wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 05:15 PM EDT

PDB ID	:	6Q8W
Title	:	Respiratory complex I from Thermus thermophilus with bound Aureothin.
Authors	:	Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.
Deposited on	:	2018-12-16
Resolution	:	3.40 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

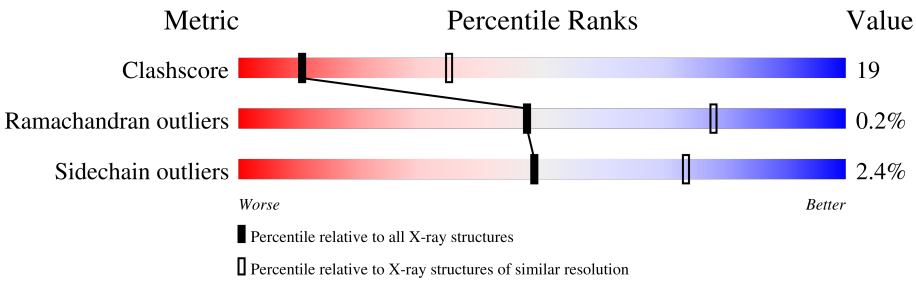
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	64% 34% •
1	B	438	57% 41% •
2	2	181	66% 30% • •
2	C	181	62% 34% • •
3	3	783	59% 37% • •
3	D	783	62% 34% • •
4	4	409	51% 43% 6%
4	E	409	50% 42% • 6%

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Mol	Chain	Length	Quality of chain
5	5	207	57% 36% 5%
5	F	207	60% 33% 5%
6	6	181	35% 54% 8%
6	G	181	44% 45% 8%
7	9	182	61% 37%
7	O	182	60% 38%
8	7	129	71% 27%
8	I	129	70% 28%
9	W	131	68% 28%
9	X	131	76% 20%
10	A	119	51% 45%
10	P	119	55% 40%
11	J	176	53% 37% 9%
11	R	176	55% 35% 9%
12	K	95	64% 34%
12	S	95	69% 29%
13	L	606	66% 33%
13	T	606	66% 33%
14	M	469	65% 34%
14	U	469	64% 35%
15	N	427	67% 32%
15	V	427	69% 30%
16	H	365	50% 43%
16	Q	365	50% 43%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	1	501	-	-	X	-
17	SF4	B	501	-	-	X	-
19	FES	3	804	-	-	X	-
19	FES	C	201	-	-	X	-
19	FES	D	804	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 74144 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
			Total	C	N	O	S			
5	5	196	1607	1043	273	288	3	0	0	0
5	F	196	1607	1043	273	288	3	0	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	6	166	1289	815	235	226	13	0	0	0
6	G	166	1289	815	235	226	13	0	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	9	180	1388	890	232	255	11	0	0	0
7	O	180	1388	890	232	255	11	0	0	0

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	7	127	1031	664	183	181	3	0	0	0
8	I	127	1031	664	183	181	3	0	0	0

- Molecule 9 is a protein called Uncharacterized protein.

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

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

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

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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

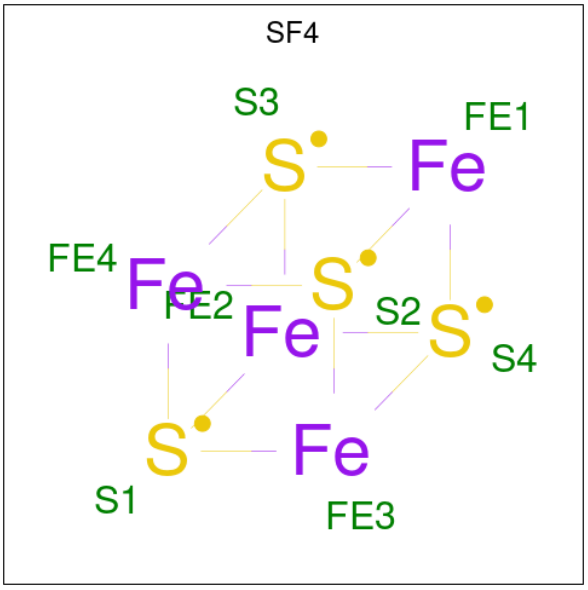
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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	2838	1943	431	457	7	0	0	0
			Total	C	N	O	S			
16	Q	353	2838	1943	431	457	7	0	0	0

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



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

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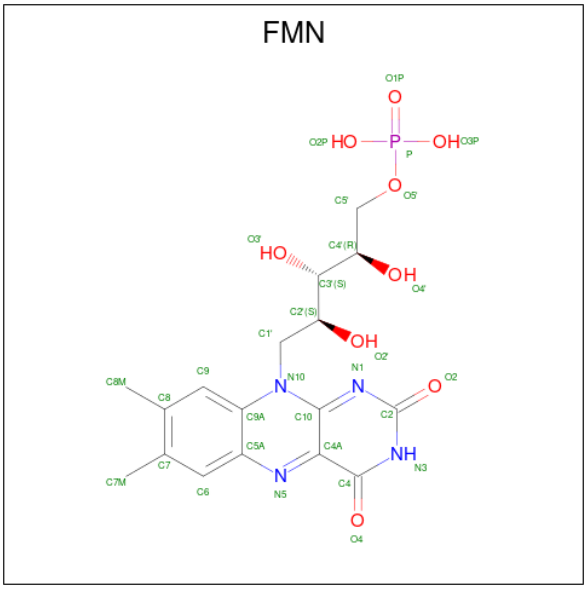
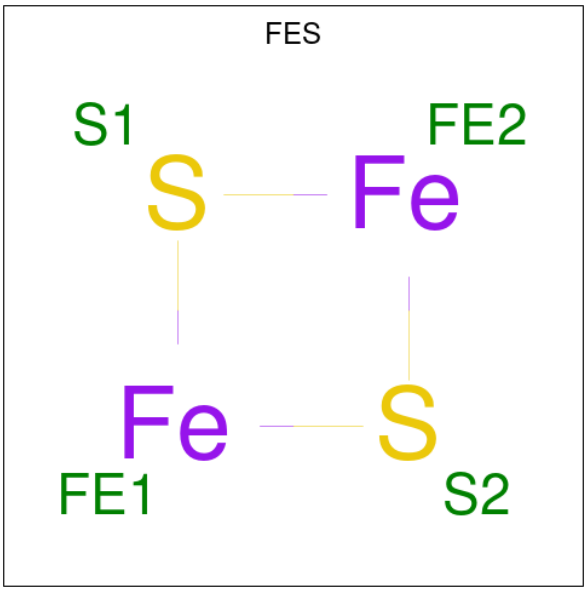
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	D	1	Total	Fe	S		0	0
			8	4	4			
17	G	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			
17	O	1	Total	Fe	S		0	0
			8	4	4			

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



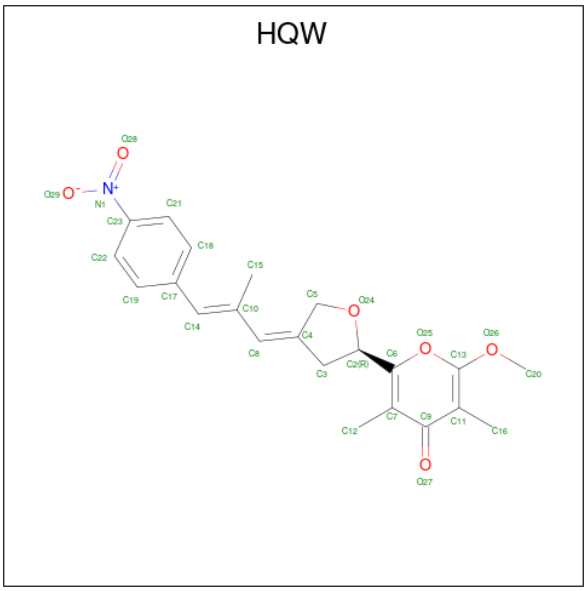
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
18	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



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

- Molecule 20 is Aureothin (three-letter code: HQW) (formula: $C_{22}H_{23}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
20	4	1	29	22	1	6	0	0
			Total	C	N	O		
20	E	1	29	22	1	6	0	0

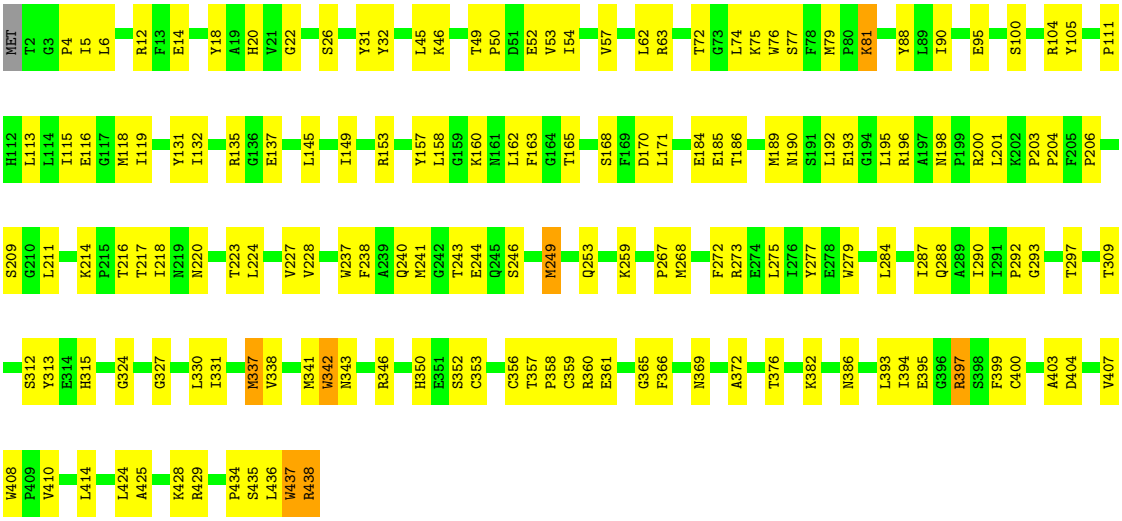
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

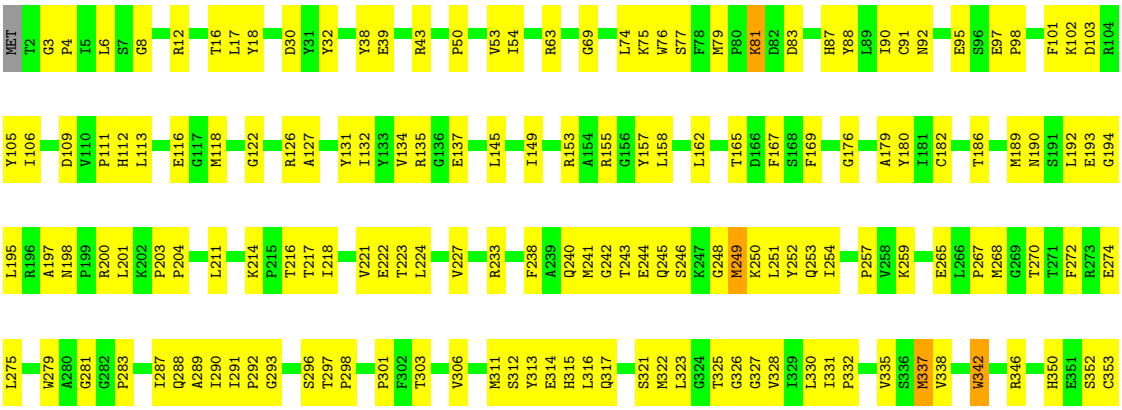
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain 1:



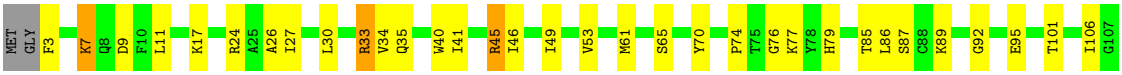
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain B:



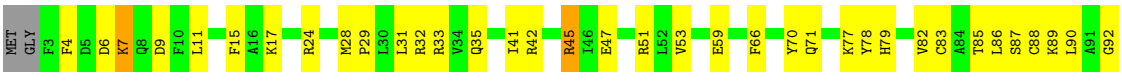
• Molecule 2: NADH-quinone oxidoreductase subunit 2

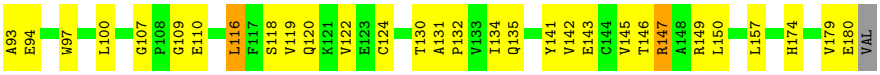
Chain 2:



• Molecule 2: NADH-quinone oxidoreductase subunit 2

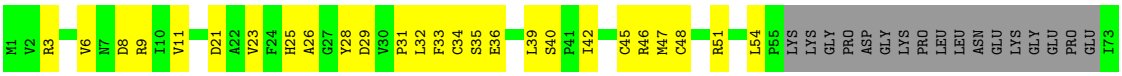
Chain C:

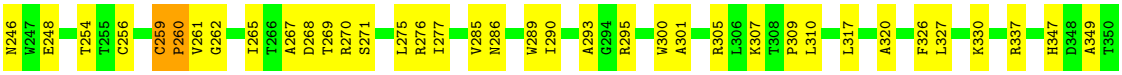


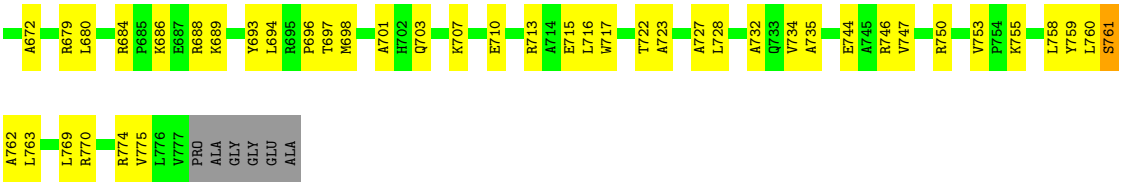


• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3:

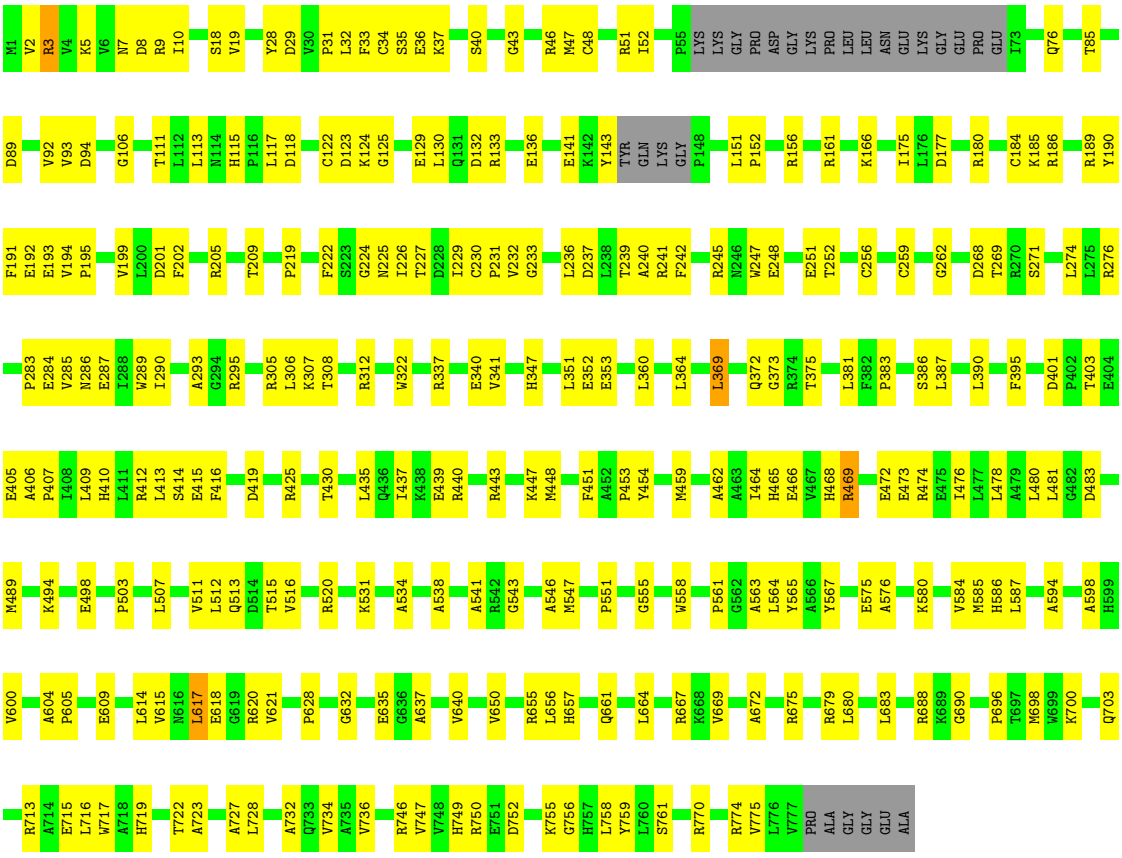






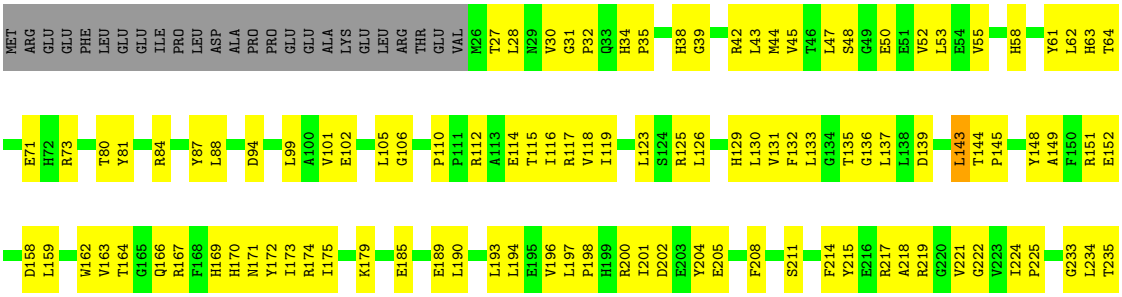
• Molecule 3: NADH-quinone oxidoreductase subunit 3

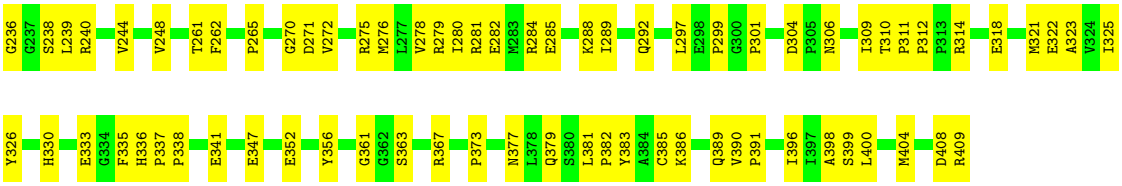
Chain D:



• Molecule 4: NADH-quinone oxidoreductase subunit 4

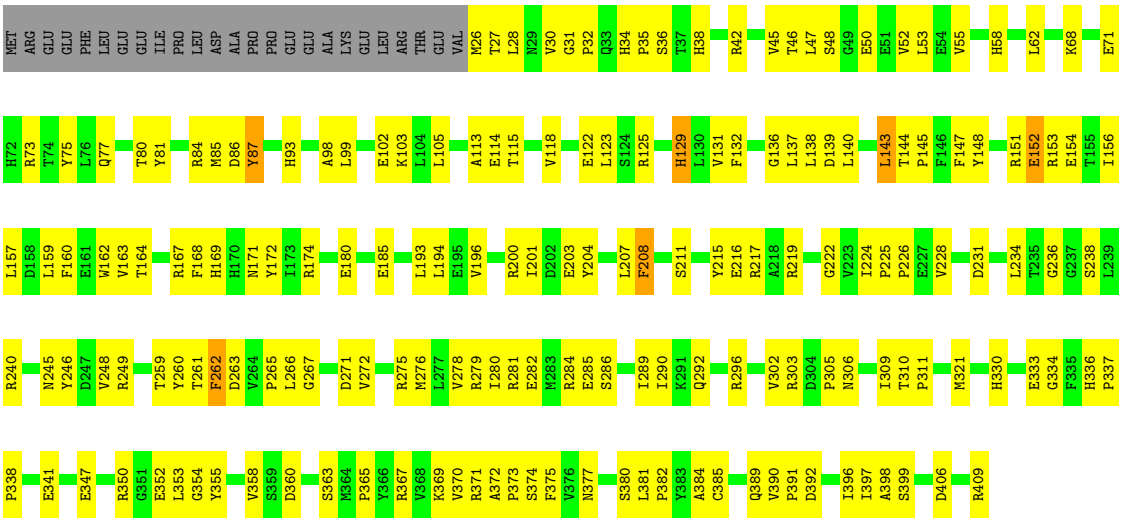
Chain 4:





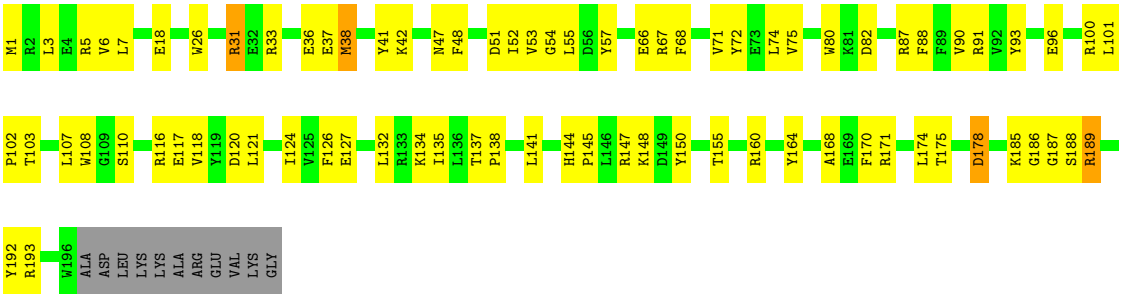
- Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E:



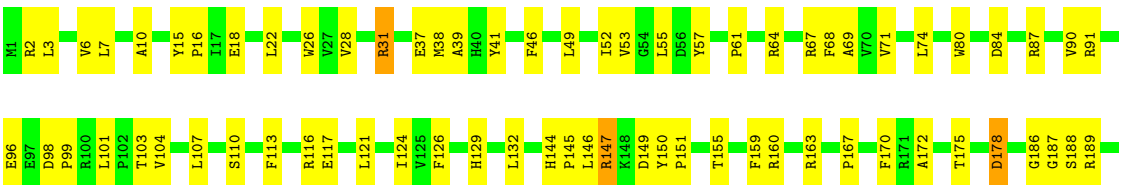
- Molecule 5: NADH-quinone oxidoreductase subunit 5

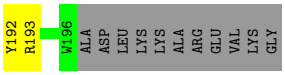
Chain 5:



- Molecule 5: NADH-quinone oxidoreductase subunit 5

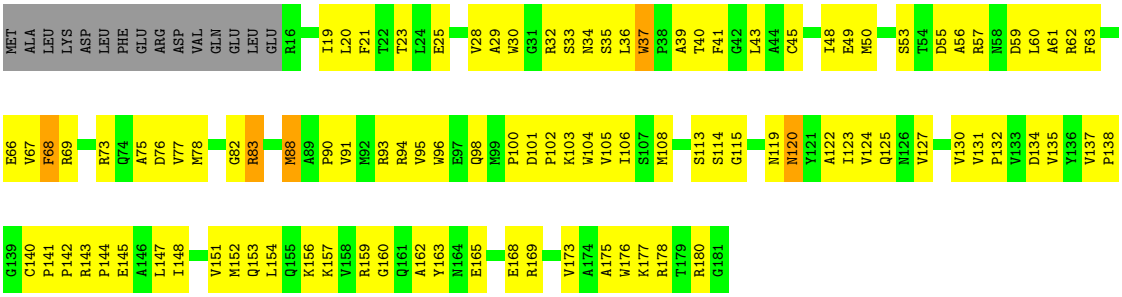
Chain F:





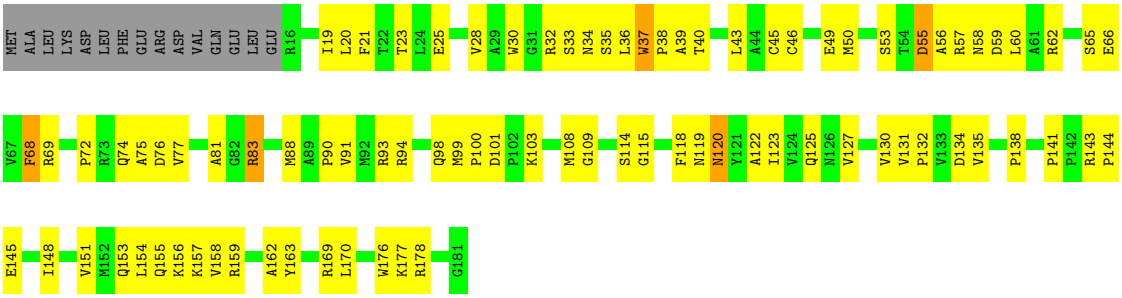
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6:



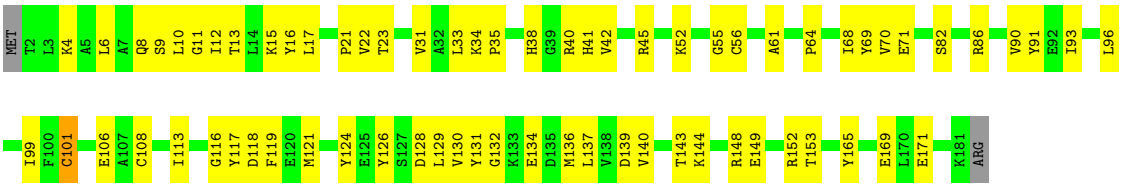
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G:



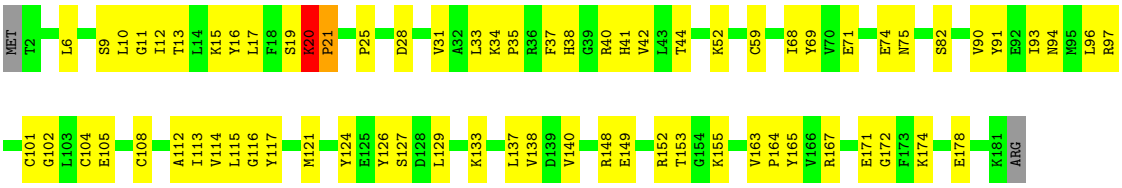
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain 9:



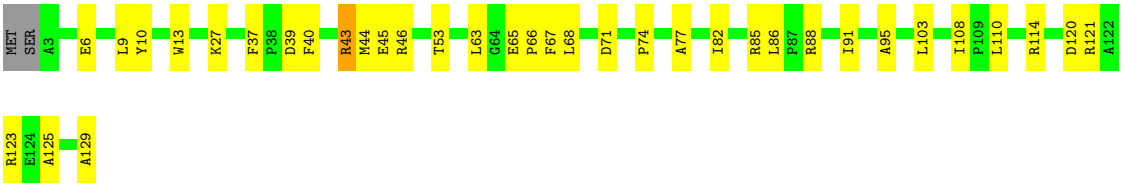
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O:



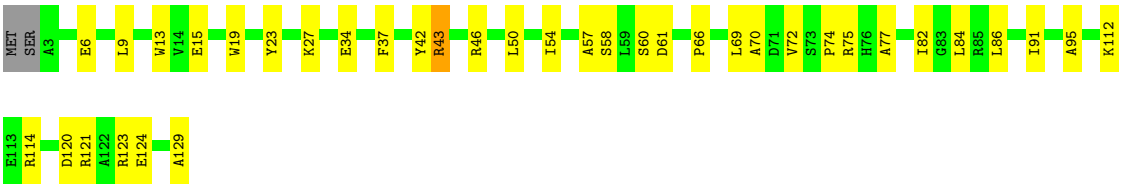
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:



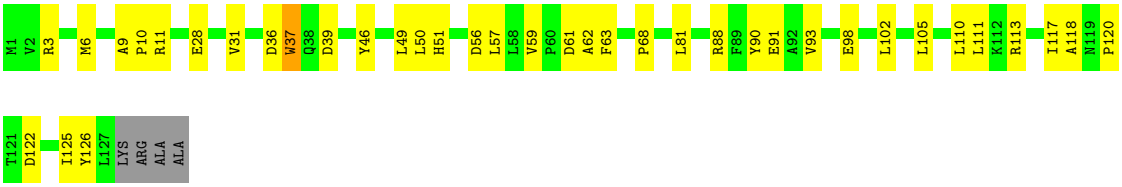
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I:



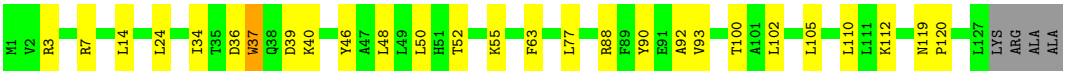
• Molecule 9: Uncharacterized protein

Chain W:



• Molecule 9: Uncharacterized protein

Chain X:



• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:

• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P: 55% 40%

M1 A2 P3 Y7 V8 G9 T10 L11 I12 Y13 V14 A23 V27 G28 K35 K40 Y44 E45 S46 G47 N48 D49 P50 A51 G52 E53 V54 K55 R56 F57 Y62 V63 V64 A65 M66 L67 F68 I69 L70 F71 E74 V75 A76 F77 L78 W79 P80 Y81 A82 V83 S84

L90 F93 L94 G95 V96 F107 L108 Y109 K113 G114 V115 M116 R117 TRP HIS

• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J: 53% 37% 9%

M1 S2 E5 L9 F10 L11 S15 N24 H27 A28 A29 L30 A31 L32 I33 F36 L37 V38 L39 A40 V44 D47 A48 R49 F50 F53 V58 Y59 A62 I63 V64 V65 L66 F67 L68 F69 V70 I71 M72 L73 L74 F75 A76 A77 Q78 G79 E80 F83

D84 L92 L95 L96 A97 V100 L104 A105 W109 L113 D118 L119 G122 L123 P124 L127 L131 Y132 G133 D134 W135 L136 L139 L146 T150 V151 V152 A153 V154 A155 L156 V157 E158 P159 G160 LYS ALA SER ARG ALA LYS GLU ALA GLU LYS ARG GLU

GLU VAL ALA ARG

• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R: 55% 35% 9%

M1 S2 E5 L9 S15 G16 V19 L22 R23 N24 H27 A28 A29 L32 I33 L34 N35 V44 D47 A48 R49 F50 Q55 V58 Y59 A60 G61 A62 I63 V64 V65 L66 F67 L68 F69 V70 I71 M72 L73 L74 F75 Q78 F83 D84 R88

P91 L92 L95 L96 A97 I103 L104 G107 L108 W109 Q117 D118 L119 G122 L123 P124 L127 L131 Y132 G133 D134 W135 L136 T150 V151 V152 A155 L156 P159 G160 LYS ALA SER ARG ALA LYS GLU ALA GLU LYS ARG GLU GLU VAL ALA ARG

• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K: 64% 34%

M1 S2 Y3 L4 L5 T6 S7 A12 V15 Y16 L19 T20 R21 I25 L26 V27 F28 L29 L40 S41 L42 A46 R47 A48 Y49 G50 L51 D52 G53 Q54 V55 A56 M59 V60 I61 A62 V63 V68 A69 V70 F79 R80 H81 R82 T85 D88 G95

• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S: 69% 29%

M1 S2 Y3 L4 L5 Y16 L19 T20 R21 R22 T23 L26 V27 F28 L29 L42 A46 R47 G50 G53 L58 I61 V68 A69 I78 F79 R80 H81 R82 T85 D88 R94 G95

• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L: 66% 33%

M1 A2 L3 I7 L8 L9 P10 L11 L12 G13 L16 L17 M24 R25 E26 P27 L28 P29 G30 L36 F41 L42 L43 G44 A53 E58 W59 L60 F65 S66 L67 S73 L77 T81 G82 V83 G84 F85 L86 I87 H88 I92 R103 F104 F105 A106 Y107

F108 N109 M115 L120 A121 D122 F128 I129 F139 L140 L141 F144 K147 Y151 F159 I160 V161 N162 R163 I164 G165 D166 L167 G168 F169 M170 L171 G172 M173 A174 I175 T182 L183 S184 I185 S186 E187 E190 N198 L201 V214 G215 K216 Q219 L222

W225 A231 P235 V236 L239 I240 H241 T244 M245 V246 R255 P264 S267 Y268 V272 L275 A278 A285 F286 Q287 Q288 I291 K292 K293 I294 Y297 S298 S301 Q302 L303 G304 Y305 M306 G311 V312 G313 A314 Y315 W316 V317 H321 H325

A326 F327 F328 K329 A335 S336 V339 I340 G345 L355 W356 L359 P360 Q361 T362 R363 W364 H365 I368 L371 A372 L373 L376 P377 S380 D386 A387 I388 A391 T392 L393 T394 Y395 P396 F397 F402 G405 V409 A410 V411 L412 T413 Y416 R419

H432 H433 H434 P435 H436 E437 A438 P439 M442 L443 W444 H447 A450 L451 G452 S453 V454 L455 A456 G457 Y458 L459 A460 L461 P462 H463 P464 L465 P466 N467 V468 L477 H484 L487 E490 W491 I494 A496 L496 V500 A501 L502 W506 F511 F512 K515 V516

F517 E525 S528 N539 I542 L546 L549 F554 D557 L561 Y564 F565 G575 Q582 T583 G584 Y585 L586 R587 L591 L598 L599 L600 M604 R605 TRP

• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain T: 66% 33%

M1 L9 P10 L11 L12 G13 F14 A15 L16 L17 F20 G21 K22 R23 M24 R25 E26 P27 L28 P29 A33 V37 F41 L42 L43 G44 L49 A53 Q56 W59 L60 P61 G62 I63 L69 D70 N71 L72 S73 G74 L77 L78 T81 G84 I87 H88

V89 Y90 A91 I92 G93 Y94 G100 F105 A106 Y107 F108 N109 M115 S123 Y124 P125 V126 M127 F128 I129 E132 F139 L140 L141 K147 Y151 R156 K157 A158 F159 I160 R163 I164 G165 D166 F169 T182 L183 S184 E187 E190 G194 P195 L202

A213 V214 G215 K216 Q219 W225 M230 A231 V236 S237 A238 L239 I240 H241 A242 A243 T244 A248 R255 S256 S267 L275 L276 T277 A278 A285 F286 D290 I291 K292 K293 I294 Y297 S298 T299 I300 S301 Q302 L303 G304 Y305 M306 F307 L308 A309 A310 G311 V312

G313 A314 Y315 W316 V317 T324 H325 K329 F333 L334 A335 S336 G337 S338 V339 I340 H341 G345 E346 Q347 D348 V349 G354 L355 W356 K357 H358 I359 P360 R363 A366 L371 A372 L373 G374 G375 L376 L379 S380 K385 I388 L389 A390 A391 T394 Y395 P396 F397

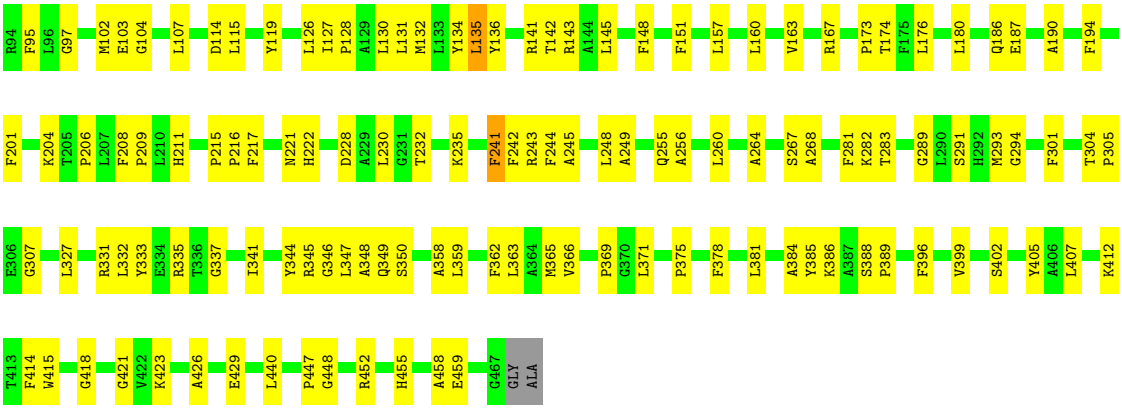
F402 G405 A406 L407 L408 V409 A410 T413 Y416 R419 W420 L423 E428 H433 H434 P435 H436 E437 A438 P439 M442 L443 W444 H447 G452 S453 V454 L455 A456 G457 Y458 L459 A460 L461 P462 H463 P464 L469 H484 L487 E490 W491 I494

W506 F511 F512 K515 V516 F517 E525 D535 N539 V543 F554 D557 Q582 T583 G584 Y585 L586 R587 L591 V594 L598 L599 L600 M604 R605 TRP

• Molecule 14: NADH-quinone oxidoreductase subunit 13

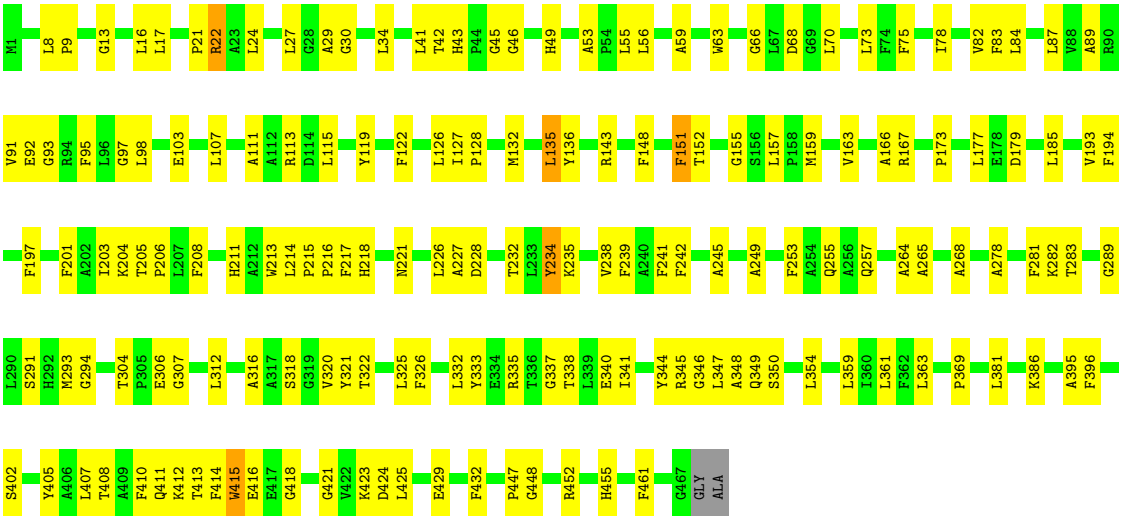
Chain M: 65% 34%

M1 P9 V10 G13 L16 P21 R22 A23 L24 G25 V26 L27 G30 F33 L34 L39 F40 L41 T42 H43 P44 G45 A48 A53 L56 A59 Y62 W63 L67 D68 G69 L70 L73 F74 I78 A79 V82 V88 A89 R90 V91 E92 G93



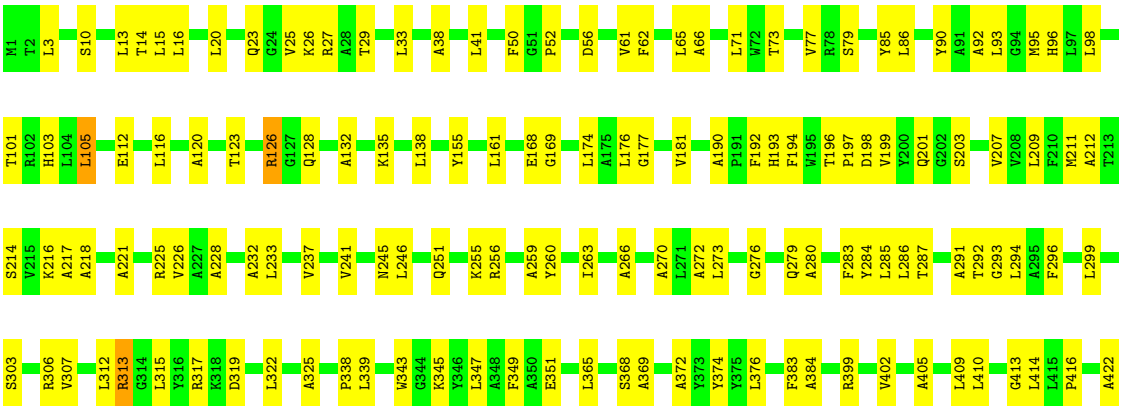
- Molecule 14: NADH-quinone oxidoreductase subunit 13

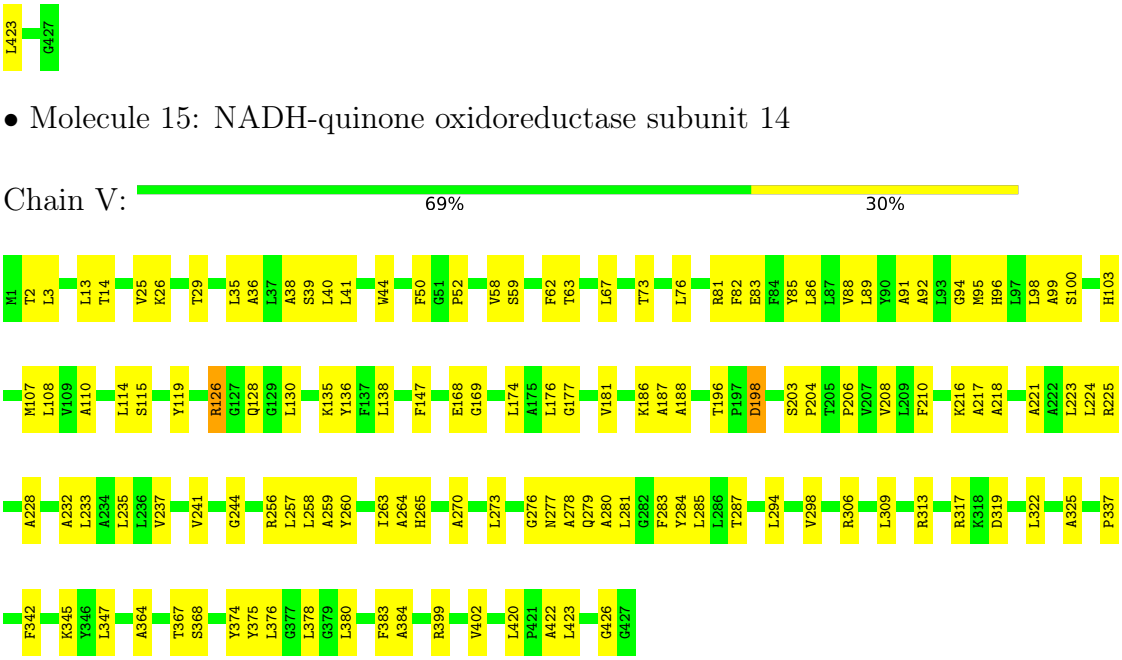
Chain U: 64% 35%

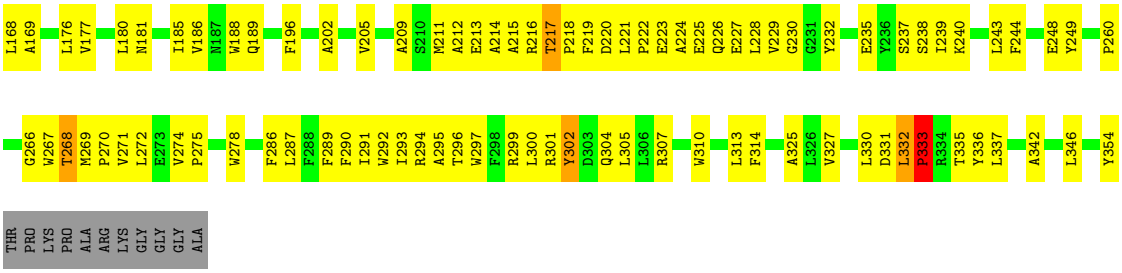


- Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N: 67% 32%




L423 G427
• Molecule 15: NADH-quinone oxidoreductase subunit 14
Chain V:
69%
30%
M1 T2 L3 L13 T14 V25 K26 T29 L35 A36 L37 A38 S39 L40 L41 W44 F50 G51 P52 V58 S59 F62 T63 L67 T73 L76 R81 F82 E83 F84 Y85 L86 L87 V88 L89 Y90 A91 A92 L93 G94 M95 H96 L97 L98 A99 S100 H103
M107 L108 V109 A110 L114 S115 Y119 R126 G127 Q128 G129 L130 K135 Y136 F137 L138 F147 E168 G169 L174 A175 L176 G177 V181 K186 A187 A188 T196 P197 D198 S203 P204 T205 P206 V207 V208 L209 F210 K216 A217 A218 A221 A222 L223 L224 R225
A228 A232 L233 A234 L235 L236 V237 V241 G244 R256 L257 L258 A259 Y260 I263 A264 H265 A270 L273 G276 N277 A278 Q279 A280 L281 G282 F283 Y284 L285 L286 T287 L294 V298 R306 L309 R313 R317 K318 D319 L322 A325 P337
F342 K345 Y346 L347 A364 T367 S368 Y374 Y375 L376 G377 L378 G379 L380 F383 A384 R399 V402 L420 P421 A422 L423 G426 G427
• Molecule 16: NADH-quinone oxidoreductase subunit 8
Chain H:
50%
43%
MET T2 Y5 P6 P9 Y10 W11 K16 F28 A29 T32 L33 R36 R37 L38 L39 A40 R41 F42 Q43 V44 R45 M46 G47 P48 N49 R50 V51 G52 P53 F54 G55 P59 L60 I64 K65 S66 I67 F68 K69 E70 D71 I72 P86 V90 L95 A96 F97 G98
L99 G103 Q112 P113 W114 V115 I116 N117 L118 D119 L120 G121 I122 L123 A127 V128 L131 A132 V133 Y134 G135 I136 F137 L138 S139 S143 K146 Y147 S148 L149 L150 G151 S152 L153 R154 S155 S156 A157 S158 L159 I160 S161 Y162 E163 L164 A169 L180 N181 D184 I185
Q189 K190 G193 W194 L195 F196 L197 Y198 P201 A202 F203 L204 V205 Y206 E213 A214 A215 R216 T217 P218 F219 D220 L221 P222 E223 A224 E225 Q226 E227 L228 V229 G230 G231 Y232 H233 T234 E235 Y236 S237 S238 L243 F244 A247 E248 Y249 A255 S256 A257 L258 I259 P260 G265 G266
W267 T268 M269 P270 V274 P275 W278 K282 F286 L287 F290 I291 W292 I293 R294 A295 T296 W297 F298 R299 L300 R301 Y302 L305 L306 R307 F308 G309 W310 G311 F312 L313 F314 A317 L326 V327 L330 D331 L332 P333 Y336 L337 S341 A342 F345 L346 L349
Y354 THR PRO LYS PRO ALA ARG LYS GLY GLY GLY GLY ALA
• Molecule 16: NADH-quinone oxidoreductase subunit 8
Chain Q:
50%
43%
MET T2 P6 M12 L15 K16 A17 V21 F28 A29 T32 E35 R36 R37 L38 L39 A40 R41 F42 Q43 V44 R45 M46 G47 P48 N49 R50 V51 G52 P53 F54 G55 Q58 D62 K65 S66 K69 E70 D71 I72 V73 V74 V83 P86 V90 V91
L94 L95 G98 L99 S107 F108 Y111 Q112 P113 W114 V115 I116 N117 L118 D119 L120 G121 I122 L123 Y124 L125 F126 A127 L131 A132 Y133 Y134 G135 I136 F137 W141 A142 S143 K146 Y147 S148 L149 L150 L153 R154 S155 S156 L159 I160 S161 Y162 E163 L164 G165 L166 G167


L168
A169
L176
V177
L180
N181
I185
V186
N187
W188
Q189
F196
A202
V205
A209
S210
M211
A212
E213
A214
A215
R216
T217
P218
F219
D220
L221
P222
E223
A224
E225
Q226
E227
L228
V229
G230
G231
Y232
E235
Y236
S237
S238
I239
K240
L243
F244
E248
Y249
P260
G266
W267
T268
M269
P270
V271
L272
E273
V274
P275
W278
F286
L287
F288
F289
F290
I291
W292
I293
R294
A295
T296
W297
F298
R299
L300
R301
Y302
D303
Q304
L305
L306
R307
W310
L313
F314
A325
L326
V327
L330
D331
L332
P333
R334
T335
Y336
L337
A342
L346
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 is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.98Å 340.50Å 264.27Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	49.71 – 3.40	Depositor
% Data completeness (in resolution range)	84.1 (49.71-3.40)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.40Å)	Xtriage
Refinement program	PHENIX (dev_3026: ???)	Depositor
R, R_{free}	0.213 , 0.234	Depositor
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.027	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.379 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 191608 reflections	Xtriage
Total number of atoms	74144	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.36	0/3506	0.54	0/4745
1	B	0.29	0/3506	0.49	0/4745
2	2	0.33	0/1439	0.50	0/1953
2	C	0.29	0/1439	0.47	0/1953
3	3	0.43	0/6035	0.66	0/8185
3	D	0.41	0/6035	0.62	1/8185 (0.0%)
4	4	0.39	0/3150	0.60	1/4284 (0.0%)
4	E	0.32	0/3150	0.52	0/4284
5	5	0.40	0/1656	0.60	1/2246 (0.0%)
5	F	0.36	0/1656	0.57	0/2246
6	6	0.46	0/1319	0.66	0/1786
6	G	0.40	0/1319	0.63	1/1786 (0.1%)
7	9	0.51	1/1423 (0.1%)	0.64	0/1933
7	O	0.38	0/1423	0.71	1/1933 (0.1%)
8	7	0.34	0/1059	0.56	1/1429 (0.1%)
8	I	0.31	0/1059	0.53	0/1429
9	W	0.41	0/985	0.68	1/1335 (0.1%)
9	X	0.38	0/985	0.57	0/1335
10	A	0.34	0/940	0.53	0/1280
10	P	0.33	0/940	0.53	0/1280
11	J	0.33	0/1206	0.54	0/1649
11	R	0.29	0/1206	0.49	0/1649
12	K	0.31	0/710	0.51	0/962
12	S	0.30	0/710	0.50	0/962
13	L	0.31	0/4741	0.49	0/6460
13	T	0.28	0/4741	0.46	0/6460
14	M	0.33	0/3591	0.53	0/4896
14	U	0.28	0/3591	0.47	0/4896
15	N	0.34	0/3238	0.50	0/4434
15	V	0.31	0/3238	0.47	0/4434
16	H	0.33	0/2935	0.55	0/4014
16	Q	0.33	0/2935	0.57	1/4014 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.35	1/75866 (0.0%)	0.55	8/103182 (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
10	A	0	1
10	P	0	1
13	T	0	2
16	H	0	2
16	Q	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	101	CYS	CB-SG	-5.81	1.72	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	20	LYS	C-N-CD	-16.21	84.94	120.60
4	4	133	LEU	CA-CB-CG	6.46	130.16	115.30
6	G	169	ARG	C-N-CA	-6.21	106.17	121.70
5	5	189	ARG	NE-CZ-NH1	5.99	123.29	120.30
16	Q	332	LEU	CA-CB-CG	5.45	127.83	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	21	PRO	Peptide
10	A	45	GLU	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
10	P	45	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3389	122	0
1	B	3417	0	3389	155	0
2	2	1406	0	1373	63	0
2	C	1406	0	1373	58	0
3	3	5895	0	5931	235	0
3	D	5895	0	5930	196	0
4	4	3067	0	3049	166	0
4	E	3067	0	3049	166	0
5	5	1607	0	1574	81	0
5	F	1607	0	1574	65	0
6	6	1289	0	1299	104	0
6	G	1289	0	1298	99	0
7	9	1388	0	1383	70	0
7	O	1388	0	1383	65	0
8	7	1031	0	1029	35	0
8	I	1031	0	1029	30	0
9	W	967	0	1010	32	0
9	X	967	0	1010	20	0
10	A	910	0	939	59	0
10	P	910	0	939	56	0
11	J	1183	0	1286	55	0
11	R	1183	0	1286	61	0
12	K	703	0	747	34	0
12	S	703	0	747	29	0
13	L	4604	0	4734	170	0
13	T	4604	0	4734	169	0
14	M	3489	0	3606	127	0
14	U	3489	0	3606	125	0
15	N	3154	0	3343	109	0
15	V	3154	0	3343	104	0
16	H	2838	0	2903	173	0
16	Q	2838	0	2903	179	0
17	1	8	0	0	2	0
17	3	24	0	0	1	0
17	6	8	0	0	1	0
17	9	16	0	0	2	0
17	B	8	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	24	0	0	2	0
17	G	8	0	0	1	0
17	O	16	0	0	2	0
18	1	31	0	19	1	0
18	B	31	0	19	2	0
19	2	4	0	0	1	0
19	3	4	0	0	2	0
19	C	4	0	0	2	0
19	D	4	0	0	2	0
20	4	29	0	0	0	0
20	E	29	0	0	0	0
All	All	74144	0	75226	2779	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 2779 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)
9:W:102:LEU:O	9:W:110:LEU:HD13	1.16	1.26
3:D:283:PRO:HG3	3:D:425:ARG:HH21	1.00	1.13
7:O:20:LYS:N	7:O:21:PRO:HD3	1.64	1.08
3:D:283:PRO:CG	3:D:425:ARG:HH21	1.68	1.04
6:6:56:ALA:HB1	16:H:44:VAL:CG1	1.87	1.02

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	435/438 (99%)	399 (92%)	36 (8%)	0	100	100
2	2	176/181 (97%)	170 (97%)	6 (3%)	0	100	100
2	C	176/181 (97%)	169 (96%)	7 (4%)	0	100	100
3	3	750/783 (96%)	702 (94%)	48 (6%)	0	100	100
3	D	750/783 (96%)	700 (93%)	50 (7%)	0	100	100
4	4	382/409 (93%)	361 (94%)	21 (6%)	0	100	100
4	E	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
5	5	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
5	F	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
6	6	164/181 (91%)	144 (88%)	20 (12%)	0	100	100
6	G	164/181 (91%)	148 (90%)	16 (10%)	0	100	100
7	9	178/182 (98%)	166 (93%)	12 (7%)	0	100	100
7	O	178/182 (98%)	172 (97%)	5 (3%)	1 (1%)	25	57
8	7	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
8	I	125/129 (97%)	116 (93%)	9 (7%)	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%)	105 (91%)	10 (9%)	0	100	100
10	P	115/119 (97%)	105 (91%)	10 (9%)	0	100	100
11	J	158/176 (90%)	148 (94%)	10 (6%)	0	100	100
11	R	158/176 (90%)	146 (92%)	12 (8%)	0	100	100
12	K	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
12	S	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
13	L	603/606 (100%)	568 (94%)	34 (6%)	1 (0%)	47	78
13	T	603/606 (100%)	569 (94%)	33 (6%)	1 (0%)	47	78
14	M	465/469 (99%)	438 (94%)	27 (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%)	402 (95%)	23 (5%)	0	100	100
16	H	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	7	30
16	Q	351/365 (96%)	302 (86%)	42 (12%)	7 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9478/9796 (97%)	8826 (93%)	635 (7%)	17 (0%)	47	78

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	45	ARG
16	H	51	VAL
7	O	21	PRO
16	Q	51	VAL
16	H	44	VAL

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%)	344 (97%)	11 (3%)	40	68
1	B	355/356 (100%)	345 (97%)	10 (3%)	43	70
2	2	150/152 (99%)	144 (96%)	6 (4%)	31	60
2	C	150/152 (99%)	144 (96%)	6 (4%)	31	60
3	3	609/628 (97%)	599 (98%)	10 (2%)	62	81
3	D	609/628 (97%)	598 (98%)	11 (2%)	59	79
4	4	332/355 (94%)	328 (99%)	4 (1%)	71	85
4	E	332/355 (94%)	326 (98%)	6 (2%)	59	79
5	5	167/175 (95%)	163 (98%)	4 (2%)	49	74
5	F	167/175 (95%)	164 (98%)	3 (2%)	59	79
6	6	135/149 (91%)	125 (93%)	10 (7%)	13	42
6	G	135/149 (91%)	126 (93%)	9 (7%)	16	46
7	9	148/150 (99%)	147 (99%)	1 (1%)	84	92
7	O	148/150 (99%)	146 (99%)	2 (1%)	67	83
8	7	104/106 (98%)	103 (99%)	1 (1%)	76	88
8	I	104/106 (98%)	103 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	99/101 (98%)	98 (99%)	1 (1%)	76	88
9	X	99/101 (98%)	98 (99%)	1 (1%)	76	88
10	A	90/92 (98%)	88 (98%)	2 (2%)	52	75
10	P	90/92 (98%)	87 (97%)	3 (3%)	38	66
11	J	118/130 (91%)	114 (97%)	4 (3%)	37	65
11	R	118/130 (91%)	115 (98%)	3 (2%)	47	72
12	K	71/71 (100%)	69 (97%)	2 (3%)	43	70
12	S	71/71 (100%)	69 (97%)	2 (3%)	43	70
13	L	453/454 (100%)	445 (98%)	8 (2%)	59	79
13	T	453/454 (100%)	445 (98%)	8 (2%)	59	79
14	M	332/332 (100%)	324 (98%)	8 (2%)	49	74
14	U	332/332 (100%)	323 (97%)	9 (3%)	44	70
15	N	302/302 (100%)	297 (98%)	5 (2%)	60	80
15	V	302/302 (100%)	297 (98%)	5 (2%)	60	80
16	H	293/300 (98%)	280 (96%)	13 (4%)	28	58
16	Q	293/300 (98%)	282 (96%)	11 (4%)	33	61
All	All	7516/7706 (98%)	7336 (98%)	180 (2%)	49	74

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	761	SER
11	R	84	ASP
4	E	143	LEU
6	G	83	ARG
13	T	169	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	92	ASN
3	D	168	HIS
16	Q	251	HIS
14	U	255	GLN
1	B	219	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 monosaccharides 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	$\#\|Z\| > 2$
20	HQW	4	501	-	29,31,31	1.30	4 (13%)	29,44,44	1.49	6 (20%)
18	FMN	1	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.29	9 (18%)
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
20	HQW	E	501	-	29,31,31	1.01	1 (3%)	29,44,44	1.58	6 (20%)
17	SF4	D	801	3	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		
18	FMN	B	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.31	7 (14%)
17	SF4	6	201	6	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SF4	G	201	6	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	3	801	3	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		

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
20	HQW	4	501	-	-	4/13/27/27	0/3/3/3
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
20	HQW	E	501	-	-	4/13/27/27	0/3/3/3
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	6	201	6	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	502	FMN	C4A-N5	4.23	1.39	1.30
18	B	502	FMN	C4A-N5	3.90	1.38	1.30
20	E	501	HQW	C23-N1	2.87	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	501	HQW	C23-N1	2.72	1.51	1.45
20	4	501	HQW	O25-C13	2.69	1.40	1.35

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	E	501	HQW	C17-C14-C10	-4.13	123.70	130.74
20	E	501	HQW	O24-C5-C4	3.26	109.16	105.58
20	4	501	HQW	C17-C14-C10	-3.06	125.53	130.74
18	1	502	FMN	C4-N3-C2	-2.98	120.14	125.64
18	B	502	FMN	C4-N3-C2	-2.96	120.17	125.64

There are no chirality outliers.

5 of 24 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.

17 monomers are involved in 24 short contacts:

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

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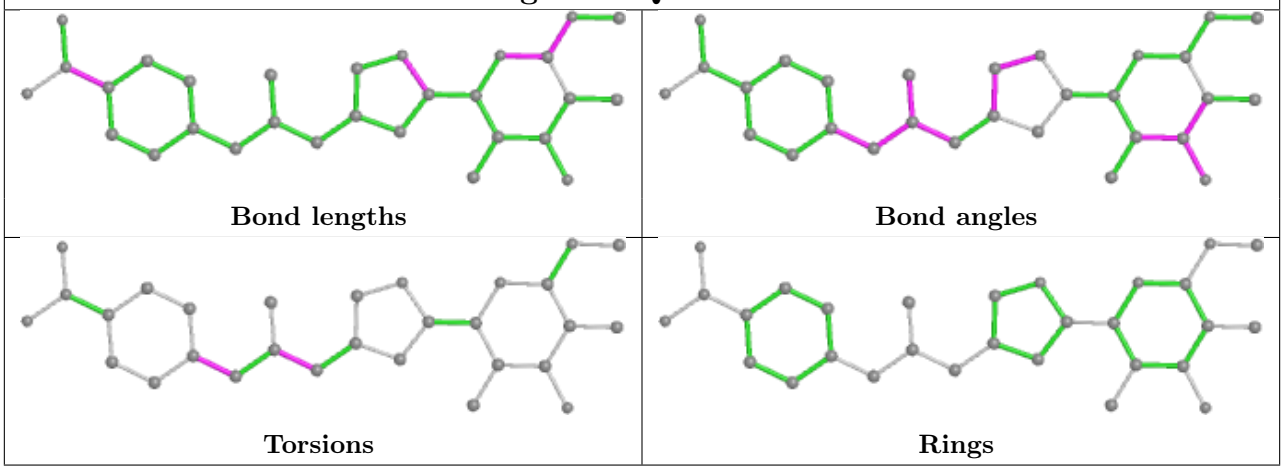
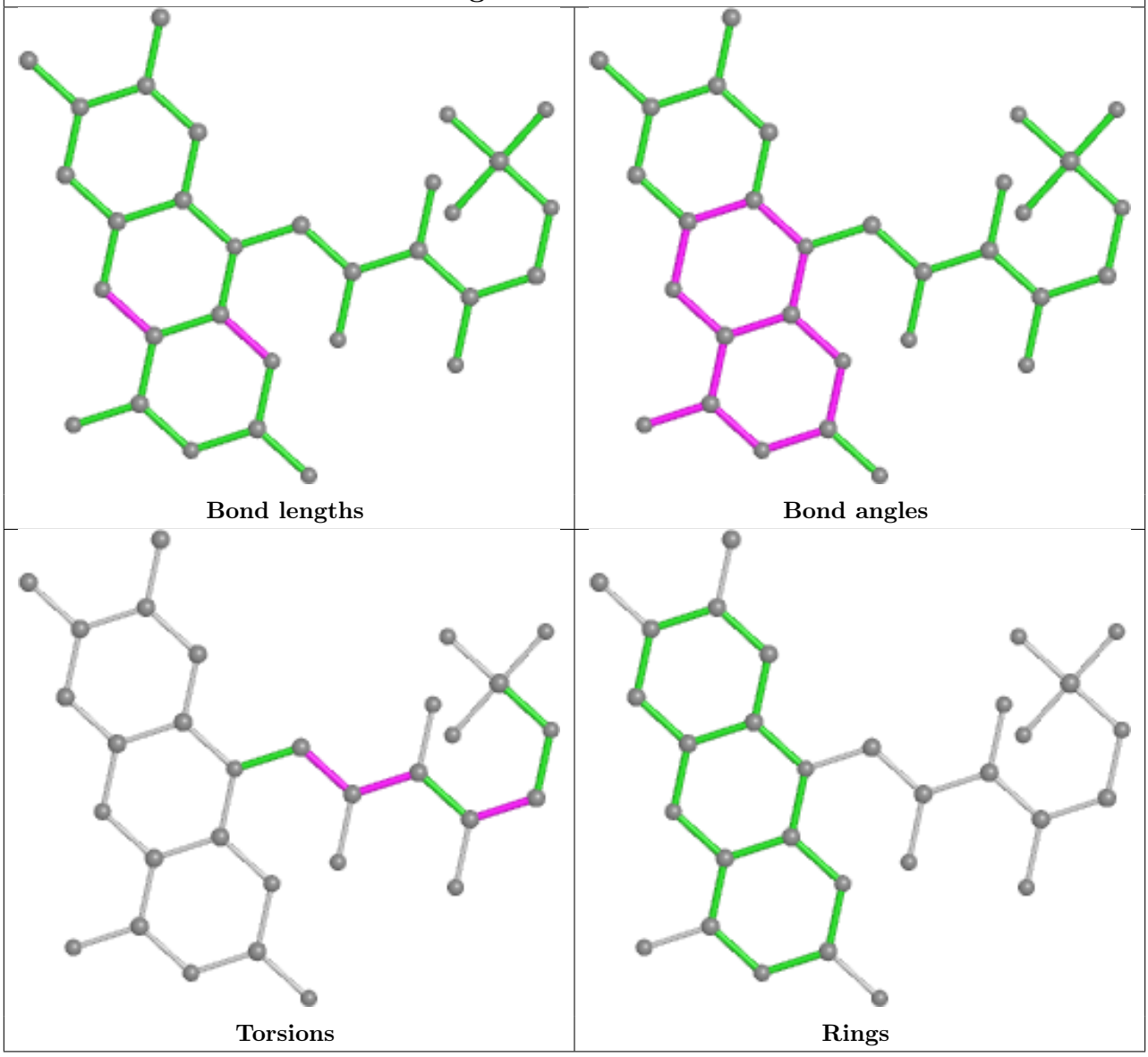
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	501	SF4	2	0
19	C	201	FES	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

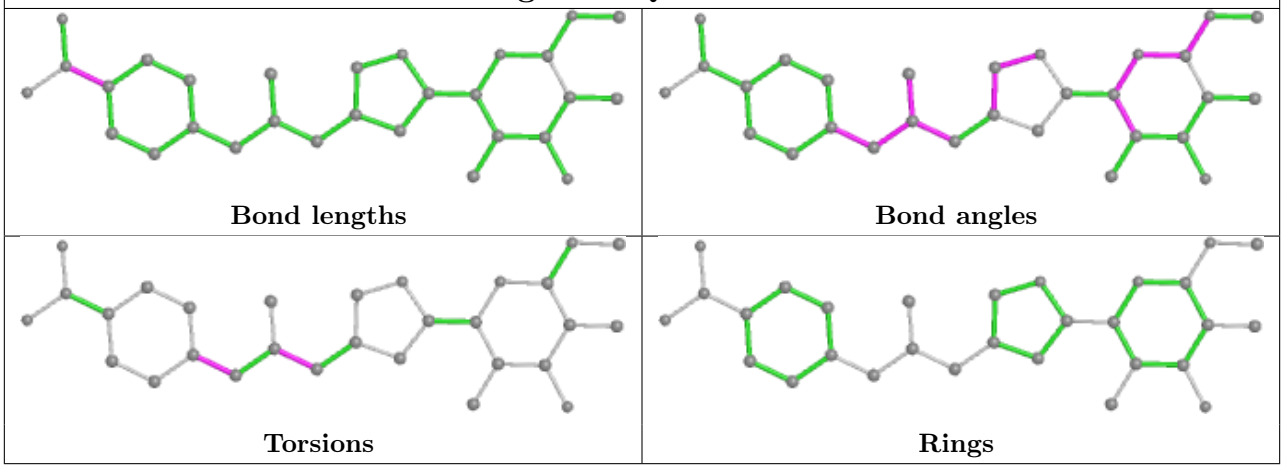
Ligand HQW 4 501



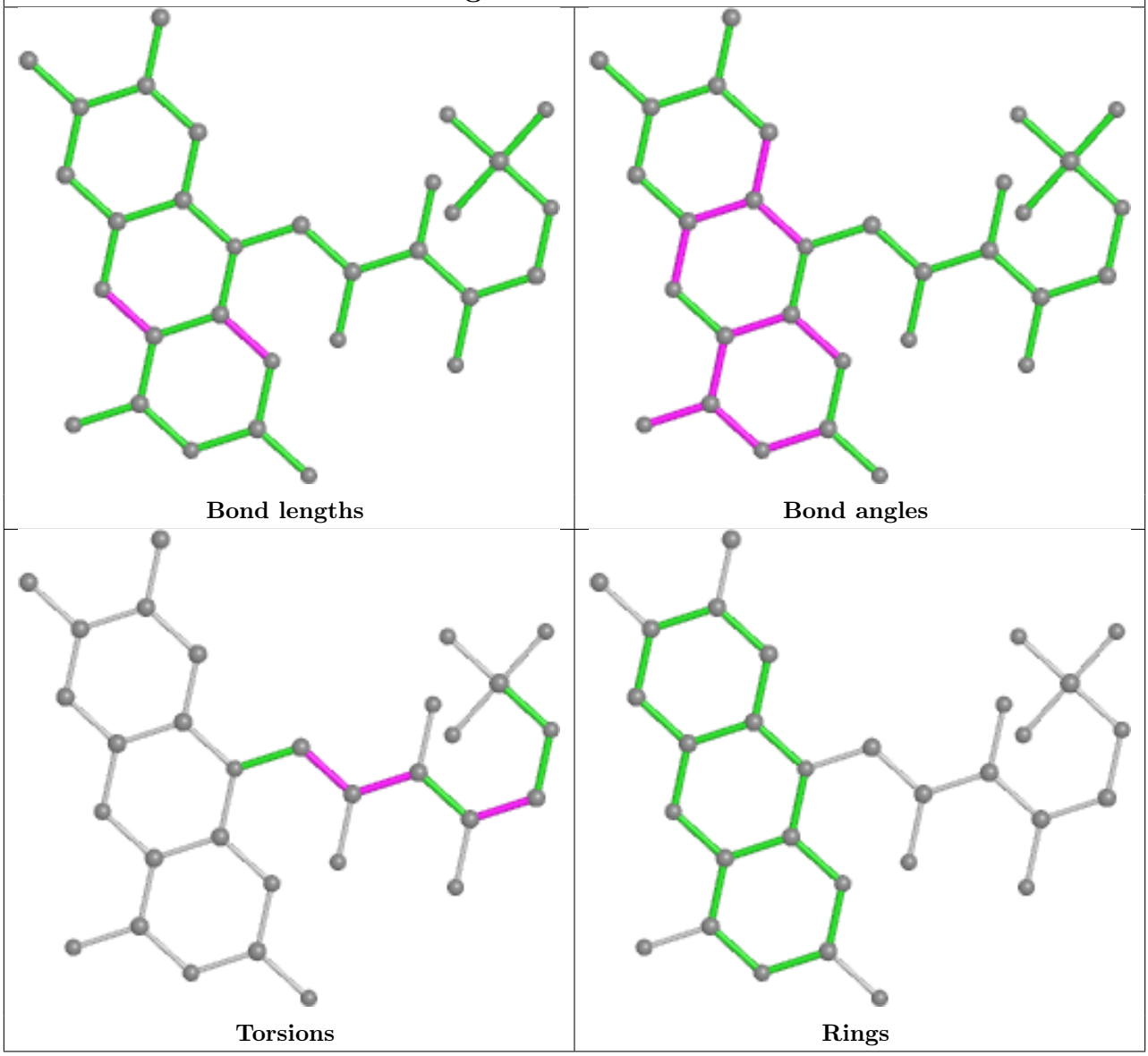
Ligand FMN 1 502



Ligand HQW E 501



Ligand FMN B 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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