



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 12:16 am BST

PDB ID : 1PJL  
Title : Crystal structure of human m-NAD-ME in ternary complex with NAD and Lu<sup>3+</sup>  
Authors : Yang, Z.; Batra, R.; Floyd, D.L.; Hung, H.-C.; Chang, G.-G.; Tong, L.  
Deposited on : 2003-06-03  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.11

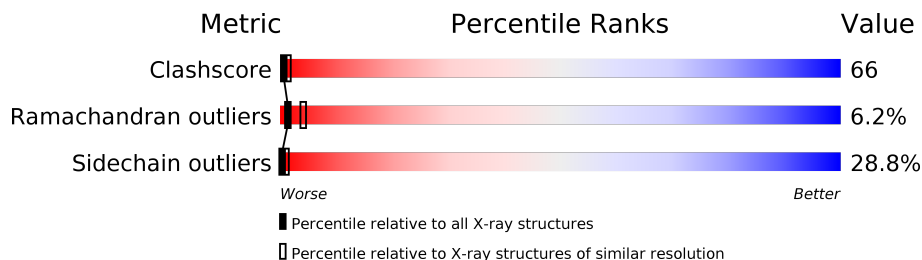
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	21% 52% 21% • 6%
1	B	584	20% 49% 25% • 6%
1	C	584	23% 47% 23% • 6%
1	D	584	20% 49% 24% • 6%
1	E	584	22% 53% 19% • 6%
1	F	584	24% 50% 19% • 6%
1	G	584	17% 54% 22% • 6%
1	H	584	23% 50% 20% • 6%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 35527 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 NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	551	4344	2781	738	802	9	14	0	0	0
1	B	551	4344	2781	738	802	9	14	0	0	0
1	C	551	4344	2781	738	802	9	14	0	0	0
1	D	551	4344	2781	738	802	9	14	0	0	0
1	E	551	4344	2781	738	802	9	14	0	0	0
1	F	551	4344	2781	738	802	9	14	0	0	0
1	G	551	4344	2781	738	802	9	14	0	0	0
1	H	551	4344	2781	738	802	9	14	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1001	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1029	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1038	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1047	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1075	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1086	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1177	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1327	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1539	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2001	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2029	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2038	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2047	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2075	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2086	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2108	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2177	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2219	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2239	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2325	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2327	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2343	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2407	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2539	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3001	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3029	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3038	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3047	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3075	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3086	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3108	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3177	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3219	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3239	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3325	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3327	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3343	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3407	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3539	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4001	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4029	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4038	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4047	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4075	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4086	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4108	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4177	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4219	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4239	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4325	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4327	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4343	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4407	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4539	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5001	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5029	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5038	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5047	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5075	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5086	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5108	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5177	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5219	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5239	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5325	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5327	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5343	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5407	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5539	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6001	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6029	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6038	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6047	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6075	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6086	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6108	MSE	MET	MODIFIED RESIDUE	UNP P23368

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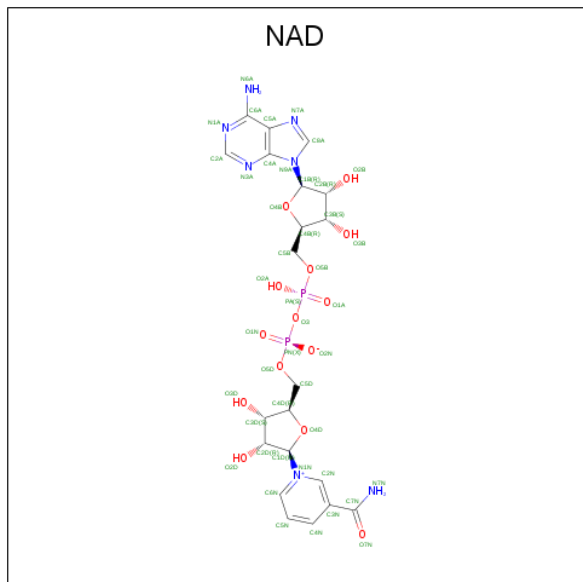
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Chain	Residue	Modelled	Actual	Comment	Reference
G	6177	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6219	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6239	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6325	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6327	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6343	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6407	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6539	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7001	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7029	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7038	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7047	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7075	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7086	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7108	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7177	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7219	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7239	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7325	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7327	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7343	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7407	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Lu 1 1	0	0
2	D	1	Total Lu 1 1	0	0
2	E	1	Total Lu 1 1	0	0
2	H	1	Total Lu 1 1	0	0
2	B	1	Total Lu 1 1	0	0
2	C	1	Total Lu 1 1	0	0
2	A	1	Total Lu 1 1	0	0
2	F	1	Total Lu 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	17	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	18	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	18	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	6	Total	O	0	0
			6	6		
4	C	11	Total	O	0	0
			11	11		
4	D	6	Total	O	0	0
			6	6		
4	E	6	Total	O	0	0
			6	6		
4	F	10	Total	O	0	0
			10	10		
4	G	5	Total	O	0	0
			5	5		
4	H	10	Total	O	0	0
			10	10		

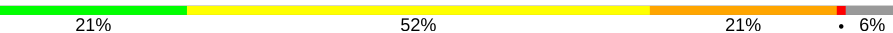


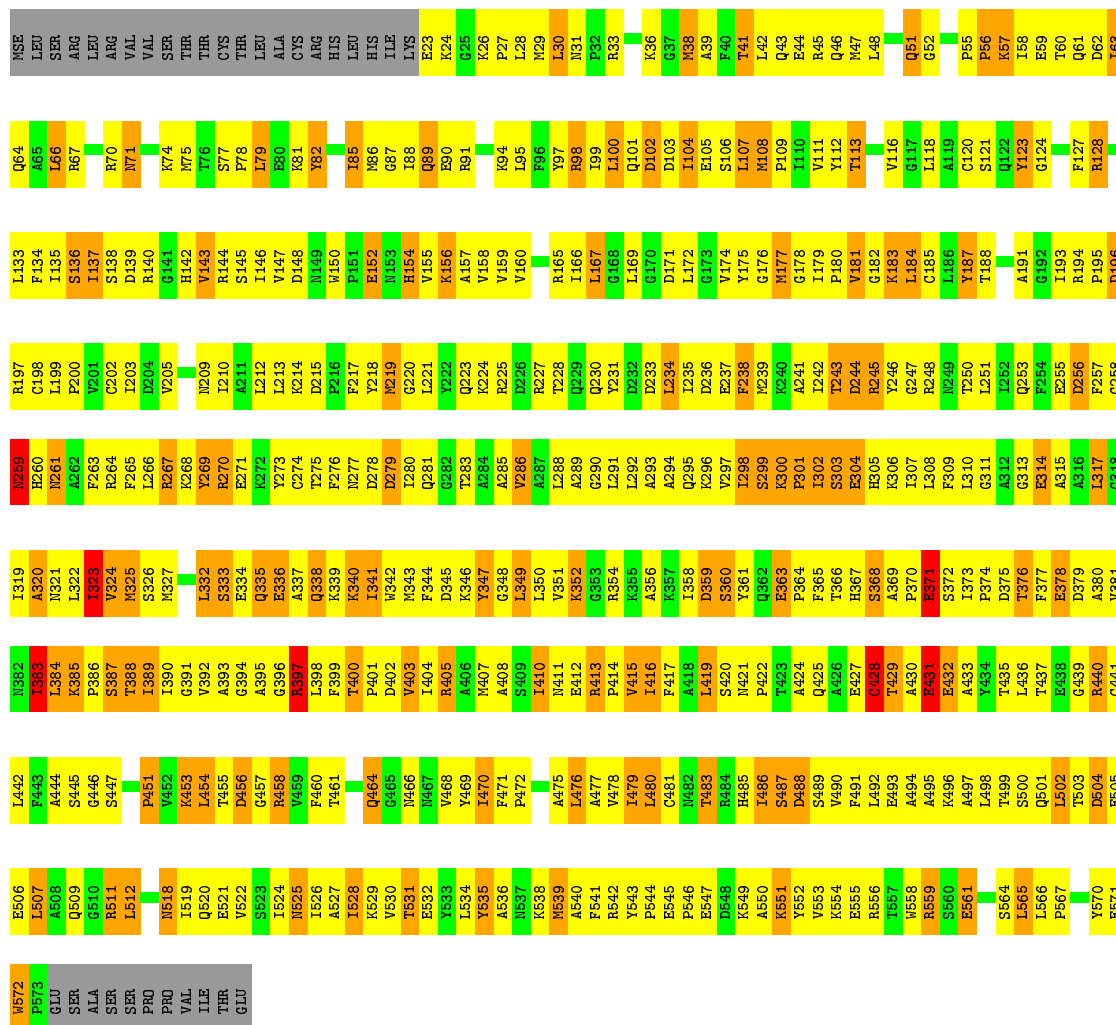
### 3 Residue-property plots

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.

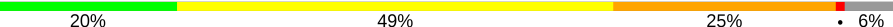
Note EDS was not executed.

- Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain A: 

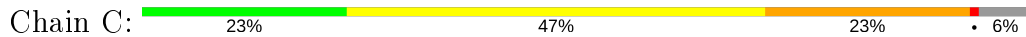


- Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain B: 

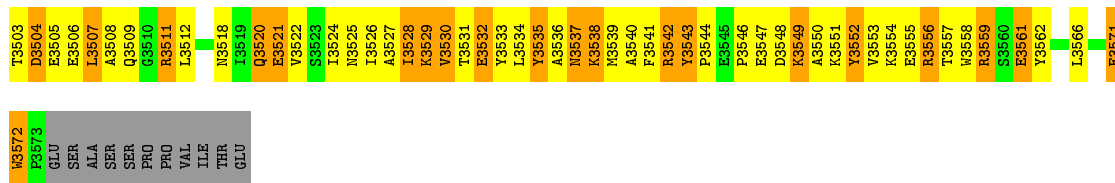
MSE	LEU	ARG	ARG	LEU	ARG	VAL	VAL	SER	THR	THR	CYS	THR	THR	LEU	ALA	CYS	ARG	HIS	HIS	HIS	LYS	E1023	K1024	K1026	K1027	L1028	E1029	L1030	M1031	R1032	R1033	T1034	M1035	K1036	G1037	M1038	A1039	F1040	T1041	L1042	L1043	E1044	R1045	Q1046	M1047	L1048	G1049	L1050	Q1051	G1052	L1053	L1054	P1055	P1056	K1057	L1058	E1059	T1060																																																															
Q1061	R1129	F1150	K1131	G1132	F1133	L1134	L1135	S1136	I1137	S1138	D1139	R1140	V1143	R1144	S1145	S1146	L1147	V1147	D1148	M1149	W1150	E1151	H1152	H1153	H1154	V1155	K1156	M1159	V1160	T1161	D1162	G1163	R1164	R1165	Q1166	L1167	G1168	L1169	G1170	D1171	L1172	L1173	M1174	G1175	Y1176	T1113	Y1112	M1116	G1117	L1118	S1121	Q1122	L1123	G1124	P1125	H1125	L1126	F1127	R1128																																																														
R1194	P1195	D1196	R1197	C1198	L1199	P1200	V1201	C1202	I1203	D1204	V1205	G1206	T1207	D1208	M1209	I1210	A1211	L1212	L1213	K1214	D1215	P1216	F1217	Y1218	M1219	G1220	L1221	Q1222	Q1223	K1224	R1225	D1226	R1227	T1228	Q1229	Q1230	L1231	D1232	D1233	L1234	I1235	D1236	E1237	F1238	M1239	K1240	A1241	I1242	T1243	D1244	R1245	Y1246	L1247	K1248	M1249	T1250	L1251	L1252	Q1253																																																														
F1254	E1255	D1256	F1257	M1258	H1259	H1260	M1261	A1262	F1263	R1264	F1265	L1266	R1267	Y1268	Y1269	R1270	E1271	K1272	Y1273	D1274	F1275	T1276	M1277	D1278	D1279	I1280	Q1281	G1282	Y1283	L1284	A1285	V1286	A1287	L1288	A1289	G1290	L1291	R1292	A1293	A1294	Q1295	L1296	V1297	L1298	S1299	K1300	P1301	I1302	S1303	E1304	H1305	K1306	I1307	A1308	L1309	P1310	L1311	G1312	L1313	P1314	L1315	E1316	L1317	E1318	L1319	A1320	M1321	L1322	L1323	V1324	M1325	S1326	M1327	V1328	E1329	L1330	L1331	L1332	S1333	E1334	Q1335	E1336	Q1337	K1338	K1339	K1340	L1341	W1342	M1343	F1344	D1345	K1346	K1347	G1348	G1349	L1350	V1351	K1352	L1353	R1354	R1355	K1356	A1357	K1358	D1359	S1360	Y1361	Q1362	E1363	P1364	F1365	L1366	H1367	S1368	A1369	P1370	E1371	L1372	G1373	A1374	D1375
T1376	F1377	D1378	D1379	A1380	L1381	M1382	I1383	L1384	K1385	P1386	S1387	I1388	I1389	I1390	G1391	V1392	A1393	G1394	A1395	G1396	R1397	L1398	F1399	T1400	P1401	D1402	V1403	F1404	R1405	R1406	M1407	A1408	S1409	I1410	M1411	E1412	R1413	P1414	V1415	I1416	A1417	L1418	L1419	I1420	M1421	P1422	T1423	L1424	Q1425	A1426	E1427	T1428	T1429	A1429	A1430	E1431	E1432	A1433	Y1434	T1435																																																													
L1436	T1437	R1440	L1441	L1442	F1443	A1444	S1445	R1446	G1447	P1448	P1451	V1452	K1453	L1454	T1455	D1456	G1457	R1458	F1459	F1460	T1461	M1466	M1467	V1468	Y1469	L1470	F1471	F1472	G1473	V1474	A1475	L1476	M1477	V1478	I1479	L1480	C1481	M1482	L1483	F1484	H1485	I1486	S1487	D1488	S1489	V1490	F1491	L1492	R1493	A1494	A1495	K1496	T1499	S1500	Q1501																																																																		
L1502	T1503	D1504	E1505	ALA	LEU	SER	VAL	PRO	PRO	THR	GLU	A1517	M1518	I1519	Q1520	L1521	V1522	S1523	I1524	I1525	M1526	A1527	L1528	K1529	V1530	V1531	E1532	Y1533	L1534	Y1535	A1536	M1537	M1538	M1539	A1540	F1541	Y1542	Y1543	P1546	E1547	D1548	K1549	K1550	K1551	Y1552	Y1553	E1554	E1555	R1556	T1557	M1558	A1559	A1560	K1561	Y1570	E1571																																																																	

• Molecule 1: NAD-dependent malic enzyme, mitochondrial

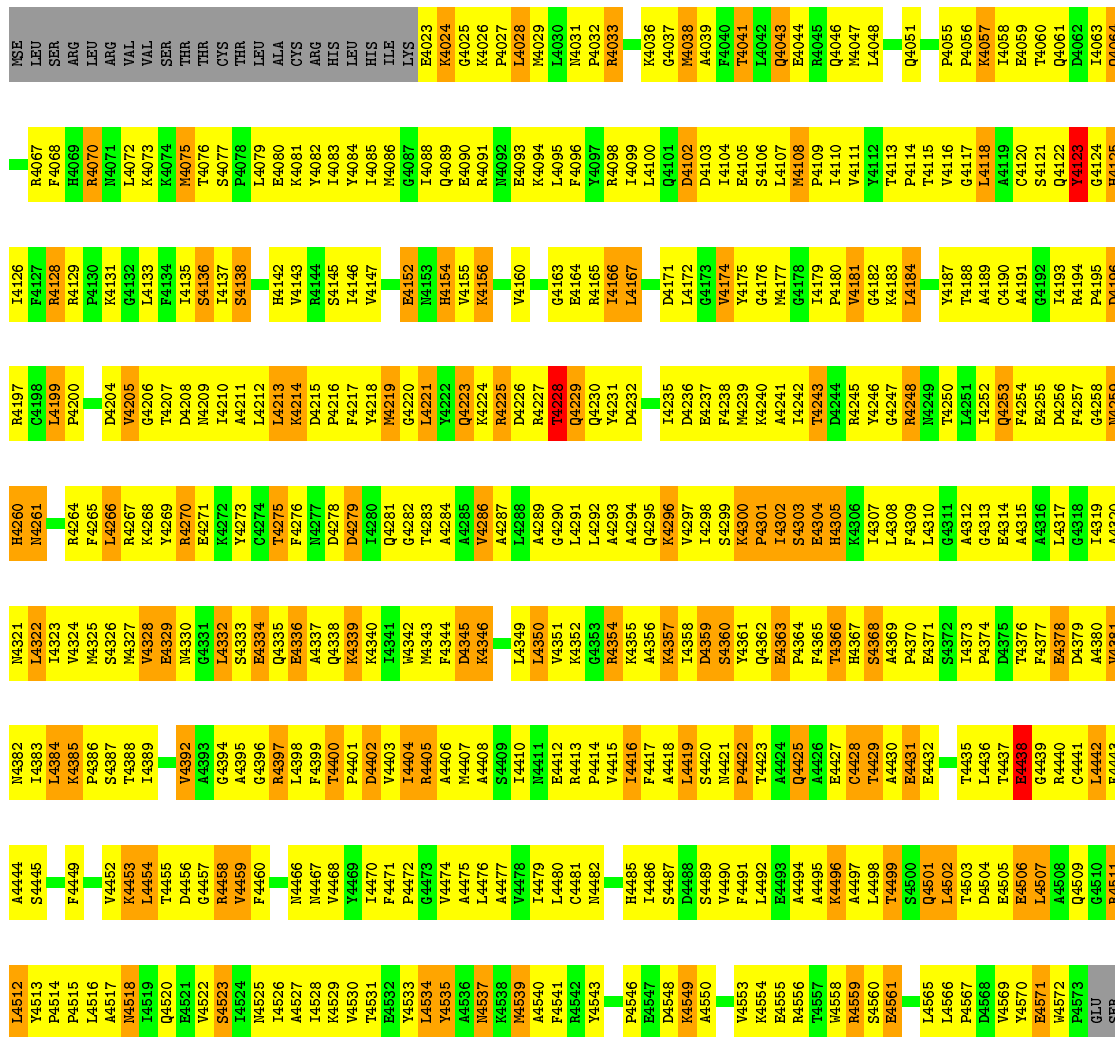


MSE	LEU	SER	ARG	LEU	ARG	VAL	VAL	SER	THR	THR	CYS	THR	THR	LEU	ALA	CYS	ARG	HIS	HIS	HIS	LYS	E2023	K2024	G2025	K2026	P2027	M2028	P2029	L2030	K2036	G2037	M2038	A2039	F2040	T2041	E2044	R2045	L2046	G2048	L2050	Q2051	L2054	P2055	P2056	K2057	L2058	E2059	T2060	Q2061	Q2062	L2063	Q2064	L2065	R2066	R2067
F2068	R2069	R2070	M2071	L2072	M2075	T2076	S2077	F2078	L2079	R2080	K2081	Y2082	L2085	M2086	G2087	L2088	Q2089	E2090	E2093	K2094	L2095	F2096	Y2097	L2099	L2100	Q2101	D2102	D2103	L2104	E2105	S2106	L2107	R2108	F2109	L2110	V2111	Y2112	T2113	P2114	T2115	L2118	A2119	C2120	S2121	Q2122	Y2123	G2124	H2125	Q2126	F2127	R2128	R2129	F2130	L2131	P2200
G2132	L2133	S2136	T2137	S2138	D2139	R2140	R2144	S2145	L2146	Y2147	D2148	M2149	W2150	P2151	E2152	L2153	H2154	V2155	K2156	V2160	T2161	D2162	E2164	L2169	G2170	D2171	L2172	G2173	Y2174	G2175	G2176	R2177	G2178	L2179	P2180	G2182	K2183	L2184	C2185	L2186	Y2187	T2188	A2189	C2190	A2191	G2192	L2193	R2194	P2195	D2196	R2197	R2200			
Y2201	G2205	G2206	T2207	D2208	N2209	T2210	A2211	L2212	L2213	K2214	F2217	Y2218	N2219	G2220	E2221	L2222	Q2223	R2224	D2225	V2226	R2227	Q2230	Y2231	D2232	D2233	L2234	L2235	F2238	Y2239	K2240	A2241	L2242	T2243	D2244	R2245	Y2246	R2248	N2249	T2250	L2251	L2252	Q2253	F2254	E2255	D2256	F2257	G2258	K2259	R2260	N2261	A2262	F2263	F2265		

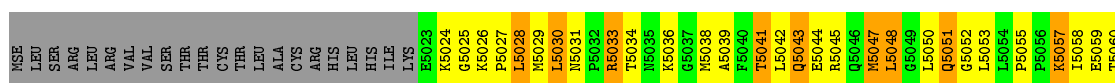
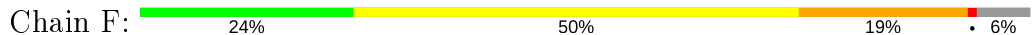




• Molecule 1: NAD-dependent malic enzyme, mitochondrial

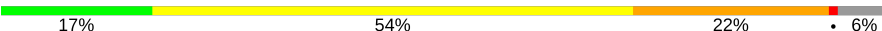


• Molecule 1: NAD-dependent malic enzyme, mitochondrial



Q5061	Y5123	G5198	N5261	L5323	P5488	R5511	SER	Q6064	L6126	I6186	M6249
R5062	G5124	L5199	R5264	Y5324	P5481	L5122	SER	A6065	F6127	Y6187	T6250
Q5064	R5125	T5388	F5265	R5327	Y5482	P5515	PRO	L6066	R6128	T6188	L6250
A5065	I5126	I5390	F5266	M6327	V5483	P5516	PRO	R6067	R6129	A6189	L6251
	R5128	G5320	R5267	E5329	K5483	L5516	VAL	F6068	F6130	G6190	Q6252
	L5133	G5204	R5268	E5391	L5454	A5517	ILE	R6069	K6131	A6191	Q6253
F5068	L5134	R5205	R5269	M5390	T5485	M5518	THR	R6070	G6132	G6192	E6255
R5070	F5135	G5206	R5270	G5331	D5486	Q5520	GLU	M6071	L6133	I6193	D6256
N5071	I5136	T5207	R5271	L5332	G5487	Q5521	SER	L6072	F6134	R6194	F6257
L5072	S5136	E5271	K5272	S5333	R5488	E5521	THR	K6073	I6135	P6195	G6258
K5073	I5137	D5208	K5273	G5334	V5489	V5522	THR	K6074	S6136	D6196	N6259
K5074	I5138	N5209	E5274	E5335	F5490	S5523	CYS	M6075	I6137	R6197	H6260
L5075	R5138	L5210	C6274	E5336	T5481	L5524	THR	T6076	S6138	C6198	M6261
	D5139	A5211	T5275	A5337	P5482	M5525	LEU	S6077	D6139	L6199	A6262
	G5140	L5212	R5276	P5401	G5483	L5526	ALA	F6078	R6140	P6200	F6263
	R5141	L5213	E5277	D5402	G5484	A5527	CYS	L6079	G6141	V6201	R6264
	H5142	K5214	D5278	V5340	G5485	I5528	ARG	E6080	K6142	D6202	L6265
	Y5143	R5279	D5279	I5341	I5404	S5529	HIS	K6081	H6143	D6203	L6266
	R5144	F5217	I5280	N5342	R5405	V5530	ARG	Y6082	R6144	V6204	L6267
	S5145	I5218	Q5281	M5343	A5406	E5531	ILE	I6083	S6145	G6206	R6268
	V5146	N5219	G5282	R5344	V5467	T5532	LEU	M6086	G6146	T6207	Y6269
	V5147	R5219	T5283	F5344	V5468	E5533	LEU	E6089	H6147	D6208	M6270
	D5148	L5221	A5284	K5346	I5470	Y5533	LYS	E6090	K6148	N6209	E6271
	N5149	Y5222	A5285	K5346	F5471	L5534	ARG	M6091	L6149	I6210	R6272
		G5223	A5286	L5349	P5472	Y5535	HIS	R6092	G6150	A6211	G6273
		K5224	E5287	L5350	G5473	A5536	ILE	R6093	R6151	L6212	C6274
		R5225	L5288	L5351	V5474	M5537		M6092	G6152	L6213	T6275
		R5226	L5289	V5351	A5477	K5538		E6093	R6153	K6214	F6276
		G5227	A5290	K5352	V5478	M5539		E6094	H6154	R6215	N6277
		G5228	G5291	E5353	V5479	E5540		K6095	L6155	F6217	D6278
		T5228	L5291	E5354	L5479	F5541		L6096	V6156	Y6218	D6279
		G5229	L5292	K5355	L5480	R5542		F6097	A6157	M6219	L6280
		Q5230	A5293	K5356	C5481	Y5543		R6098	G6158	G6220	G6281
		Y5231	A5294	K5357	S5420	P5544		L6099	V6159	V6158	G6282
			L5234	D5359	R5484	K5549		L6100	L6160	L6160	G6283
			L5235	S5360	E5485	A5550		Q6101	Q6101	Y6222	A6284
				Y5361	S5487	K5551		D6102	D6162	K6224	A6285
				Q5362	R5488	Y5552		D6103	G6163	R6225	V6286
				E5363	S5489	K5553		E6104	R6165	D6226	A6287
				E5364	V5490	K5554		L6106	I6166	R6227	L6288
				F5365	L5492	E5555		L6107	L6167	G6230	A6289
				E5366	F5491	L5492		L6108	L6168	Y6231	G6290
				E5367	E5493	E5493		P6109	L6169	D6232	L6291
				S5368	A5494	A5494		I6110	G6170	D6233	L6292
				A5369	R5496	Y5496		V6111	L6171	L6234	A6294
				S5372	A5497	D5562		Y6112	L6172	I6235	Q6295
				L5373	L5498	S5564		T6113	G6173	D6236	G6296
				P5374	T5499	L5565		P6114	V6174	E6237	V6297
				Y5375	S5500	L5566		T6115	G6175	F6238	L6298
				R5376	Q5501	P5567		V6116	G6176	M6239	S6299
				F5377	L5502	D5568		G6117	M6177	K6240	R6300
				E5378	T5503	L6568		L6118	O6178	A6241	P6301
				D5379	D6504	Y5570		A6119	I6179	I6242	L6302
				L5442	E5505	E5571		G6120	P6180	T6243	S6303
				V5381	E5506	M5572		S6121	G6181	D6244	B6304
				M5382	L5507	F6573		Q6122	G6182	R6245	H6305
				L5383	S5445	GLU		Y6123	L6183	Y6246	R6306
				L5384	L5364	SER		G6124	L6184	L6247	L6307
				L5385	K5385	ALA		H6125	L6063	R6248	L6308

- Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain G:  17% 54% 22% 6%

NSE	L6024	Q6064	L6126	I6186	M6249
LEU	G6024	A6065	F6127	Y6187	T6250
SER	L6024	L6066	R6128	T6188	L6250
PRO	L6024	R6067	R6129	A6189	L6251
VAL	L6024	F6068	F6130	G6190	Q6252
THR	L6024	R6069	K6131	A6191	Q6253
ILE	L6024	R6070	G6132	G6192	E6255
GLU	L6024	M6071	L6133	I6193	D6256
	L6024	L6072	F6134	R6194	F6257
	L6024	K6073	I6135	P6195	G6258
	L6024	K6074	S6136	D6196	N6259
	L6024	M6075	I6137	R6197	H6260
	L6024	T6076	S6138	C6198	M6261
	L6024	S6077	D6139	L6199	A6262
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	L6024	L6079	G6141	V6201	R6264
	L6024	E6080	H6142	D6202	L6265
	L6024	K6081	H6143	D6203	L6266
	L6024	Y6082	R6144	V6204	L6267
	L6024	I6083	S6145	G6206	R6268
	L6024	M6086	G6146	T6207	Y6269
	L6024	Q6089	H6147	D6208	M6270
	L6024	E6090	K6148	N6209	E6271
	L6024	R6091	L6149	I6210	R6272
	L6024	R6092	G6150	A6211	G6273
	L6024	R6093	R6151	L6212	C6274
	L6024	M6092	G6152	L6213	T6275
	L6024	E6093	R6153	K6214	F6276
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	L6024	F6096	V6156	Y6218	D6279
	L6024	Y6097	A6157	M6219	L6280
	L6024	R6098	G6158	G6220	G6281
	L6024	L6099	V6159	V6158	G6282
	L6024	L6100	L6160	L6160	G6283
	L6024	Q6101	Q6101	Y6222	A6284
	L6024	D6102	D6162	K6224	A6285
	L6024	D6103	G6163	R6225	V6286
	L6024	E6104	R6165	D6226	A6287
	L6024	L6106	I6166	R6227	L6288
	L6024	L6107	L6167	G6230	A6289
	L6024	L6108	L6168	Y6231	G6290
	L6024	P6109	L6169	D6232	L6291
	L6024	I6110	G6170	D6233	L6292
	L6024	V6111	L6171	L6234	A6294
	L6024	Y6112	L6172	I6235	Q6295
	L6024	T6113	G6173	D6236	G6296
	L6024	P6114	V6174	E6237	V6297
	L6024	T6115	G6175	F6238	L6298
	L6024	V6116	G6176	M6239	S6299
	L6024	G6117	M6177	K6240	R6300
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	L6024	Y6123	L6183	Y6246	R6306
	L6024	G6124	L6184	L6247	L6307
	L6024	H6125	L6063	R6248	L6308

L6309	L6310	L6311	L6312	L6313	L6314	L6315	L6316	L6317	L6318	L6319	L6320	L6321	L6322	L6323	L6324	L6325	L6326	L6327	L6328	L6329	L6330	L6331	L6332	L6333	L6334	L6335	L6336	L6337	L6338	L6339	L6340	L6341	L6342	L6343	L6344	L6345	L6346	L6347	L6348	L6349	L6350	L6351	L6352	L6353	L6354	L6355	L6356	L6357	L6358	L6359	L6360	L6361	L6362	L6363	L6364	L6365	L6366	L6367	L6368	L6369										
P6370	E6371	S6372	I6373	P6374	D6375	T6376	F6377	D6378	D6379	A6380	V6381	I6382	I6383	L6384	L6385	L6386	S6387	S6388	I6389	I6390	G6391	V6392	A6393	G6394	A6395	G6396	G6397	L6398	L6399	T6400	P6401	D6402	V6403	I6404	R6405	A6406	L6407	A6408	S6409	I6410	N6411	E6412	R6413	P6414	V6415	I6416	F6417	K6418	L6419	S6420	N6421	P6422	T6423	A6424	V6425	A6426	E6427	C6428	T6429											
A6430	E6431	E6432	A6433	V6434	T6435	L6436	L6437	E6438	E6439	R6440	C6441	R6442	F6443	G6444	G6445	G6446	S6447	P6448	P6449	V6450	L6451	L6452	L6453	L6454	D6455	G6456	G6457	R6458	V6459	F6460	I6461	L6462	F6471	E6472	G6473	V6474	A6475	L6476	A6477	V6478	L6479	G6480	C6481	N6482	P6483	P6484	R6485	L6486	S6487	D6488	K6489	K6490	S6491	V6492	V6493	V6494	L6495	E6496	E6497	E6498	E6499	A6495								
K6496	A6497	L6498	L6499	S6500	G6501	L6502	L6503	D6504	E6505	R6506	L6507	A6508	Q6509	R6510	R6511	R6512	L6513	P6514	R6515	N6518	I6519	Q6520	E6521	V6522	S6523	I6524	I6525	N6526	I6527	I6528	E6529	L6530	L6531	E6532	L6533	Y6534	L6535	L6536	L6537	L6538	L6539	L6540	L6541	L6542	L6543	L6544	L6545	L6546	L6547	L6548	L6549	L6550	L6551	L6552	L6553	L6554	L6555	L6556	L6557											
L6558	R6559	S6560	E6561	V6562	L6563	E6564	E6565	E6566	E6567	E6568	E6569	E6570	E6571	E6572	E6573	GLU	SER	ALA	SER	SER	PRO	PRO	PRO	VAL	LEU	HIS	HIS	ILE	THR	GLU	N6518	I6519	Q6520	E6521	V6522	S6523	I6524	I6525	N6526	I6527	I6528	E6529	L6530	L6531	E6532	L6533	Y6534	L6535	L6536	L6537	L6538	L6539	L6540	L6541	L6542	L6543	L6544	L6545	L6546	L6547	L6548	L6549	L6550	L6551	L6552	L6553	L6554	L6555	L6556	L6557

● Molecule 1: NAD-dependent malic enzyme, mitochondrial



R5E	L5U	S5R	A5R	L5U	A5R	V5L	V5L	S5R	S5R	T5H	T5R	C5Y	T5H	L5U	A5A	A5A	C5Y	A5R	H5I	V5L	H5I	I5L	T5H	G5L	L5S	K5O24	G5O25	K5O26	F5O27	L5O28	N5O29	L5O30	I5O31	F5O32	R5O33	T5O34	R5O35	K5O36	G5O37	M5O38	A5O39	F5O40	L5O41	L5O42	L5O43	E5O44	R5O45	Q5O46	M5O47	L5O48	G5O49	L5O50	Q5O51	L5O52	L5O53	L5O54	K5O57	L5O58	E5O59	S5O60	L5O61	
D7062	I7063	L7064	L7065	L7066	L7067	F7068	H7069	R7070	N7071	L7072	M7073	T7074	S7075	F7076	P7077	L7078	L7079	E7080	K7081	Y7082	L7083	L7084	L7085	L7086	G7087	I7088	Q7089	E7090	R7091	N7092	L7093	K7094	L7095	F7096	Y7097	R7098	L7099	L7100	Q7101	D7102	L7103	L7104	E7105	S7106	L7107	M7108	P7109	I7110	I7111	L7112	L7113	P7114	L7115	L7116	L7117	L7118	L7119	C7120	S7121	L7122	Y7123	
H7124	H7125	L7126	F7127	L7128	R7129	L7130	L7131	G7132	L7133	F7134	L7135	S7136	D7139	R7140	N7141	L7142	L7143	R7144	S7145	L7146	L7147	L7148	L7149	E7150	R7151	E7152	N7153	L7154	L7155	L7156	A7157	V7158	L7159	V7160	L7161	Q7228	Q7229	Q7230	Q7231	D7232	D7233	F7238	L7239	L7240	L7241	L7242	L7243	D7244	L7245	G7246	L7247	R7248	H7249	L7250	L7251	L7252	Q7253	F7254	E7255	D7256	L7257	G7258
N7259	H7260	N7261	A7262	L7263	L7264	F7265	L7266	R7267	K7268	L7269	L7270	L7271	K7272	Y7273	C7274	L7275	F7276	N7277	D7278	D7279	Q7280	L7281	L7282	L7283	V7286	L7287	L7288	L7289	G7290	L7291	L7292	A7293	L7294	L7295	L7296	L7297	L7298	S7299	K7300	P7301	L7302	S7303	E7304	H7305	L7306	L7307	L7308	L7309	L7310	L7311	L7312	L7313	E7314	L7315	L7316	L7317	L7318	L7319				
A7320	N7321	L7322	L7323	L7324	L7325	L7326	N7327	V7328	E7329	L7332	S7333	E7334	Q7335	E7336	A7337	D7402	V7403	L7404	L7405	R7406	M7407	L7408	L7409	L7410	E7411	E7412	R7413	L7414	L7415	L7416	F7417	L7418	L7419	L7420	L7421	L7422	L7423	A7424	Q7425	L7426	L7427	C7428	L7429	A7430	E7431	E7432	L7433	L7434	L7435	L7436	L7437	L7438	L7439	L7440	L7441	L7442	L7443	L7444				
S7445	L7446	S7447	L7448	F7449	K7453	L7454	L7455	L7456	L7457	L7458	L7459	L7460	L7461	L7462	L7463	L7464	L7465	L7466	L7467	L7468	L7469	L7470	L7471	L7472	L7476	L7477	L7478	L7479	L7480	L7481	L7482	L7483	L7484	L7485	L7486	L7487	L7488	L7489	L7490	L7491	L7492	L7493	L7496	L7497	L7498	T7499	S7500	Q7501	L7502	L7503	D7504	L7505	L7506	L7507	L7508	Q7509	L7510					
R7511	L7512	Y7513	L7516	L7517	N7518	I7519	Q7520	E7521	L7522	L7523	L7524	L7525	L7526	L7527	L7528	K7529	L7530	L7531	E7532	L7533	L7534	L7535	L7538	L7539	R7542	L7543	L7544	D7548	K7549	A7550	H7551	L7552	L7553	L7554	L7555	L7556	L7559	S7560	E7561	L7565	L7566	L7567	L7570	E7571	M7572	P7573	GLU	SER	ALA	SER	SER	PRO										

PRO  
VAL  
ILE  
THR  
GLU

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.30Å 119.00Å 125.90Å 116.50° 94.80° 102.80°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	35527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LU, NAD

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	A	0.46	0/4424	0.67	0/5969
1	B	0.46	0/4424	0.66	0/5969
1	C	0.46	0/4424	0.66	0/5969
1	D	0.49	0/4424	0.69	0/5969
1	E	0.47	0/4424	0.68	1/5969 (0.0%)
1	F	0.47	0/4424	0.66	0/5969
1	G	0.46	0/4424	0.69	0/5969
1	H	0.46	0/4424	0.68	0/5969
All	All	0.47	0/35392	0.67	1/47752 (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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4442	LEU	CA-CB-CG	-5.11	103.55	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	TYR	Sidechain

## 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	A	4344	0	4372	604	0
1	B	4344	0	4372	618	0
1	C	4344	0	4372	594	0
1	D	4344	0	4372	650	0
1	E	4344	0	4372	543	0
1	F	4344	0	4372	504	0
1	G	4344	0	4372	654	0
1	H	4344	0	4372	560	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	88	0	52	3	0
3	B	88	0	52	5	0
3	C	88	0	52	2	0
3	D	88	0	52	4	0
3	E	88	0	52	3	0
3	F	88	0	52	3	0
3	G	88	0	52	4	0
3	H	88	0	52	3	0
4	A	9	0	0	3	0
4	B	6	0	0	1	0
4	C	11	0	0	1	0
4	D	6	0	0	6	0
4	E	6	0	0	0	0
4	F	10	0	0	1	0
4	G	5	0	0	3	0
4	H	10	0	0	1	0
All	All	35527	0	35392	4647	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 66.

The worst 5 of 4647 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)
1:D:3061:GLN:HA	1:D:3064:GLN:HE21	1.04	1.18
1:D:3388:THR:HG23	1:D:3415:VAL:HB	1.27	1.15
1:H:7388:THR:HG23	1:H:7415:VAL:HB	1.27	1.14
1:D:3253:GLN:HE22	1:D:3255:GLU:HG2	1.13	1.13
1:D:3263:PHE:HA	4:D:8022:HOH:O	1.48	1.13

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	A	549/584 (94%)	415 (76%)	99 (18%)	35 (6%)	1	4
1	B	549/584 (94%)	406 (74%)	107 (20%)	36 (7%)	1	3
1	C	549/584 (94%)	407 (74%)	102 (19%)	40 (7%)	1	3
1	D	549/584 (94%)	394 (72%)	119 (22%)	36 (7%)	1	3
1	E	549/584 (94%)	429 (78%)	94 (17%)	26 (5%)	2	8
1	F	549/584 (94%)	437 (80%)	83 (15%)	29 (5%)	2	6
1	G	549/584 (94%)	398 (72%)	111 (20%)	40 (7%)	1	3
1	H	549/584 (94%)	398 (72%)	120 (22%)	31 (6%)	2	5
All	All	4392/4672 (94%)	3284 (75%)	835 (19%)	273 (6%)	1	4

5 of 273 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ILE
1	A	167	LEU
1	A	256	ASP
1	A	259	ASN

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Mol	Chain	Res	Type
1	A	268	LYS

### 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	A	466/483 (96%)	332 (71%)	134 (29%)	0	1
1	B	466/483 (96%)	318 (68%)	148 (32%)	0	0
1	C	466/483 (96%)	327 (70%)	139 (30%)	0	1
1	D	466/483 (96%)	318 (68%)	148 (32%)	0	0
1	E	466/483 (96%)	340 (73%)	126 (27%)	0	1
1	F	466/483 (96%)	341 (73%)	125 (27%)	0	1
1	G	466/483 (96%)	335 (72%)	131 (28%)	0	1
1	H	466/483 (96%)	344 (74%)	122 (26%)	0	1
All	All	3728/3864 (96%)	2655 (71%)	1073 (29%)	0	1

5 of 1073 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3268	LYS
1	E	4183	LYS
1	H	7225	ARG
1	D	3306	LYS
1	D	3487	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3330	ASN
1	E	4125	HIS
1	H	7069	HIS
1	D	3335	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	D	3509	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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$
3	NAD	C	2601	-	42,48,48	2.03	11 (26%)	50,73,73	1.42	7 (14%)
3	NAD	E	4602	-	42,48,48	2.01	11 (26%)	50,73,73	1.42	6 (12%)
3	NAD	D	3602	-	42,48,48	2.00	10 (23%)	50,73,73	1.49	6 (12%)
3	NAD	F	5602	-	42,48,48	1.98	10 (23%)	50,73,73	1.45	5 (10%)
3	NAD	H	7601	-	42,48,48	2.24	11 (26%)	50,73,73	1.39	6 (12%)
3	NAD	B	1602	-	42,48,48	2.08	9 (21%)	50,73,73	1.41	5 (10%)
3	NAD	G	6602	-	42,48,48	2.02	9 (21%)	50,73,73	1.41	5 (10%)
3	NAD	A	601	-	42,48,48	2.09	12 (28%)	50,73,73	1.49	6 (12%)
3	NAD	A	602	-	42,48,48	2.11	10 (23%)	50,73,73	1.41	4 (8%)
3	NAD	D	3601	-	42,48,48	2.38	14 (33%)	50,73,73	1.48	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAD	F	5601	-	42,48,48	1.94	11 (26%)	50,73,73	1.38	5 (10%)
3	NAD	E	4601	-	42,48,48	2.16	12 (28%)	50,73,73	1.33	4 (8%)
3	NAD	H	7602	-	42,48,48	1.99	9 (21%)	50,73,73	1.48	6 (12%)
3	NAD	B	1601	-	42,48,48	1.97	11 (26%)	50,73,73	1.40	4 (8%)
3	NAD	C	2602	-	42,48,48	2.10	9 (21%)	50,73,73	1.42	6 (12%)
3	NAD	G	6601	-	42,48,48	2.02	11 (26%)	50,73,73	1.49	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	2601	-	-	5/26/62/62	0/5/5/5
3	NAD	E	4602	-	-	6/26/62/62	0/5/5/5
3	NAD	D	3602	-	-	8/26/62/62	0/5/5/5
3	NAD	F	5602	-	-	6/26/62/62	0/5/5/5
3	NAD	H	7601	-	-	1/26/62/62	0/5/5/5
3	NAD	B	1602	-	-	7/26/62/62	0/5/5/5
3	NAD	G	6602	-	-	7/26/62/62	0/5/5/5
3	NAD	A	601	-	-	1/26/62/62	0/5/5/5
3	NAD	A	602	-	-	6/26/62/62	0/5/5/5
3	NAD	D	3601	-	-	5/26/62/62	0/5/5/5
3	NAD	F	5601	-	-	2/26/62/62	0/5/5/5
3	NAD	E	4601	-	-	2/26/62/62	0/5/5/5
3	NAD	H	7602	-	-	6/26/62/62	0/5/5/5
3	NAD	B	1601	-	-	9/26/62/62	0/5/5/5
3	NAD	C	2602	-	-	5/26/62/62	0/5/5/5
3	NAD	G	6601	-	-	1/26/62/62	0/5/5/5

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	NAD	C2N-N1N	8.07	1.44	1.35
3	D	3601	NAD	C2N-N1N	7.62	1.44	1.35
3	C	2602	NAD	C2N-N1N	7.46	1.44	1.35
3	H	7601	NAD	C2N-N1N	7.25	1.43	1.35
3	D	3602	NAD	C2N-N1N	7.16	1.43	1.35

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5601	NAD	N3A-C2A-N1A	-5.44	120.17	128.68
3	E	4601	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
3	G	6601	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
3	C	2601	NAD	N3A-C2A-N1A	-5.34	120.33	128.68
3	A	601	NAD	N3A-C2A-N1A	-5.31	120.37	128.68

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAD	C5B-O5B-PA-O1A
3	F	5601	NAD	PN-O3-PA-O5B
3	E	4602	NAD	C5B-O5B-PA-O1A
3	E	4602	NAD	C5D-O5D-PN-O1N
3	E	4602	NAD	C3D-C4D-C5D-O5D

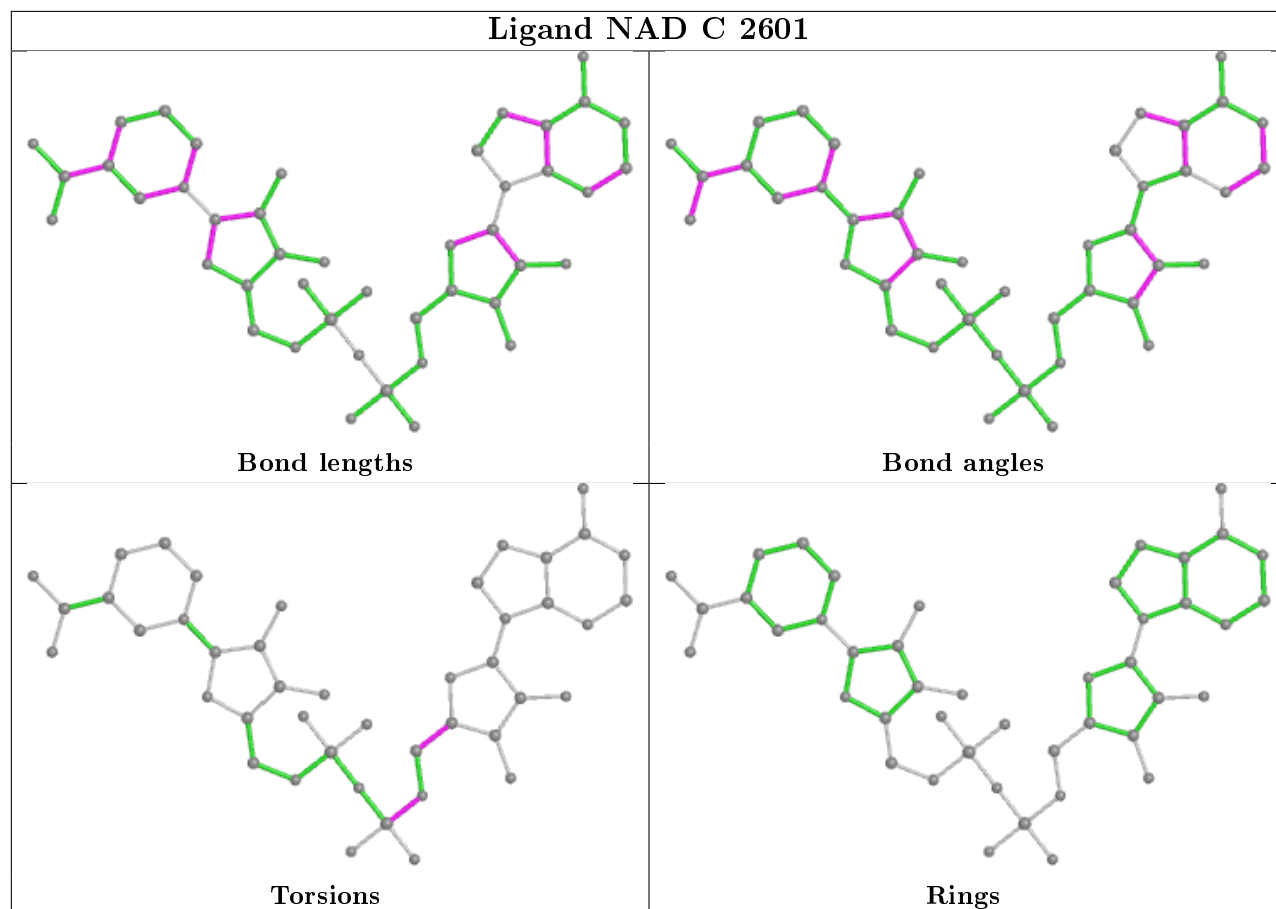
There are no ring outliers.

11 monomers are involved in 27 short contacts:

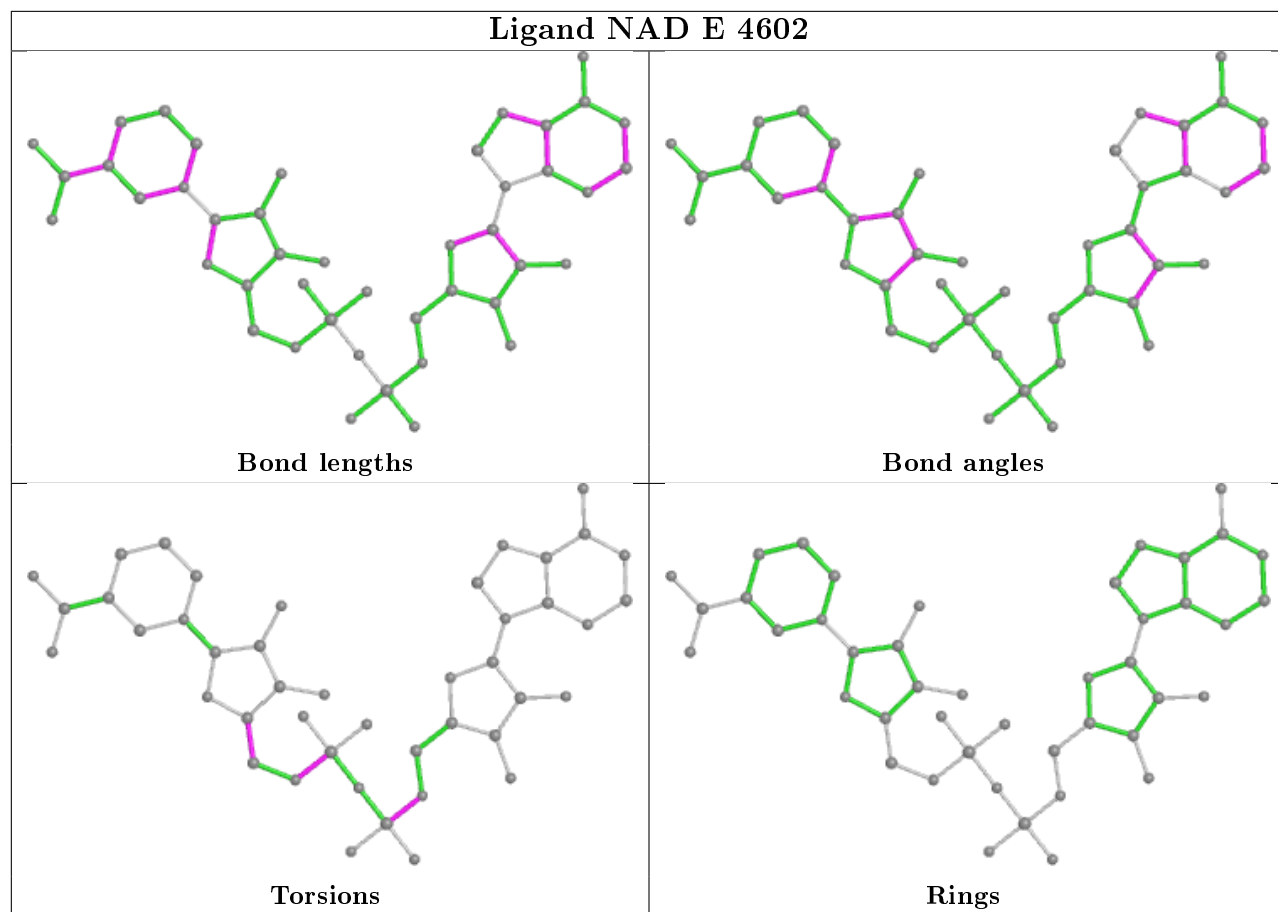
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2601	NAD	2	0
3	D	3602	NAD	1	0
3	H	7601	NAD	2	0
3	B	1602	NAD	1	0
3	A	601	NAD	3	0
3	D	3601	NAD	3	0
3	F	5601	NAD	3	0
3	E	4601	NAD	3	0
3	H	7602	NAD	1	0
3	B	1601	NAD	4	0
3	G	6601	NAD	4	0

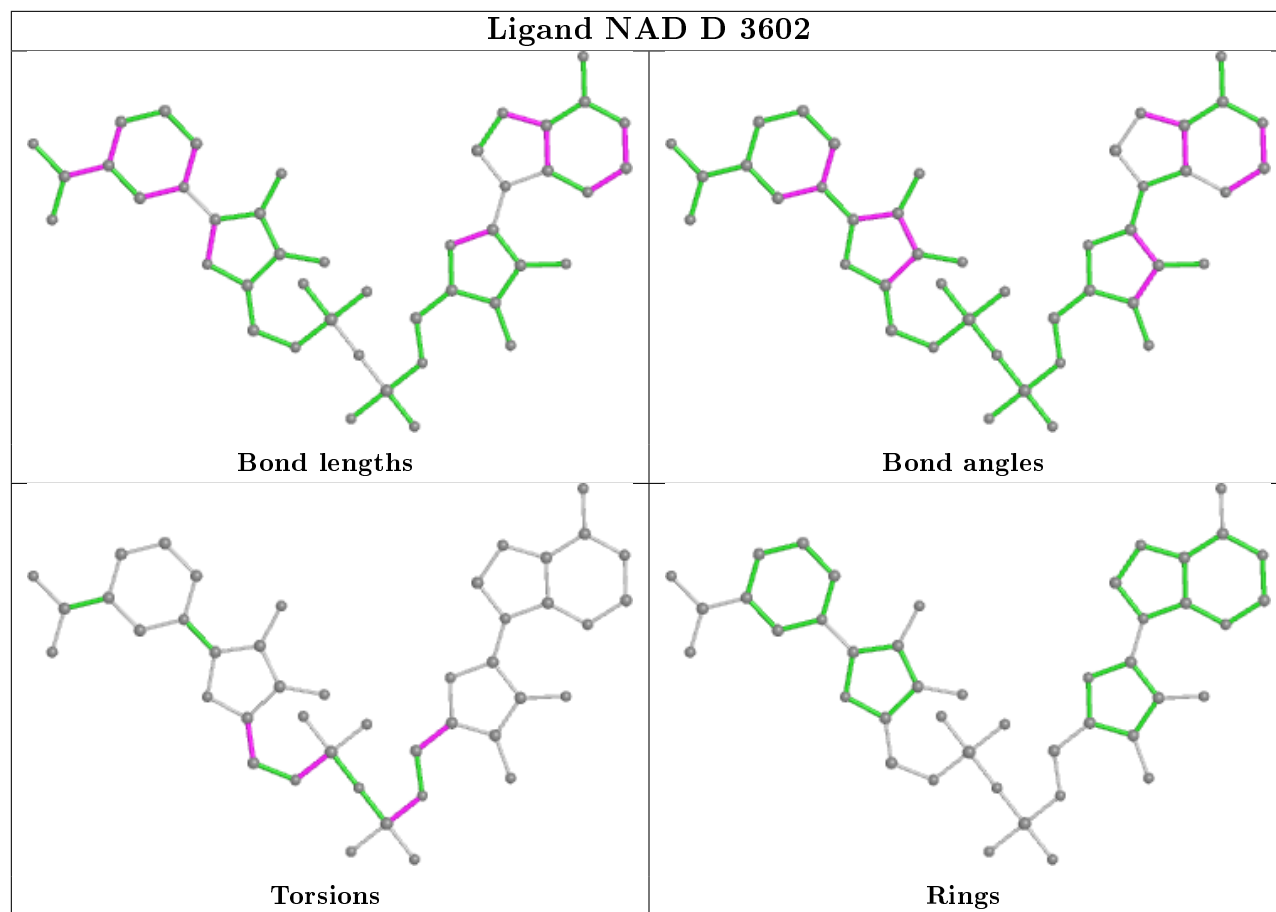
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

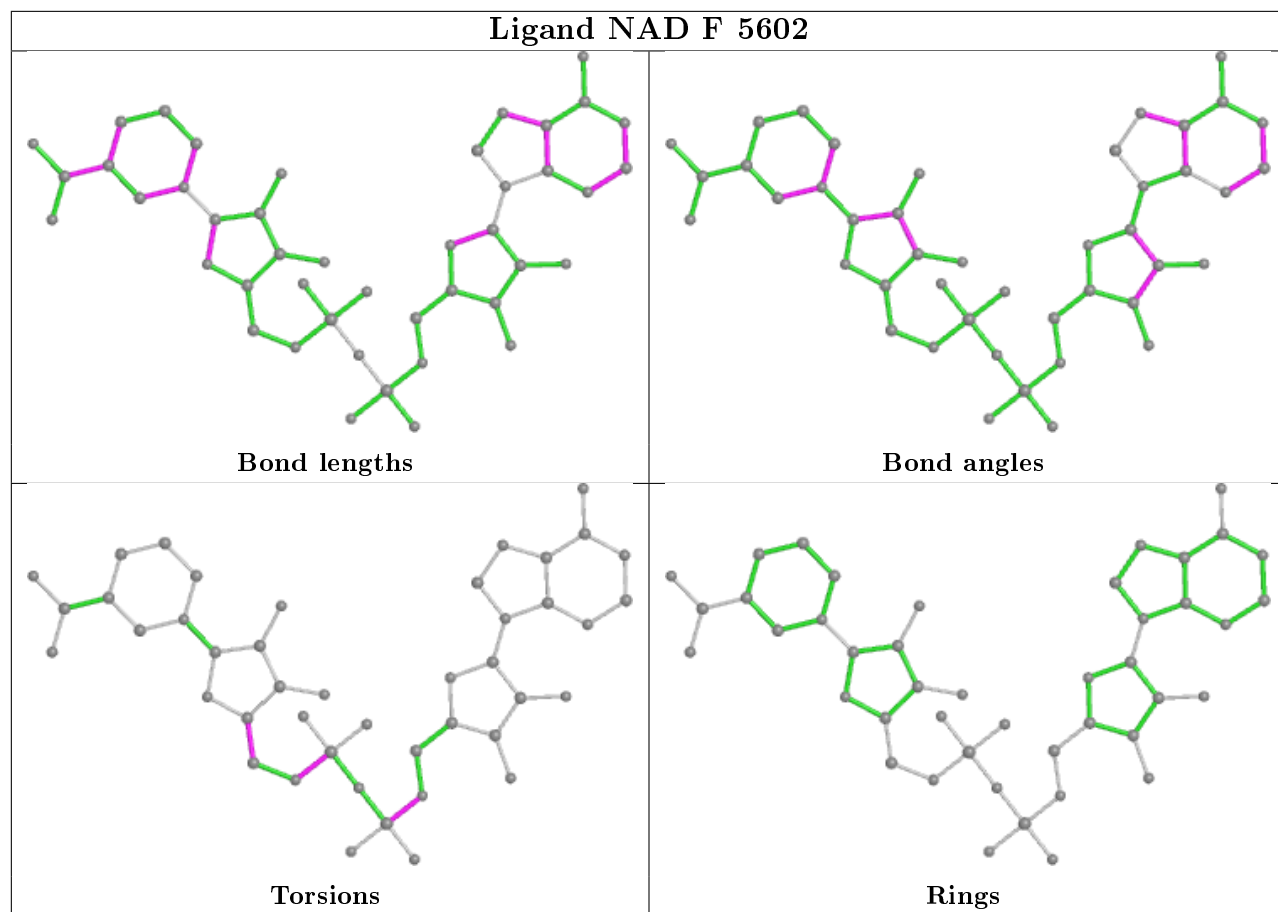
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

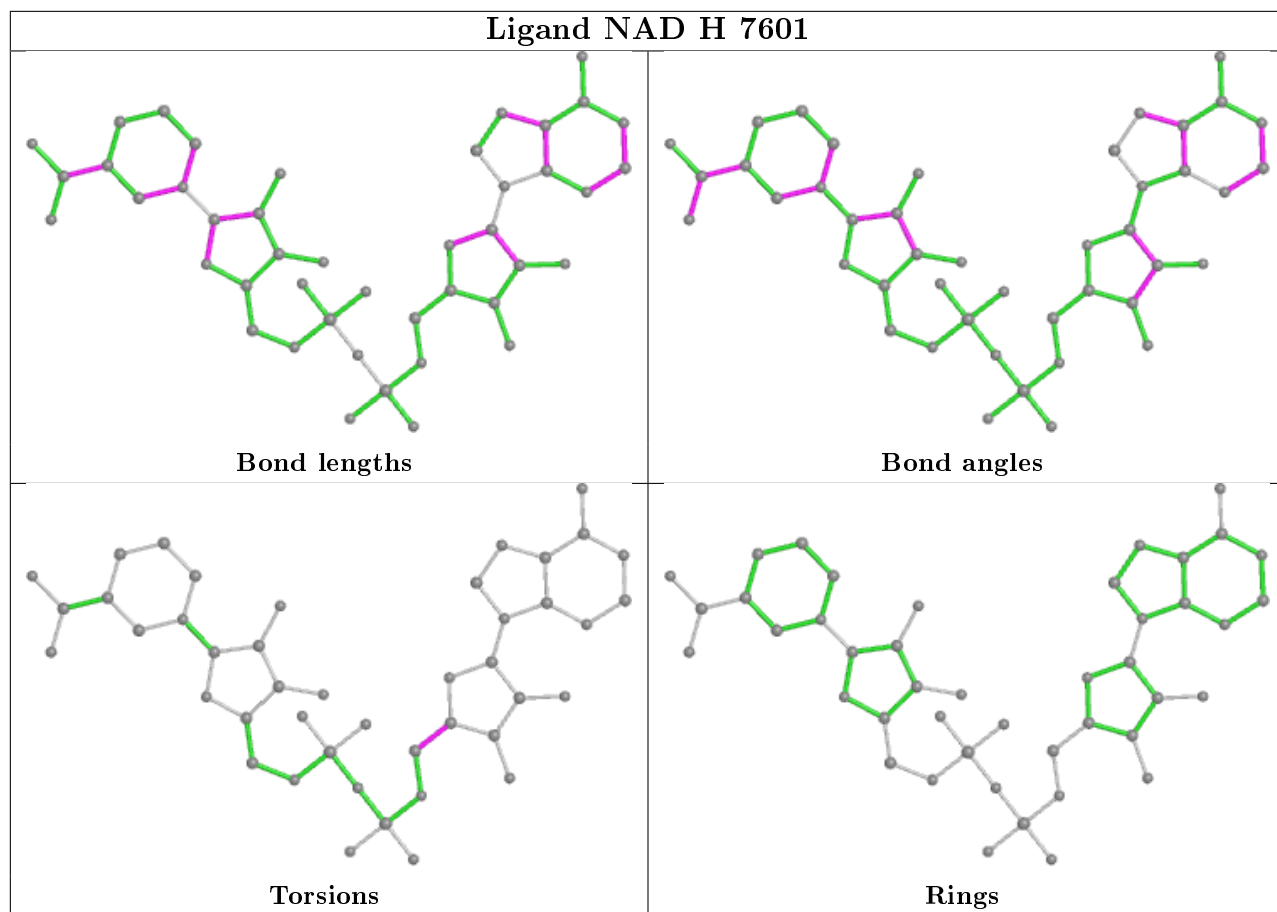


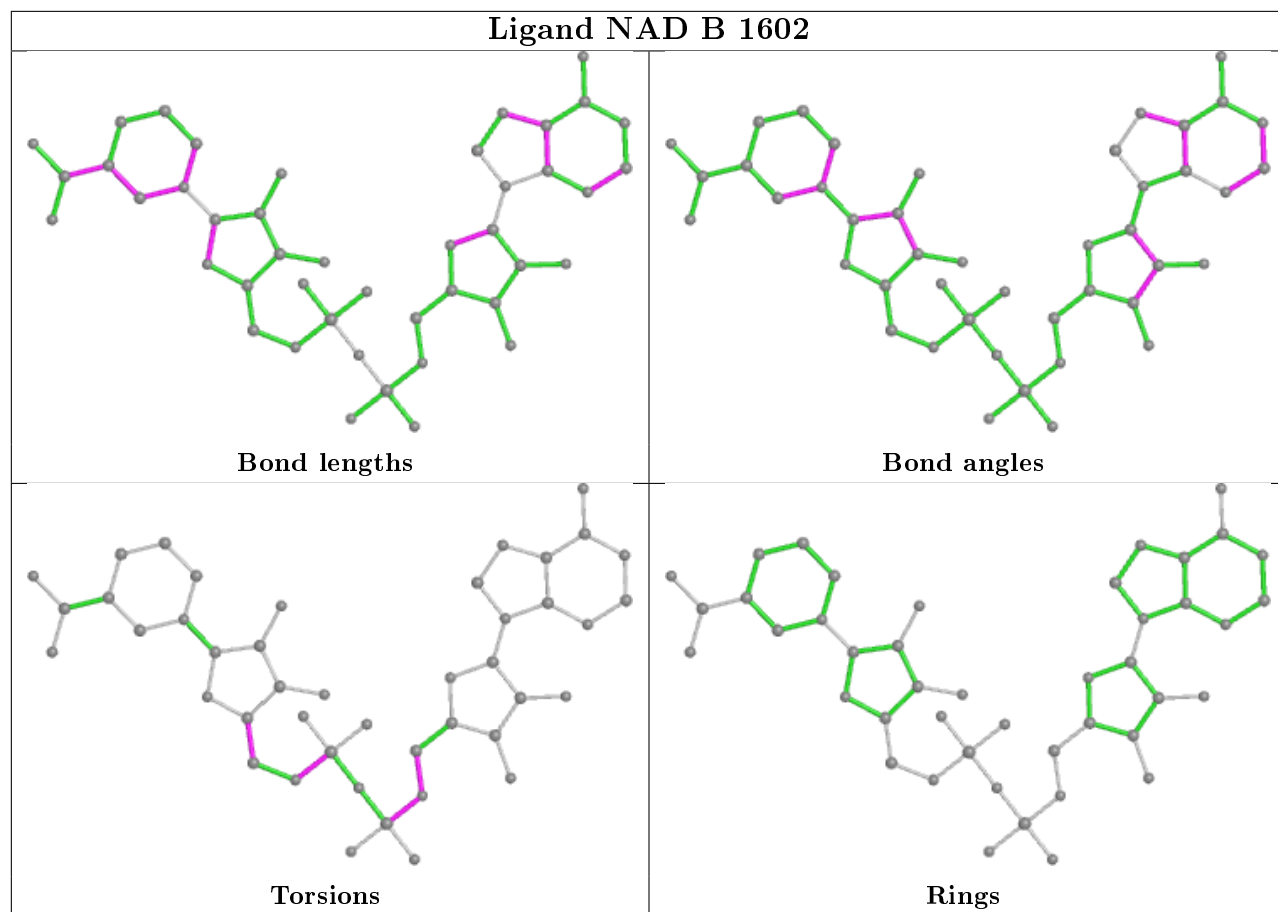


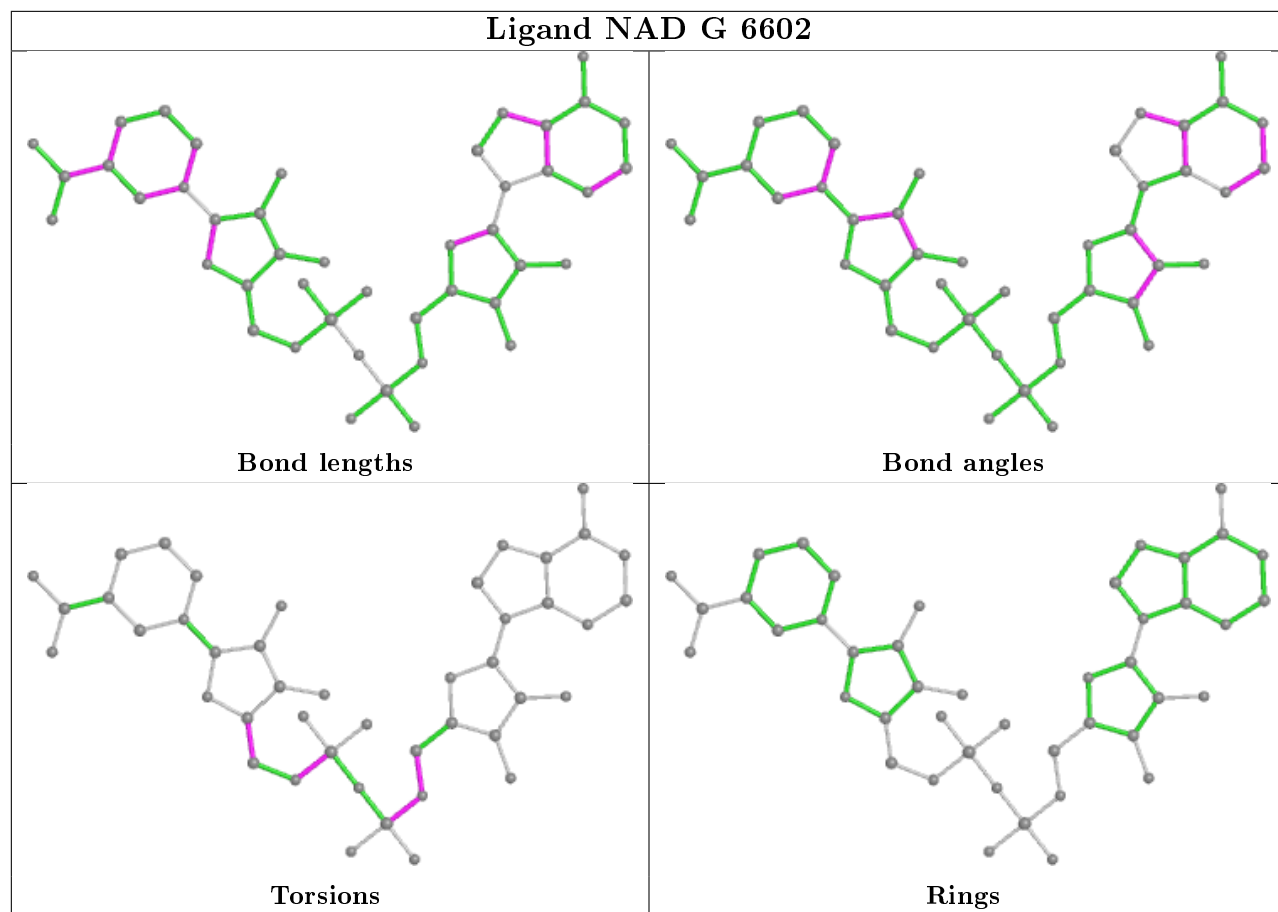


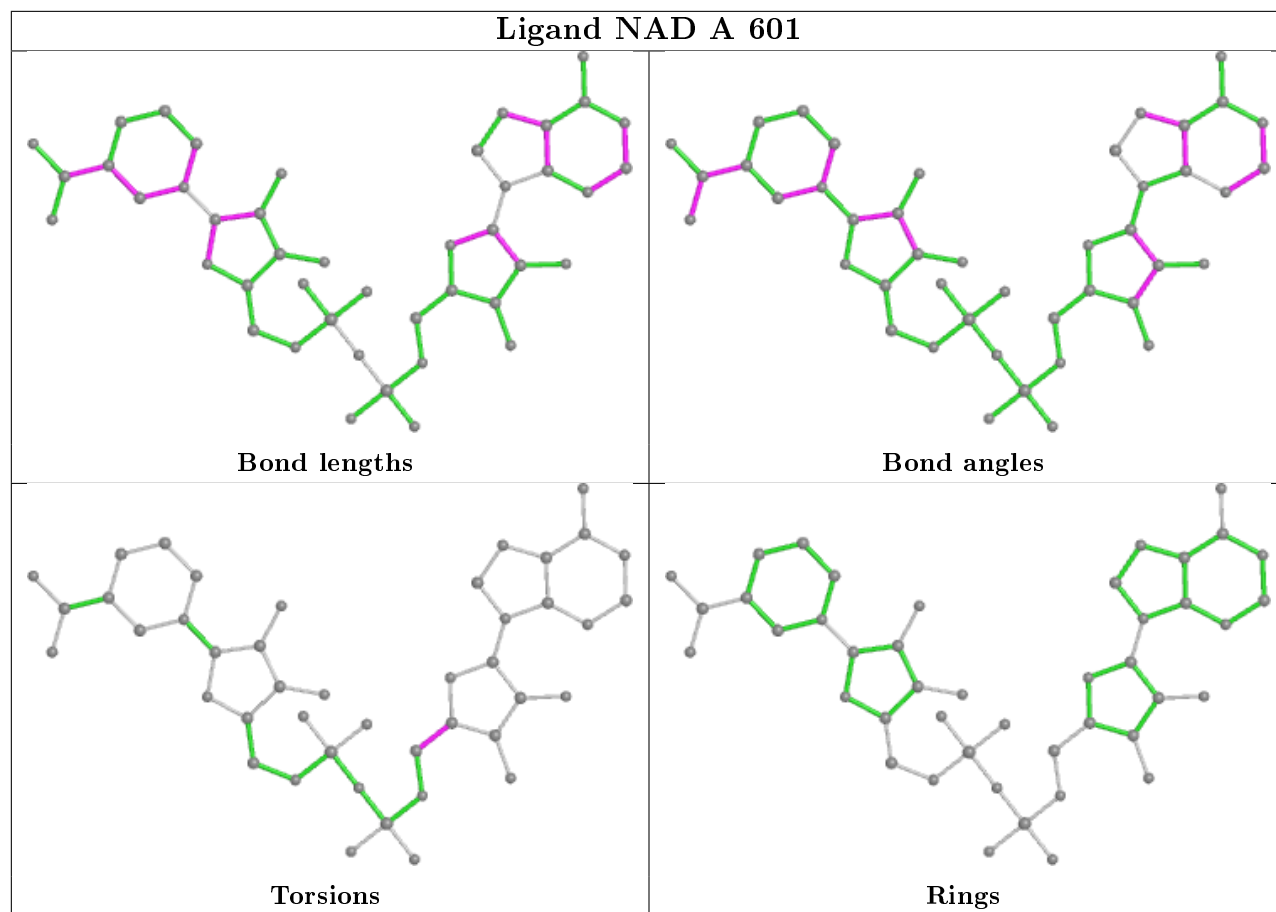


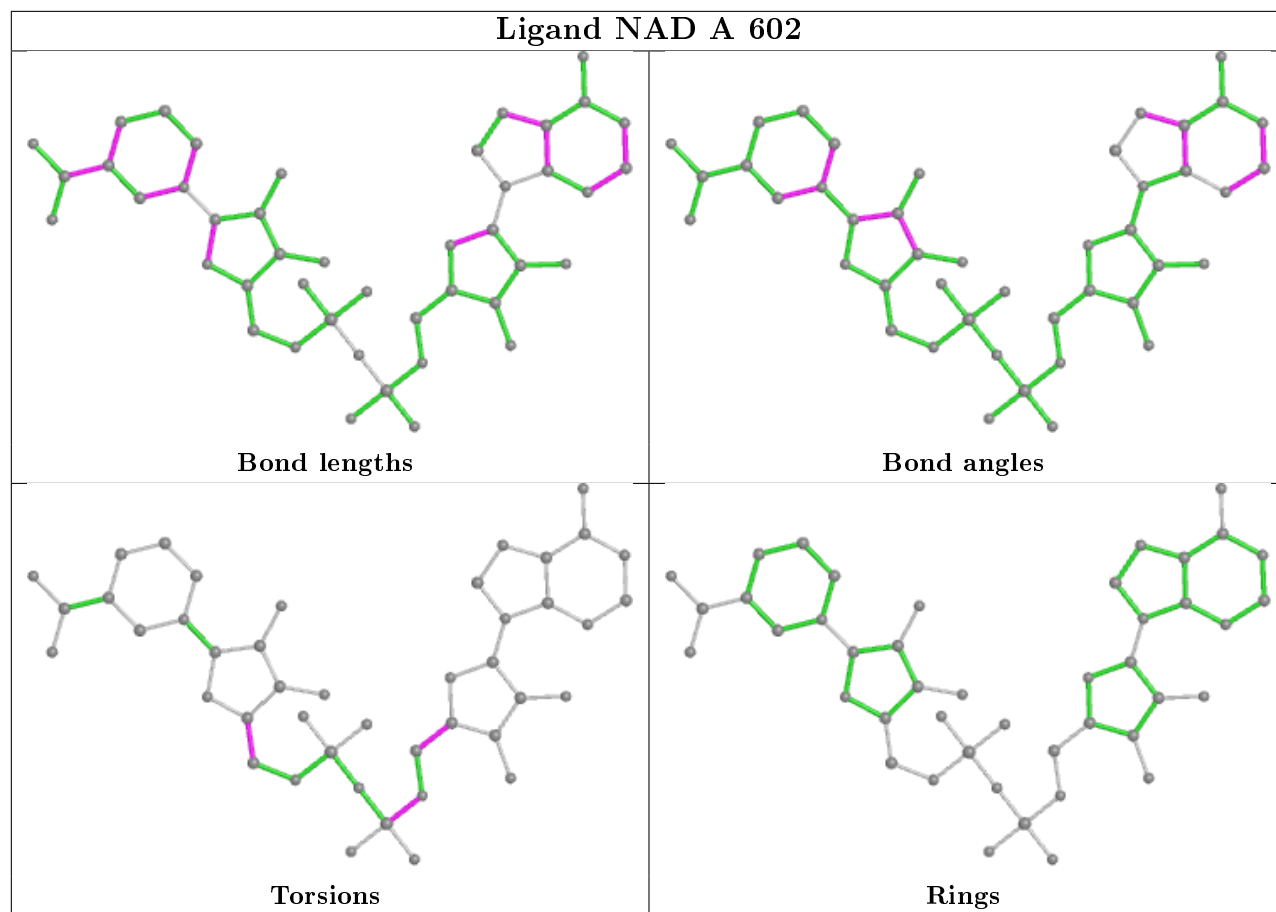




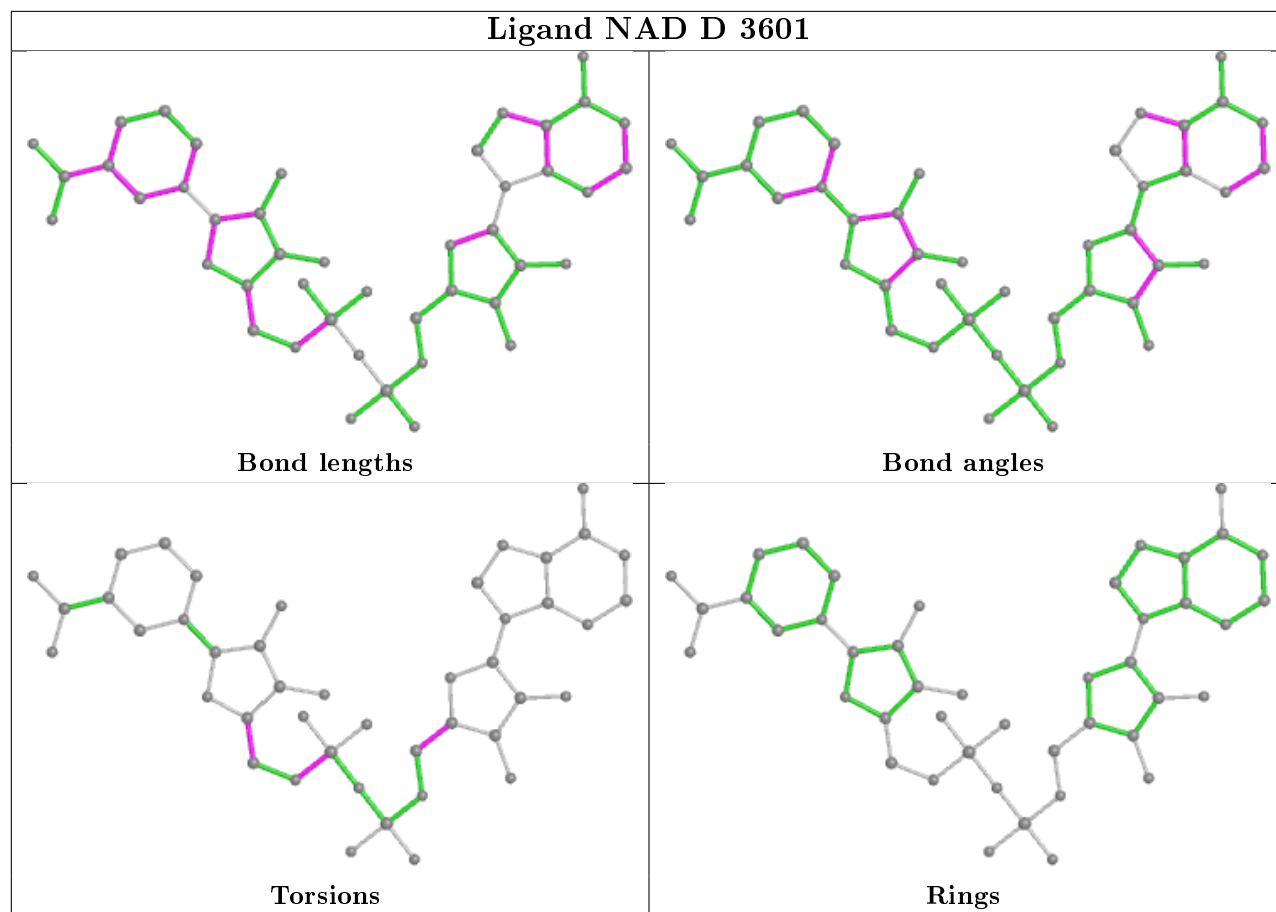


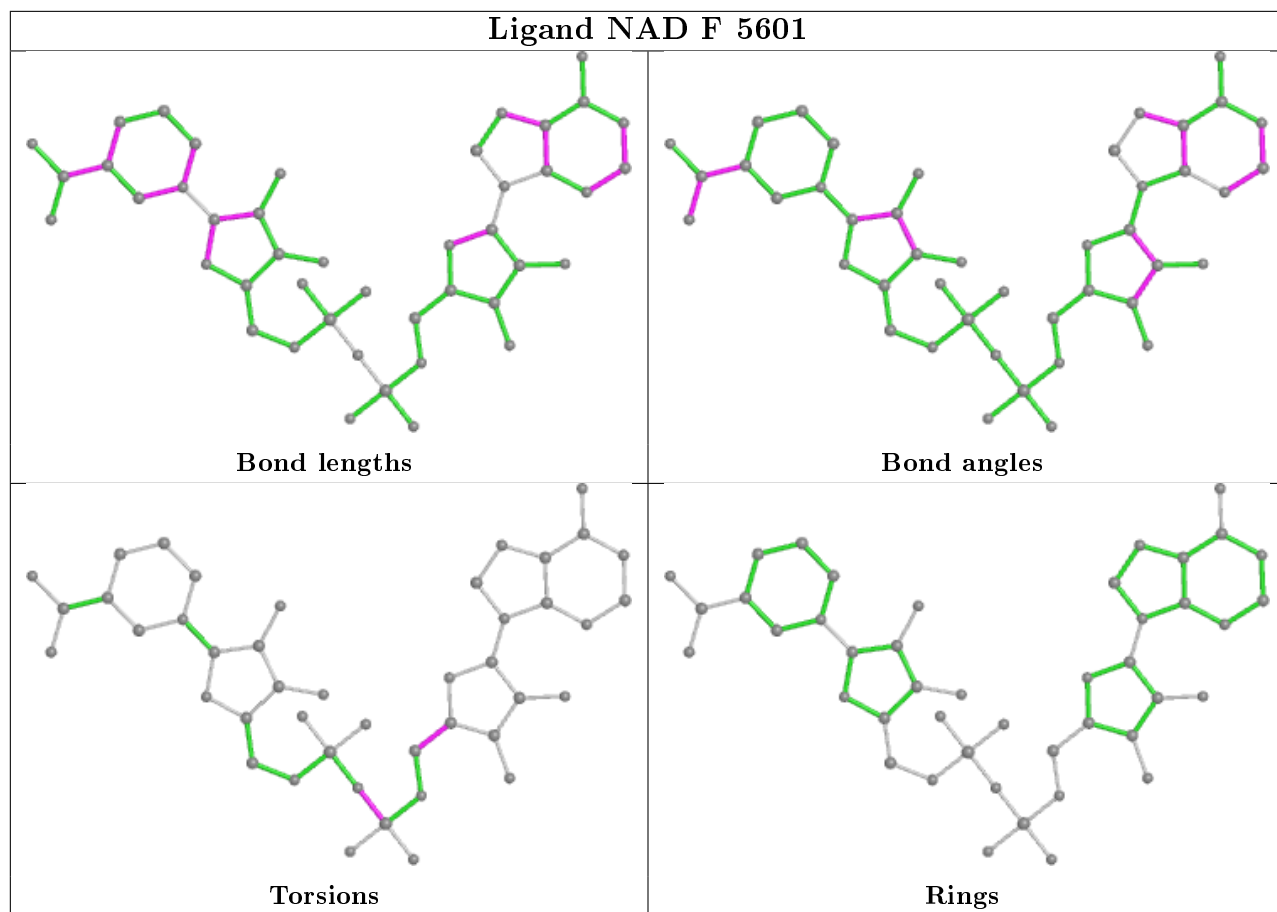


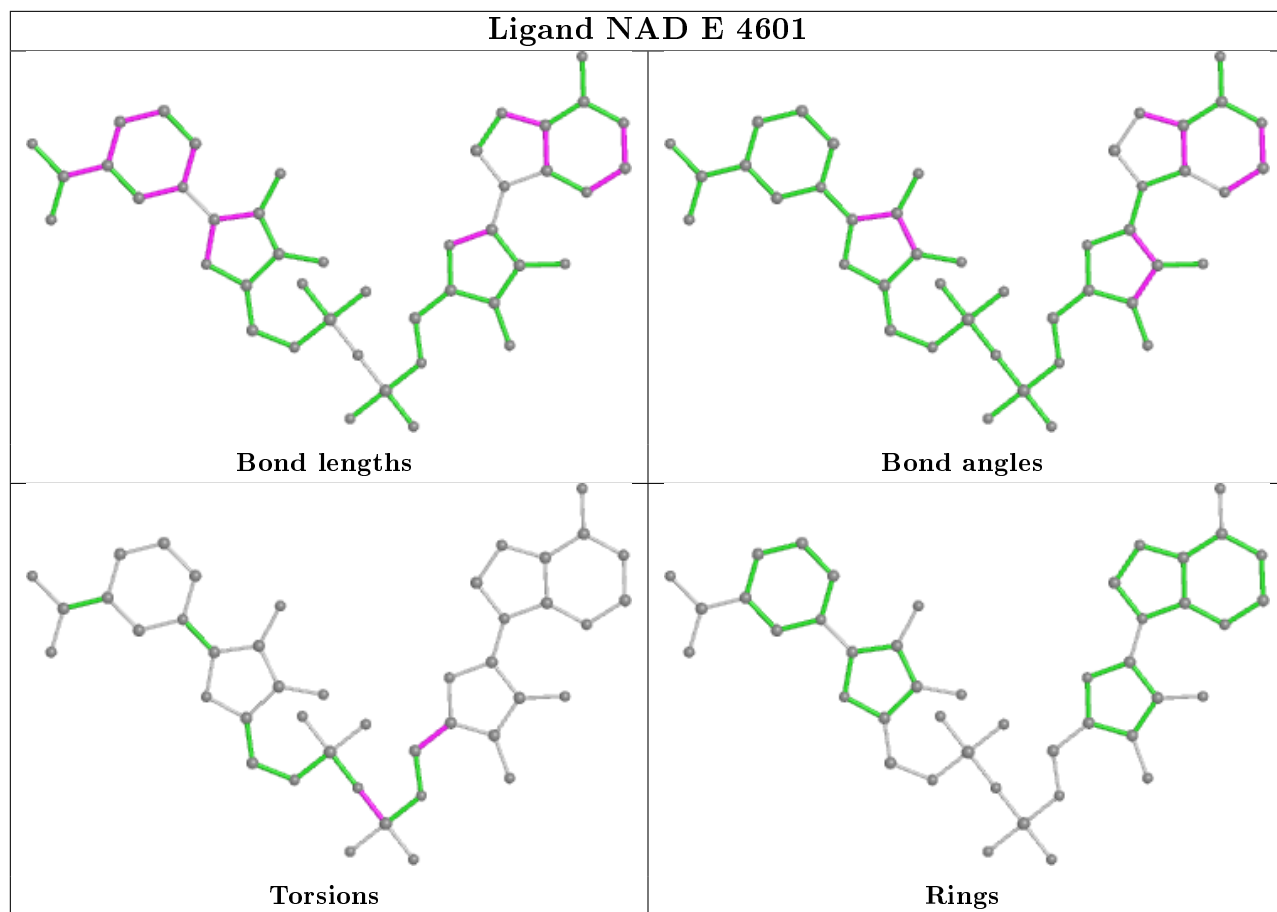


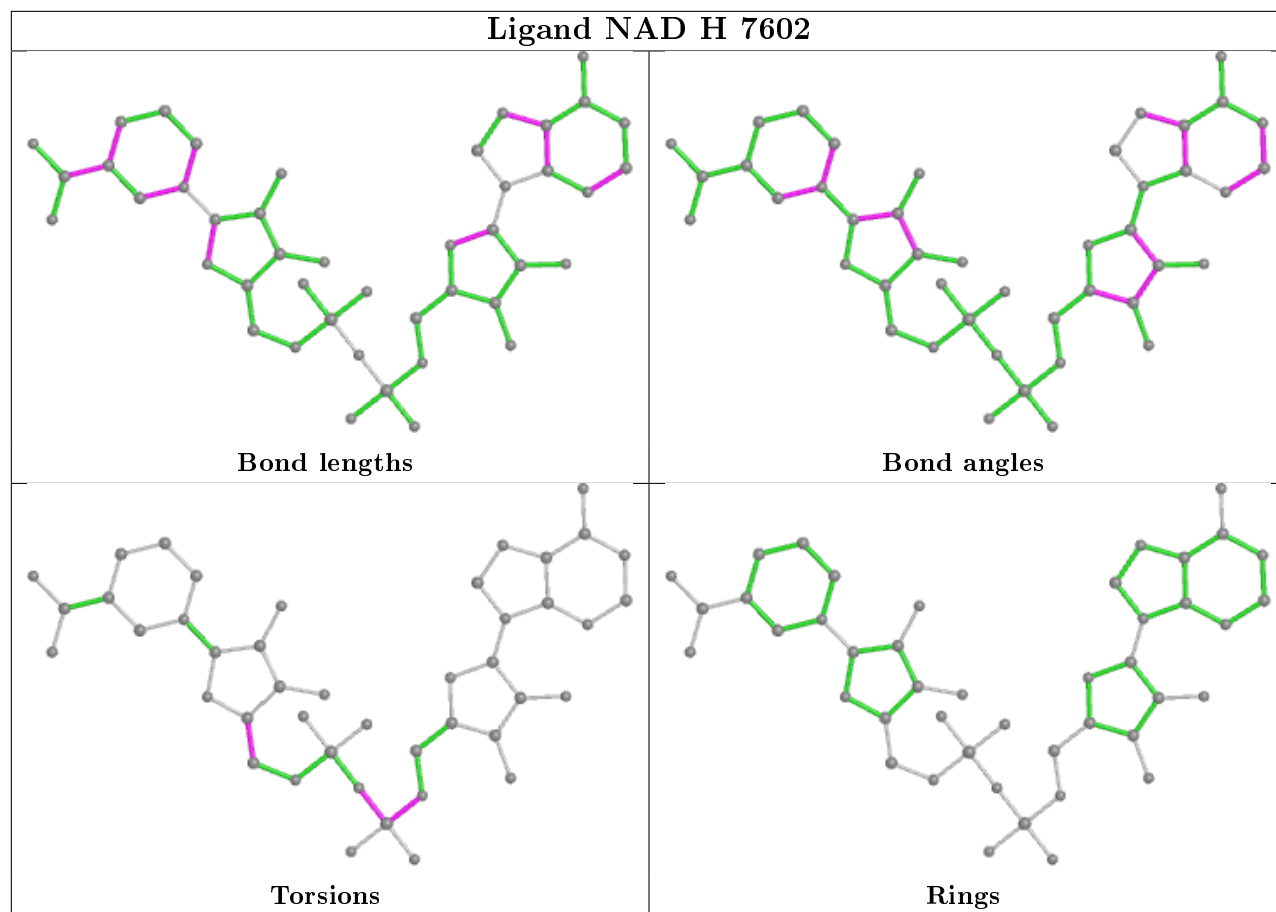


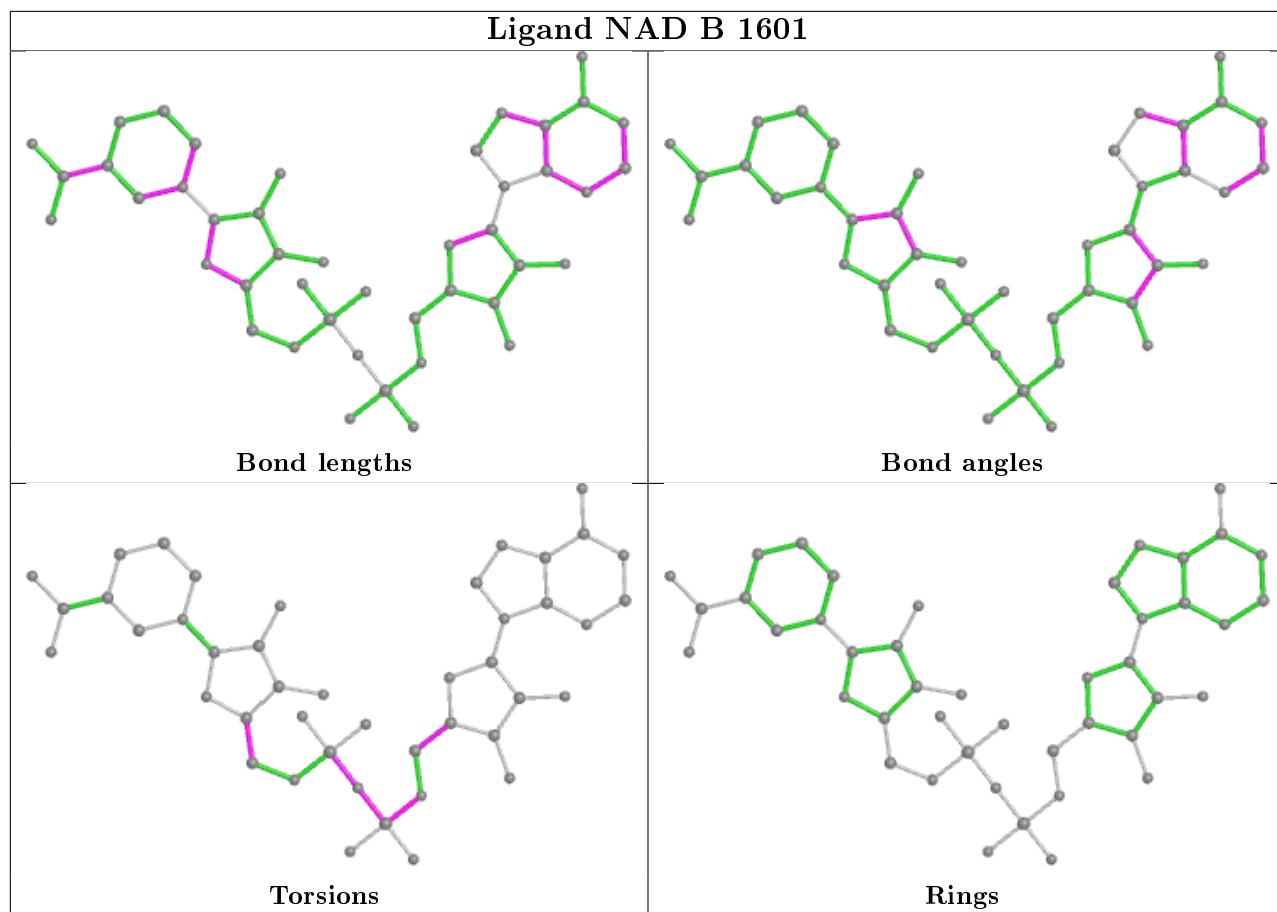


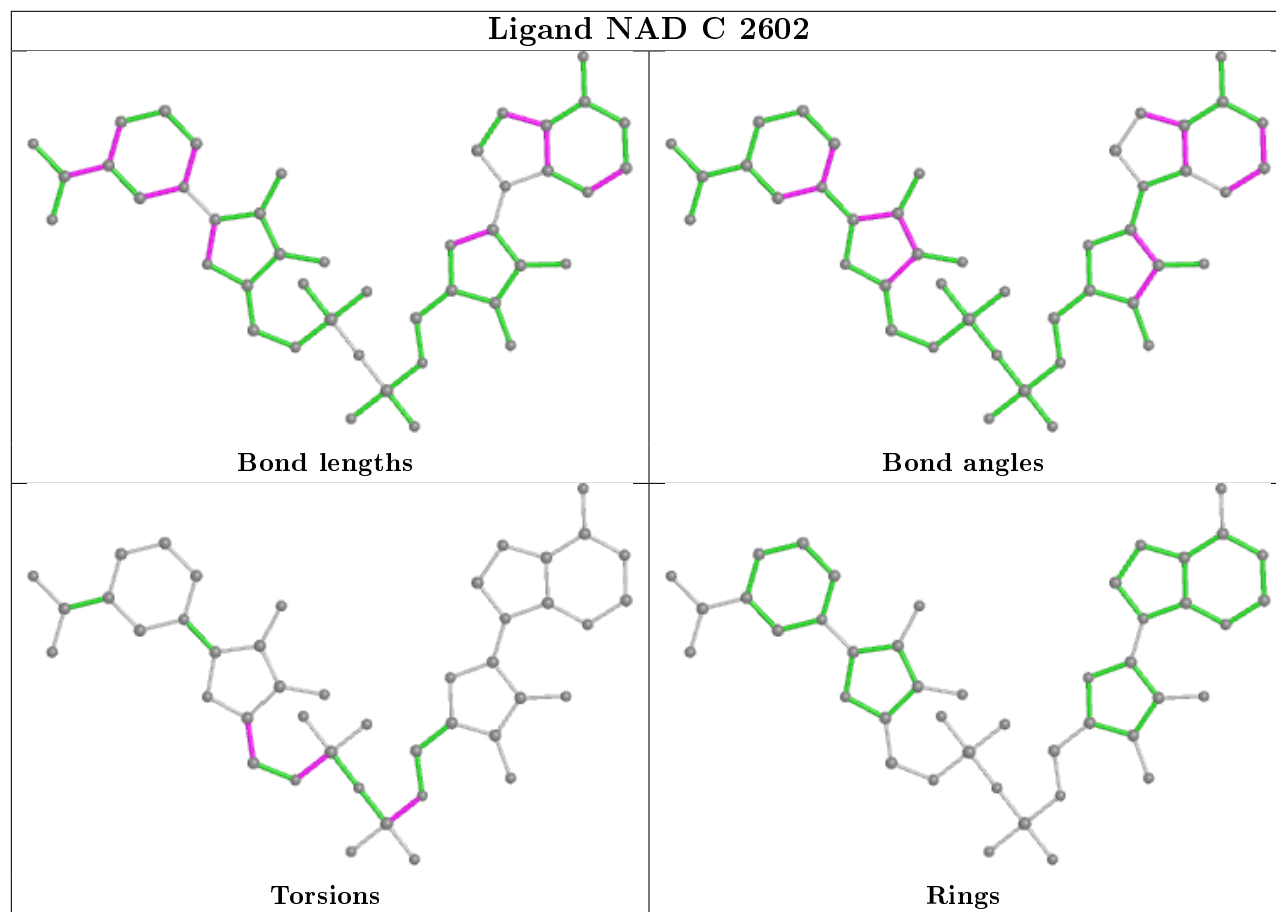


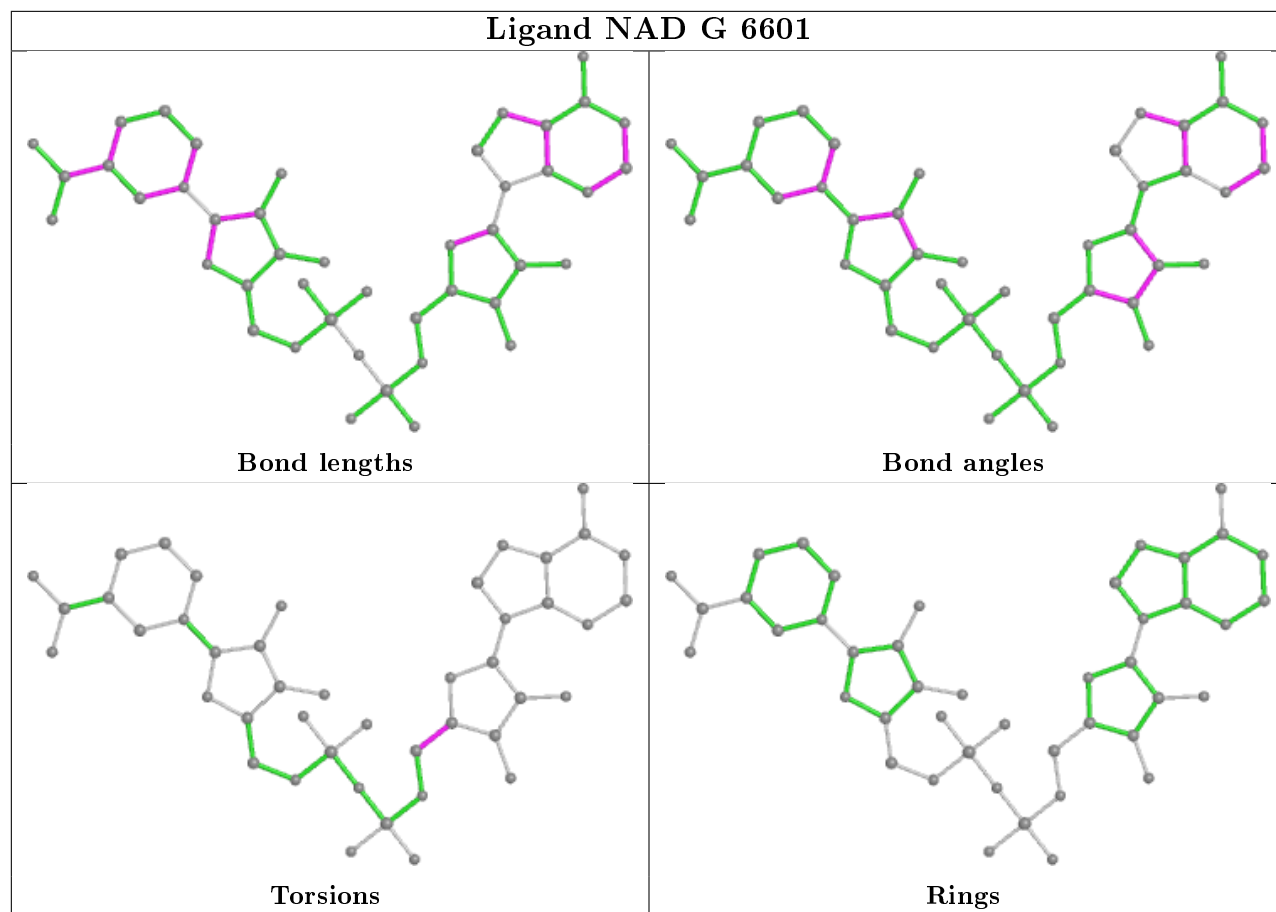












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.