



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:49 PM UTC

PDB ID : 6I1P / pdb_00006i1p
Title : Respiratory complex I from Thermus thermophilus with bound NADH
Authors : Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on : 2018-10-29
Resolution : 3.21 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

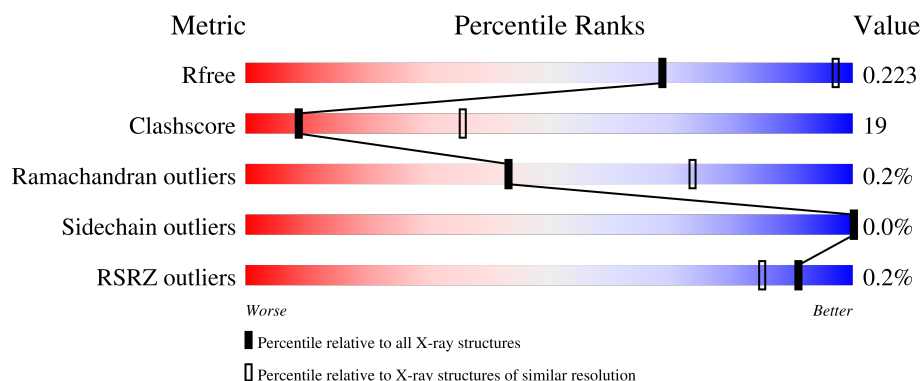
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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.



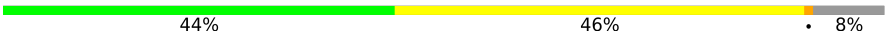
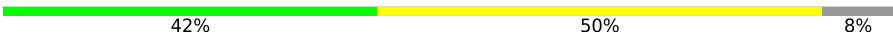
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	 61% 39%
1	B	438	 56% 43%
2	2	181	 72% 26% .
2	C	181	 62% 36% .
3	3	783	 58% 39% .

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Mol	Chain	Length	Quality of chain
3	D	783	
4	4	409	
4	E	409	
5	5	207	
5	F	207	
6	6	181	
6	G	181	
7	9	182	
7	O	182	
8	7	129	
8	I	129	
9	W	131	
9	X	131	
10	A	119	
10	P	119	
11	J	176	
11	R	176	
12	K	95	
12	S	95	
13	L	606	
13	T	606	
14	M	469	
14	U	469	
15	N	427	
15	V	427	

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Mol	Chain	Length	Quality of chain
16	H	365	 % 52% 44% . .
16	Q	365	 49% 45% . .

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	1	501	-	-	X	-
17	SF4	3	803	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	202	-	-	X	-
20	FES	C	201	-	-	X	-
20	FES	D	804	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 74174 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 NADH-quinone oxidoreductase subunit 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	W	127	Total	C	N	O	S	0	0	0
			967	623	165	175	4			
9	X	127	Total	C	N	O	S	0	0	0
			967	623	165	175	4			

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A	117	Total	C	N	O	S	0	0	0
			910	624	138	144	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	P	117	Total	C	N	O	S	0	0	0
			910	624	138	144	4			

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

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

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

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

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

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

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

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

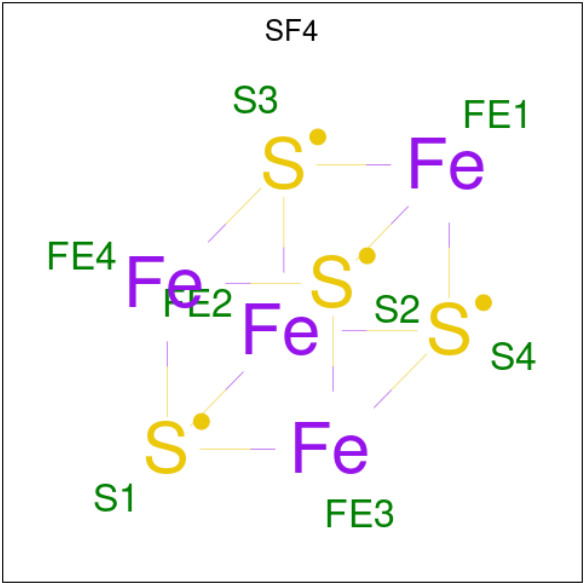
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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

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

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

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



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		

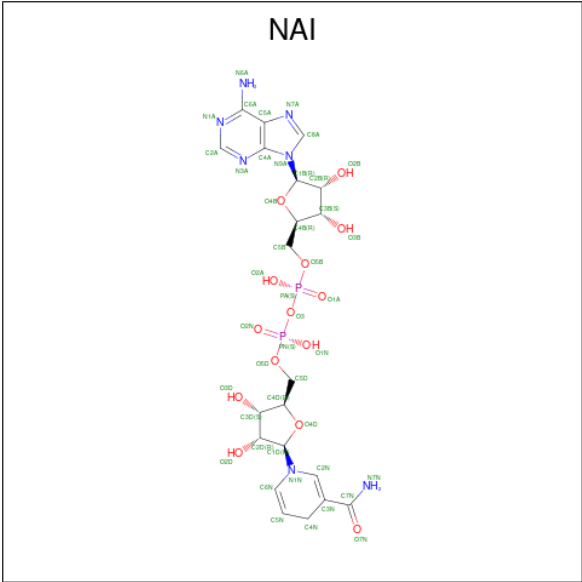
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	D	1	Total 8	Fe 4	S 4	0	0
17	D	1	Total 8	Fe 4	S 4	0	0
17	G	1	Total 8	Fe 4	S 4	0	0
17	O	1	Total 8	Fe 4	S 4	0	0
17	O	1	Total 8	Fe 4	S 4	0	0

-
- 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 (C1' to C5') with hydroxyl groups at C1', C2', C3', and C4'. The C5' carbon is attached to a phosphate group (O1P, O2P, O3P, O4P). The ribitol chain is shown in a specific conformation with stereochemistry indicated by wedges and dashes. The isoalloxazine ring system is shown with atoms labeled C6, C7, C8, C9, C10, C4A, C5A, N1, N5, N3, and N4. The phosphate group is shown with atoms labeled O1P, O2P, O3P, and O4P.

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

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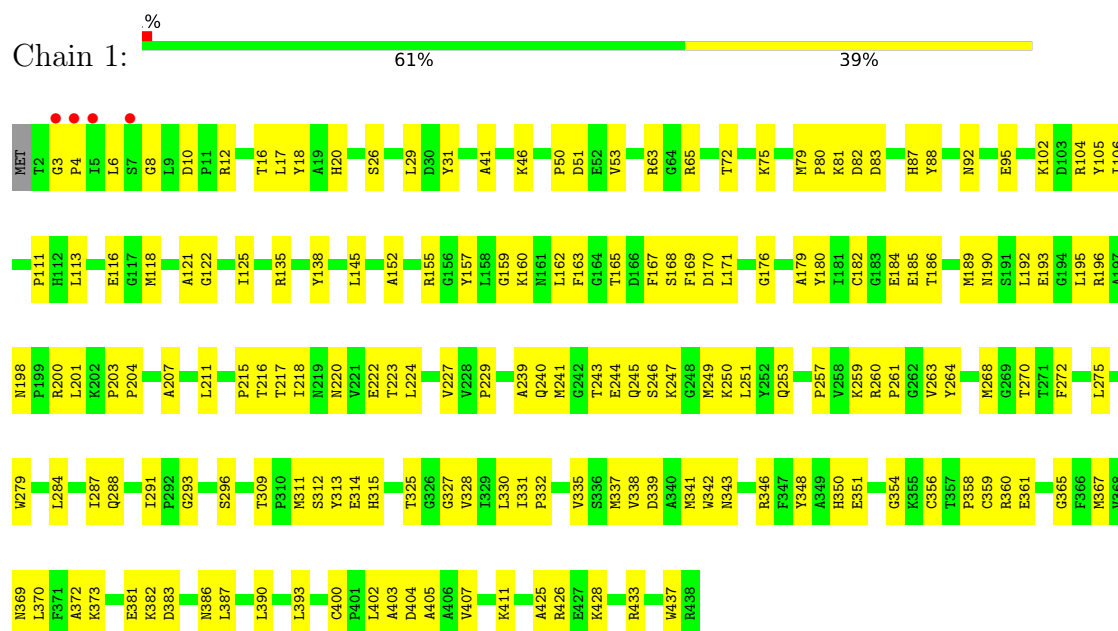
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	C	1	Total	Fe	S	0	0
			4	2	2		
20	D	1	Total	Fe	S	0	0
			4	2	2		

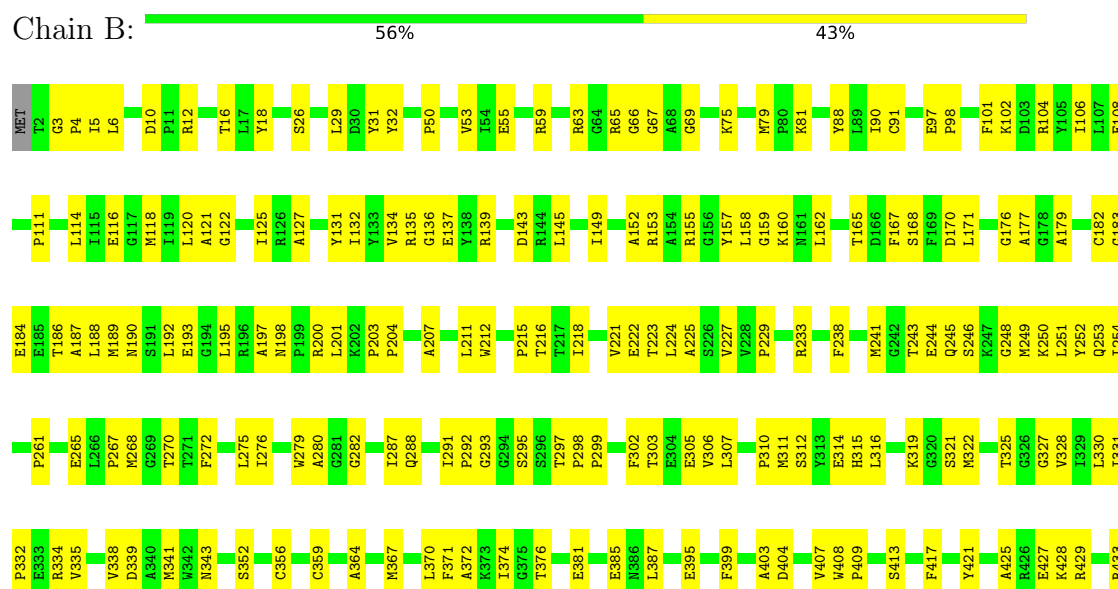
3 Residue-property plots

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



P434
W437
R438

• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2:  72% 26%

MET GLY F3 F4 D9 F10 L11 E12 E13 T14 F15 A16 K17 R24 A25 A26 P29 L30 L31 R32 R33 V34 Q35 R45 I49 V53 K77 Y78 H79 T85 L86 S87 C88 K89 G92 A93 E94 G107 P108 G109 E110 T112 G115 L116 F117 S118 V119 A131 E143 T146 R147 R148 R149 L154 K161 R162 E165 I166 K171 H177 E178 V179 E180 VAL

• Molecule 2: NADH-quinone oxidoreductase subunit 2

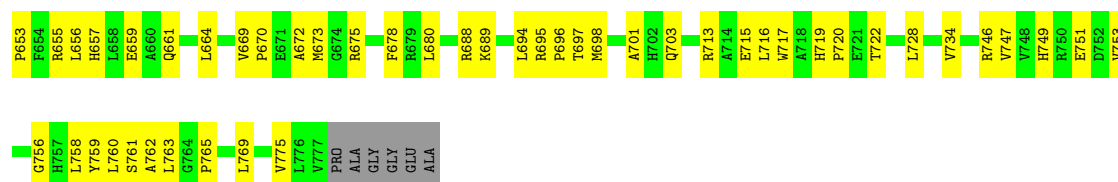
Chain C:  62% 36%

MET GLY F3 F4 D5 D6 K7 Q8 D9 L11 F10 L12 K17 R24 C24 I27 L31 R32 I41 E48 I49 A50 V53 G54 T55 M61 S65 P66 Q71 P74 T75 G76 H79 L80 Q81 V82 C83 A84 T85 L86 S87 K89 G92 E95 L96 W97 I106 G107 P108 G109 E110 V111 T112 F117 S118 V119 K120 Q121 V122 E123 C124 L125 H129 T130 A131 P132 Q135 V136 N137 Y141 G142 E143 C144 V145 T146 R149 L154 K161 R162 E165 I166 G173 V176 H177 E180 VAL

• Molecule 3: NADH-quinone oxidoreductase subunit 3

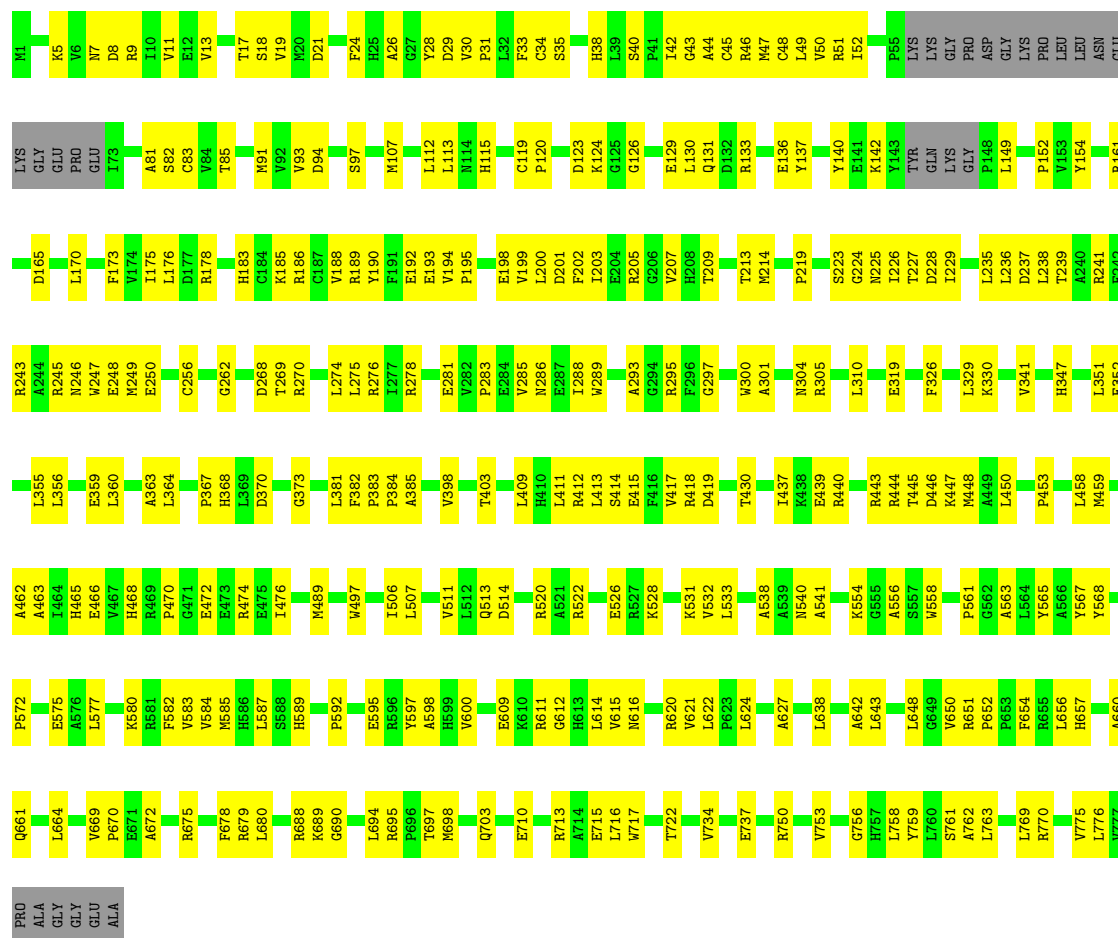
Chain 3:  58% 39%

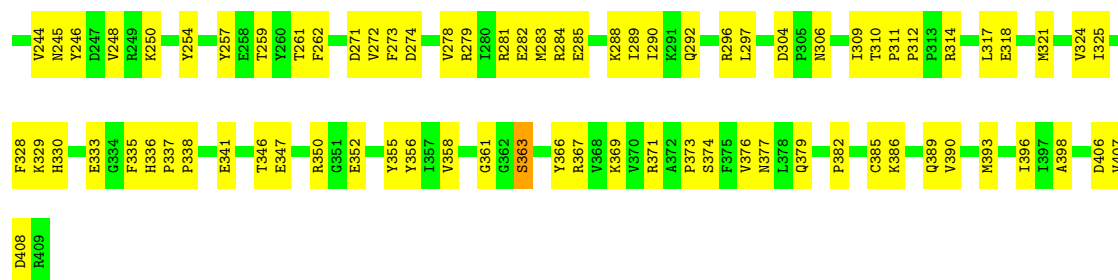
M1 V2 D8 R9 M20 A26 G27 Y28 D29 V30 P31 L32 F33 C34 S35 L39 G43 A44 C45 R46 M47 C48 V50 R51 P55 LYS LYS GLY PRO ASP GLY LYS PRO LEU LEU ASN GLY LYS GLY TYR GLN GLY P148 Y154 R161 R162 D165 K166 P169 L170 I175 T85 A86 D89 G90 M91 V92 V93 D94 T95 L96 S97 D98 R101 M107 L113 N114 H115 P116 L117 C119 G122 D123 A124 G125 C126 A127 C128 E129 L130 Q131 D132 R133 E136 Y137 Y143 GLN GLY P148 Y154 R161 R162 D165 K166 P169 L170 I175 T85 A86 E179 R180 K185 R186 R189 Y190 V194 P195 V199 L200 D201 F202 I203 E204 R205 P219 F222 S223 G224 N225 T226 T227 D228 L229 C230 P231 V232 G233 A234 L235 L236 D237 L238 T239 R241 F242 R243 A244 R245 N246 W247 E248 C256 C259 P260 V261 I265 T266 A267 D268 T269 S271 L274 L275 R278 A279 R280 E281 V285 N286 E287 I288 W289 I290 R295 F296 H298 F299 W300 A301 D302 R305 L306 K307 L317 L327 L337 K330 L343 Y344 H347 E352 L355 L356 A357 S358 E359 L360 A361 L364 P367 H368 L369 K460 A463 I464 H465 F363 P384 R468 P470 S386 G569 G570 E473 L476 L477 L478 A479 A576 K580 M489 V583 V584 M585 H586 L587 K501 N502 P503 L593 V504 L505 I506 L507 H599 A509 V511 L512 A521 R522 L523 R527 V615 M616 R620 V621 L622 P623 L624 A627 P628 I629 G632 E635 V640 A645 V650 S557 E466 Y467 R468 P470 S386 G569 G570 E473 L476 L477 L478 A479 A576 K580 M489 V583 V584 M585 H586 L587 K501 N502 P503 L593 V504 L505 I506 L507 H599 A509 V511 L512 A521 R522 L523 R527 V615 M616 R620 V621 L622 P623 L624 A627 P628 I629 G632 E635 V640 A645 V650 S557



• Molecule 3: NADH-quinone oxidoreductase subunit 3

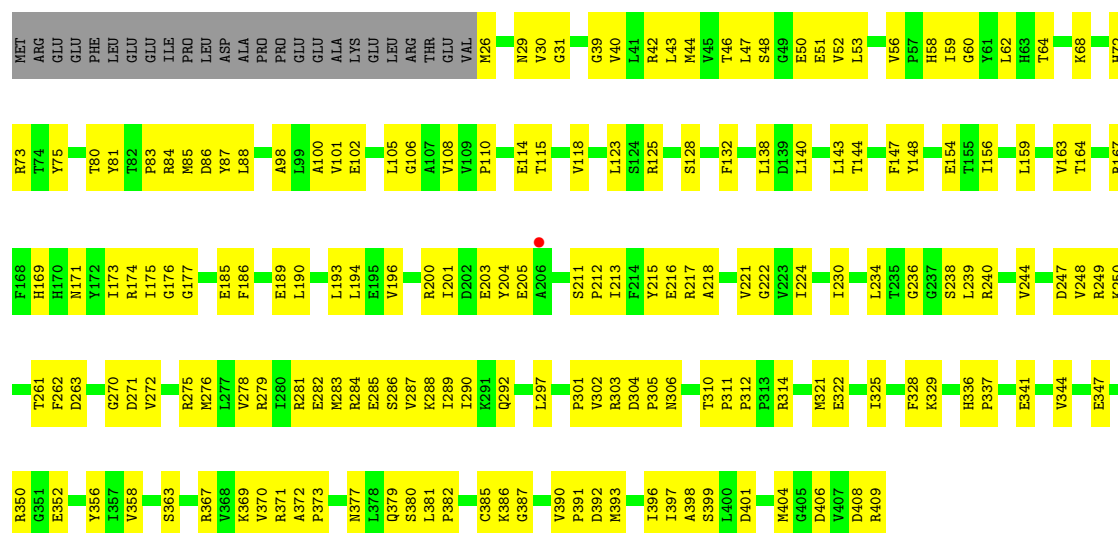
Chain D: 60% 37%





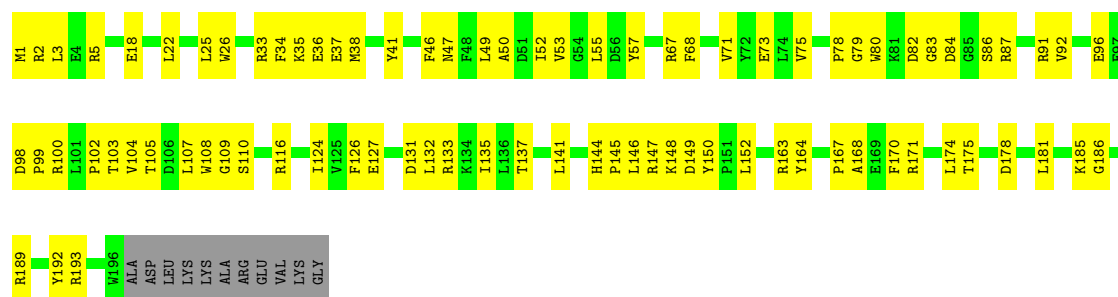
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E: 51% 43% 6%



• Molecule 5: NADH-quinone oxidoreductase subunit 5

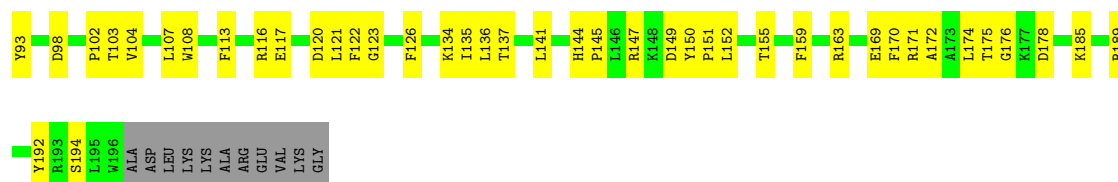
Chain 5: 55% 40% 5%



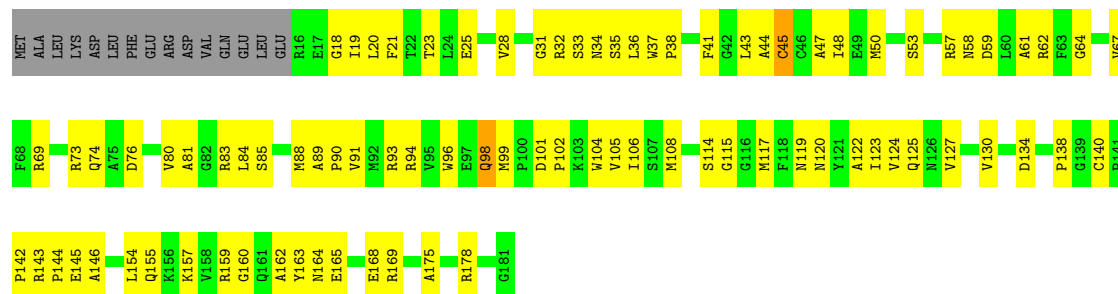
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F: 57% 38% 5%

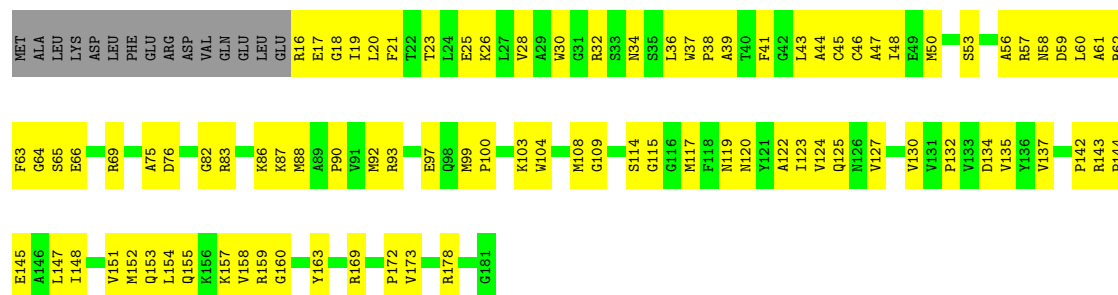




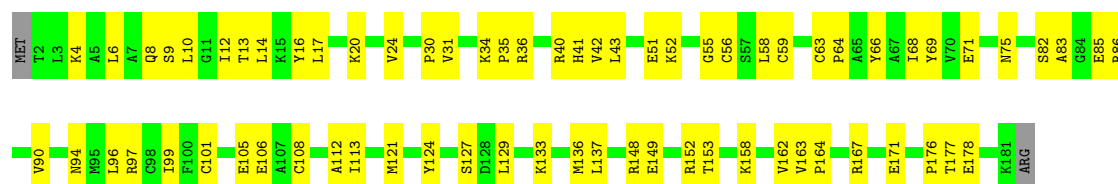
• Molecule 6: NADH-quinone oxidoreductase subunit 6



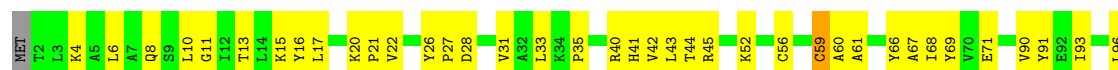
• Molecule 6: NADH-quinone oxidoreductase subunit 6



• Molecule 7: NADH-quinone oxidoreductase subunit 9



• Molecule 7: NADH-quinone oxidoreductase subunit 9

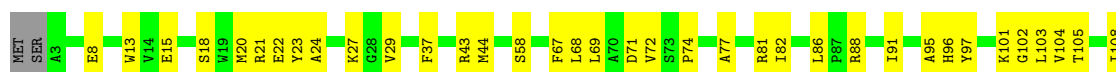




- Molecule 8: NADH-quinone oxidoreductase subunit 15



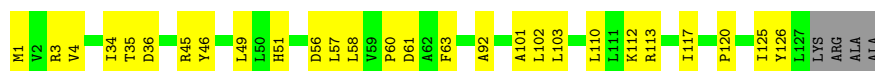
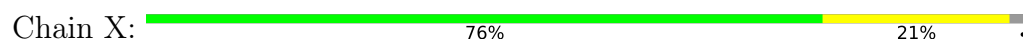
- Molecule 8: NADH-quinone oxidoreductase subunit 15



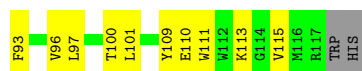
- Molecule 9: NADH-quinone oxidoreductase subunit 16



- Molecule 9: NADH-quinone oxidoreductase subunit 16



- Molecule 10: NADH-quinone oxidoreductase subunit 7



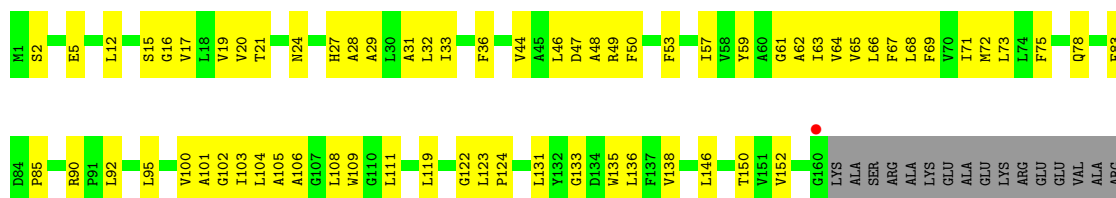
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:  61% 36% ..



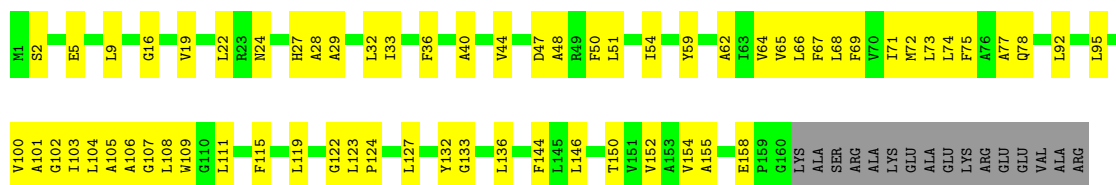
- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:  53% 38% 9%



- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:  55% 36% 9%



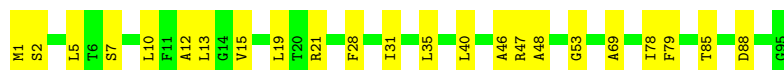
- Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:  69% 31%



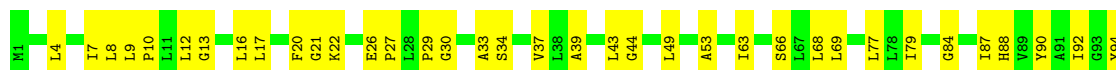
- Molecule 12: NADH-quinone oxidoreductase subunit 11

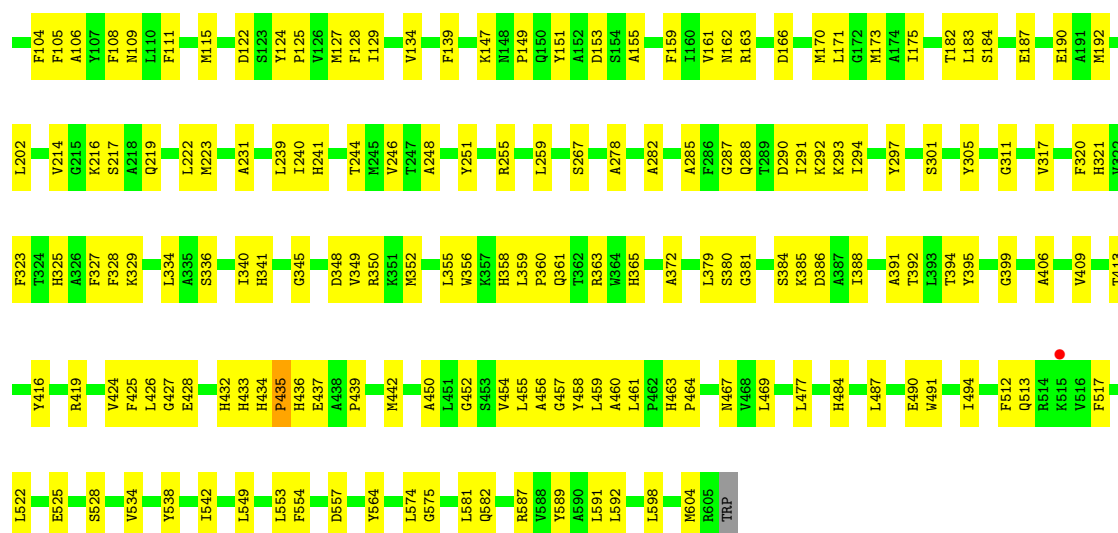
Chain S:  76% 24%



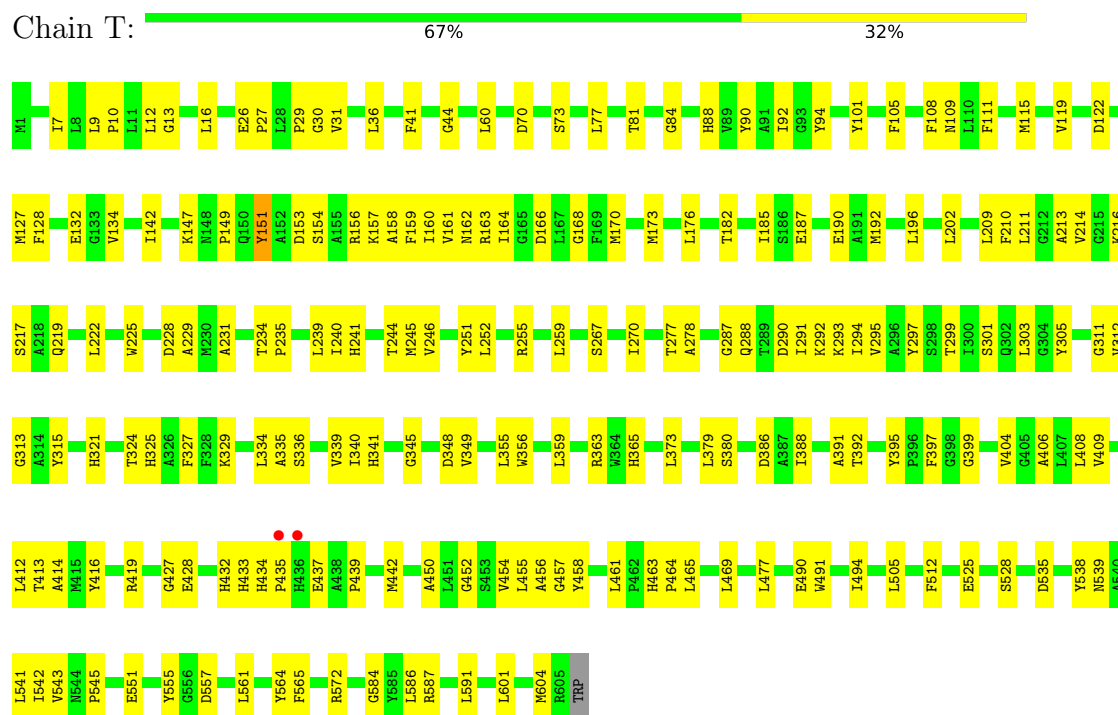
- Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:  66% 33%

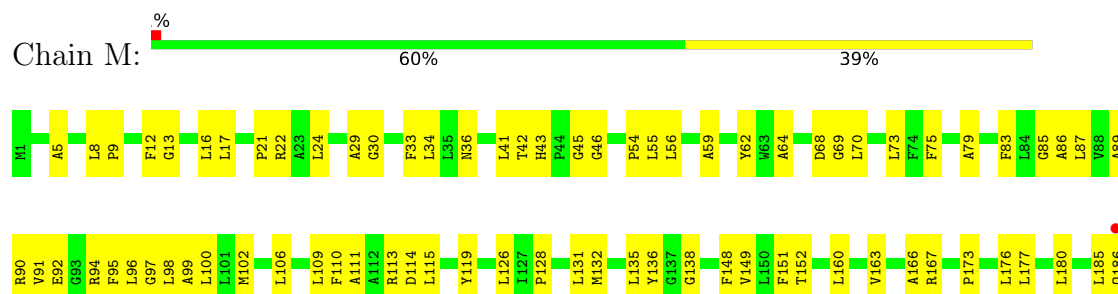




• Molecule 13: NADH-quinone oxidoreductase subunit 12

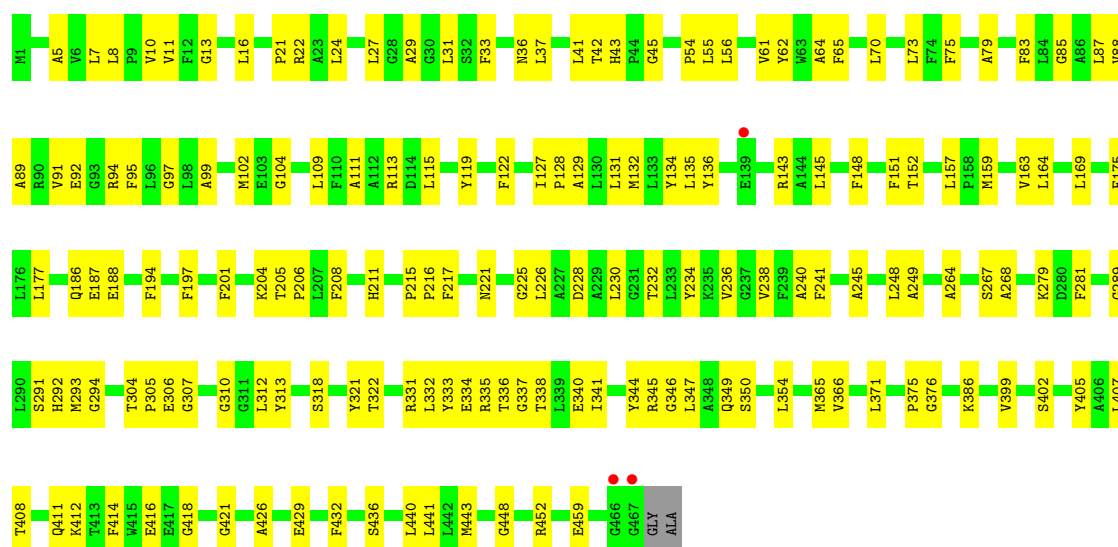


• Molecule 14: NADH-quinone oxidoreductase subunit 13

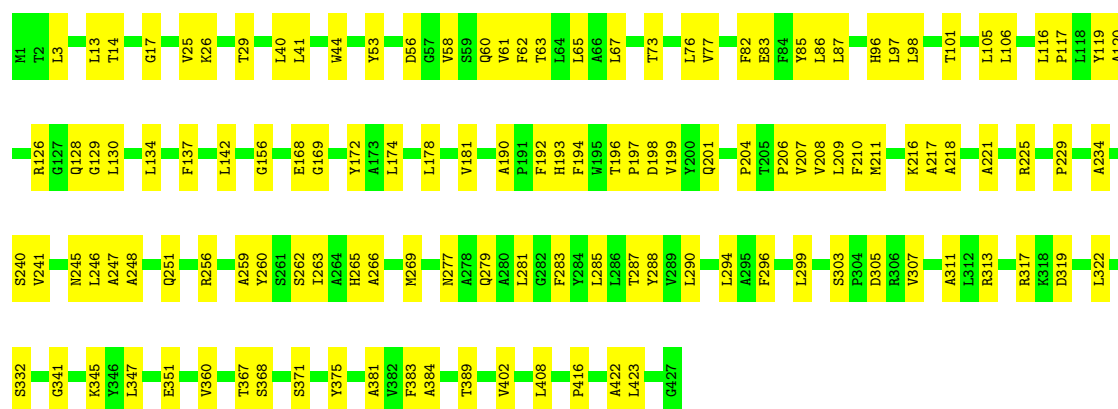




• Molecule 14: NADH-quinone oxidoreductase subunit 13

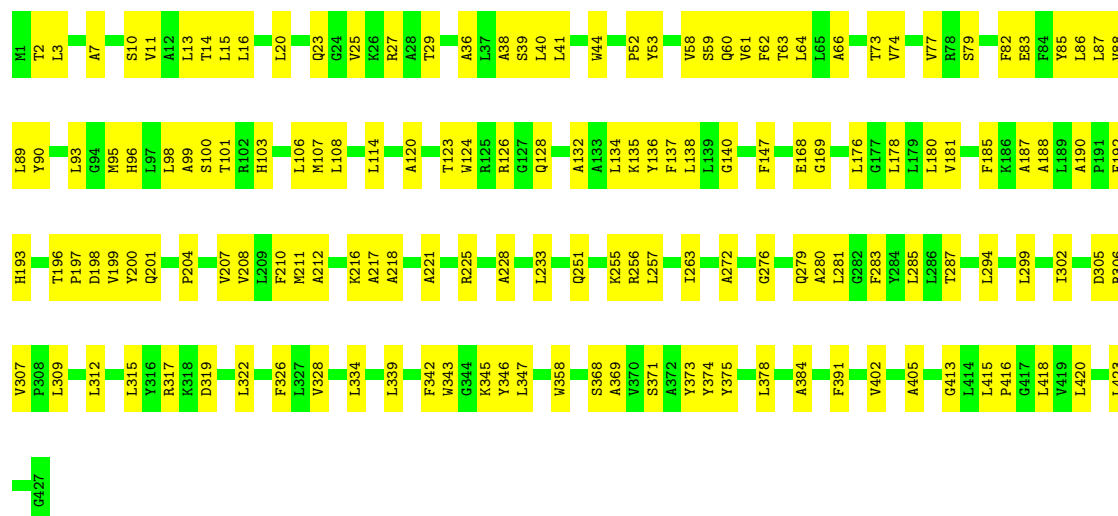


• Molecule 15: NADH-quinone oxidoreductase subunit 14

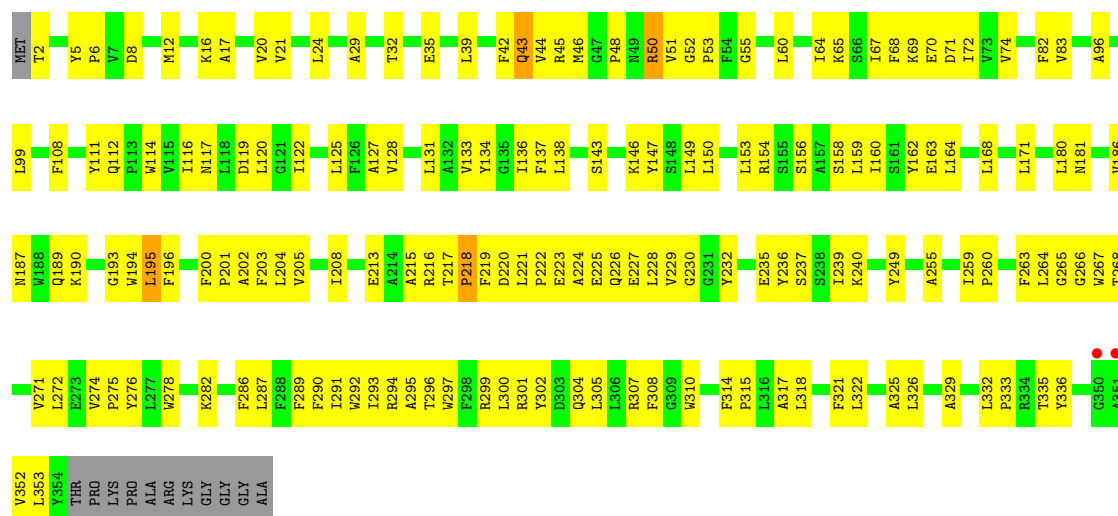


• Molecule 15: NADH-quinone oxidoreductase subunit 14

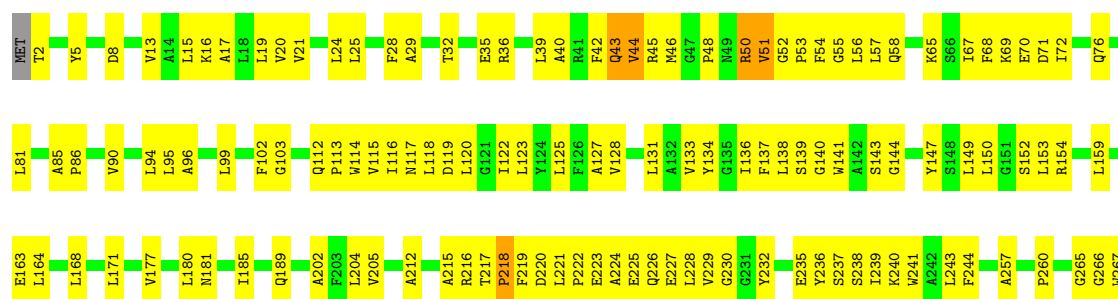


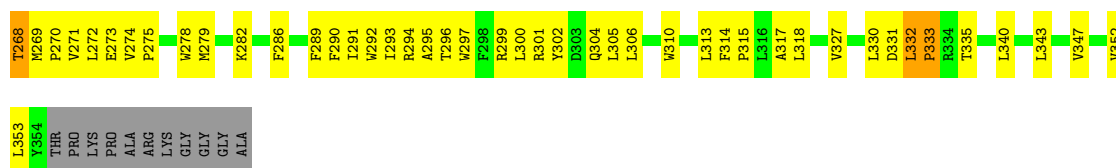


• Molecule 16: NADH-quinone oxidoreductase subunit 8



• Molecule 16: NADH-quinone oxidoreductase subunit 8





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.11Å 341.45Å 263.89Å 90.00° 100.52° 90.00°	Depositor
Resolution (Å)	58.71 – 3.21 58.71 – 3.21	Depositor EDS
% Data completeness (in resolution range)	76.1 (58.71-3.21) 76.1 (58.71-3.21)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13rc1_2961: ???)	Depositor
R, R_{free}	0.210 , 0.231 0.214 , 0.223	Depositor DCC
R_{free} test set	2117 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 3.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.357 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.470 for -H,-K,H+L	Depositor
Outliers	0 of 207039 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	74174	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 2.75% 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: SF4, FMN, FES, NAI

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	0.24	0/3506	0.46	0/4745
1	B	0.21	0/3506	0.42	0/4745
2	2	0.26	0/1439	0.47	0/1953
2	C	0.24	0/1439	0.47	0/1953
3	3	0.45	0/6035	0.71	0/8185
3	D	0.33	0/6035	0.56	0/8185
4	4	0.37	0/3150	0.60	0/4284
4	E	0.28	0/3150	0.49	0/4284
5	5	0.38	0/1656	0.64	0/2246
5	F	0.29	0/1656	0.51	0/2246
6	6	0.39	0/1319	0.64	0/1786
6	G	0.37	0/1319	0.62	0/1786
7	9	0.40	0/1423	0.63	0/1933
7	O	0.38	0/1423	0.62	1/1933 (0.1%)
8	7	0.26	0/1059	0.51	0/1429
8	I	0.31	0/1059	0.53	0/1429
9	W	0.38	0/985	0.59	0/1335
9	X	0.29	0/985	0.51	0/1335
10	A	0.27	0/940	0.49	0/1280
10	P	0.28	0/940	0.52	0/1280
11	J	0.25	0/1206	0.44	0/1649
11	R	0.27	0/1206	0.50	0/1649
12	K	0.26	0/710	0.49	0/962
12	S	0.25	0/710	0.47	0/962
13	L	0.22	0/4741	0.43	0/6460
13	T	0.22	0/4741	0.46	2/6460 (0.0%)
14	M	0.23	0/3591	0.43	0/4896
14	U	0.25	0/3591	0.48	0/4896
15	N	0.24	0/3238	0.43	0/4434
15	V	0.28	0/3238	0.49	0/4434
16	H	0.28	0/2935	0.56	0/4014
16	Q	0.30	0/2935	0.58	0/4014

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.30	0/75866	0.53	3/103182 (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	2
10	P	0	1
16	H	0	3
16	Q	0	3
All	All	0	10

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	149	PRO	N-CA-C	6.82	122.86	113.65
13	T	151	TYR	N-CA-CB	6.66	121.08	110.22
7	O	59	CYS	CA-CB-SG	5.86	127.88	114.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	20	LYS	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
16	H	43	GLN	Peptide
7	O	20	LYS	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	3389	117	0
1	B	3417	0	3388	154	0
2	2	1406	0	1373	37	0
2	C	1406	0	1373	73	0
3	3	5895	0	5930	237	0
3	D	5895	0	5930	222	0
4	4	3067	0	3049	175	0
4	E	3067	0	3049	166	0
5	5	1607	0	1574	79	0
5	F	1607	0	1574	78	0
6	6	1289	0	1298	89	0
6	G	1289	0	1298	104	0
7	9	1388	0	1383	75	0
7	O	1388	0	1383	69	0
8	7	1031	0	1029	34	0
8	I	1031	0	1029	35	0
9	W	967	0	1010	35	0
9	X	967	0	1010	23	0
10	A	910	0	939	54	0
10	P	910	0	939	55	0
11	J	1183	0	1286	65	0
11	R	1183	0	1286	57	0
12	K	703	0	747	30	0
12	S	703	0	747	18	0
13	L	4604	0	4734	172	0
13	T	4604	0	4734	142	0
14	M	3489	0	3606	136	0
14	U	3489	0	3606	126	0
15	N	3154	0	3343	103	0
15	V	3154	0	3343	114	0
16	H	2838	0	2903	159	0
16	Q	2838	0	2903	180	0
17	1	8	0	0	3	0
17	3	24	0	0	2	0
17	6	8	0	0	0	0
17	9	16	0	0	6	0
17	B	8	0	0	1	0
17	D	24	0	0	1	0
17	G	8	0	0	2	0
17	O	16	0	0	3	0
18	1	31	0	19	7	0
18	B	31	0	19	2	0
19	1	44	0	27	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	44	0	27	4	0
20	2	4	0	0	1	0
20	3	4	0	0	0	0
20	C	4	0	0	2	0
20	D	4	0	0	2	0
All	All	74174	0	75277	2797	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 19.

The worst 5 of 2797 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)
4:4:190:LEU:O	4:4:194:LEU:HD13	1.54	1.05
7:9:133:LYS:O	7:9:137:LEU:HD13	1.57	1.04
3:D:286:ASN:ND2	3:D:289:TRP:O	1.96	0.98
4:E:47:LEU:HD13	4:E:51:GLU:O	1.62	0.97
3:3:42:ILE:HD12	3:3:42:ILE:O	1.65	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%)	403 (93%)	32 (7%)	0	100	100
1	B	435/438 (99%)	404 (93%)	31 (7%)	0	100	100
2	2	176/181 (97%)	168 (96%)	8 (4%)	0	100	100
2	C	176/181 (97%)	168 (96%)	8 (4%)	0	100	100
3	3	750/783 (96%)	696 (93%)	54 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	750/783 (96%)	703 (94%)	47 (6%)	0	100	100
4	4	382/409 (93%)	359 (94%)	23 (6%)	0	100	100
4	E	382/409 (93%)	360 (94%)	22 (6%)	0	100	100
5	5	194/207 (94%)	185 (95%)	9 (5%)	0	100	100
5	F	194/207 (94%)	187 (96%)	7 (4%)	0	100	100
6	6	164/181 (91%)	147 (90%)	16 (10%)	1 (1%)	21	56
6	G	164/181 (91%)	145 (88%)	19 (12%)	0	100	100
7	9	178/182 (98%)	172 (97%)	6 (3%)	0	100	100
7	O	178/182 (98%)	171 (96%)	7 (4%)	0	100	100
8	7	125/129 (97%)	116 (93%)	9 (7%)	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%)	121 (97%)	4 (3%)	0	100	100
10	A	115/119 (97%)	106 (92%)	9 (8%)	0	100	100
10	P	115/119 (97%)	106 (92%)	9 (8%)	0	100	100
11	J	158/176 (90%)	147 (93%)	11 (7%)	0	100	100
11	R	158/176 (90%)	146 (92%)	12 (8%)	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%)	569 (94%)	33 (6%)	1 (0%)	43	73
13	T	603/606 (100%)	569 (94%)	33 (6%)	1 (0%)	43	73
14	M	465/469 (99%)	437 (94%)	28 (6%)	0	100	100
14	U	465/469 (99%)	437 (94%)	28 (6%)	0	100	100
15	N	425/427 (100%)	400 (94%)	25 (6%)	0	100	100
15	V	425/427 (100%)	404 (95%)	21 (5%)	0	100	100
16	H	351/365 (96%)	303 (86%)	42 (12%)	6 (2%)	7	35
16	Q	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	6	31
All	All	9478/9796 (97%)	8845 (93%)	617 (6%)	16 (0%)	43	73

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL

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Mol	Chain	Res	Type
16	Q	51	VAL
16	H	50	ARG
16	H	218	PRO
16	H	44	VAL

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%)	355 (100%)	0	100	100
1	B	355/356 (100%)	355 (100%)	0	100	100
2	2	150/152 (99%)	150 (100%)	0	100	100
2	C	150/152 (99%)	150 (100%)	0	100	100
3	3	609/628 (97%)	609 (100%)	0	100	100
3	D	609/628 (97%)	609 (100%)	0	100	100
4	4	332/355 (94%)	331 (100%)	1 (0%)	86	88
4	E	332/355 (94%)	332 (100%)	0	100	100
5	5	167/175 (95%)	167 (100%)	0	100	100
5	F	167/175 (95%)	167 (100%)	0	100	100
6	6	135/149 (91%)	134 (99%)	1 (1%)	76	83
6	G	135/149 (91%)	135 (100%)	0	100	100
7	9	148/150 (99%)	148 (100%)	0	100	100
7	O	148/150 (99%)	148 (100%)	0	100	100
8	7	104/106 (98%)	104 (100%)	0	100	100
8	I	104/106 (98%)	104 (100%)	0	100	100
9	W	99/101 (98%)	99 (100%)	0	100	100
9	X	99/101 (98%)	99 (100%)	0	100	100
10	A	90/92 (98%)	90 (100%)	0	100	100
10	P	90/92 (98%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	118/130 (91%)	118 (100%)	0	100	100
11	R	118/130 (91%)	118 (100%)	0	100	100
12	K	71/71 (100%)	71 (100%)	0	100	100
12	S	71/71 (100%)	71 (100%)	0	100	100
13	L	453/454 (100%)	453 (100%)	0	100	100
13	T	453/454 (100%)	453 (100%)	0	100	100
14	M	332/332 (100%)	332 (100%)	0	100	100
14	U	332/332 (100%)	332 (100%)	0	100	100
15	N	302/302 (100%)	302 (100%)	0	100	100
15	V	302/302 (100%)	302 (100%)	0	100	100
16	H	293/300 (98%)	293 (100%)	0	100	100
16	Q	293/300 (98%)	293 (100%)	0	100	100
All	All	7516/7706 (98%)	7514 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	363	SER
6	6	98	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	29	ASN
13	T	325	HIS
4	E	292	GLN
9	X	43	GLN
14	U	218	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	501	1	0,12,12	-	-	-		
20	FES	2	201	2	0,4,4	-	-	-		
20	FES	C	201	2	0,4,4	-	-	-		
20	FES	D	804	3	0,4,4	-	-	-		
17	SF4	G	201	6	0,12,12	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
19	NAI	1	503	-	47,48,48	0.34	0	64,73,73	0.53	0
17	SF4	6	201	6	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
19	NAI	B	503	-	47,48,48	0.40	0	64,73,73	0.51	1 (1%)
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
18	FMN	1	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.30	9 (18%)
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.26	8 (16%)
20	FES	3	804	3	0,4,4	-	-	-		
17	SF4	D	801	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
17	SF4	B	501	1	-	-	0/6/5/5
20	FES	2	201	2	-	-	0/1/1/1
20	FES	C	201	2	-	-	0/1/1/1
20	FES	D	804	3	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
19	NAI	1	503	-	-	11/29/72/72	0/5/5/5
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
19	NAI	B	503	-	-	9/29/72/72	0/5/5/5
17	SF4	9	201	7	-	-	0/6/5/5
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
20	FES	3	804	3	-	-	0/1/1/1
17	SF4	D	801	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	3.45	1.38	1.30
18	1	502	FMN	C4A-N5	3.32	1.37	1.30
18	B	502	FMN	C10-N1	2.72	1.38	1.33
18	1	502	FMN	C10-N1	2.33	1.37	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	502	FMN	C4-N3-C2	-3.17	120.02	125.64
18	1	502	FMN	C4-N3-C2	-2.99	120.32	125.64
18	B	502	FMN	O4-C4-C4A	-2.89	118.92	126.53
18	B	502	FMN	C4A-C4-N3	2.76	120.27	113.25
18	1	502	FMN	C5A-C9A-N10	2.61	120.33	117.97

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

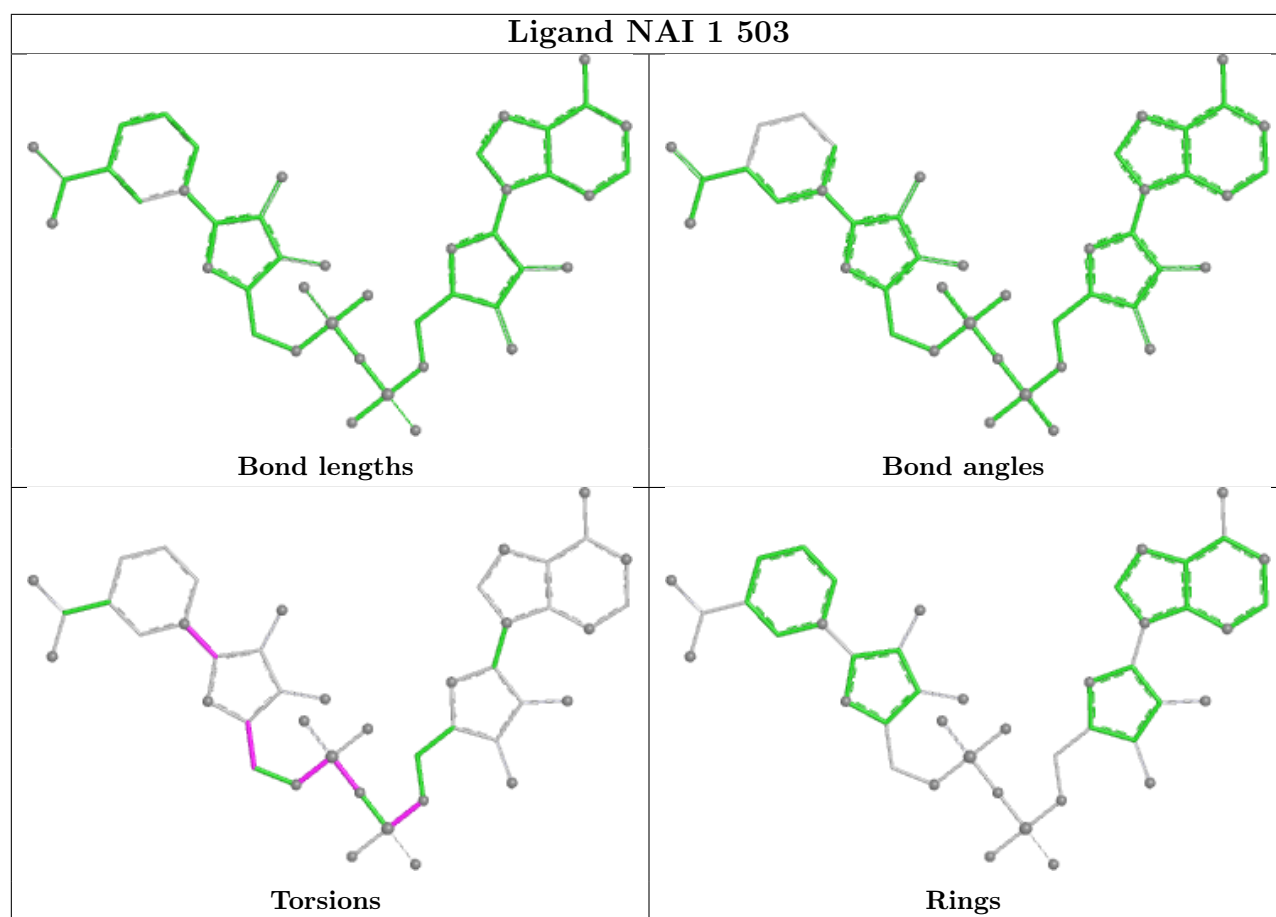
Mol	Chain	Res	Type	Atoms
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	N10-C1'-C2'-C3'
18	1	502	FMN	C1'-C2'-C3'-O3'
18	1	502	FMN	C1'-C2'-C3'-C4'
18	1	502	FMN	O2'-C2'-C3'-O3'

There are no ring outliers.

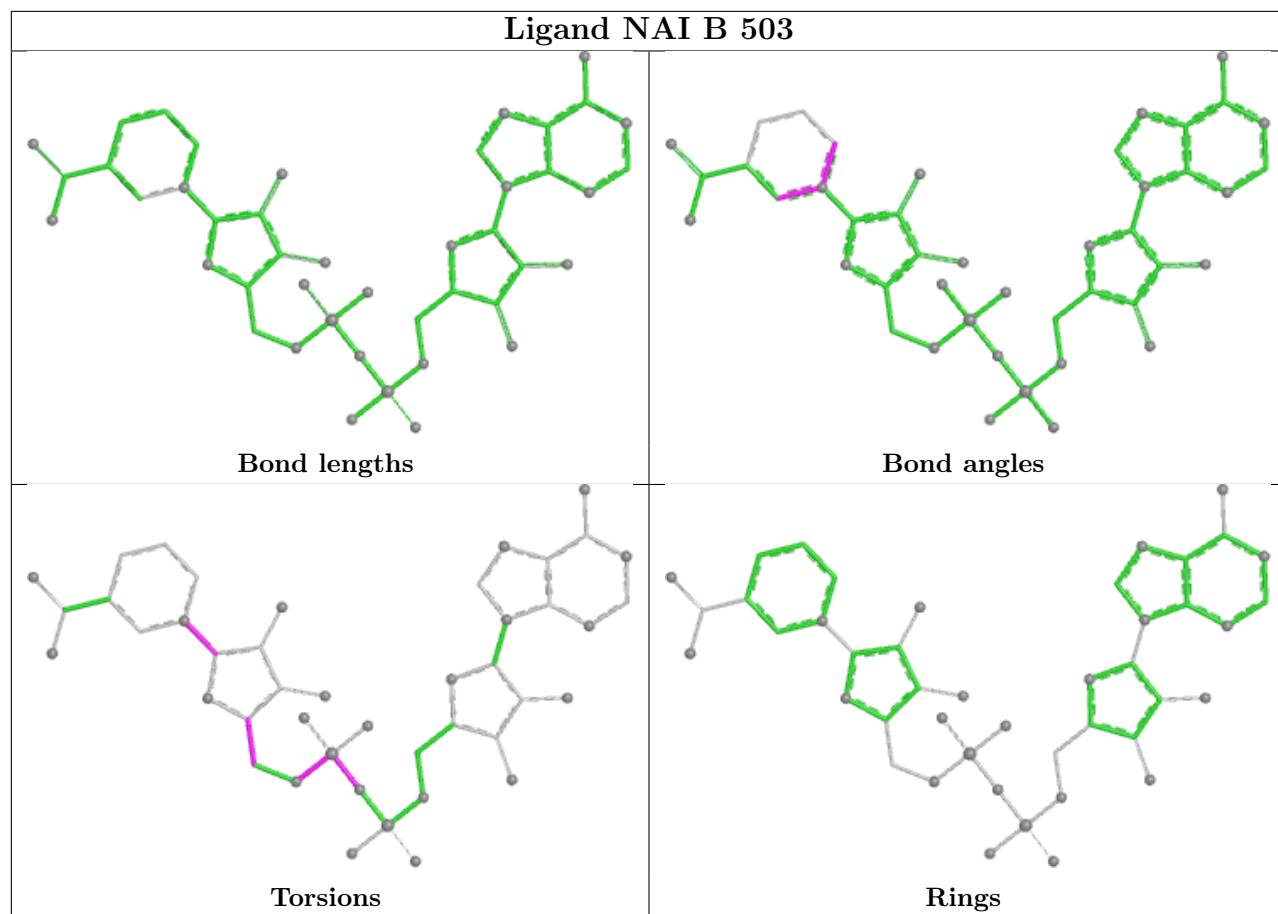
16 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	501	SF4	1	0
20	2	201	FES	1	0
20	C	201	FES	2	0
20	D	804	FES	2	0
17	G	201	SF4	2	0
19	1	503	NAI	3	0
17	3	803	SF4	2	0
17	9	202	SF4	2	0
17	9	201	SF4	4	0
19	B	503	NAI	4	0
17	O	202	SF4	2	0
17	O	201	SF4	1	0
18	1	502	FMN	7	0
17	1	501	SF4	3	0
18	B	502	FMN	2	0
17	D	801	SF4	1	0

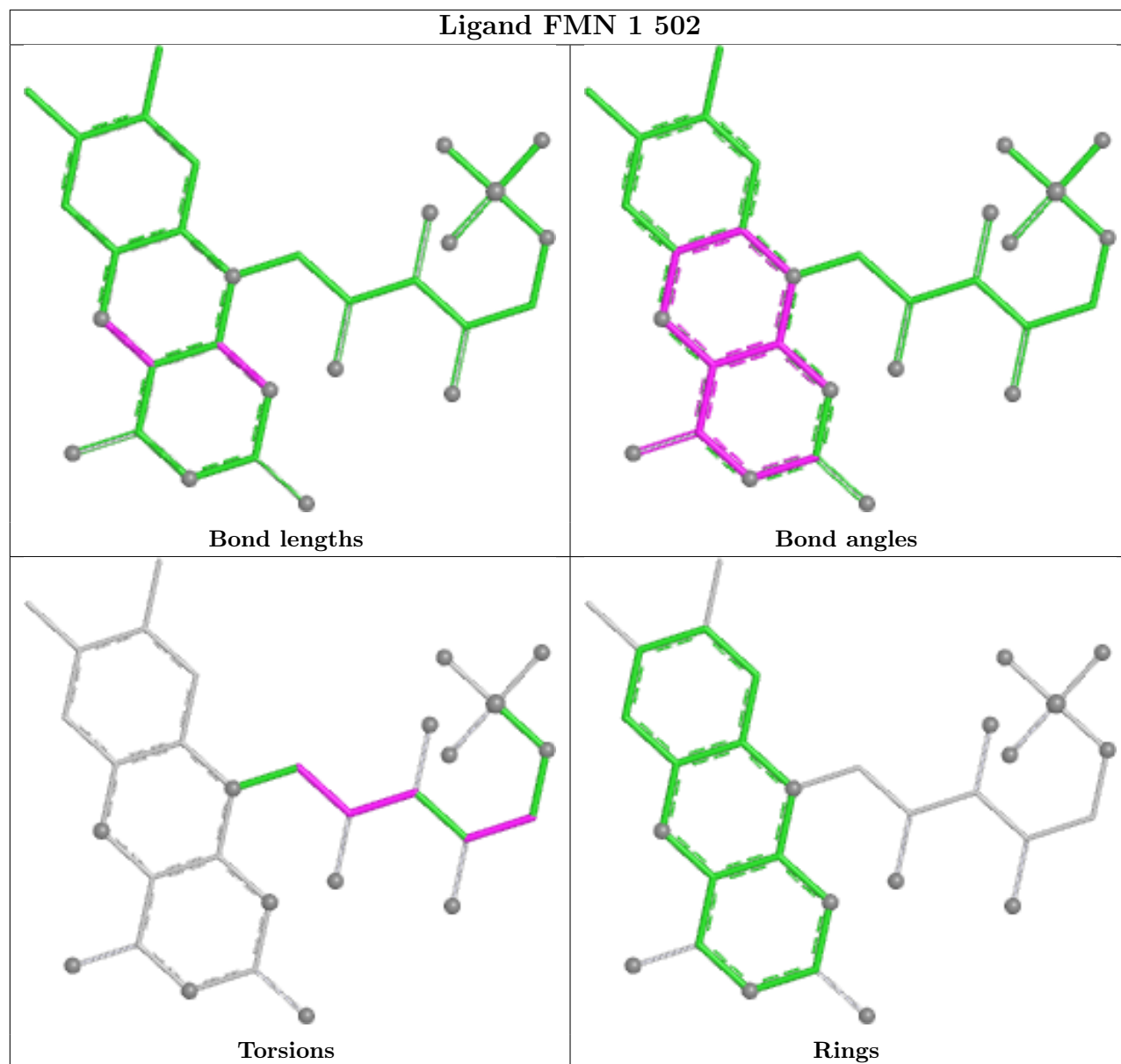
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

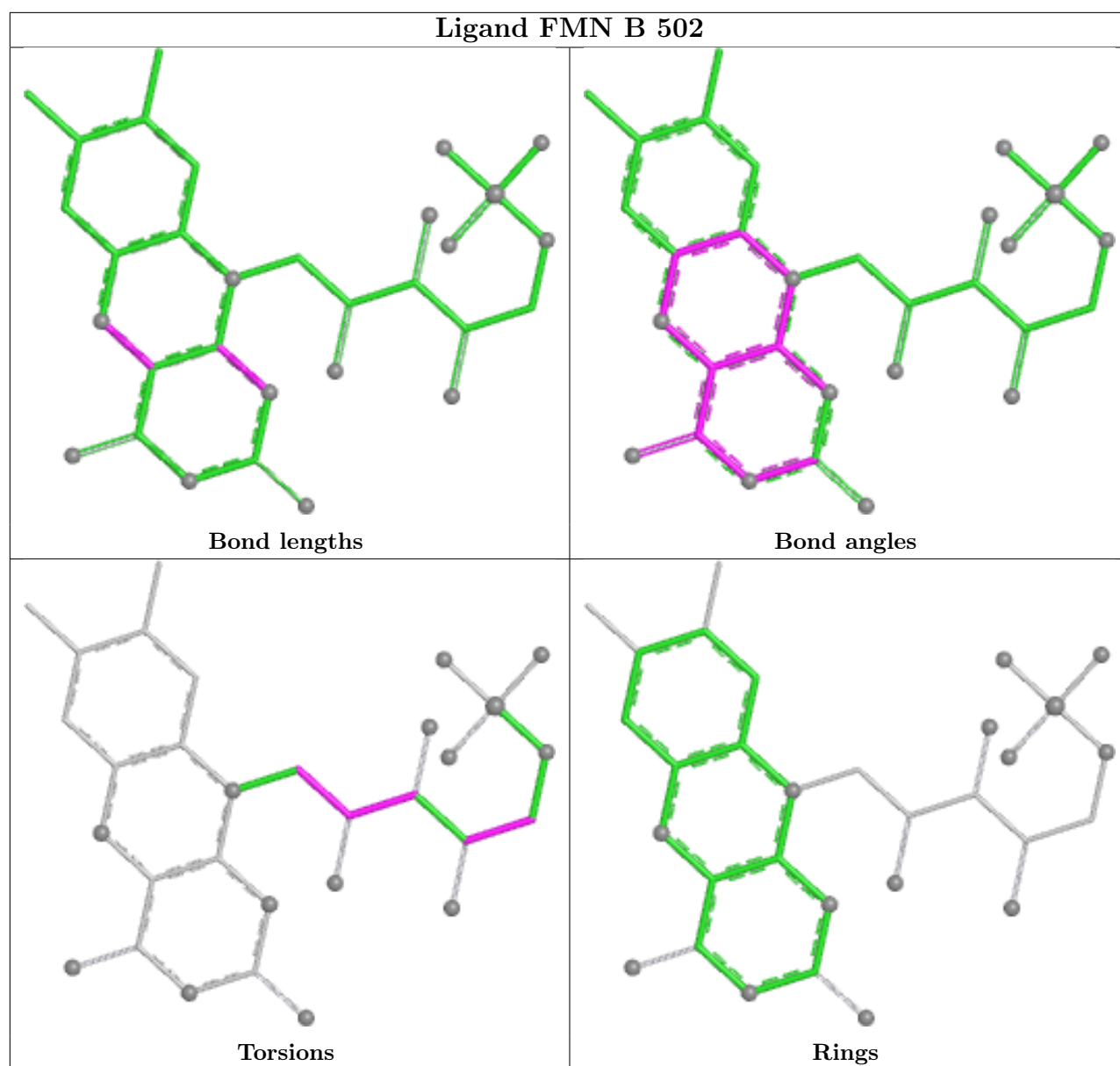


Ligand NAI B 503



Ligand FMN 1 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	437/438 (99%)	-1.31	4 (0%) 81 64	27, 82, 137, 228	0
1	B	437/438 (99%)	-1.31	0 100 100	46, 105, 150, 215	0
2	2	178/181 (98%)	-1.39	0 100 100	15, 74, 130, 148	0
2	C	178/181 (98%)	-1.55	0 100 100	23, 90, 131, 157	0
3	3	756/783 (96%)	-1.54	0 100 100	9, 32, 72, 170	0
3	D	756/783 (96%)	-1.40	0 100 100	12, 53, 98, 200	0
4	4	384/409 (93%)	-1.43	0 100 100	25, 54, 100, 141	0
4	E	384/409 (93%)	-1.25	1 (0%) 90 81	20, 81, 120, 171	0
5	5	196/207 (94%)	-1.44	0 100 100	9, 46, 126, 197	0
5	F	196/207 (94%)	-1.43	0 100 100	19, 63, 111, 174	0
6	6	166/181 (91%)	-1.40	0 100 100	21, 45, 133, 178	0
6	G	166/181 (91%)	-1.34	0 100 100	14, 55, 155, 212	0
7	9	180/182 (98%)	-1.50	0 100 100	13, 41, 86, 103	0
7	O	180/182 (98%)	-1.40	0 100 100	9, 55, 106, 142	0
8	7	127/129 (98%)	-1.47	0 100 100	31, 77, 107, 121	0
8	I	127/129 (98%)	-1.33	0 100 100	23, 59, 102, 110	0
9	W	127/131 (96%)	-1.58	0 100 100	7, 48, 99, 185	0
9	X	127/131 (96%)	-1.51	0 100 100	11, 61, 160, 217	0
10	A	117/119 (98%)	-1.21	0 100 100	38, 75, 174, 218	0
10	P	117/119 (98%)	-1.18	0 100 100	24, 70, 174, 217	0
11	J	160/176 (90%)	-1.48	1 (0%) 85 73	30, 68, 126, 140	0
11	R	160/176 (90%)	-1.35	0 100 100	16, 70, 122, 161	0
12	K	95/95 (100%)	-1.44	0 100 100	32, 67, 126, 138	0
12	S	95/95 (100%)	-1.53	0 100 100	32, 68, 106, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	L	605/606 (99%)	-1.26	1 (0%) 91 85	28, 96, 148, 297	0
13	T	605/606 (99%)	-1.31	2 (0%) 90 81	46, 91, 154, 291	0
14	M	467/469 (99%)	-1.30	3 (0%) 85 73	44, 86, 130, 149	0
14	U	467/469 (99%)	-1.37	3 (0%) 85 73	20, 73, 116, 137	0
15	N	427/427 (100%)	-1.43	0 100 100	27, 76, 120, 184	0
15	V	427/427 (100%)	-1.43	0 100 100	22, 65, 111, 179	0
16	H	353/365 (96%)	-1.22	2 (0%) 85 73	20, 79, 123, 178	0
16	Q	353/365 (96%)	-1.37	0 100 100	19, 71, 114, 205	0
All	All	9550/9796 (97%)	-1.38	17 (0%) 91 85	7, 71, 132, 297	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	U	467	GLY	5.5
14	M	467	GLY	5.4
16	H	350	GLY	4.3
1	1	5	ILE	3.6
1	1	7	SER	3.5

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
19	NAI	1	503	44/44	0.99	0.04	34,88,93,93	0
19	NAI	B	503	44/44	0.99	0.03	30,64,73,80	0

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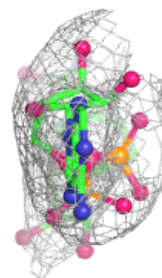
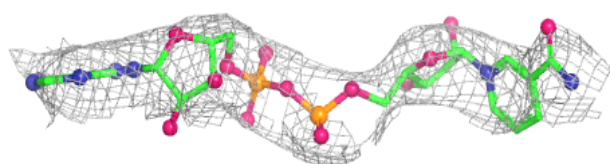
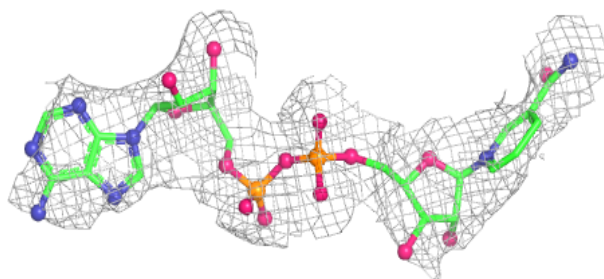
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	SF4	3	802	8/8	1.00	0.02	31,31,31,31	0
17	SF4	3	803	8/8	1.00	0.01	15,15,15,15	0
17	SF4	6	201	8/8	1.00	0.01	31,31,31,31	0
17	SF4	9	201	8/8	1.00	0.02	17,17,17,17	0
17	SF4	9	202	8/8	1.00	0.03	19,19,19,19	0
17	SF4	B	501	8/8	1.00	0.02	47,47,47,47	0
17	SF4	D	801	8/8	1.00	0.02	24,24,24,24	0
17	SF4	D	802	8/8	1.00	0.02	31,31,31,31	0
17	SF4	D	803	8/8	1.00	0.02	15,15,15,15	0
17	SF4	G	201	8/8	1.00	0.02	32,32,32,32	0
17	SF4	O	201	8/8	1.00	0.02	18,18,18,18	0
17	SF4	O	202	8/8	1.00	0.03	20,20,20,20	0
18	FMN	1	502	31/31	1.00	0.03	10,47,106,108	0
18	FMN	B	502	31/31	1.00	0.02	99,107,114,118	0
17	SF4	1	501	8/8	1.00	0.01	46,46,46,46	0
17	SF4	3	801	8/8	1.00	0.01	23,23,23,23	0
20	FES	2	201	4/4	1.00	0.01	46,46,46,46	0
20	FES	3	804	4/4	1.00	0.01	31,31,31,31	0
20	FES	C	201	4/4	1.00	0.01	47,47,47,47	0
20	FES	D	804	4/4	1.00	0.01	31,31,31,31	0

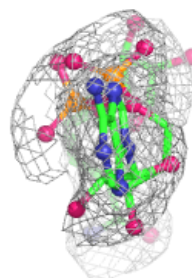
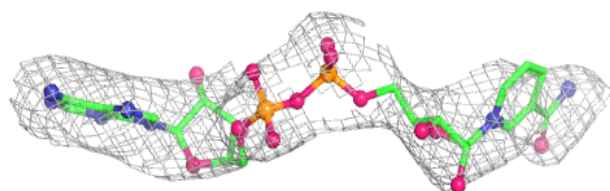
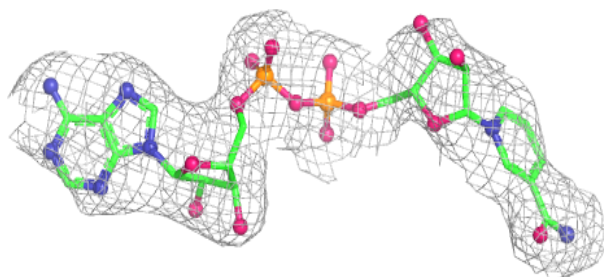
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI 1 503:

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

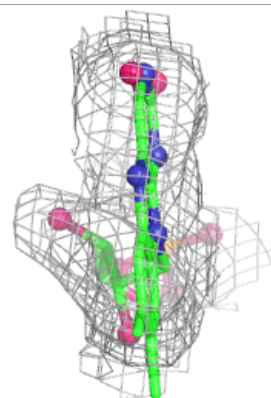
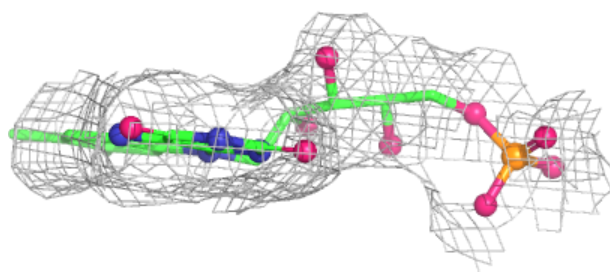
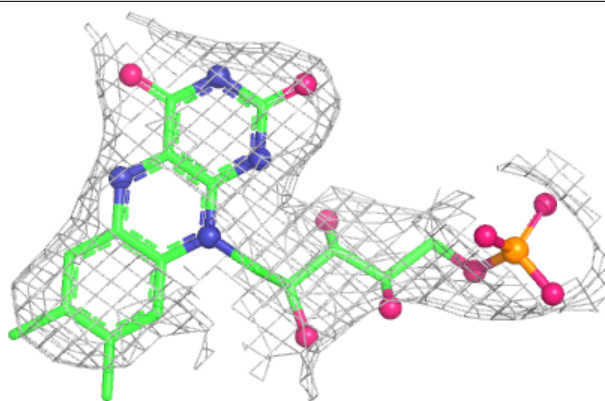
**Electron density around NAI B 503:**

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

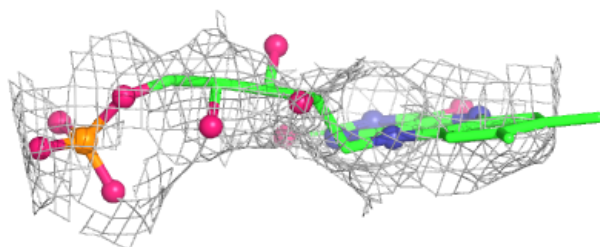
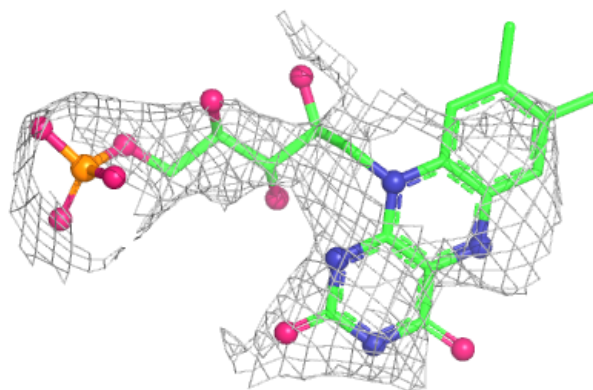


Electron density around FMN 1 502:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.