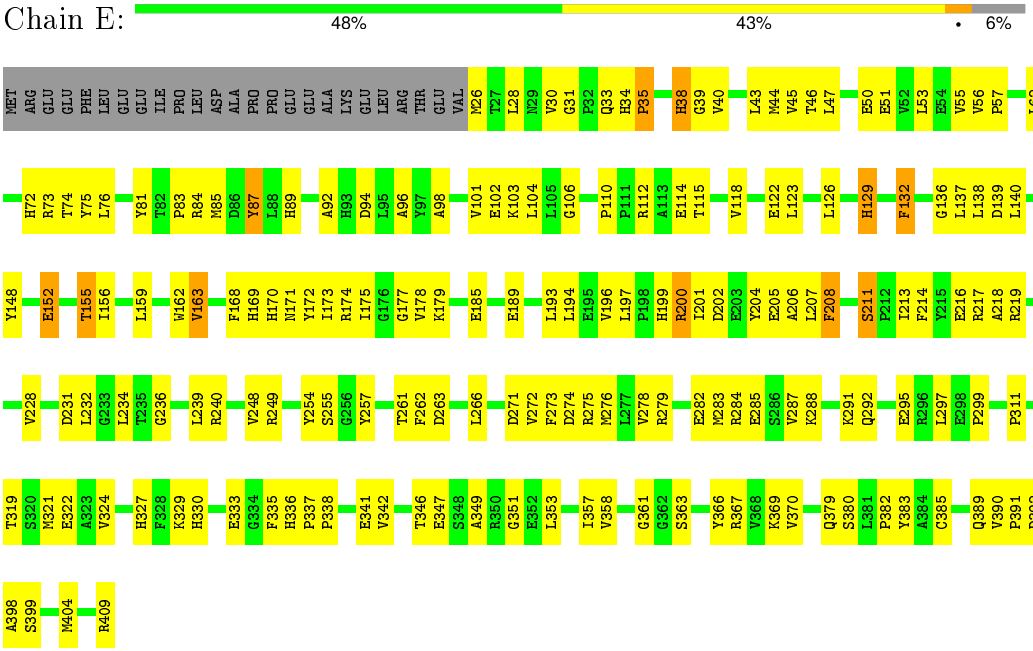
Chain 4:





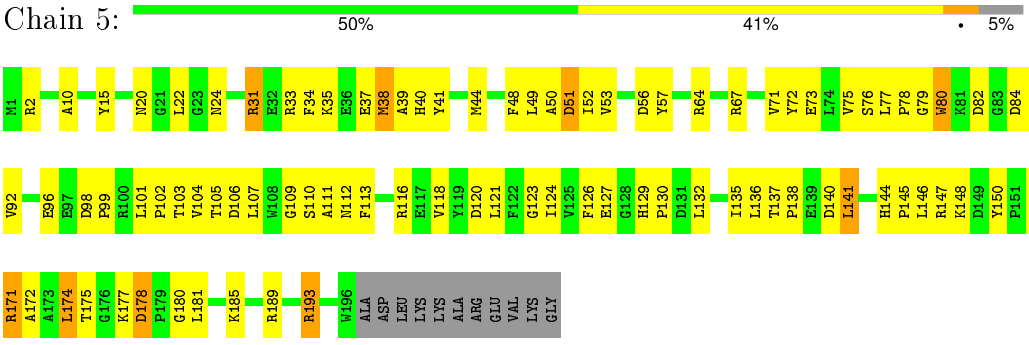
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E:



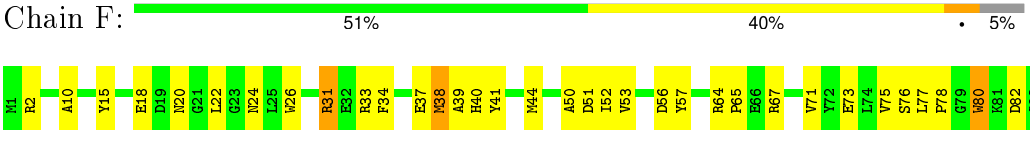
• Molecule 5: NADH-quinone oxidoreductase subunit 5

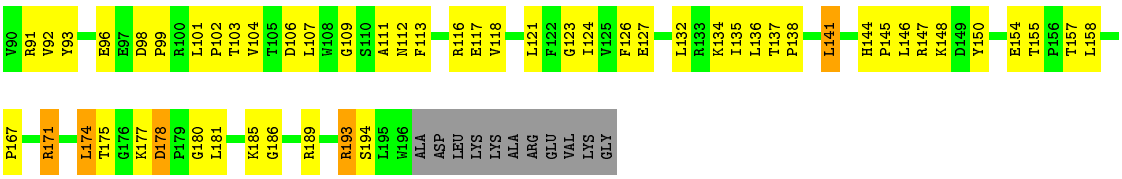
Chain 5:



• Molecule 5: NADH-quinone oxidoreductase subunit 5

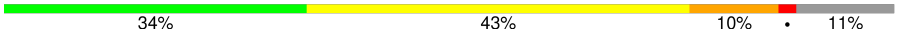
Chain F:

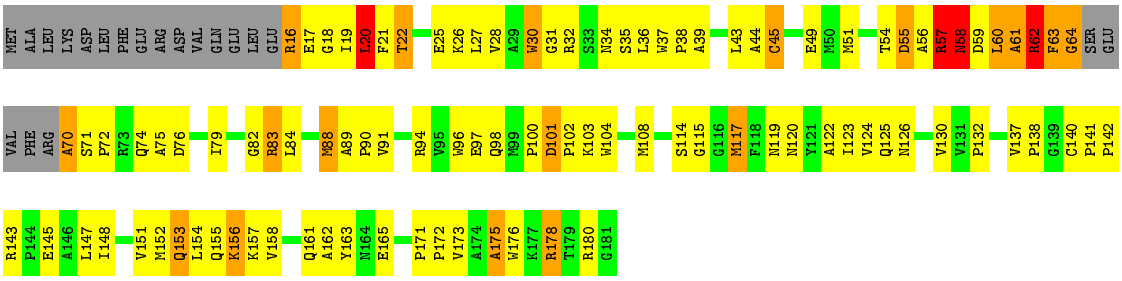




- Molecule 6: NADH-quinone oxidoreductase subunit 6

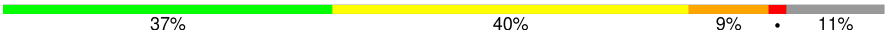
Chain 6:

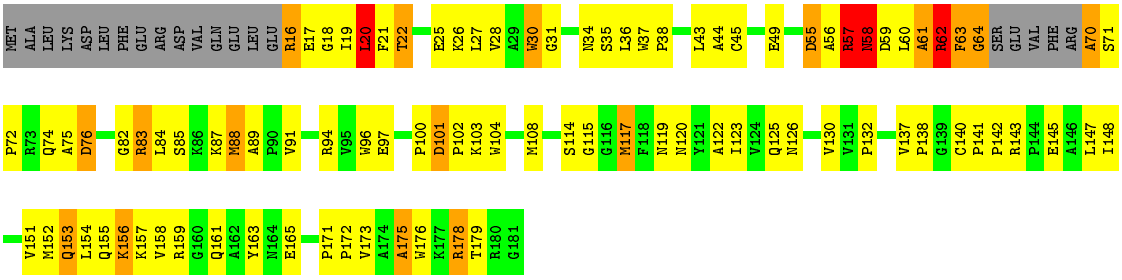




- Molecule 6: NADH-quinone oxidoreductase subunit 6

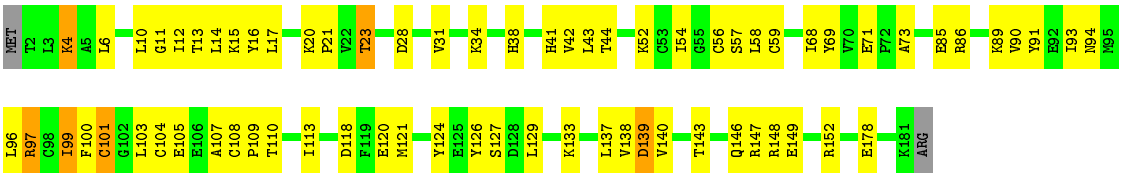
Chain G:





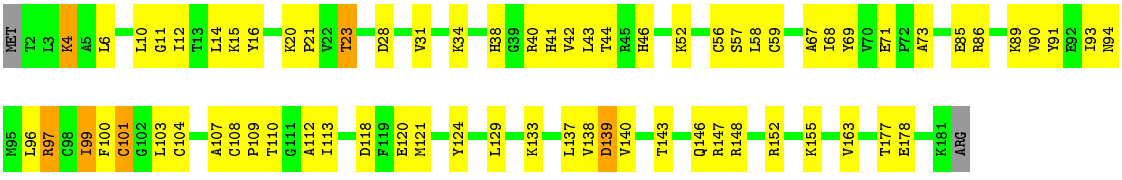
- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:



- Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:

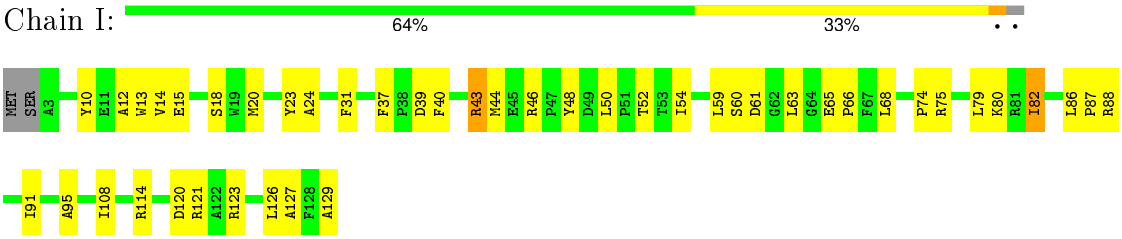


• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:

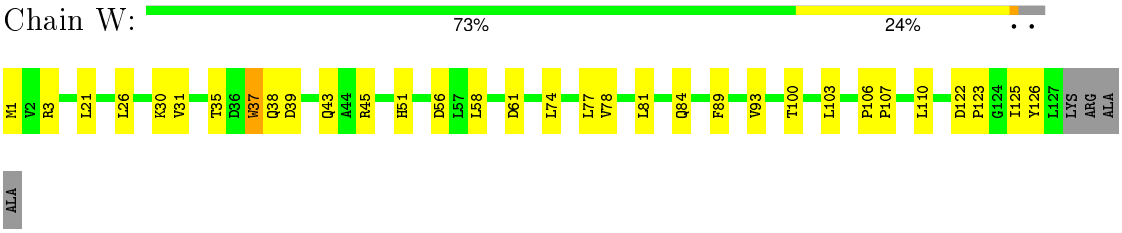
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:



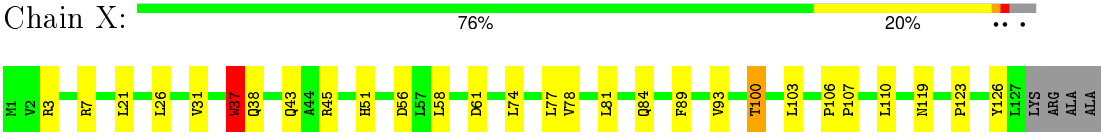
• Molecule 9: Putative uncharacterized protein TTHA1528

Chain W:



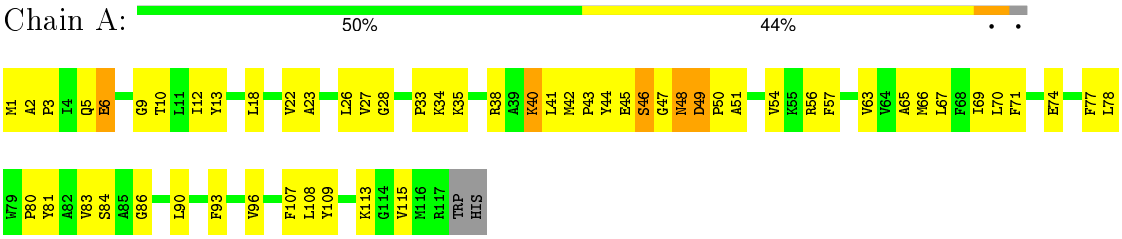
• Molecule 9: Putative uncharacterized protein TTHA1528

Chain X:



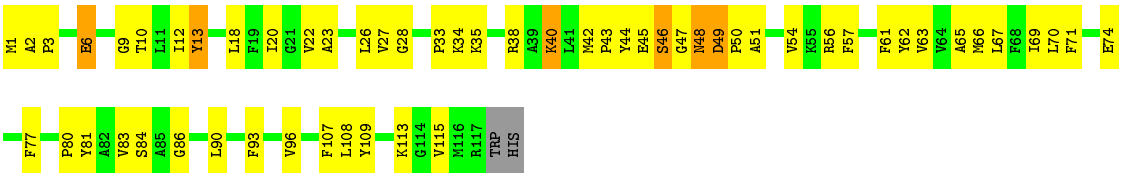
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:



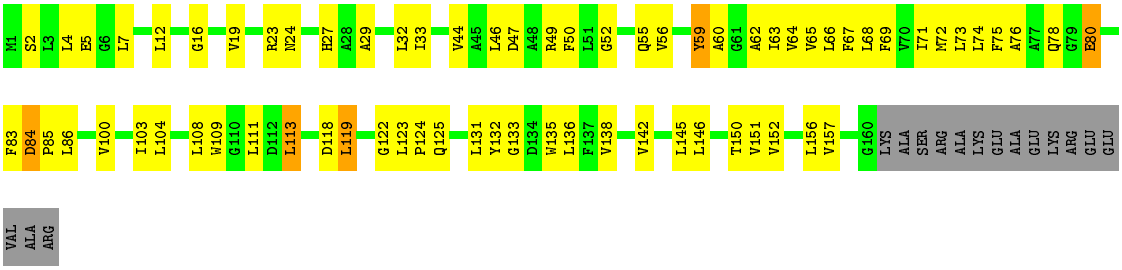
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:



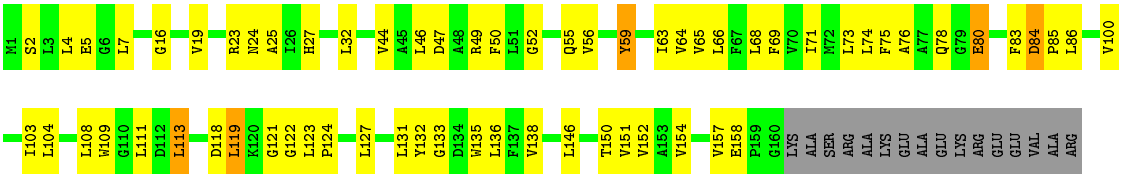
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:



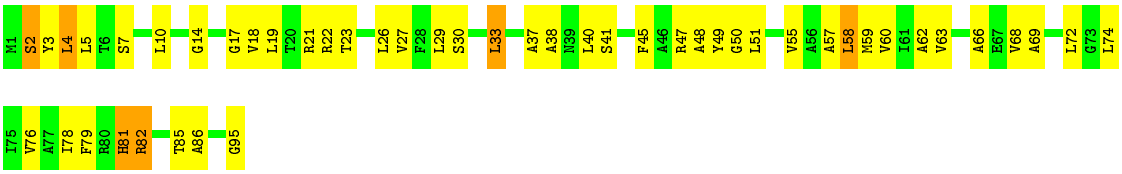
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:



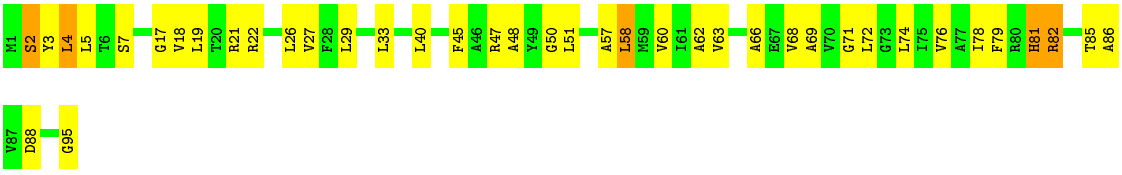
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:



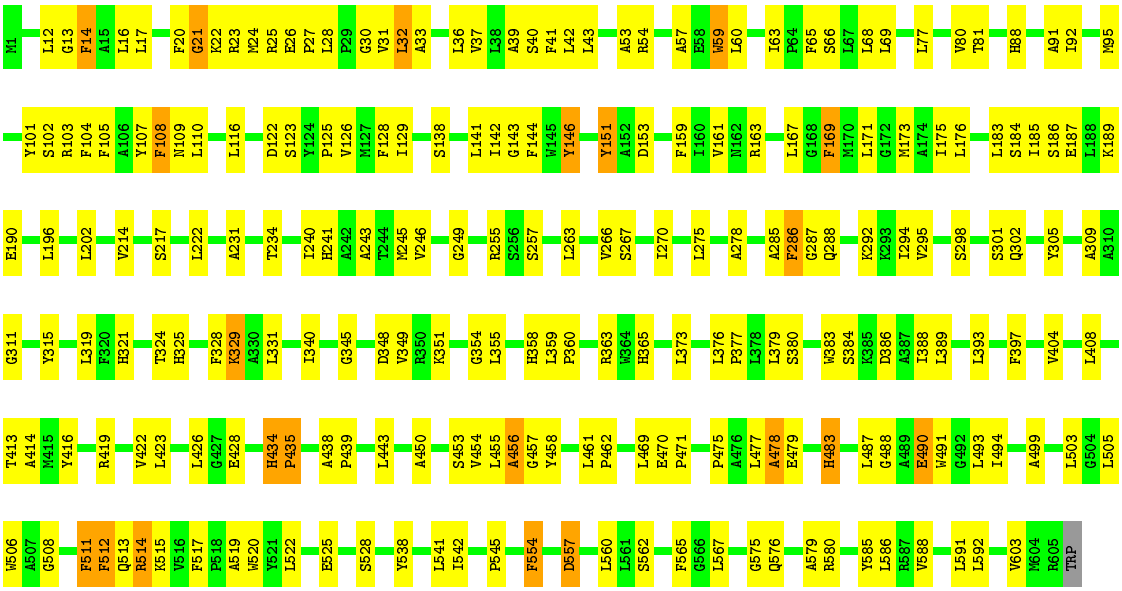
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S:



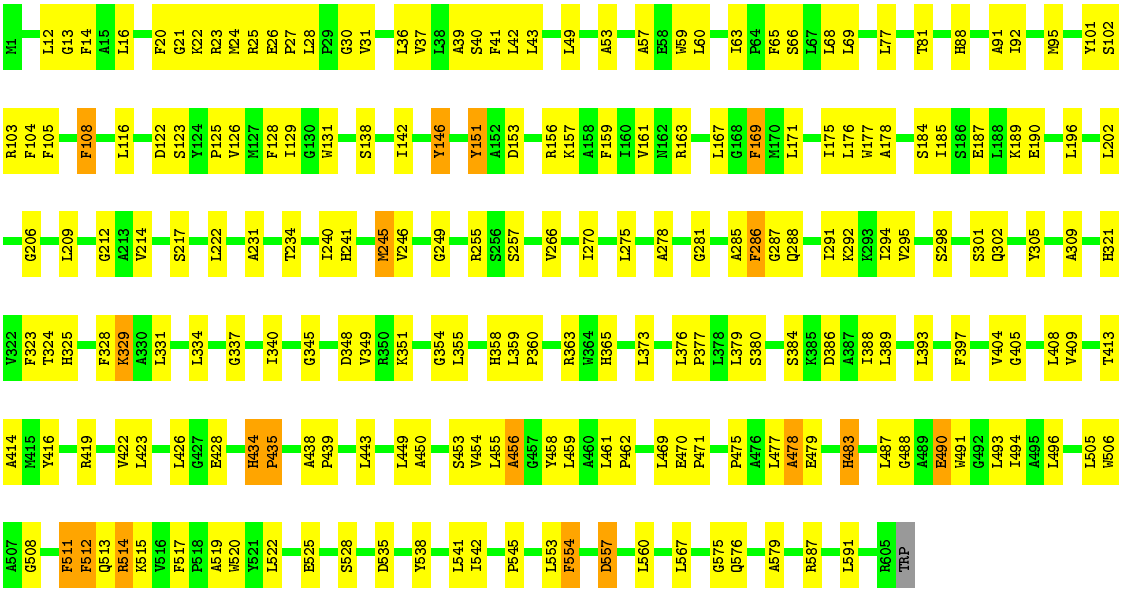
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:



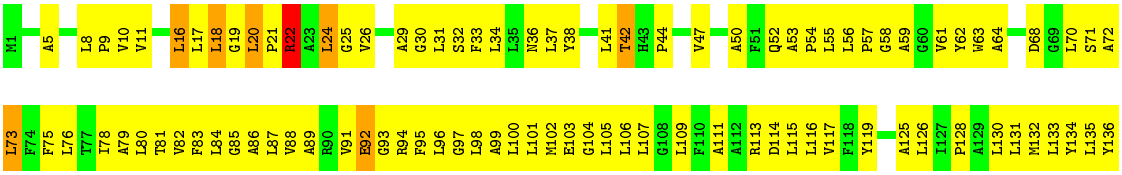
- Molecule 13: NADH-quinone oxidoreductase subunit 12

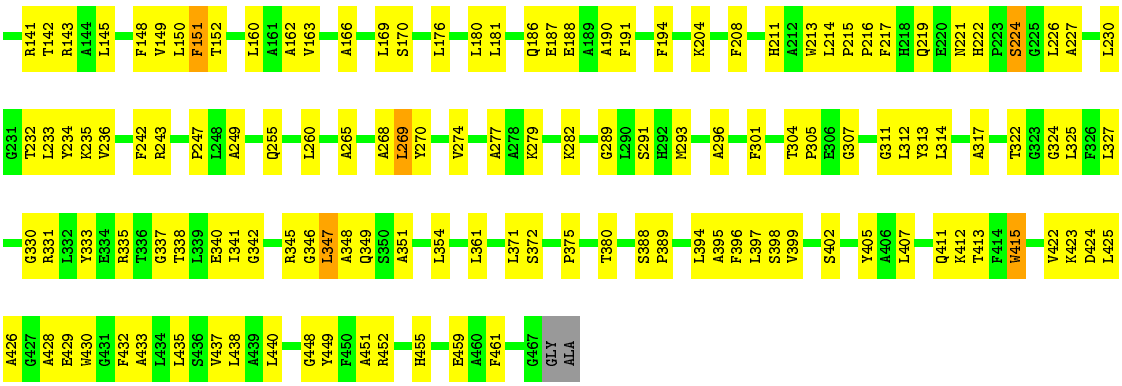
Chain T:



- Molecule 14: NADH-quinone oxidoreductase subunit 13

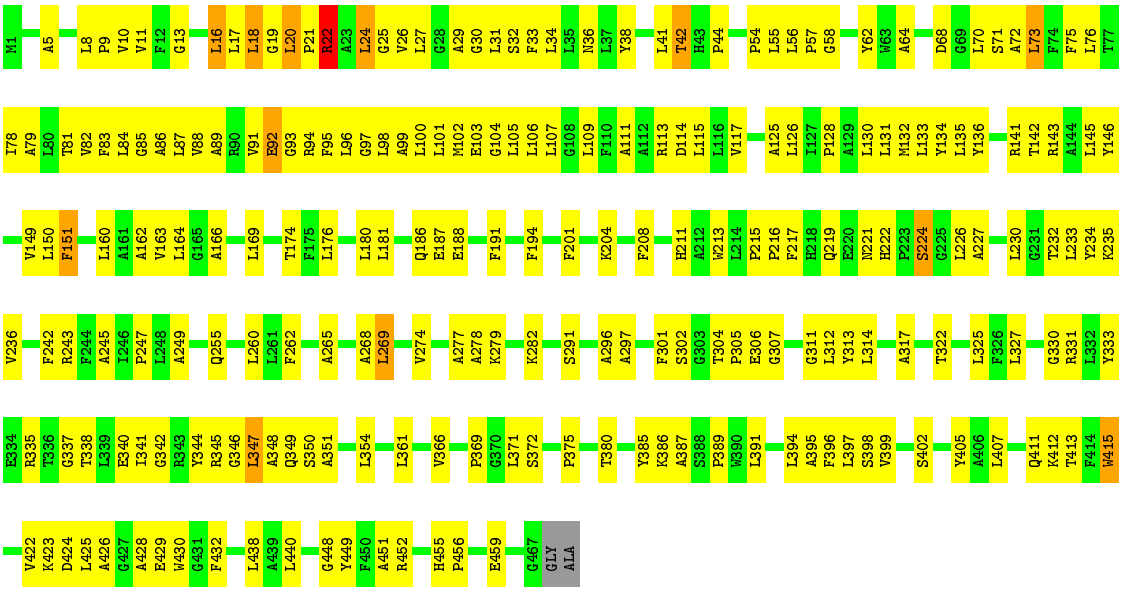
Chain M:





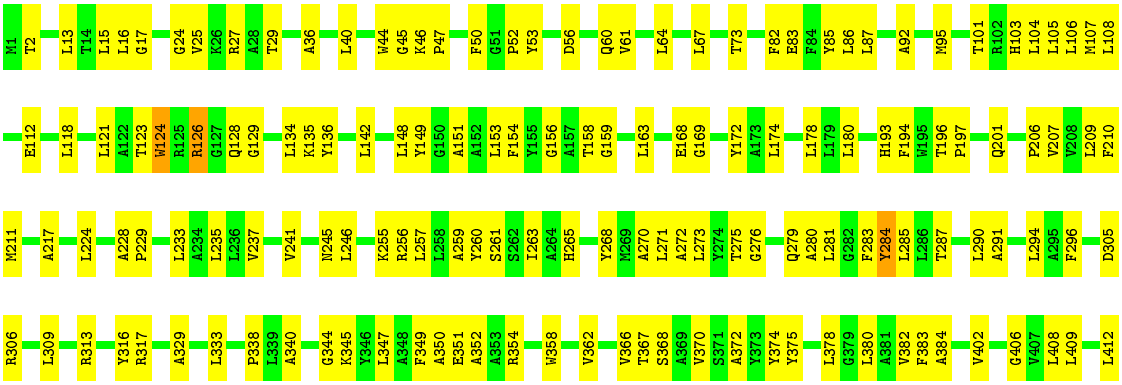
• Molecule 14: NADH-quinone oxidoreductase subunit 13

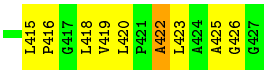
Chain U:



• Molecule 15: NADH-quinone oxidoreductase subunit 14

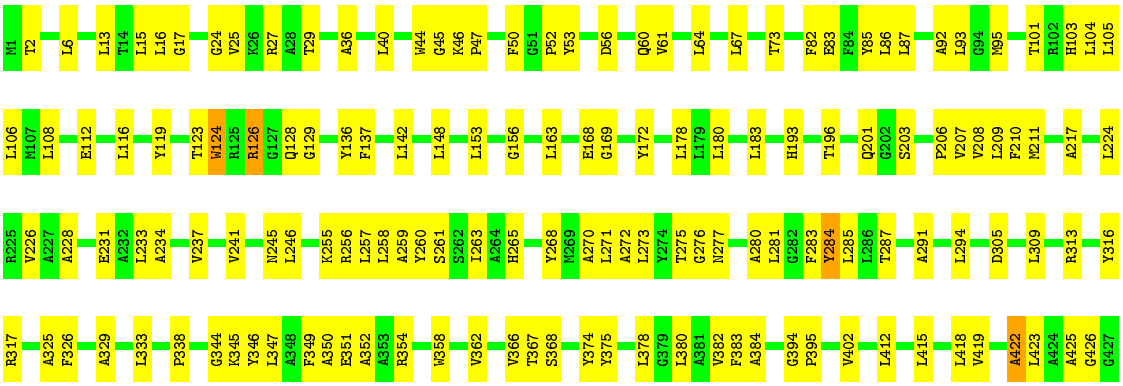
Chain N:





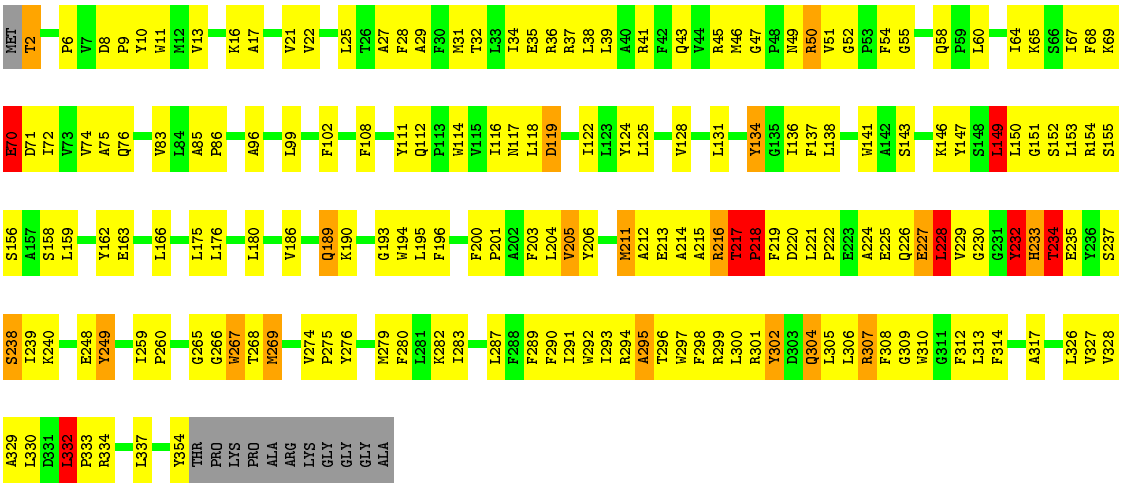
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V:



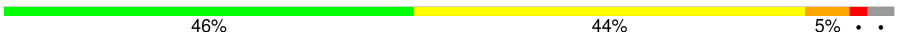
• Molecule 16: NADH-quinone oxidoreductase subunit 8

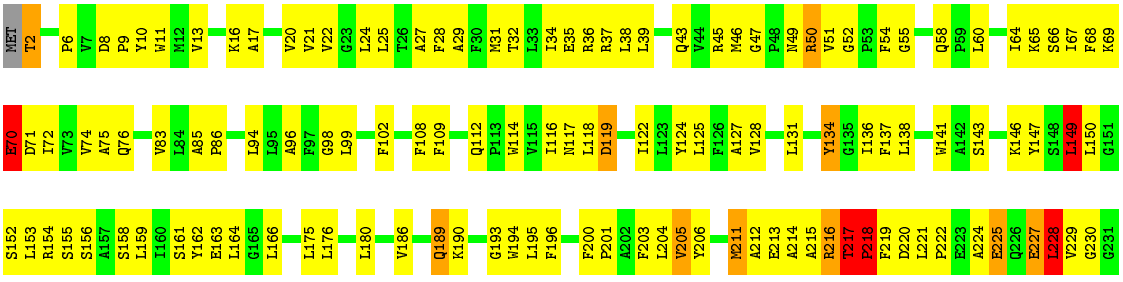
Chain H:

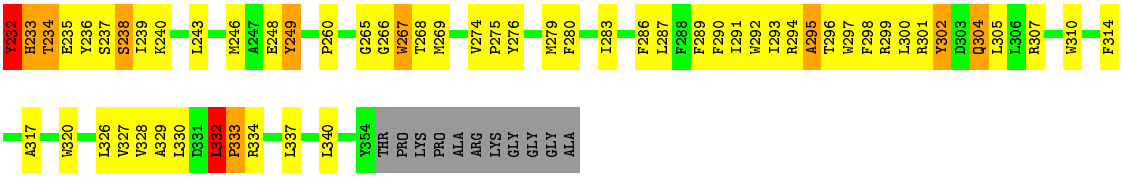


• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q:






Y232
H233
T234
E235
Y236
S237
S238
I239
K240
L243
M246
A247
E248
Y249
P260
G265
G266
W267
T268
M269
V274
P275
Y276
M279
F280
I283
F286
L287
F288
F289
F290
I291
W292
I293
R294
A295
T296
W297
F298
R299
L300
R301
Y302
D303
Q304
L305
L306
R307
W310
F314
A317
W320
L326
V327
V328
A329
L330
D331
L332
P333
R334
L337
L340
Y354
THR
PRO
LYS
PRO
ALA
ARG
LYS
GLY
GLY
GLY
ALA

4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	93.7 (40.00-3.30)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1041)	Depositor
R, R_{free}	0.202 , 0.239	Depositor
Wilson B-factor (Å^2)	76.0	Xtriage
Anisotropy	0.003	Xtriage
Estimated twinning fraction	0.470 for -h,-k,h+l 0.377 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,h+l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Outliers	0 of 233384 reflections	Xtriage
Total number of atoms	73998	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.34	0/3506	0.61	0/4745
1	B	0.33	1/3506 (0.0%)	0.59	0/4745
2	2	0.39	0/1439	0.63	0/1953
2	C	0.38	0/1439	0.61	0/1953
3	3	0.42	0/6035	0.71	0/8185
3	D	0.41	0/6035	0.71	0/8185
4	4	0.38	0/3150	0.70	1/4284 (0.0%)
4	E	0.37	0/3150	0.67	0/4284
5	5	0.36	0/1656	0.68	0/2246
5	F	0.35	0/1656	0.67	0/2246
6	6	0.57	0/1273	0.93	4/1723 (0.2%)
6	G	0.56	0/1273	0.92	5/1723 (0.3%)
7	9	0.46	0/1423	0.71	0/1933
7	O	0.42	0/1423	0.69	0/1933
8	7	0.37	0/1059	0.66	1/1429 (0.1%)
8	I	0.31	0/1059	0.63	1/1429 (0.1%)
9	W	0.37	0/985	0.62	0/1335
9	X	0.36	0/985	0.61	0/1335
10	A	0.41	0/940	0.70	0/1280
10	P	0.41	0/940	0.69	0/1280
11	J	0.35	0/1206	0.64	0/1649
11	R	0.36	0/1206	0.64	0/1649
12	K	0.37	0/710	0.59	0/962
12	S	0.38	0/710	0.59	0/962
13	L	0.33	0/4741	0.63	1/6460 (0.0%)
13	T	0.33	0/4741	0.62	2/6460 (0.0%)
14	M	0.39	0/3591	0.70	3/4896 (0.1%)
14	U	0.39	0/3591	0.70	3/4896 (0.1%)
15	N	0.34	0/3238	0.59	0/4434
15	V	0.34	0/3238	0.57	0/4434
16	H	0.48	1/2935 (0.0%)	0.79	5/4014 (0.1%)
16	Q	0.48	0/2935	0.79	5/4014 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.39	2/75774 (0.0%)	0.68	31/103056 (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
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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	225	GLU	CG-CD	-5.04	1.44	1.51
1	B	356	CYS	CB-SG	-5.02	1.73	1.81

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	U	22	ARG	NE-CZ-NH2	-12.89	113.85	120.30
14	M	22	ARG	NE-CZ-NH2	-12.73	113.93	120.30
14	U	22	ARG	NE-CZ-NH1	10.89	125.74	120.30
14	M	22	ARG	NE-CZ-NH1	10.39	125.49	120.30
16	Q	149	LEU	CB-CG-CD1	-8.27	96.95	111.00

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 (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	128	0
2	2	1406	0	1373	81	0
2	C	1406	0	1373	78	0
3	3	5895	0	5930	232	0
3	D	5895	0	5930	236	0
4	4	3067	0	3049	193	0
4	E	3067	0	3049	179	0
5	5	1607	0	1574	99	0
5	F	1607	0	1574	84	0
6	6	1245	0	1255	148	0
6	G	1245	0	1255	139	0
7	9	1388	0	1383	65	0
7	O	1388	0	1383	58	0
8	7	1031	0	1029	42	0
8	I	1031	0	1029	42	0
9	W	967	0	1010	27	0
9	X	967	0	1010	23	0
10	A	910	0	939	79	0
10	P	910	0	939	80	0
11	J	1183	0	1286	69	0
11	R	1183	0	1286	62	0
12	K	703	0	747	47	0
12	S	703	0	747	36	0
13	L	4604	0	4734	164	0
13	T	4604	0	4734	150	0
14	M	3489	0	3606	199	0
14	U	3489	0	3606	184	0
15	N	3154	0	3343	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	V	3154	0	3343	107	0
16	H	2838	0	2903	208	0
16	Q	2838	0	2903	205	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	3243	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 3243 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 (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%)	405 (93%)	28 (6%)	2 (0%)	34 71
1	B	435/438 (99%)	406 (93%)	27 (6%)	2 (0%)	34 71
2	2	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	30 68
2	C	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	30 68
3	3	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	56 89
3	D	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	56 89
4	4	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	34 71
4	E	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	34 71
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%)	15 52
6	G	157/181 (87%)	141 (90%)	14 (9%)	2 (1%)	15 52
7	9	178/182 (98%)	166 (93%)	11 (6%)	1 (1%)	30 68
7	O	178/182 (98%)	167 (94%)	10 (6%)	1 (1%)	30 68
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%)	24 62
9	X	125/131 (95%)	121 (97%)	3 (2%)	1 (1%)	24 62
10	A	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	7 36
10	P	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	7 36
11	J	158/176 (90%)	143 (90%)	14 (9%)	1 (1%)	30 68
11	R	158/176 (90%)	142 (90%)	15 (10%)	1 (1%)	30 68
12	K	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	17 57
12	S	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	17 57
13	L	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	24 62
13	T	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	24 62
14	M	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	21 60
14	U	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	21 60
15	N	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	34 71
15	V	425/427 (100%)	396 (93%)	27 (6%)	2 (0%)	34 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	H	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	7 36
16	Q	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	7 36
All	All	9464/9796 (97%)	8730 (92%)	664 (7%)	70 (1%)	26 66

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%)	342 (96%)	13 (4%)	41 76
1	B	355/356 (100%)	343 (97%)	12 (3%)	44 77
2	2	150/152 (99%)	140 (93%)	10 (7%)	20 58
2	C	150/152 (99%)	139 (93%)	11 (7%)	17 53
3	3	609/628 (97%)	574 (94%)	35 (6%)	25 65
3	D	609/628 (97%)	573 (94%)	36 (6%)	24 63
4	4	332/355 (94%)	315 (95%)	17 (5%)	29 68
4	E	332/355 (94%)	314 (95%)	18 (5%)	27 66
5	5	167/175 (95%)	158 (95%)	9 (5%)	27 66
5	F	167/175 (95%)	158 (95%)	9 (5%)	27 66
6	6	130/149 (87%)	109 (84%)	21 (16%)	3 14
6	G	130/149 (87%)	109 (84%)	21 (16%)	3 14
7	9	148/150 (99%)	138 (93%)	10 (7%)	20 57
7	O	148/150 (99%)	138 (93%)	10 (7%)	20 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	7	104/106 (98%)	101 (97%)	3 (3%)	50 80
8	I	104/106 (98%)	102 (98%)	2 (2%)	65 85
9	W	99/101 (98%)	96 (97%)	3 (3%)	48 79
9	X	99/101 (98%)	96 (97%)	3 (3%)	48 79
10	A	90/92 (98%)	85 (94%)	5 (6%)	26 65
10	P	90/92 (98%)	85 (94%)	5 (6%)	26 65
11	J	118/130 (91%)	108 (92%)	10 (8%)	13 46
11	R	118/130 (91%)	108 (92%)	10 (8%)	13 46
12	K	71/71 (100%)	64 (90%)	7 (10%)	10 37
12	S	71/71 (100%)	64 (90%)	7 (10%)	10 37
13	L	453/454 (100%)	434 (96%)	19 (4%)	36 73
13	T	453/454 (100%)	435 (96%)	18 (4%)	38 74
14	M	332/332 (100%)	315 (95%)	17 (5%)	29 68
14	U	332/332 (100%)	315 (95%)	17 (5%)	29 68
15	N	302/302 (100%)	296 (98%)	6 (2%)	63 84
15	V	302/302 (100%)	296 (98%)	6 (2%)	63 84
16	H	293/300 (98%)	270 (92%)	23 (8%)	16 50
16	Q	293/300 (98%)	271 (92%)	22 (8%)	17 52
All	All	7506/7706 (97%)	7091 (94%)	415 (6%)	27 66

5 of 415 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	H	28	PHE
3	D	11	VAL
14	U	349	GLN
16	H	180	LEU
1	B	217	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	386	ASN
2	C	71	GLN
6	G	34	ASN

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Mol	Chain	Res	Type
12	K	81	HIS
15	N	245	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 carbohydrates 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	1	501	1	0,12,12	0.00	-	0,24,24	0.00	-
18	FMN	1	502	-	32,33,33	1.21	3 (9%)	34,50,50	1.69	6 (17%)
19	FES	2	201	2	0,4,4	0.00	-	0,4,4	0.00	-
17	SF4	3	801	3	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	3	802	3	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	3	803	3	0,12,12	0.00	-	0,24,24	0.00	-
19	FES	3	804	3	0,4,4	0.00	-	0,4,4	0.00	-
17	SF4	6	201	6	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	9	201	7	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	9	202	7	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	B	501	1	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	FMN	B	502	-	32,33,33	1.19	3 (9%)	34,50,50	1.63	6 (17%)
19	FES	C	201	2	0,4,4	0.00	-	0,4,4	0.00	-
17	SF4	D	801	3	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	D	802	3	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	D	803	3	0,12,12	0.00	-	0,24,24	0.00	-
19	FES	D	804	3	0,4,4	0.00	-	0,4,4	0.00	-
17	SF4	G	201	6	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	O	201	7	0,12,12	0.00	-	0,24,24	0.00	-
17	SF4	O	202	7	0,12,12	0.00	-	0,24,24	0.00	-

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	1	501	1	-	0/0/48/48	0/6/5/5
18	FMN	1	502	-	-	0/18/18/18	0/3/3/3
19	FES	2	201	2	-	0/0/4/4	0/1/1/1
17	SF4	3	801	3	-	0/0/48/48	0/6/5/5
17	SF4	3	802	3	-	0/0/48/48	0/6/5/5
17	SF4	3	803	3	-	0/0/48/48	0/6/5/5
19	FES	3	804	3	-	0/0/4/4	0/1/1/1
17	SF4	6	201	6	-	0/0/48/48	0/6/5/5
17	SF4	9	201	7	-	0/0/48/48	0/6/5/5
17	SF4	9	202	7	-	0/0/48/48	0/6/5/5
17	SF4	B	501	1	-	0/0/48/48	0/6/5/5
18	FMN	B	502	-	-	0/18/18/18	0/3/3/3
19	FES	C	201	2	-	0/0/4/4	0/1/1/1
17	SF4	D	801	3	-	0/0/48/48	0/6/5/5
17	SF4	D	802	3	-	0/0/48/48	0/6/5/5
17	SF4	D	803	3	-	0/0/48/48	0/6/5/5
19	FES	D	804	3	-	0/0/4/4	0/1/1/1
17	SF4	G	201	6	-	0/0/48/48	0/6/5/5
17	SF4	O	201	7	-	0/0/48/48	0/6/5/5
17	SF4	O	202	7	-	0/0/48/48	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	502	FMN	C4-N3	2.73	1.38	1.33
18	B	502	FMN	C1'-N10	2.77	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4-N3	2.92	1.38	1.33
18	1	502	FMN	C4A-N5	2.97	1.37	1.33
18	B	502	FMN	C4A-N5	3.05	1.38	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	1	502	FMN	N3-C2-N1	-4.20	120.61	127.69
18	B	502	FMN	N3-C2-N1	-4.14	120.71	127.69
18	1	502	FMN	C1'-N10-C9A	-2.92	115.44	118.83
18	1	502	FMN	C4A-C4-N3	-2.71	119.98	123.52
18	B	502	FMN	C1'-N10-C9A	-2.65	115.76	118.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 32 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers

EDS failed to run properly - this section will therefore be empty.