



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 9, 2019 – 01:01 AM EST

PDB ID : 6QA9
EMDB ID: : EMD-4482
Title : Isolated complex I class refinement from Ovine respiratory supercomplex I+III2
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-19
Resolution : 4.10 Å(reported)
Based on PDB ID : 1PPJ

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

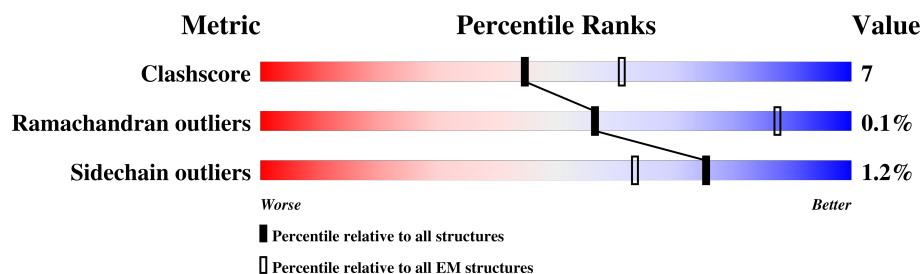
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	V1	445	
2	V2	217	
3	S1	704	
4	S2	430	
5	S3	228	
6	S7	179	
7	S8	176	
8	V3	75	
9	S6	96	

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Mol	Chain	Length	Quality of chain
10	S4	133	
11	A9	338	
12	A2	98	
13	A5	115	
14	A6	127	
15	A7	112	
16	AL	145	
17	AA	88	
17	AB	88	
18	D3	115	
19	D1	318	
20	D6	175	
21	4L	98	
22	D5	606	
23	D4	459	
24	D2	347	
25	AK	140	
26	B5	143	
27	A8	171	
28	BJ	175	
29	AJ	320	
30	S5	105	
31	A3	83	
32	B3	97	
33	C2	120	

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Mol	Chain	Length	Quality of chain
34	B4	128	
35	AM	143	
36	B6	127	
37	B7	136	
38	B9	178	
39	B2	72	
40	B8	158	
41	BK	125	
42	C1	49	
43	B1	57	
44	A1	70	

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
45	SF4	V1	500	-	-	X	-

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 65403 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V2	212	Total	C	N	O	S	0	0
			1647	1052	277	308	10		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S1	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 4 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S2	427	Total	C	N	O	S	0	0
			3436	2194	589	628	25		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S3	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 6 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	156	Total	C	N	O	S	0	0
			1248	795	225	214	14		

- Molecule 7 is a protein called NDUF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	176	Total	C	N	O	S	0	0
			1415	889	243	271	12		

- Molecule 8 is a protein called NDUFV3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V3	40	Total	C	N	O	S	0	0
			335	209	60	65	1		

- Molecule 9 is a protein called NDUF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S6	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S4	126	Total	C	N	O	S	0	0
			1025	646	182	194	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	290	Total	C	N	O	S	0	0
			2321	1483	423	410	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	82	Total	C	N	O	S	0	0
			665	419	124	120	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A5	111	Total	C	N	O	S	0	0
			902	583	151	166	2		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A6	114	Total	C	N	O	S	0	0
			970	619	180	167	4		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A7	94	Total	C	N	O	S	0	0
			752	470	143	136	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	143	Total	C	N	O	S	0	0
			1192	768	214	206	4		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AA	80	Total	C	N	O	S	0	0
			645	416	96	128	5		
17	AB	87	Total	C	N	O	S	0	0
			702	451	103	143	5		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D3	97	Total	C	N	O	S	0	0
			787	538	112	132	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D1	299	Total	C	N	O	S	0	0
			2390	1618	364	389	19		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D6	171	Total	C	N	O	S	0	0
			1308	878	187	230	13		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D5	606	Total	C	N	O	S	0	0
			4805	3187	746	828	44		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D4	459	Total	C	N	O	S	0	0
			3646	2428	571	607	40		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D2	347	Total	C	N	O	S	0	0
			2724	1808	416	460	40		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AK	140	Total	C	N	O	S	0	0
			1025	654	175	190	6		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B5	139	Total	C	N	O	S	0	0
			1156	761	194	199	2		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A8	171	Total	C	N	O	S	0	0
			1404	889	253	252	10		

- Molecule 28 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BJ	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AJ	319	Total	C	N	O	S	0	0
			2583	1653	430	490	10		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S5	99	Total	C	N	O	S	0	0
			822	520	154	142	6		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A3	74	Total	C	N	O	S	0	0
			582	379	96	105	2		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B3	73	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C2	119	Total	C	N	O	S	0	0
			997	647	174	172	4		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B4	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 35 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AM	139	Total	C	N	O	S	0	0
			1143	733	200	201	9		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B6	96	Total	C	N	O	S	0	0
			815	536	139	139	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B7	119	Total	C	N	O	S	0	0
			1026	641	196	181	8		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B9	176	Total	C	N	O	S	0	0
			1515	970	278	261	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B2	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B8	157	Total	C	N	O	S	0	0
			1324	855	217	243	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BK	102	Total	C	N	O	S	0	0
			853	547	141	161	4		

- Molecule 42 is a protein called NDUFC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	C1	46	Total	C	N	O	0	0
			391	258	67	66		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	B1	52	Total	C	N	O	0	0
			449	296	79	74		

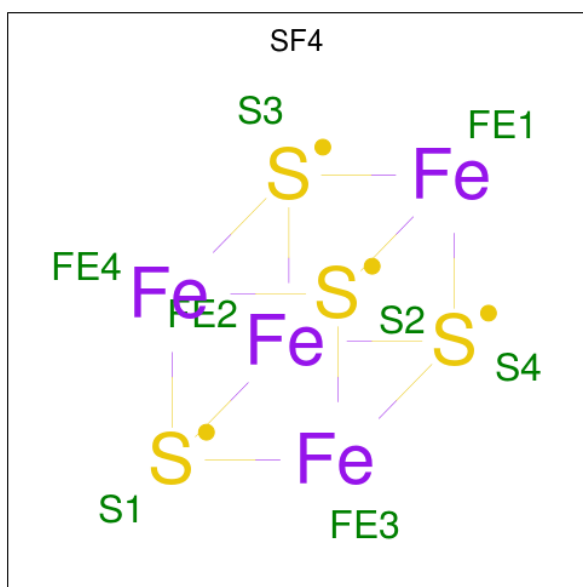
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 44 is a protein called NDUFA1.

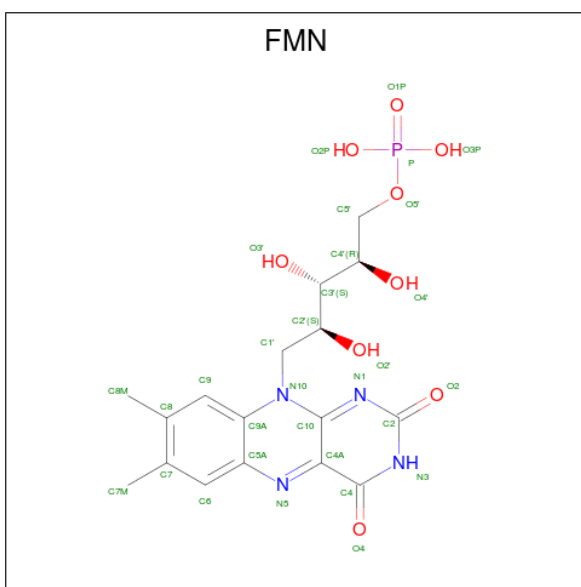
Mol	Chain	Residues	Atoms					AltConf	Trace
44	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



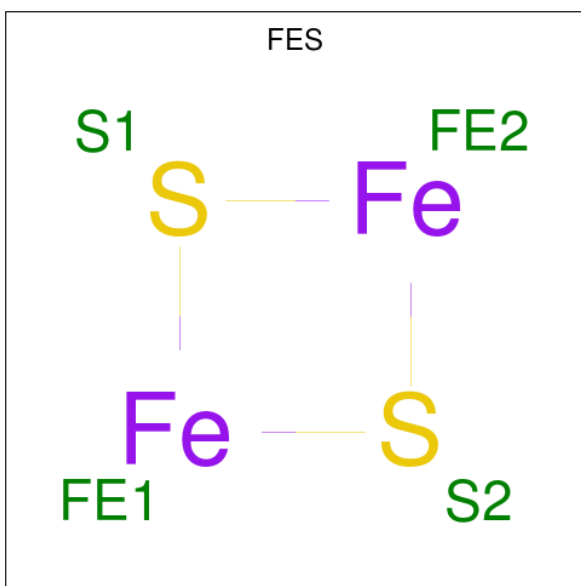
Mol	Chain	Residues	Atoms			AltConf
45	V1	1	Total	Fe	S	0
			8	4	4	
45	S1	1	Total	Fe	S	0
			16	8	8	
45	S1	1	Total	Fe	S	0
			16	8	8	
45	S7	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			16	8	8	
45	S8	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
46	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

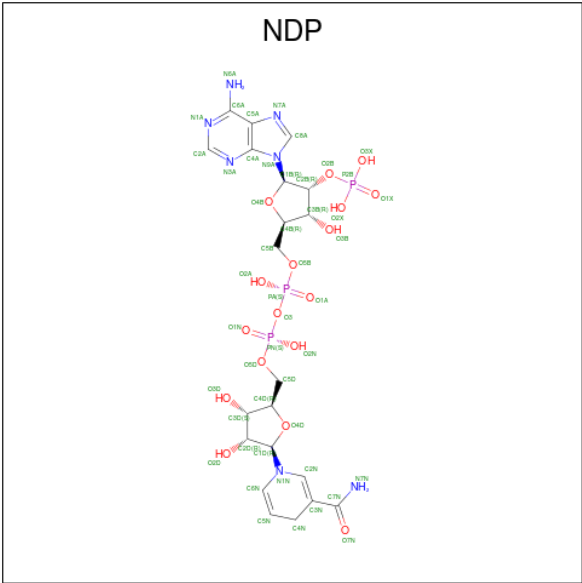


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total 4	Fe 2	S 2	0
47	S1	1	Total 4	Fe 2	S 2	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

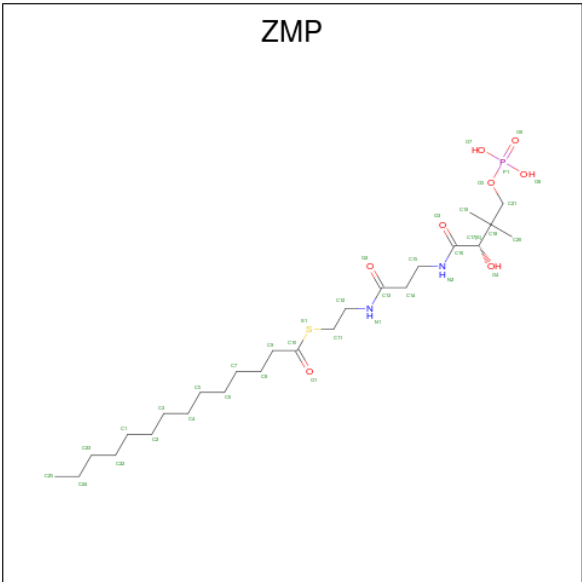
Mol	Chain	Residues	Atoms		AltConf
48	S6	1	Total	Zn	0
			1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



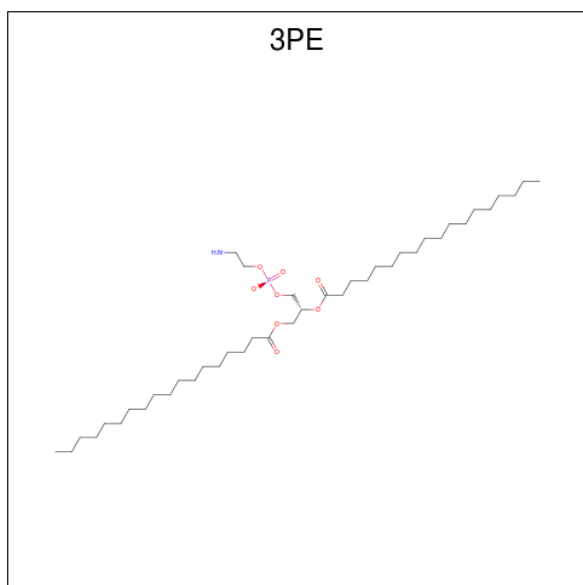
Mol	Chain	Residues	Atoms					AltConf
49	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



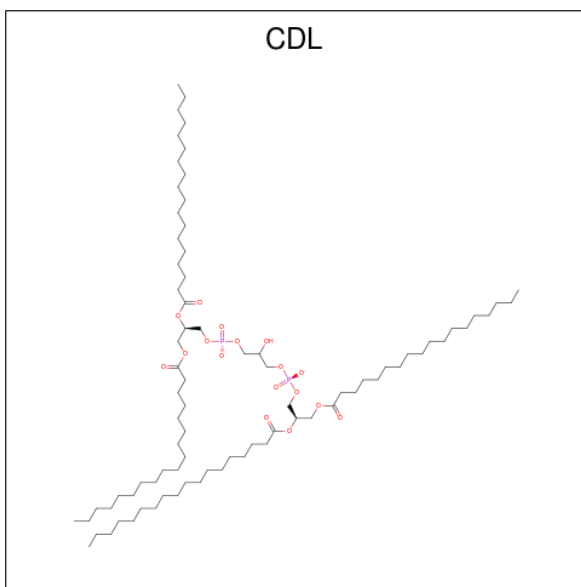
Mol	Chain	Residues	Atoms						AltConf
50	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
50	B9	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



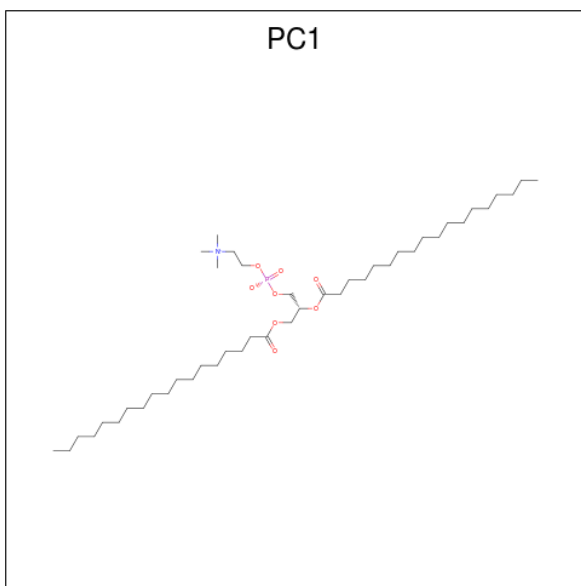
Mol	Chain	Residues	Atoms					AltConf
51	D1	1	Total	C	N	O	P	0
			19	9	1	8	1	
51	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
51	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	A8	1	Total	C	N	O	P	0
			25	15	1	8	1	

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	D5	1	36	17	17	2	0

- Molecule 53 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).

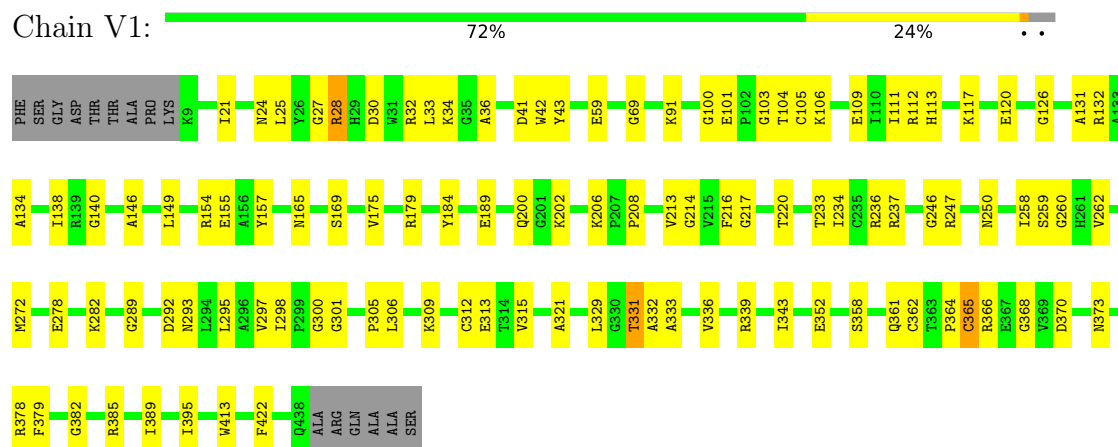


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	D4	1	28	18	1	8	1	0

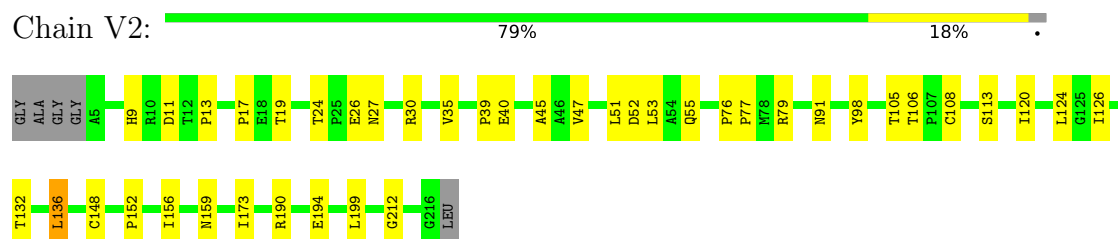
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

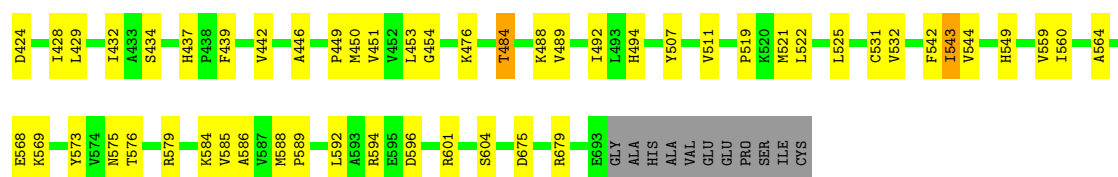


- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

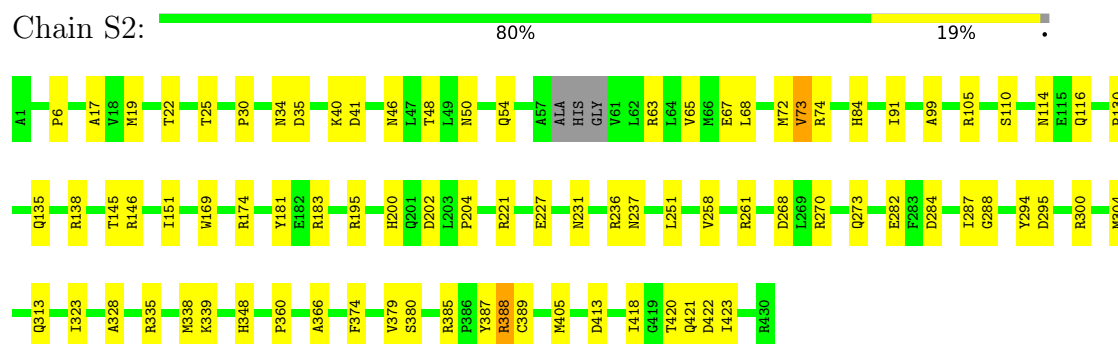


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

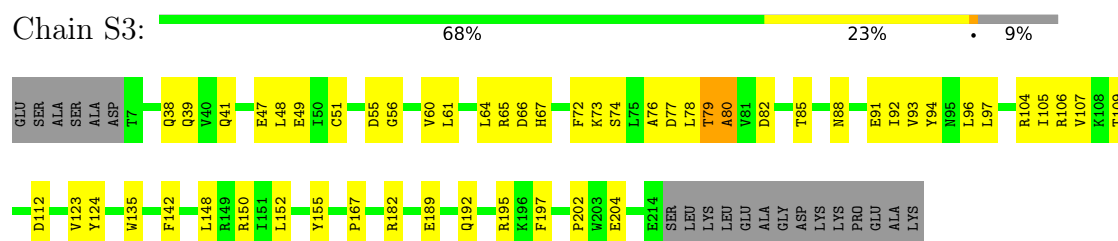




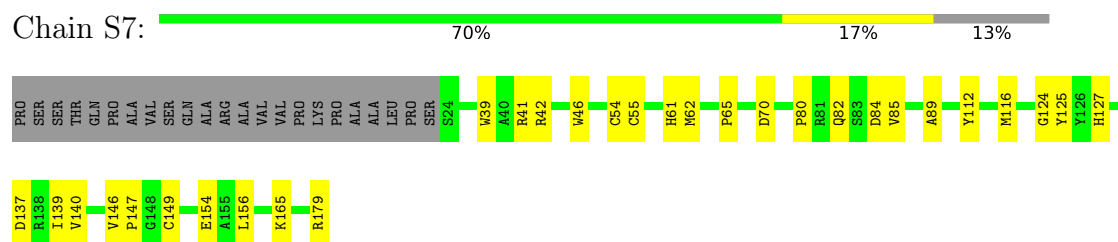
• Molecule 4: NDUF2S



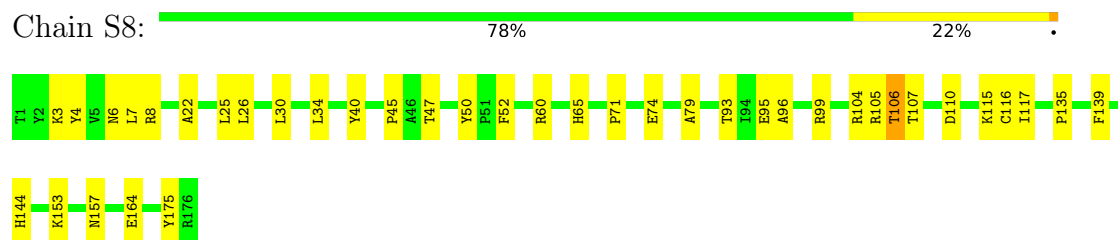
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



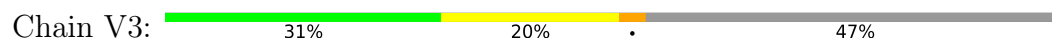
• Molecule 6: NDUF57

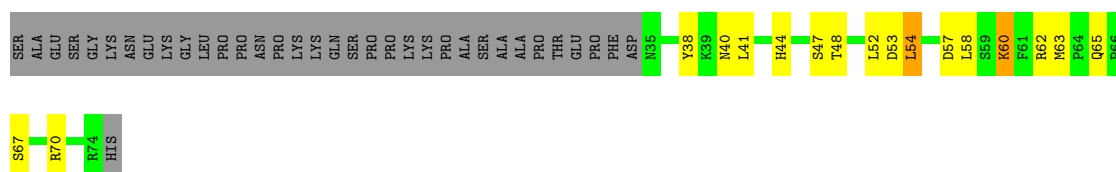


• Molecule 7: NDUF58



• Molecule 8: NDUFV3





- Molecule 9: NDUFS6

Chain S6: 77% 21% ..



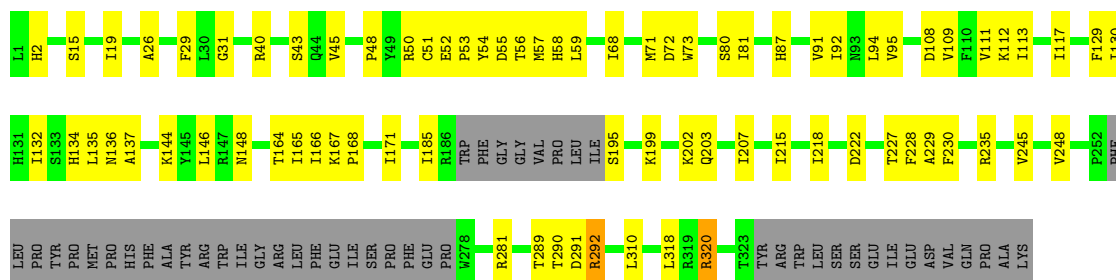
- Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

Chain S4: 77% 17% 5%



- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

Chain A9: 63% 22% 14%



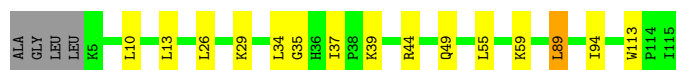
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2: 65% 18% 16%



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5: 83% 12% ..



- Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain A6: 69% 20% 10%



P127

- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain A7: 65% 19% 16%



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL: 83% 12% ..



- Molecule 17: Acyl carrier protein

Chain AA: 76% 15% 9%



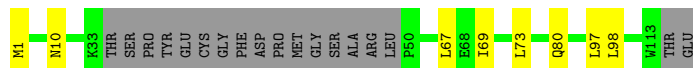
- Molecule 17: Acyl carrier protein

Chain AB: 82% 17% .



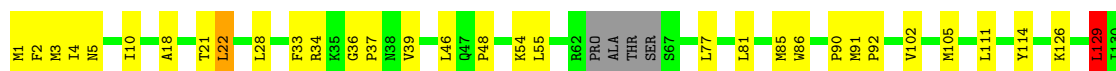
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain D3: 77% 7% 16%



- Molecule 19: NADH-ubiquinone oxidoreductase chain 1

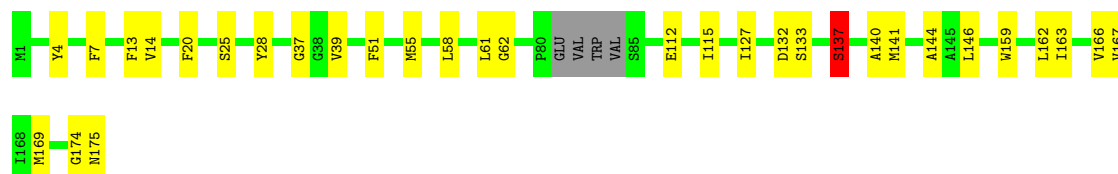
Chain D1: 70% 23% 6%





- Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain D6: 79% 18% ..



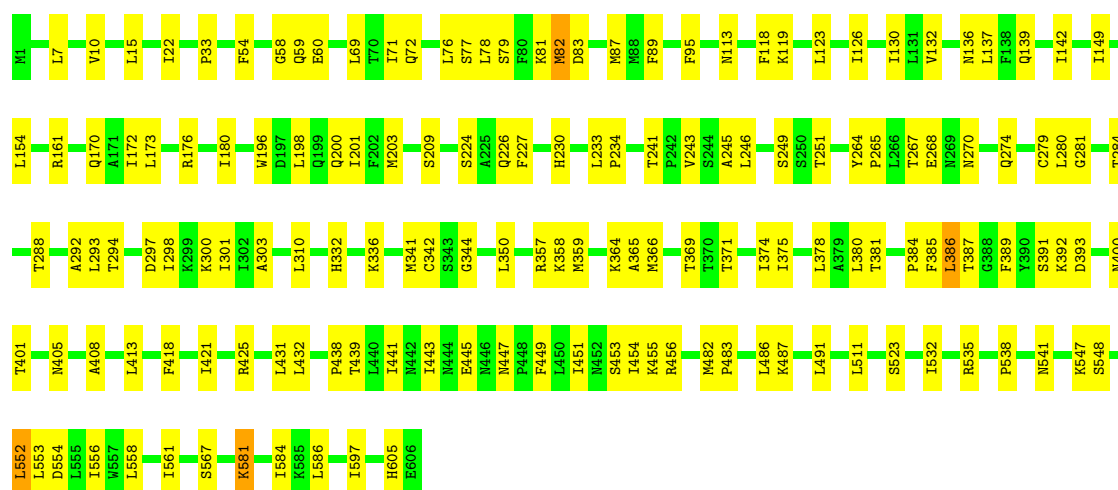
- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L: 82% 17% .



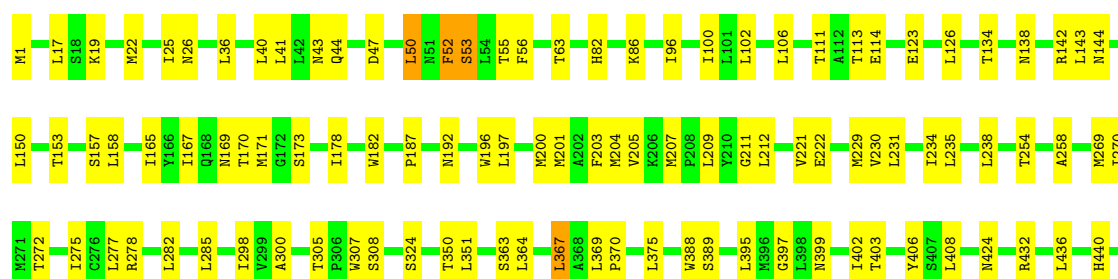
- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

Chain D5: 75% 25% .



- Molecule 23: NADH-ubiquinone oxidoreductase chain 4

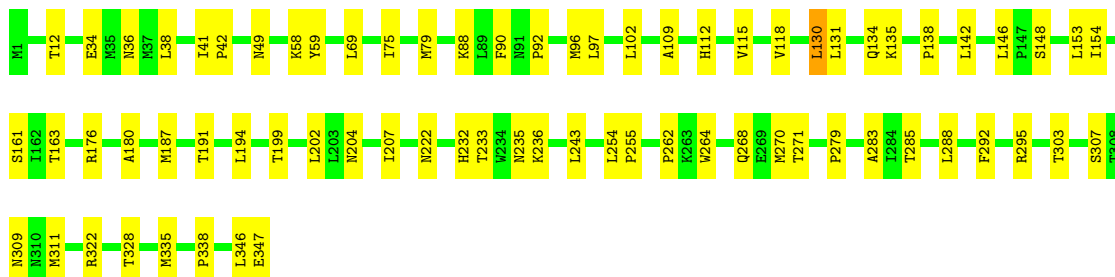
Chain D4: 77% 22% .





- Molecule 24: NADH-ubiquinone oxidoreductase chain 2

Chain D2: 79% 20%



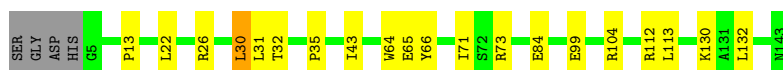
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AK: 87% 11%



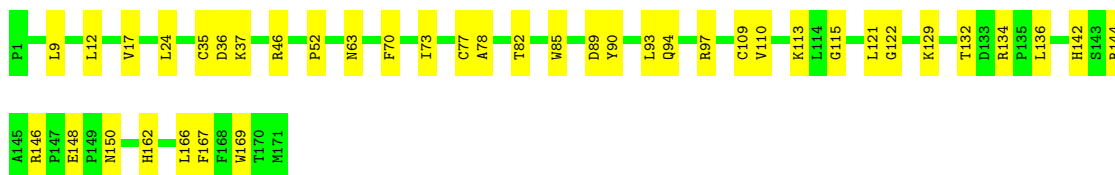
- Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

Chain B5: 83% 13%



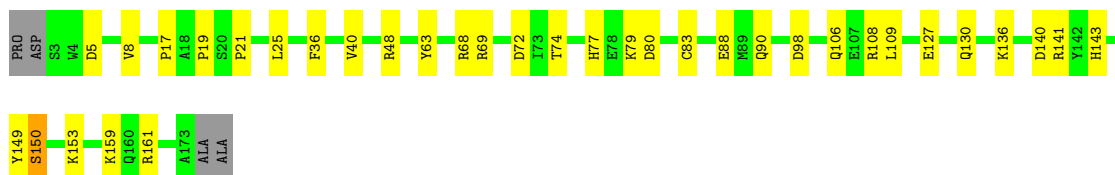
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8: 77% 23%

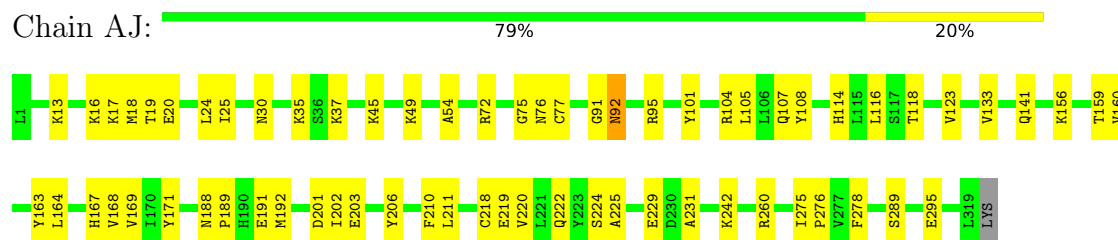


- Molecule 28: NDUFB10

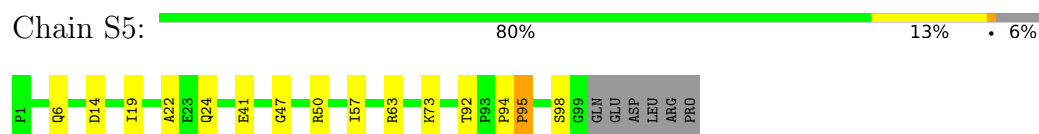
Chain BJ: 78% 19%



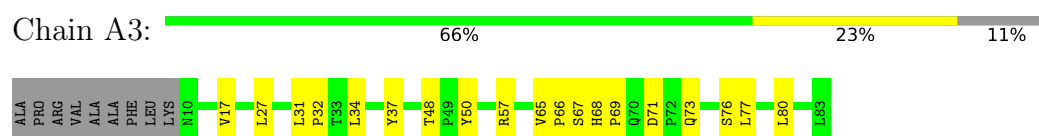
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



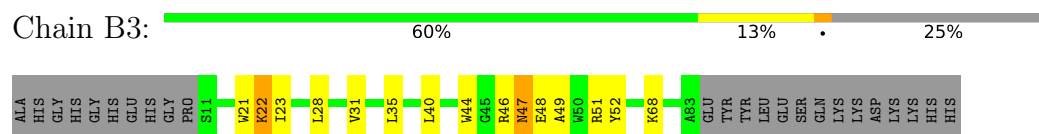
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



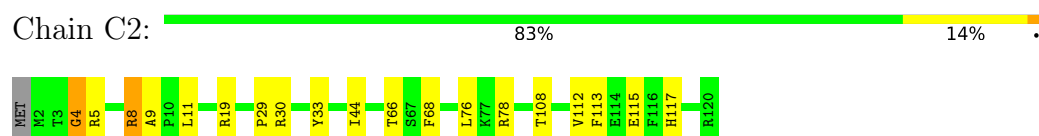
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



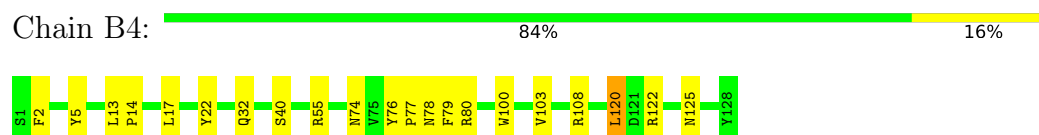
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



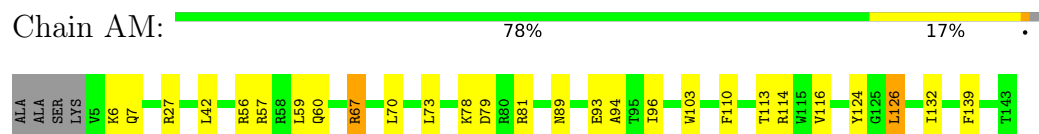
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



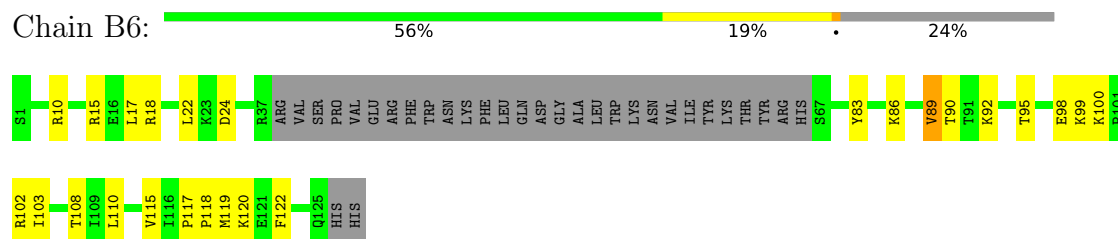
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



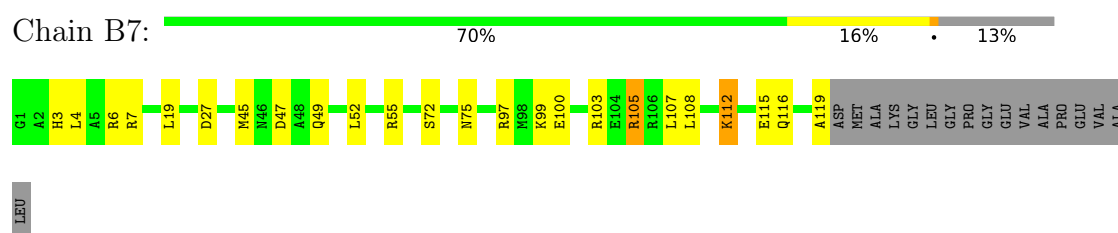
- Molecule 35: NDUFA13



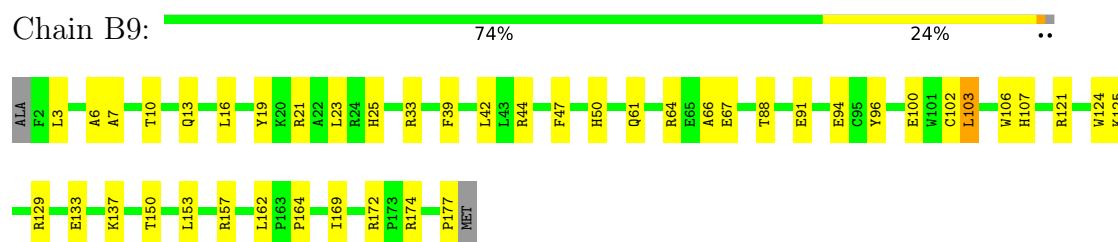
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



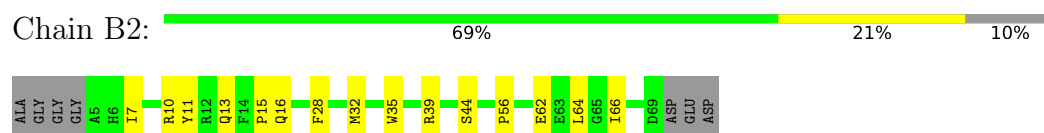
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



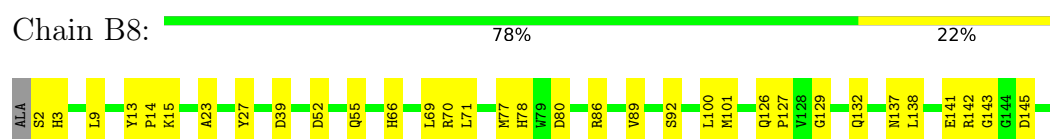
- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

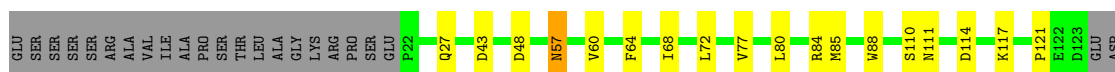


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial





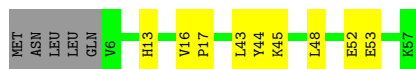
- Molecule 42: NDUFC1

Chain C1: 86% 8% 6%



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1: 75% 16% 9%



- Molecule 44: NDUFA1

Chain A1: 83% 17%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57160	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CDL, SF4, PC1, FMN, FES, NDP, ZMP, 3PE

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 >2	RMSZ	# Z >2
1	V1	0.37	0/3386	0.60	0/4575
10	S4	0.35	0/1048	0.58	0/1415
11	A9	0.35	0/2373	0.65	2/3207 (0.1%)
12	A2	0.31	0/676	0.61	0/911
13	A5	0.33	0/922	0.66	2/1249 (0.2%)
14	A6	0.32	0/994	0.55	1/1336 (0.1%)
15	A7	0.32	0/770	0.62	0/1040
16	AL	0.35	0/1233	0.62	1/1676 (0.1%)
17	AA	0.28	0/655	0.63	0/881
17	AB	0.32	0/714	0.62	0/963
18	D3	0.35	0/807	0.67	1/1103 (0.1%)
19	D1	0.40	0/2460	0.73	3/3361 (0.1%)
2	V2	0.36	0/1687	0.68	1/2295 (0.0%)
20	D6	0.38	0/1339	0.68	1/1810 (0.1%)
21	4L	0.36	0/758	0.73	0/1024
22	D5	0.37	0/4933	0.71	6/6710 (0.1%)
23	D4	0.39	0/3740	0.71	6/5095 (0.1%)
24	D2	0.40	0/2788	0.68	2/3795 (0.1%)
25	AK	0.31	0/1046	0.67	0/1419
26	B5	0.36	0/1189	0.57	1/1607 (0.1%)
27	A8	0.35	0/1441	0.66	1/1942 (0.1%)
28	BJ	0.35	0/1475	0.58	2/1989 (0.1%)
29	AJ	0.36	0/2644	0.64	2/3579 (0.1%)
3	S1	0.37	0/5362	0.63	2/7266 (0.0%)
30	S5	0.34	0/843	0.60	0/1128
31	A3	0.33	0/602	0.69	1/828 (0.1%)
32	B3	0.34	0/595	0.71	0/803
33	C2	0.37	0/1028	0.64	1/1388 (0.1%)
34	B4	0.34	0/1085	0.65	2/1467 (0.1%)
35	AM	0.36	0/1172	0.65	2/1579 (0.1%)
36	B6	0.34	0/841	0.68	0/1144
37	B7	0.34	0/1051	0.66	4/1408 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	B9	0.35	0/1568	0.60	1/2123 (0.0%)
39	B2	0.36	0/590	0.63	1/810 (0.1%)
4	S2	0.42	0/3526	0.62	0/4778
40	B8	0.37	0/1379	0.66	2/1884 (0.1%)
41	BK	0.37	0/880	0.62	1/1196 (0.1%)
42	C1	0.32	0/404	0.55	0/548
43	B1	0.32	0/462	0.61	0/624
44	A1	0.36	0/592	0.64	0/795
5	S3	0.39	0/1776	0.60	0/2417
6	S7	0.43	0/1279	0.59	0/1728
7	S8	0.47	0/1446	0.61	0/1956
8	V3	0.33	0/344	0.69	0/465
9	S6	0.37	0/749	0.56	0/1009
All	All	0.37	0/66652	0.65	49/90326 (0.1%)

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
1	V1	0	2
11	A9	0	1
13	A5	0	1
15	A7	0	1
16	AL	0	3
19	D1	0	1
2	V2	0	3
20	D6	0	2
22	D5	0	3
23	D4	0	3
25	AK	0	1
27	A8	0	1
28	BJ	0	1
29	AJ	0	1
3	S1	0	5
30	S5	0	1
32	B3	0	1
33	C2	0	2
34	B4	0	1
36	B6	0	3
39	B2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	S2	0	1
40	B8	0	1
43	B1	0	1
5	S3	0	3
7	S8	0	1
All	All	0	45

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A9	222	ASP	CB-CG-OD1	9.34	126.70	118.30
22	D5	69	LEU	CA-CB-CG	8.83	135.61	115.30
13	A5	89	LEU	CA-CB-CG	7.79	133.22	115.30
22	D5	413	LEU	CA-CB-CG	7.11	131.64	115.30
23	D4	367	LEU	CA-CB-CG	7.02	131.45	115.30

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
2	V2	13	PRO	Peptide
2	V2	194	GLU	Peptide
2	V2	35	VAL	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	V1	3312	0	3268	69	0
2	V2	1647	0	1660	28	0
3	S1	5275	0	5304	100	0
4	S2	3436	0	3379	56	0
5	S3	1726	0	1676	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S7	1248	0	1256	25	0
7	S8	1415	0	1374	32	0
8	V3	335	0	316	13	0
9	S6	737	0	710	12	0
10	S4	1025	0	1023	21	0
11	A9	2321	0	2350	47	0
12	A2	665	0	678	10	0
13	A5	902	0	936	12	0
14	A6	970	0	980	25	0
15	A7	752	0	766	18	0
16	AL	1192	0	1164	12	0
17	AA	645	0	649	7	0
17	AB	702	0	692	13	0
18	D3	787	0	832	6	0
19	D1	2390	0	2517	53	0
20	D6	1308	0	1329	23	0
21	4L	748	0	794	15	0
22	D5	4805	0	4950	107	0
23	D4	3646	0	3850	66	0
24	D2	2724	0	2930	53	0
25	AK	1025	0	1033	10	0
26	B5	1156	0	1177	15	0
27	A8	1404	0	1384	30	0
28	BJ	1441	0	1417	26	0
29	AJ	2583	0	2547	37	0
30	S5	822	0	820	13	0
31	A3	582	0	583	16	0
32	B3	578	0	570	14	0
33	C2	997	0	983	18	0
34	B4	1059	0	1062	14	0
35	AM	1143	0	1137	20	0
36	B6	815	0	837	17	0
37	B7	1026	0	995	15	0
38	B9	1515	0	1469	29	0
39	B2	563	0	509	9	0
40	B8	1324	0	1219	23	0
41	BK	853	0	800	13	0
42	C1	391	0	391	6	0
43	B1	449	0	453	9	0
44	A1	577	0	570	8	0
45	S1	16	0	0	1	0
45	S7	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	S8	16	0	0	0	0
45	V1	8	0	0	2	0
46	V1	31	0	19	1	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	5	0
50	AA	34	0	40	7	0
50	B9	31	0	34	3	0
51	A8	25	0	24	1	0
51	D1	19	0	12	0	0
51	D4	40	0	54	2	0
51	D5	38	0	50	4	0
52	D5	36	0	16	2	0
53	D4	28	0	30	0	0
All	All	65403	0	65644	970	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 7.

The worst 5 of 970 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)
5:S3:38:GLN:O	15:A7:70:SER:HA	1.62	0.98
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.62	0.97
5:S3:38:GLN:HA	15:A7:70:SER:O	1.78	0.82
3:S1:266:LYS:O	3:S1:270:ALA:HB2	1.79	0.81
37:B7:108:LEU:O	37:B7:112:LYS:HB2	1.80	0.81

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 PDB entries followed by that with respect to all EM entries.

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	V1	428/445 (96%)	380 (89%)	48 (11%)	0	100	100
2	V2	210/217 (97%)	166 (79%)	44 (21%)	0	100	100
3	S1	686/704 (97%)	619 (90%)	66 (10%)	1 (0%)	53	87
4	S2	423/430 (98%)	373 (88%)	50 (12%)	0	100	100
5	S3	206/228 (90%)	174 (84%)	32 (16%)	0	100	100
6	S7	154/179 (86%)	135 (88%)	19 (12%)	0	100	100
7	S8	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
8	V3	38/75 (51%)	29 (76%)	9 (24%)	0	100	100
9	S6	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
10	S4	124/133 (93%)	105 (85%)	19 (15%)	0	100	100
11	A9	284/338 (84%)	253 (89%)	31 (11%)	0	100	100
12	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
13	A5	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
14	A6	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
15	A7	90/112 (80%)	80 (89%)	10 (11%)	0	100	100
16	AL	141/145 (97%)	112 (79%)	29 (21%)	0	100	100
17	AA	78/88 (89%)	66 (85%)	12 (15%)	0	100	100
17	AB	85/88 (97%)	75 (88%)	10 (12%)	0	100	100
18	D3	93/115 (81%)	84 (90%)	9 (10%)	0	100	100
19	D1	293/318 (92%)	264 (90%)	29 (10%)	0	100	100
20	D6	167/175 (95%)	141 (84%)	25 (15%)	1 (1%)	27	68
21	4L	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	17	58
22	D5	604/606 (100%)	537 (89%)	67 (11%)	0	100	100
23	D4	457/459 (100%)	418 (92%)	38 (8%)	1 (0%)	49	84
24	D2	345/347 (99%)	320 (93%)	25 (7%)	0	100	100
25	AK	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
26	B5	137/143 (96%)	125 (91%)	12 (9%)	0	100	100
27	A8	169/171 (99%)	139 (82%)	30 (18%)	0	100	100
28	BJ	169/175 (97%)	153 (90%)	16 (10%)	0	100	100
29	AJ	317/320 (99%)	279 (88%)	38 (12%)	0	100	100
30	S5	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
31	A3	72/83 (87%)	63 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B3	71/97 (73%)	60 (84%)	11 (16%)	0	100	100
33	C2	117/120 (98%)	105 (90%)	12 (10%)	0	100	100
34	B4	126/128 (98%)	108 (86%)	18 (14%)	0	100	100
35	AM	137/143 (96%)	122 (89%)	15 (11%)	0	100	100
36	B6	92/127 (72%)	80 (87%)	12 (13%)	0	100	100
37	B7	117/136 (86%)	97 (83%)	20 (17%)	0	100	100
38	B9	174/178 (98%)	142 (82%)	32 (18%)	0	100	100
39	B2	63/72 (88%)	55 (87%)	8 (13%)	0	100	100
40	B8	155/158 (98%)	127 (82%)	27 (17%)	1 (1%)	27	68
41	BK	100/125 (80%)	88 (88%)	12 (12%)	0	100	100
42	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
43	B1	50/57 (88%)	43 (86%)	7 (14%)	0	100	100
44	A1	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
All	All	7983/8509 (94%)	7022 (88%)	956 (12%)	5 (0%)	56	87

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	D4	53	SER
20	D6	137	SER
21	4L	3	LEU
3	S1	359	ARG
40	B8	143	GLY

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 PDB entries followed by that with respect to all EM entries.

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	V1	344/354 (97%)	341 (99%)	3 (1%)	81	90
2	V2	182/183 (100%)	181 (100%)	1 (0%)	90	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S1	578/588 (98%)	574 (99%)	4 (1%)	85	92
4	S2	370/371 (100%)	367 (99%)	3 (1%)	83	91
5	S3	189/204 (93%)	189 (100%)	0	100	100
6	S7	132/150 (88%)	131 (99%)	1 (1%)	83	91
7	S8	151/151 (100%)	150 (99%)	1 (1%)	85	92
8	V3	39/68 (57%)	36 (92%)	3 (8%)	14	46
9	S6	79/80 (99%)	78 (99%)	1 (1%)	71	86
10	S4	113/119 (95%)	112 (99%)	1 (1%)	81	90
11	A9	249/292 (85%)	245 (98%)	4 (2%)	65	83
12	A2	73/81 (90%)	72 (99%)	1 (1%)	69	85
13	A5	99/101 (98%)	99 (100%)	0	100	100
14	A6	107/113 (95%)	107 (100%)	0	100	100
15	A7	82/94 (87%)	82 (100%)	0	100	100
16	AL	129/131 (98%)	124 (96%)	5 (4%)	35	65
17	AA	74/81 (91%)	73 (99%)	1 (1%)	69	85
17	AB	80/81 (99%)	79 (99%)	1 (1%)	71	86
18	D3	88/103 (85%)	87 (99%)	1 (1%)	76	87
19	D1	263/278 (95%)	261 (99%)	2 (1%)	83	91
20	D6	140/144 (97%)	140 (100%)	0	100	100
21	4L	87/87 (100%)	85 (98%)	2 (2%)	53	76
22	D5	539/539 (100%)	533 (99%)	6 (1%)	76	87
23	D4	412/412 (100%)	407 (99%)	5 (1%)	74	87
24	D2	315/315 (100%)	310 (98%)	5 (2%)	65	83
25	AK	101/101 (100%)	99 (98%)	2 (2%)	58	79
26	B5	122/125 (98%)	121 (99%)	1 (1%)	83	91
27	A8	154/154 (100%)	150 (97%)	4 (3%)	49	73
28	BJ	155/157 (99%)	154 (99%)	1 (1%)	87	93
29	AJ	283/284 (100%)	280 (99%)	3 (1%)	76	87
30	S5	88/94 (94%)	87 (99%)	1 (1%)	76	87
31	A3	65/71 (92%)	65 (100%)	0	100	100
32	B3	55/75 (73%)	54 (98%)	1 (2%)	62	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	C2	106/107 (99%)	106 (100%)	0	100	100
34	B4	114/114 (100%)	113 (99%)	1 (1%)	81	90
35	AM	119/121 (98%)	115 (97%)	4 (3%)	40	68
36	B6	92/121 (76%)	89 (97%)	3 (3%)	41	68
37	B7	108/119 (91%)	104 (96%)	4 (4%)	37	66
38	B9	159/160 (99%)	156 (98%)	3 (2%)	60	80
39	B2	59/62 (95%)	59 (100%)	0	100	100
40	B8	142/142 (100%)	140 (99%)	2 (1%)	69	85
41	BK	93/112 (83%)	91 (98%)	2 (2%)	55	77
42	C1	42/44 (96%)	42 (100%)	0	100	100
43	B1	48/53 (91%)	48 (100%)	0	100	100
44	A1	59/59 (100%)	56 (95%)	3 (5%)	26	59
All	All	7078/7395 (96%)	6992 (99%)	86 (1%)	75	87

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	D5	357	ARG
24	D2	311	MET
40	B8	9	LEU
23	D4	43	ASN
23	D4	144	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
22	D5	136	ASN
22	D5	580	GLN
40	B8	66	HIS
22	D5	194	ASN
22	D5	405	ASN

5.3.3 RNA ⓘ

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](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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
51	3PE	A8	301	-	24,24,50	0.43	0	27,29,55	0.36	0
49	NDP	A9	401	-	45,52,52	0.60	0	54,80,80	0.61	2 (3%)
50	ZMP	AA	101	17	27,33,36	0.73	1 (3%)	33,40,45	0.94	1 (3%)
50	ZMP	B9	201	17	24,30,36	0.72	0	30,37,45	1.00	2 (6%)
51	3PE	D1	501	-	18,18,50	0.41	0	21,23,55	0.43	0
51	3PE	D4	501	-	39,39,50	0.33	0	42,44,55	0.32	0
53	PC1	D4	502	-	27,27,53	0.39	0	33,35,61	0.38	0
52	CDL	D5	901	-	35,35,99	0.42	0	41,47,111	0.72	2 (4%)
51	3PE	D5	902	-	37,37,50	0.35	0	40,42,55	0.34	0
45	SF4	S1	801	3	0,12,12	0.00	-	-		
45	SF4	S1	802	3	0,12,12	0.00	-	-		
47	FES	S1	803	3	0,4,4	0.00	-	-		
45	SF4	S7	300	6	0,12,12	0.00	-	-		
45	SF4	S8	201	7	0,12,12	0.00	-	-		
45	SF4	S8	202	7	0,12,12	0.00	-	-		
45	SF4	V1	500	1	0,12,12	0.00	-	-		
46	FMN	V1	501	-	31,33,33	1.42	4 (12%)	40,50,50	2.58	5 (12%)
47	FES	V2	300	2	0,4,4	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
51	3PE	A8	301	-	-	5/28/28/54	-
49	NDP	A9	401	-	-	14/30/77/77	0/5/5/5
50	ZMP	AA	101	17	-	14/38/40/43	-
50	ZMP	B9	201	17	-	11/35/37/43	-
51	3PE	D1	501	-	-	10/20/20/54	-
51	3PE	D4	501	-	-	7/43/43/54	-
53	PC1	D4	502	-	-	8/31/31/57	-
52	CDL	D5	901	-	-	16/42/42/110	-
51	3PE	D5	902	-	-	9/41/41/54	-
45	SF4	S1	801	3	-	-	0/6/5/5
45	SF4	S1	802	3	-	-	0/6/5/5
47	FES	S1	803	3	-	-	0/1/1/1
45	SF4	S7	300	6	-	-	0/6/5/5
45	SF4	S8	201	7	-	-	0/6/5/5
45	SF4	S8	202	7	-	-	0/6/5/5
45	SF4	V1	500	1	-	-	0/6/5/5
46	FMN	V1	501	-	-	10/18/18/18	0/3/3/3
47	FES	V2	300	2	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	V1	501	FMN	C4A-C10	5.35	1.44	1.38
46	V1	501	FMN	C4-N3	3.06	1.38	1.33
50	AA	101	ZMP	C9-C10	2.46	1.53	1.50
46	V1	501	FMN	C4A-N5	-2.10	1.30	1.33
46	V1	501	FMN	C5A-N5	2.09	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	V1	501	FMN	C4-N3-C2	12.79	125.94	115.14
46	V1	501	FMN	C4A-C4-N3	-6.91	113.84	123.47
46	V1	501	FMN	C10-C4A-N5	4.33	124.43	121.25
46	V1	501	FMN	C4-C4A-C10	-3.41	117.43	119.95
46	V1	501	FMN	C4A-C10-N10	-3.40	116.81	120.30

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

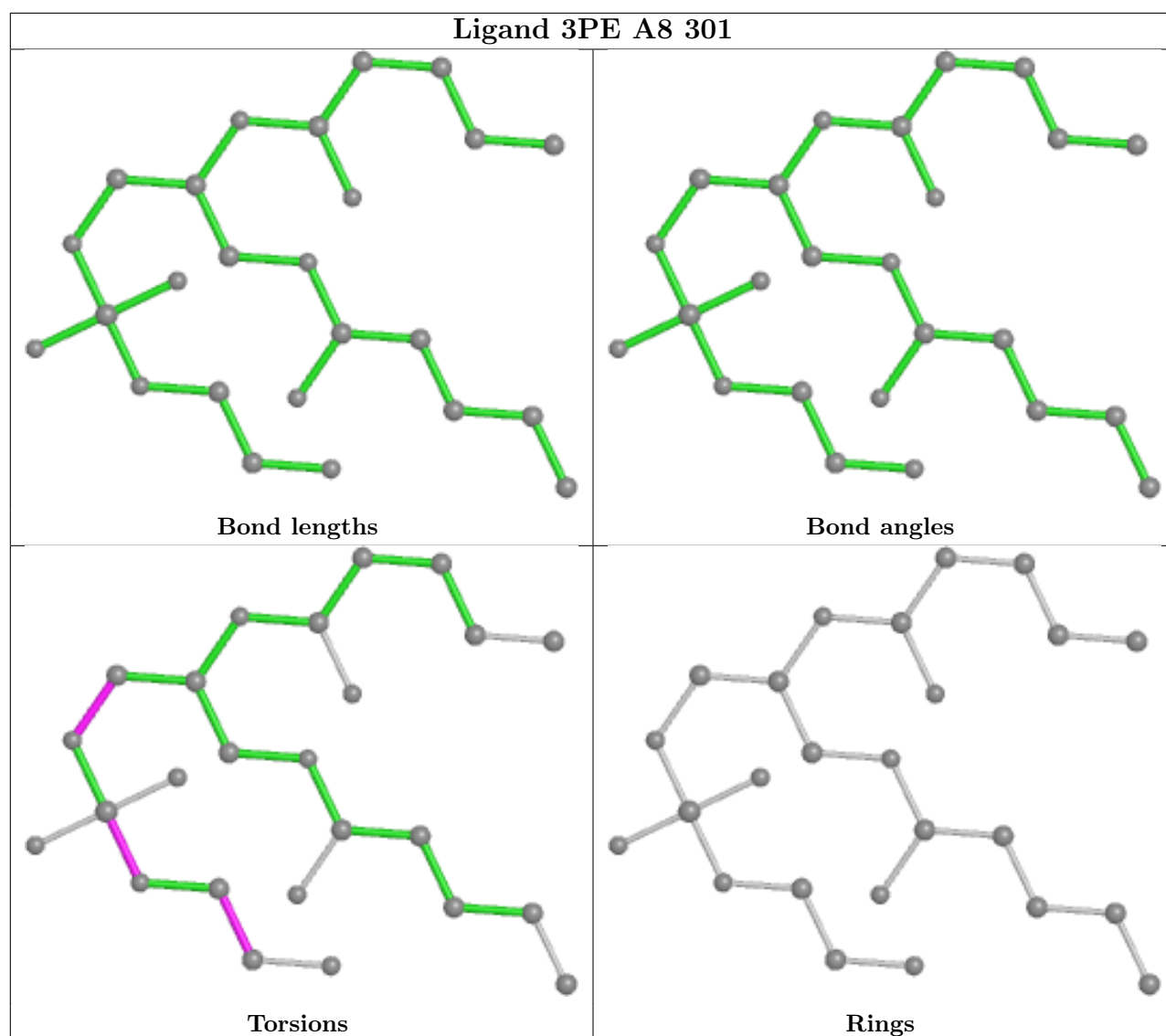
Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	N10-C1'-C2'-O2'
46	V1	501	FMN	C1'-C2'-C3'-O3'
46	V1	501	FMN	C5'-O5'-P-O1P
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P

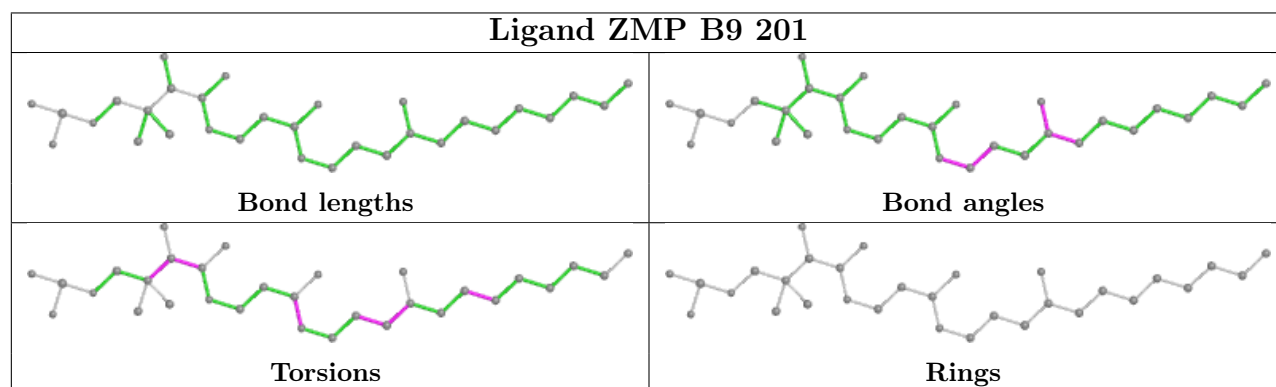
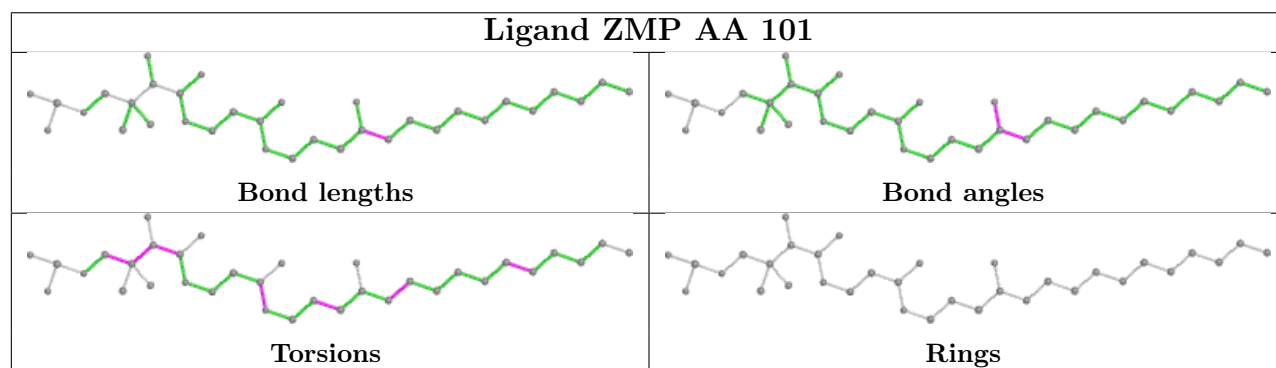
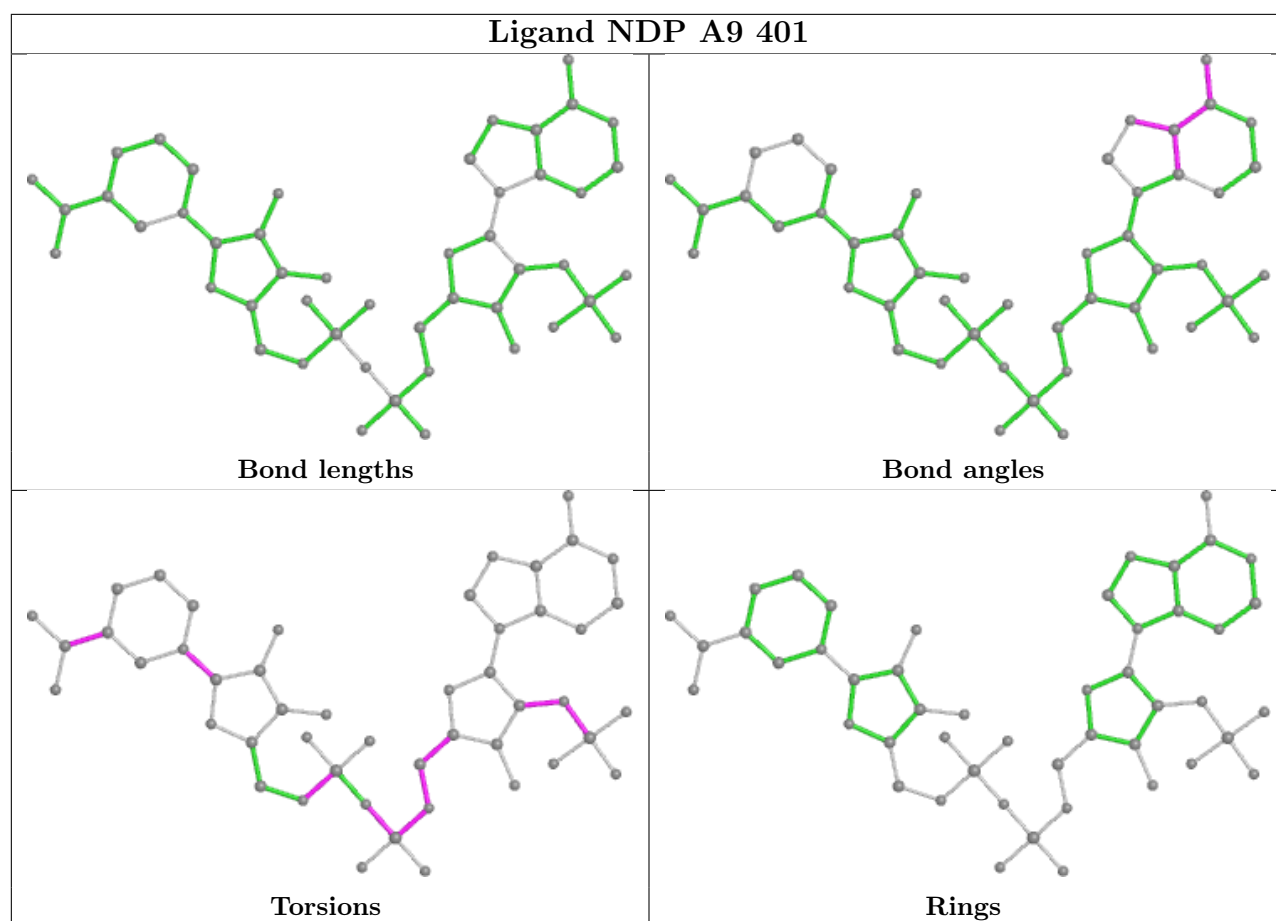
There are no ring outliers.

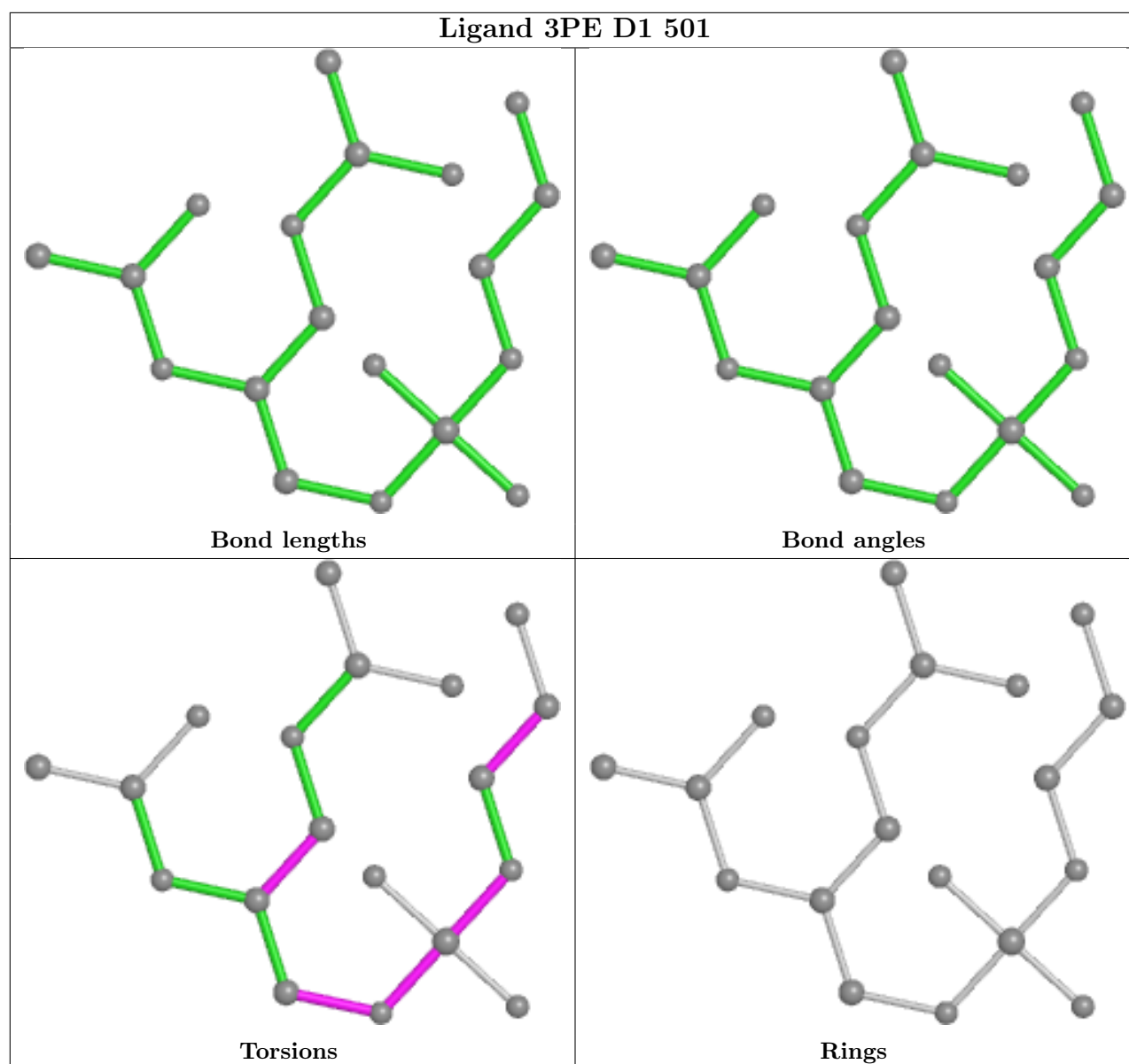
10 monomers are involved in 28 short contacts:

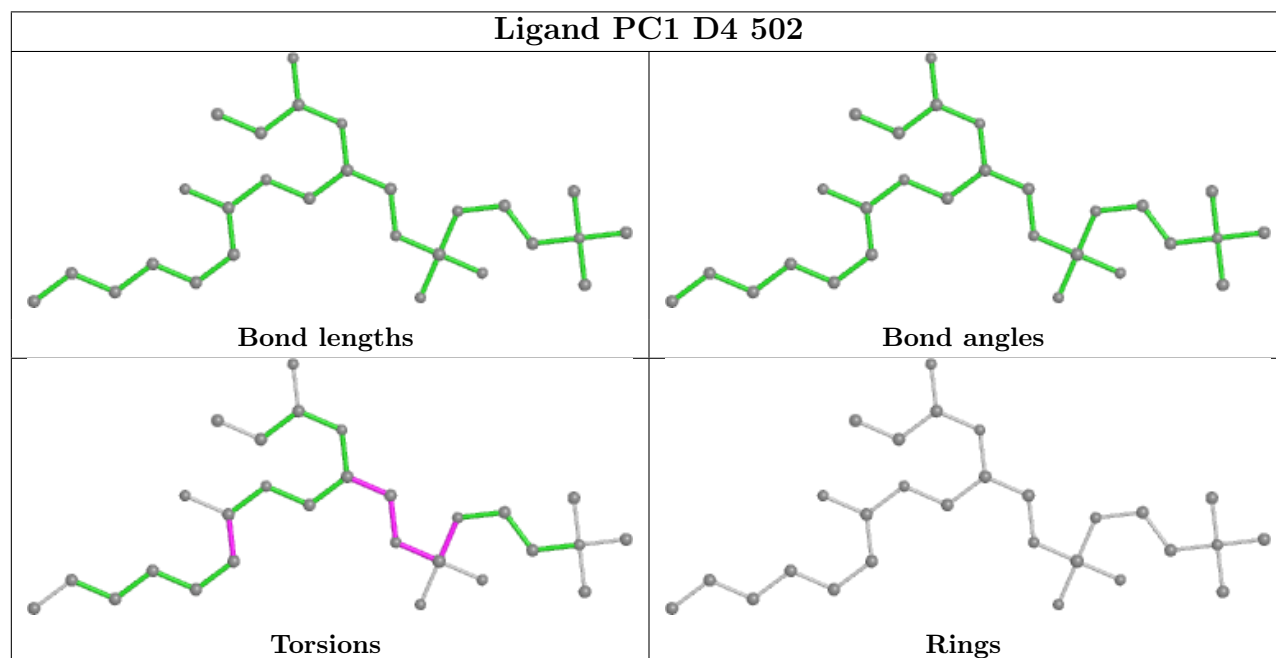
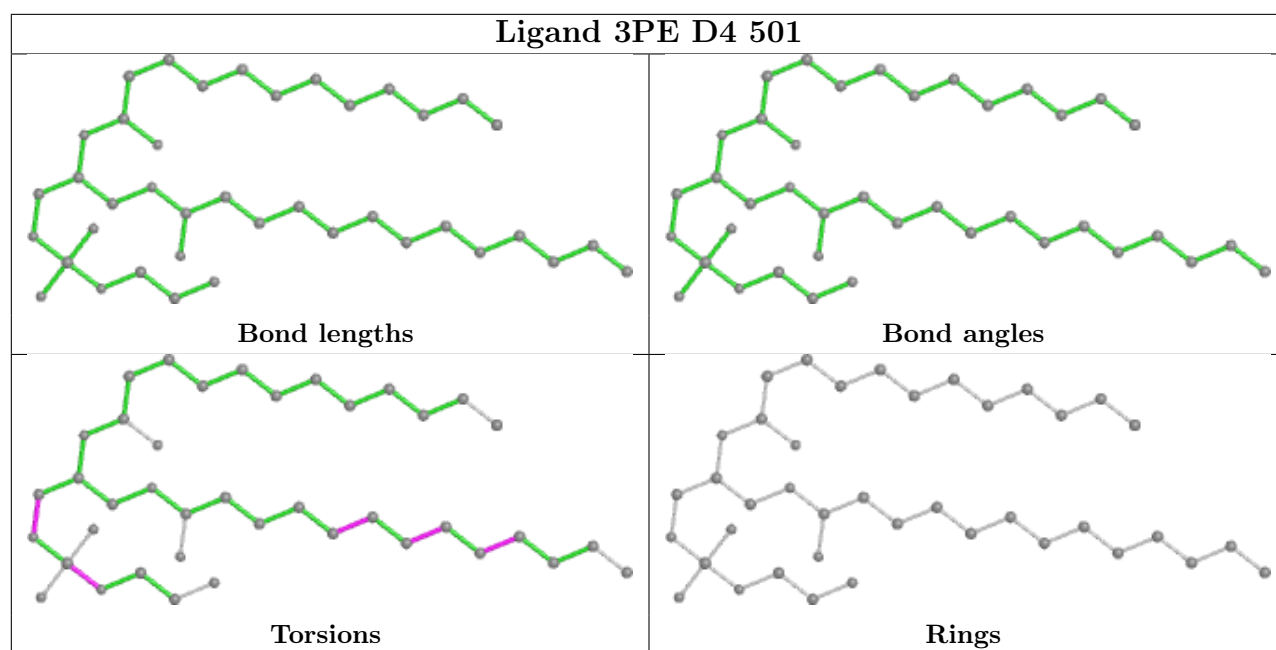
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	A8	301	3PE	1	0
49	A9	401	NDP	5	0
50	AA	101	ZMP	7	0
50	B9	201	ZMP	3	0
51	D4	501	3PE	2	0
52	D5	901	CDL	2	0
51	D5	902	3PE	4	0
45	S1	801	SF4	1	0
45	V1	500	SF4	2	0
46	V1	501	FMN	1	0

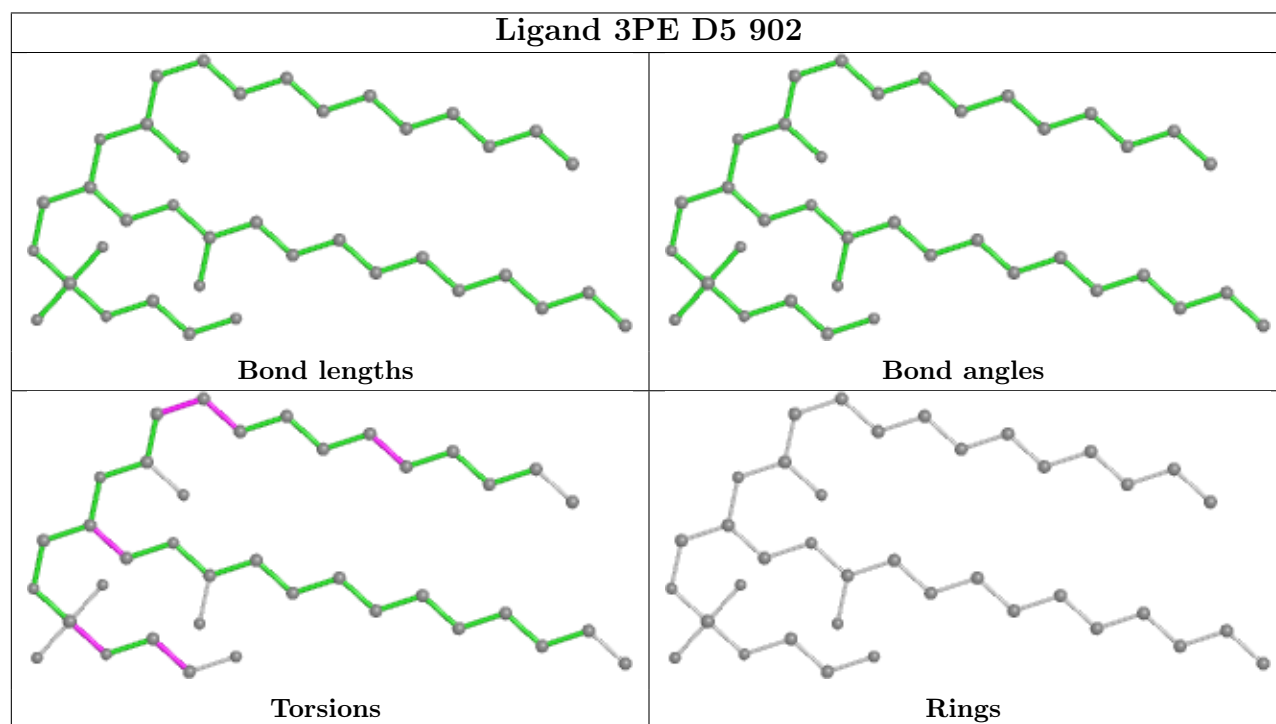
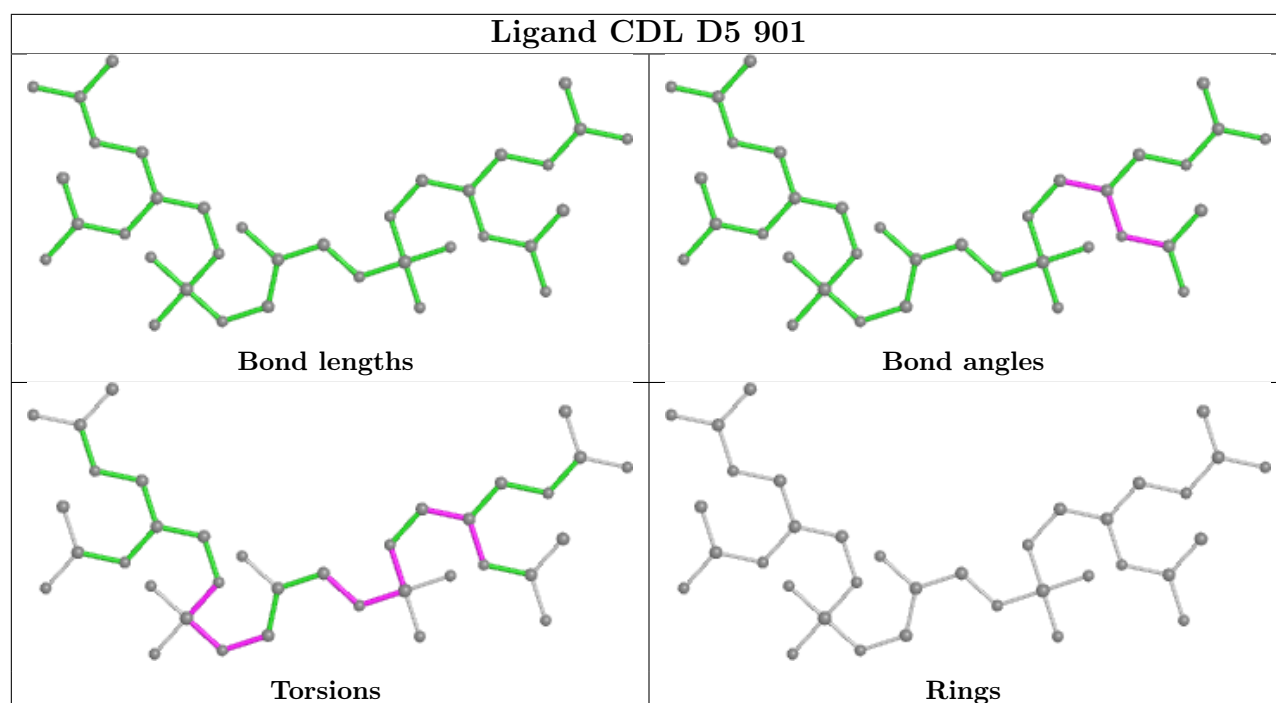
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

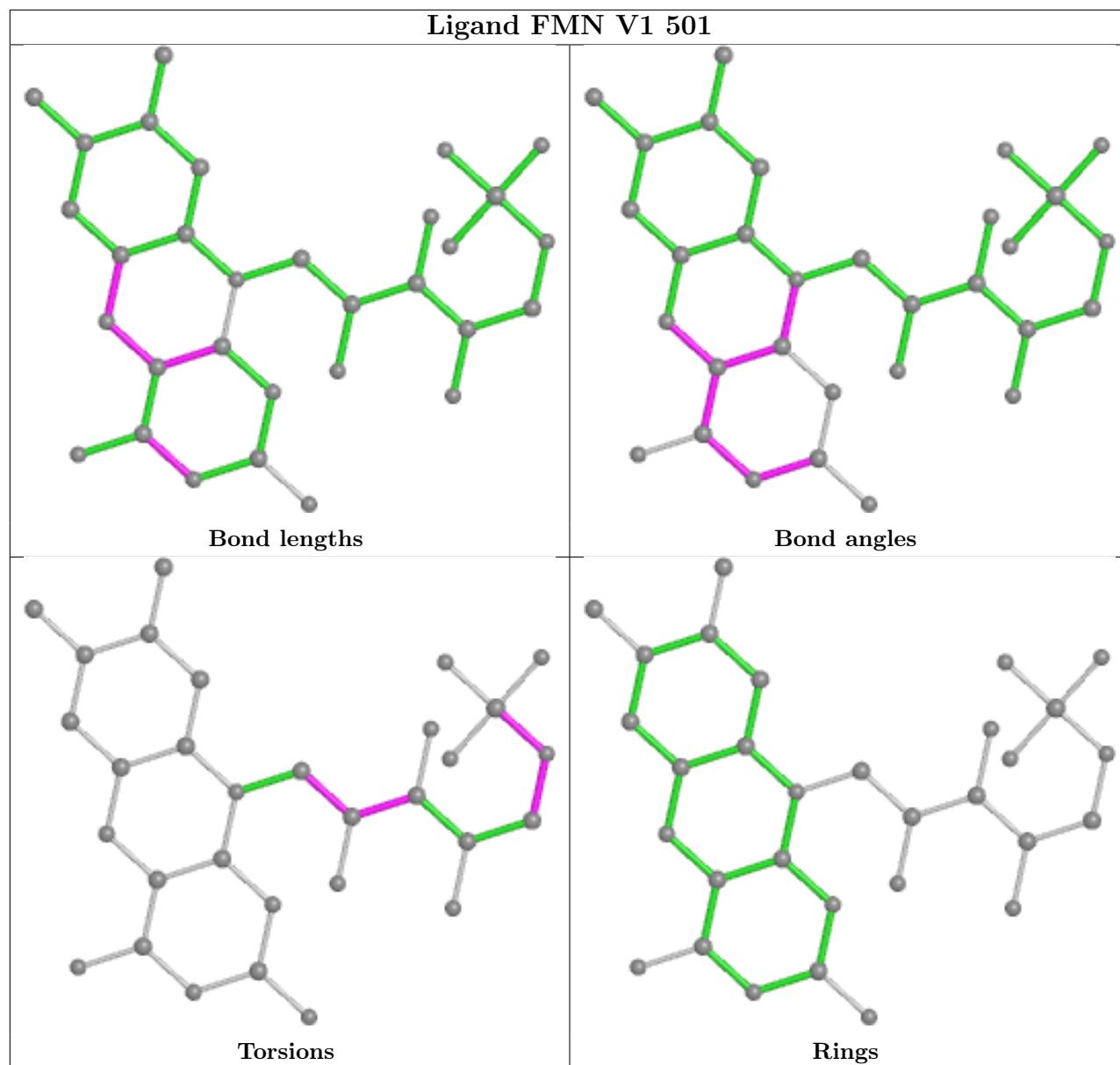












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.