



Full wwPDB NMR Structure Validation Report ⓘ

Jun 16, 2024 – 01:43 PM EDT

PDB ID : 2V93
Title : EQUILLIBRIUM MIXTURE OF OPEN AND PARTIALLY-CLOSED SPECIES IN THE APO STATE OF MALTODEXTRIN-BINDING PROTEIN BY PARAMAGNETIC RELAXATION ENHANCEMENT NMR
Authors : Clore, G.M.; Tang, C.
Deposited on : 2007-08-21

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

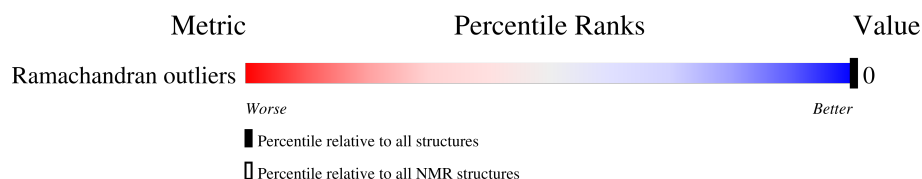
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Ramachandran outliers	154571	11451

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	A	370	 95% .

2 Ensemble composition and analysis ⓘ

This entry contains 50 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:81-A:87, A:103-A:105, A:266-A:268, A:311-A:313 (16)	0.00	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: No clusters in NmrClust output

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3792 atoms, of which 1003 are hydrogens and 0 are deuteriums.

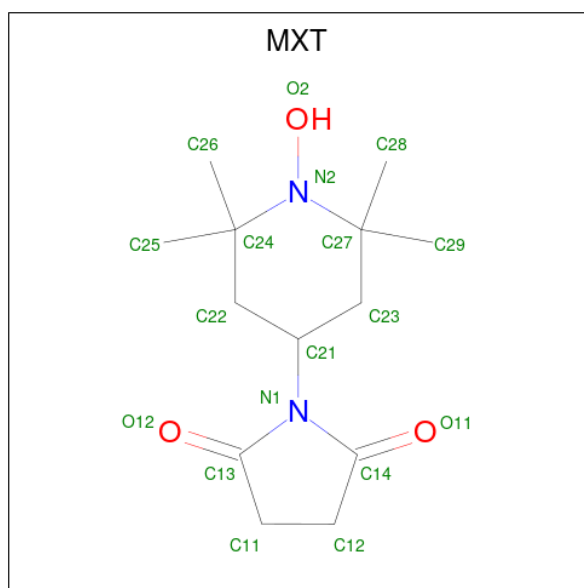
- Molecule 1 is a protein called MALTOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	366	Total	C	H	N	O	S	0
			2904	1169	547	583	581	24	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	CYS	ASP	engineered mutation	UNP P0AEY0
A	211	CYS	SER	engineered mutation	UNP P0AEY0

- Molecule 2 is 1-(1-HYDROXY-2,2,6,6-TETRAMETHYLPYRROLIDIN-4-YL)PYRROLIDIN E-2,5-DIONE (three-letter code: MXT) (formula: $C_{13}H_{22}N_2O_3$).



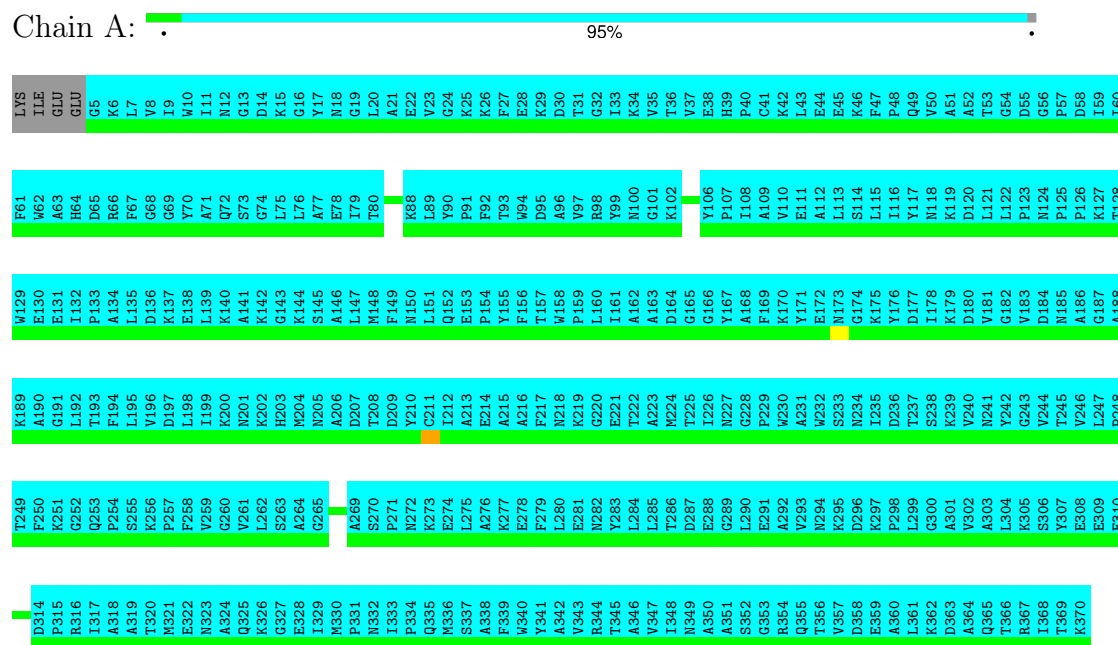
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			444	156	228	24	36
2	A	1	Total	C	H	N	O
			444	156	228	24	36

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

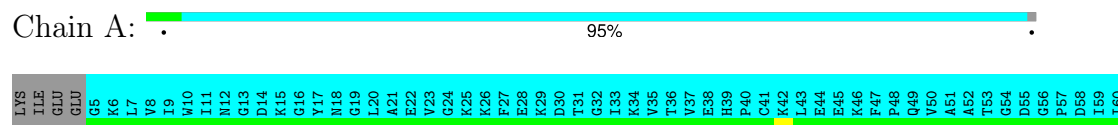


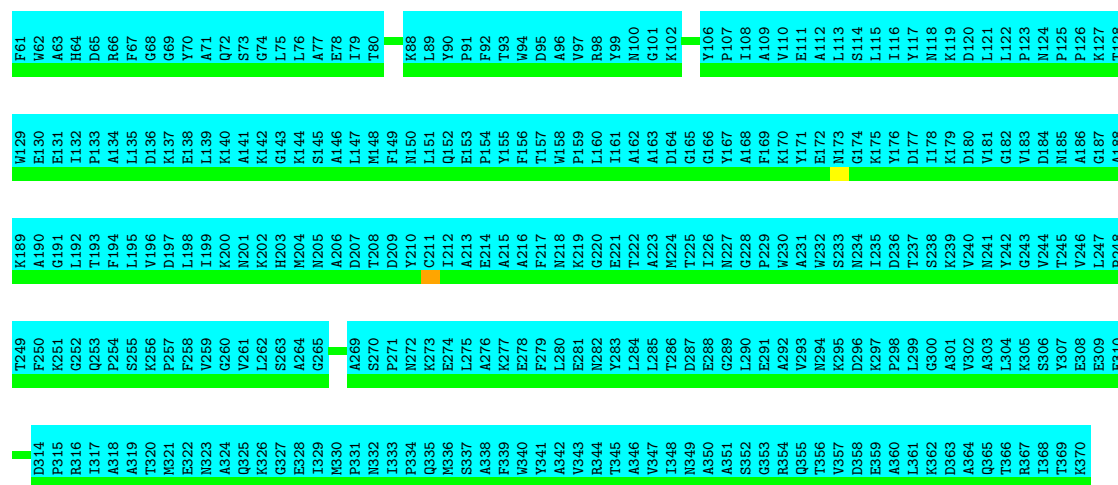
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

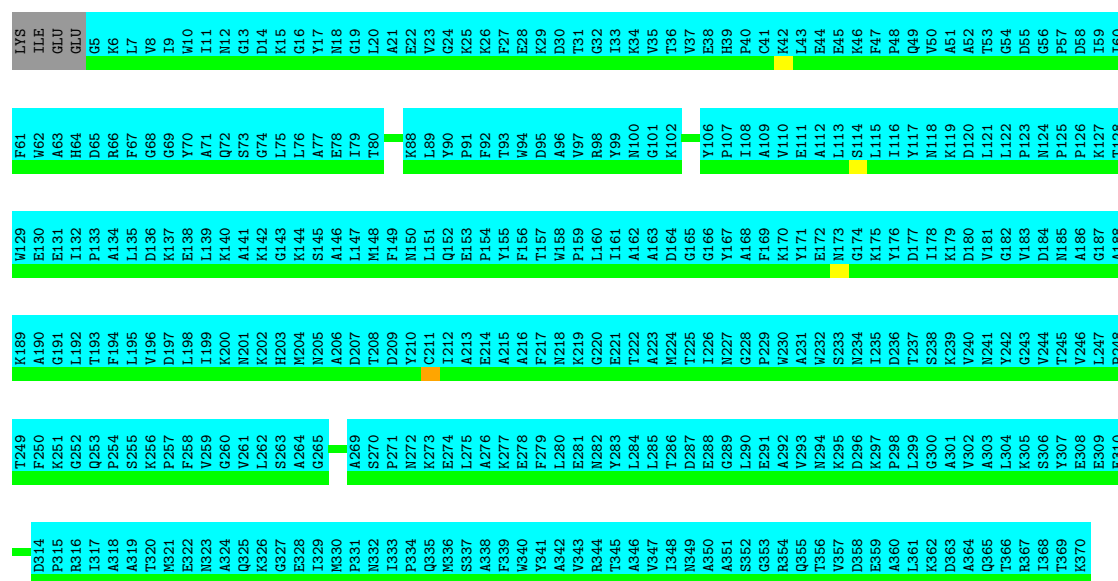




4.2.2 Score per residue for model 2

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

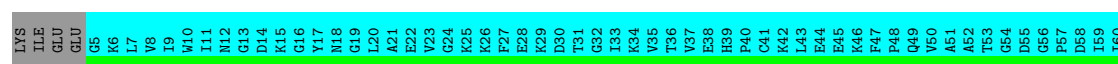
Chain A: . 95%

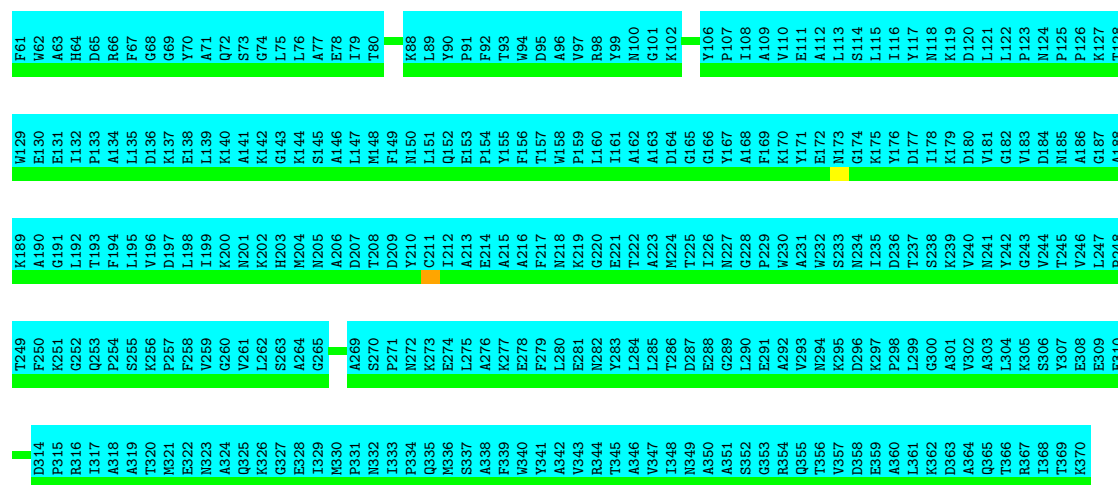


4.2.3 Score per residue for model 3

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

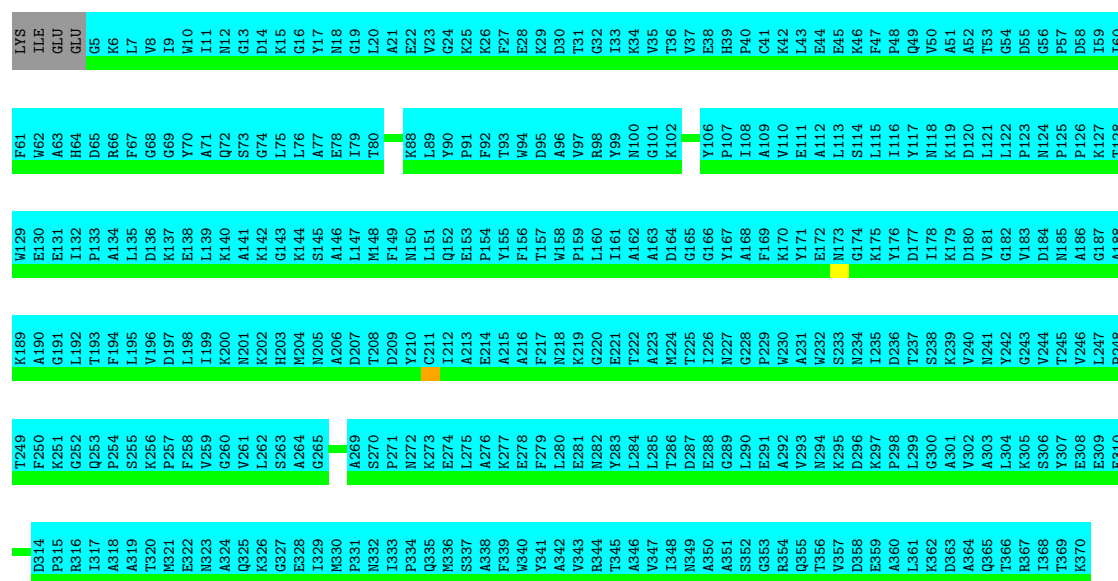




4.2.4 Score per residue for model 4

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

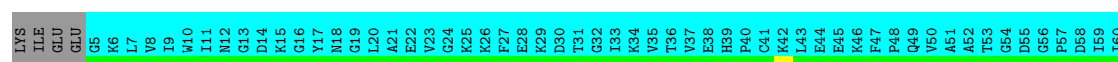
Chain A: . 95%

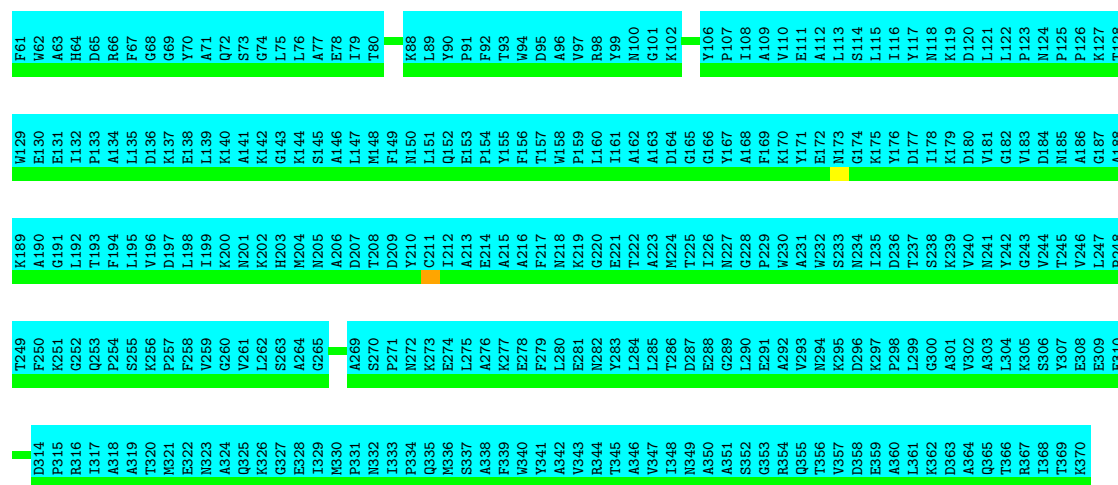


4.2.5 Score per residue for model 5

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

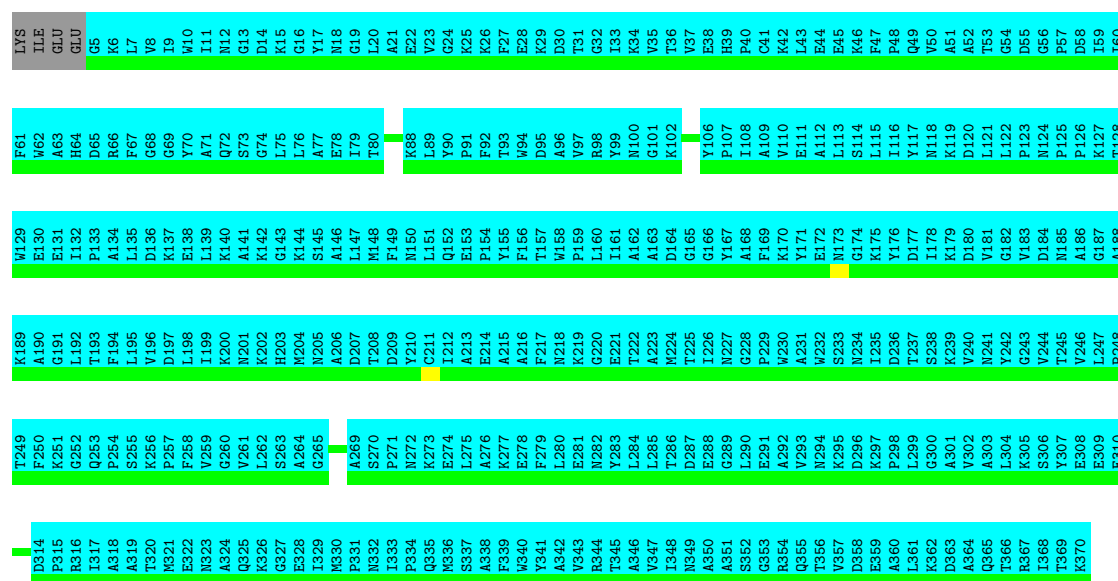




4.2.6 Score per residue for model 6

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

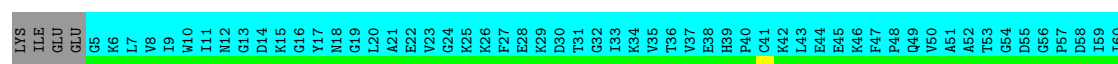
Chain A: .



4.2.7 Score per residue for model 7

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: .



F61	W429	K189	T249	D314	F61	W429	K189	T249	D314
W62	E130	A190	F250	P315	W62	E130	A190	F250	P315
A63	E131	G191	K251	R316	A63	E131	G191	K251	R316
H64	L132	G192	G252	L317	H64	L132	G192	G252	L317
D65	P133	T193	Q253	A318	D65	P133	T193	Q253	A318
R66	F194	F194	P254	A319	R66	F194	F194	P254	A319
F67	L135	L195	S255	T320	F67	L135	L195	S255	T320
G68	D136	V196	K256	G326	G68	D136	V196	K256	G326
Y70	E138	L198	P257	K326	Y70	E138	L198	P257	K326
A71	L139	I199	F258	G327	A71	L139	I199	F258	G327
A71	L139	I199	V259	K328	A71	L139	I199	V259	K328
Q72	K140	N201	G260	G325	Q72	K140	N201	G260	G325
S73	A141	N201	V261	G326	S73	A141	N201	V261	G326
G74	K142	K202	L262	K326	G74	K142	K202	L262	K326
L75	G143	H203	S263	K327	L75	G143	H203	S263	K327
L76	K144	M204	A264	G328	L76	K144	M204	A264	G328
A77	S145	N205	G265	I329	A77	S145	N205	G265	I329
E78	A146	A206	A269	M330	E78	A146	A206	A269	M330
I79	L147	D207	S270	P331	I79	L147	D207	S270	P331
T80	M148	T208	P271	N332	T80	M148	T208	P271	N332
K88	F149	D209	N272	I333	K88	F149	D209	N272	I333
L89	N150	Y210	K273	P334	L89	N150	Y210	K273	P334
Y90	L151	C211	E274	Q335	Y90	L151	C211	E274	Q335
P91	Q152	I212	L275	M336	P91	Q152	I212	L275	M336
F92	E153	A213	K276	S337	F92	E153	A213	K276	S337
T93	P154	E214	A276	A338	T93	P154	E214	A276	A338
W94	F155	A215	K277	F339	W94	F155	A215	K277	F339
D95	F156	A216	E278	W340	D95	F156	A216	E278	W340
I96	F217	F217	F279	Y341	I96	F217	F217	F279	Y341
A96	M158	N218	L280	A342	A96	M158	N218	L280	A342
V97	P159	K219	E281	V343	V97	P159	K219	E281	V343
R98	L160	G220	N282	R344	R98	L160	G220	N282	R344
Y99	I161	E221	Y283	T345	Y99	I161	E221	Y283	T345
N100	A162	T222	L284	A346	N100	A162	T222	L284	A346
G101	A163	A223	L285	V347	G101	A163	A223	L285	V347
K102	D164	M224	T286	I348	K102	D164	M224	T286	I348
Y106	G165	T225	D287	N349	Y106	G165	T225	D287	N349
P107	G166	I226	E288	A350	P107	G166	I226	E288	A350
I108	Y167	N227	G289	A351	I108	Y167	N227	G289	A351
A109	A168	G228	L290	S352	A109	A168	G228	L290	S352
K170	F169	P229	E291	G353	K170	F169	P229	E291	G353
E111	V170	W230	A292	R354	E111	V170	W230	A292	R354
A112	E171	A231	V293	Q355	A112	E171	A231	V293	Q355
L113	E172	W232	K295	T356	L113	E172	W232	K295	T356
S114	W173	S233	D296	V357	S114	W173	S233	D296	V357
L115	G174	I235	K297	D358	L115	G174	I235	K297	D358
I116	Y176	D236	P298	F47	I116	Y176	D236	P298	F47
Y117	D177	T237	L299	P48	Y117	D177	T237	L299	P48
N118	I178	S238	G300	L361	N118	I178	S238	G300	L361
K119	K179	K239	A301	K362	K119	K179	K239	A301	K362
D120	D180	V240	V302	D363	D120	D180	V240	V302	D363
L121	V181	N241	A303	A364	L121	V181	N241	A303	A364
L122	G182	Y242	T304	T365	L122	G182	Y242	T304	T365
P123	V183	G243	K305	T366	P123	V183	G243	K305	T366
N124	D184	V244	S306	I368	N124	D184	V244	S306	I368
P125	N185	T245	Y307	T369	P125	N185	T245	Y307	T369
P126	A186	V246	E308	K370	P126	A186	V246	E308	K370
K127	G187	L247	E309		K127	G187	L247	E309	
T128	A188	P248	E310		T128	A188	P248	E310	

4.2.8 Score per residue for model 8

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

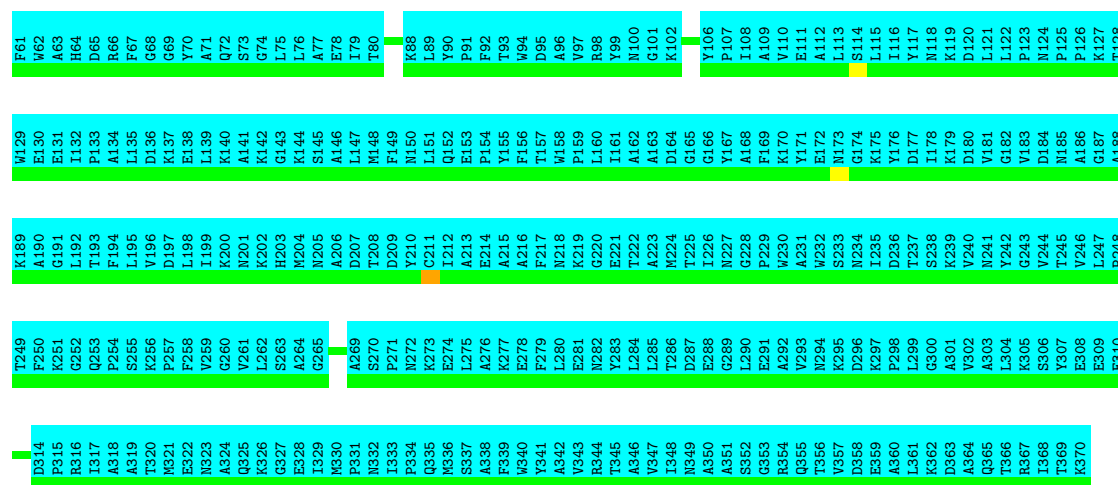
LYS	F61	W429	K189	T249	D314	F61	W429	K189	T249	D314
ILE	W62	E130	A190	F250	P315	W62	E130	A190	F250	P315
GLU	A63	E131	G191	K251	R316	A63	E131	G191	K251	R316
GLU	H64	L132	G192	G252	L317	H64	L132	G192	G252	L317
G5	D65	P133	T193	Q253	A318	D65	P133	T193	Q253	A318
K6	F194	F194	P254	P254	A319	K6	F194	F194	P254	A319
L7	L135	L195	S255	S255	T320	L7	L135	L195	S255	T320
W8	D136	V196	K256	K256	G326	W8	D136	V196	K256	G326
I9	K137	D197	P257	P257	K326	I9	K137	D197	P257	K326
W10	E138	L198	F258	F258	G327	W10	E138	L198	F258	G327
I11	L139	I199	V259	V259	K328	I11	L139	I199	V259	K328
N12	K140	N201	G260	G260	G325	N12	K140	N201	G260	G325
G13	A141	N201	V261	V261	G326	G13	A141	N201	V261	G326
D14	K142	K202	L262	L262	K326	D14	K142	K202	L262	K326
K15	G143	H203	S263	S263	K327	K15	G143	H203	S263	K327
G16	K144	M204	A264	A264	G328	G16	K144	M204	A264	G328
Y17	S145	N205	G265	G265	I329	Y17	S145	N205	G265	I329
N18	A146	A206	A269	A269	M330	N18	A146	A206	A269	M330
G19	L147	D207	S270	S270	P331	G19	L147	D207	S270	P331
L20	M148	T208	P271	P271	N332	L20	M148	T208	P271	N332
A21	F149	D209	N272	N272	I333	A21	F149	D209	N272	I333
E22	N150	Y210	K273	K273	P334	E22	N150	Y210	K273	P334
V23	L151	C211	E274	E274	Q335	V23	L151	C211	E274	Q335
G24	Q152	I212	L275	L275	M336	G24	Q152	I212	L275	M336
K25	E153	A213	K276	K276	S337	K25	E153	A213	K276	S337
K26	P154	E214	A276	A276	A338	K26	P154	E214	A276	A338
F27	F155	A215	K277	K277	F339	F27	F155	A215	K277	F339
K29	F156	A216	E278	E278	W340	K29	F156	A216	E278	W340
D30	F217	F217	F279	F279	Y341	D30	F217	F217	F279	Y341
D30	M158	N218	L280	L280	A342	D30	M158	N218	L280	A342
T31	P159	K219	E281	E281	V343	T31	P159	K219	E281	V343
G32	L160	G220	N282	N282	R344	G32	L160	G220	N282	R344
I33	I161	E221	Y283	Y283	T345	I33	I161	E221	Y283	T345
K34	A162	T222	L284	L284	A346	K34	A162	T222	L284	A346
V35	A163	A223	L285	L285	V347	V35	A163	A223	L285	V347
T36	D164	M224	T286	T286	I348	T36	D164	M224	T286	I348
V37	G165	T225	D287	D287	N349	V37	G165	T225	D287	N349
E38	G166	I226	E288	E288	A350	E38	G166	I226	E288	A350
H39	Y167	N227	G289	G289	A351	H39	Y167	N227	G289	A351
P40	A168	G228	L290	L290	S352	P40	A168	G228	L290	S352
C41	F169	P229	E291	E291	G353	C41	F169	P229	E291	G353
K42	V170	W230	A292	A292	R354	K42	V170	W230	A292	R354
L43	E171	A231	V293	V293	Q355	L43	E171	A231	V293	Q355
E44	E172	W232	K295	K295	T356	E44	E172	W232	K295	T356
E45	W173	S233	D296	D296	V357	E45	W173	S233	D296	V357
K46	G174	I235	K297	K297	D358	K46	G174	I235	K297	D358
F47	Y176	D236	P298	P298	F47	F47	Y176	D236	P298	F47
P48	D177	T237	L299	L299	P48	P48	D177	T237	L299	P48
Q49	I178	S238	G300	G300	L361	Q49	I178	S238	G300	L361
V50	K179	K239	A301	A301	K362	V50	K179	K239	A301	K362
A51	D180	V240	V302	V302	D363	A51	D180	V240	V302	D363
T53	V181	N241	A303	A303	A364	T53	V181	N241	A303	A364
G54	G182	Y242	T304	T304	T365	G54	G182	Y242	T304	T365
D55	V183	G243	K305	K305	T366	D55	V183	G243	K305	T366
G56	D184	V244	S306	S306	I368	G56	D184	V244	S306	I368
P57	N185	T245	Y307	Y307	T369	P57	N185	T245	Y307	T369
D58	A186	V246	E308	E308	K370	D58	A186	V246	E308	K370
I59	G187	L247	E309	E309		I59	G187	L247	E309	
I60	A188	P248	E310	E310		I60	A188	P248	E310	

4.2.9 Score per residue for model 9

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

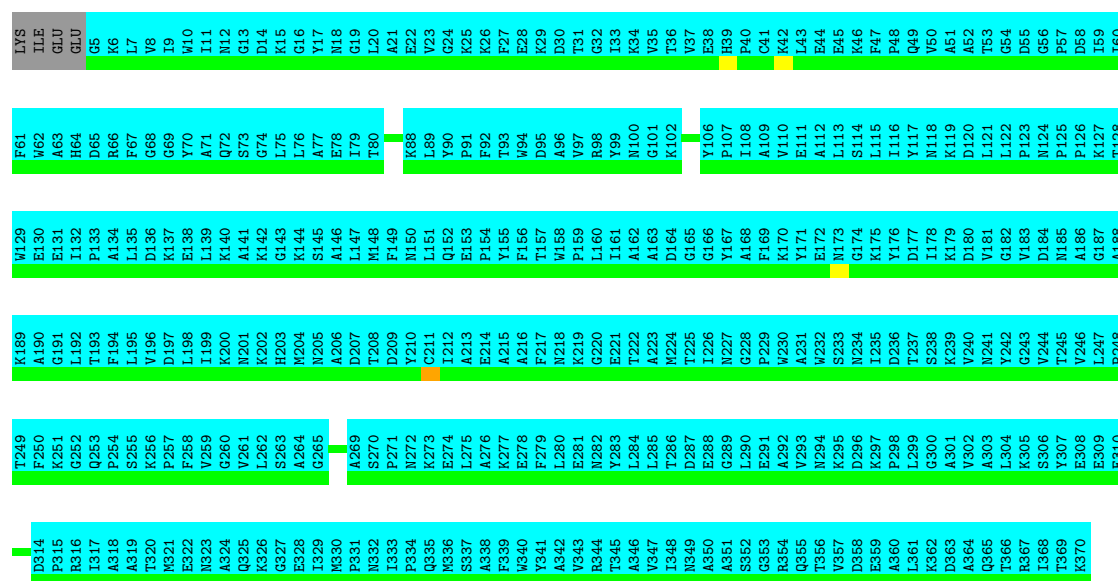
LYS	F61	W429	K189	T249	D314	F61	W429	K189	T249	D314
ILE	W62	E130	A190	F250	P315	W62	E130	A190	F250	P315
GLU	A63	E131	G191	K251	R316	A63	E131	G191	K251	R316
GLU	H64	L132	G192	G252	L317	H64	L132	G192	G252	L317
G5	D65	P133	T193	Q253	A318	D65	P133	T193	Q253	A318
K6	F194	F194	P254	P254	A319	K6	F194	F194	P254	A319
L7	L135	L195	S255	S255	T320	L7	L135	L195	S255	T320
W8	D136	V196	K256	K256	G326	W8	D136	V196	K256	G326
I9	K137	D197	P257	P257	K326	I9	K137	D197	P257	K326
W10	E138	L198	F258	F258	G327	W10	E138	L198	F258	G327
I11	L139	I199	V259	V259	K328	I11	L139	I199	V259	K328
N12	K140	N201	G260	G260	G325	N12	K140	N201	G260	G325
G13	A141	N201	V261	V261	G326	G13	A141	N201	V261	G326
D14	K142	K202	L262	L262	K326	D14	K142	K202	L262	K326
K15	G143	H203	S263	S263	K327	K15	G143	H203	S263	K327
G16	K144	M204	A264	A264	G328	G16	K144	M204	A264	G328
Y17	S145	N205	G265	G265	I329					
N18	L146	N206	L266	L266	K329	N18	L146	N206	L266	K329
G19	K147	K207	G267	G267	G330	G19	K147	K207	G267	G330
L20	L148	L208	V268	V268	K330	L20	L148	L208	V268	K330
A21	A149	A209	S269	S269	K331	A21	A149	A209	S269	K331
E22	E150	E210	F270	F270	G332	E22	E150	E210	F270	G332
D23	D151	D211	K271	K271	K333	D23	D151	D211	K271	K333
F24	F152	F212	L272	L272	L334	F24	F152	F212	L272	L334
K25	K153	K213	P273	P273	P335	K25	K153	K213	P273	P335
R26	R154	R214	A274	A274	A336	R26	R154	R214	A274	A336
E28	E155	E215	G275	G275	G337	E28	E155	E215	G275	G337
K29	K156	K216	V276	V276	K338	K29	K156	K216	V276	K338
L30	L157	L217	S277	S277	K339	L30	L157	L217	S277	K339
T31	T158	T218	F278	F278	G340	T31	T158	T218	F278	G340
D32	D159	D219	K279	K279	K341	D32	D159	D219	K279	K341
G33	G160	G220	L280	L280	L342	G33	G160	G220	L280	L342
I34	I161	I221	P281	P281	P343	I34	I161	I221	P281	P343
K35	K162	K222	A282	A282	A344	K35	K162	K222	A282	A344
V36	V163	V223	G283	G283	G345	V36	V163	V223	G283	G345
T37	T164	T224	V284	V284	K346	T37	T164	T224	V284	K346
V38	V165	V225	S285	S285	K347	V38	V165	V225	S285	K347
E39	E166	E226	F286	F286	G348	E39	E166	E226	F286	G348
H39	H167	H227	K287	K287	K349	H39	H167	H227	K287	K349
P40	P168	P228	L288	L288	L350	P40	P168	P228	L288	L350
F41	F169	F229	S289	S289	K351	F41	F169	F229	S289	K351
K42	K170	K230	A290	A290	A352	K42	K170	K230	A290	A352
L43	L171	L231	G291	G291	G353	L43	L171	L231	G291	G353
E44	E172	E232	V292	V292	K354	E44	E172	E232	V292	K354
A45	A173	A233	S293	S293	K355	A45	A173	A233	S293	K355
K46	K174	K234	F294	F294	G356	K46	K174	K234	F294	G356
F47	F175	F235	K295	K295	K357	F47	F175	F235	K295	K357
P48	P176	P236	L296	L296	L358	P48	P176	P236	L296	L358
Q49	Q177	Q237	S297	S297	K359	Q49	Q177	Q237	S297	K359
V50	V178	V238	F298	F298	G360	V50	V178	V238	F298	G360
A51	A179	A239	K299	K299	K361	A51	A179	A239	K299	K361
A52	A180	A240	L300	L300	L362	A52	A180	A240	L300	L362
T53	T181	T241	P301	P301	P363	T53	T181	T241	P301	P363
G54	G182	G242	A302	A302	A364	G54	G182	G242	A302	A364
D55	D183	D243	G303	G303	G365	D55	D183	D243	G303	G365
G56	G184	G244	V304	V304	K366	G56	G184	G244	V304	K366
F57	F185	F245	S305	S305	K367	F57	F185	F245	S305	K367
D58	D186	D246	F306	F306	G368	D58	D186	D246	F306	G368
I59	I187	I247	K307	K307	K369	I59	I187	I247	K307	K369



4.2.10 Score per residue for model 10

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

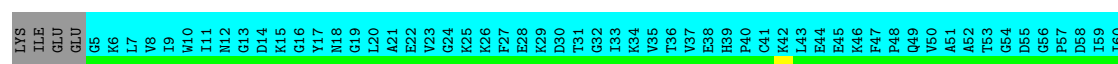
Chain A: . 95%

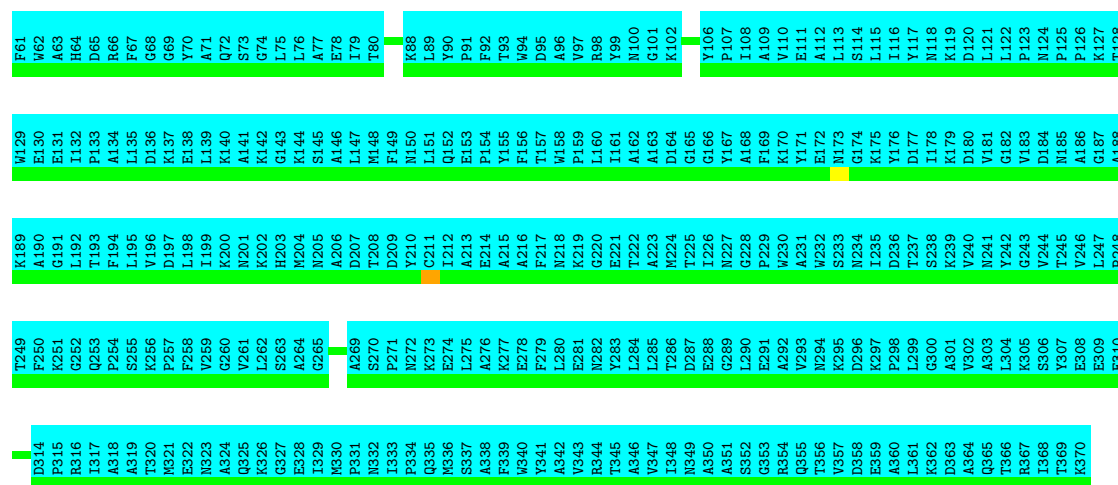


4.2.11 Score per residue for model 11

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

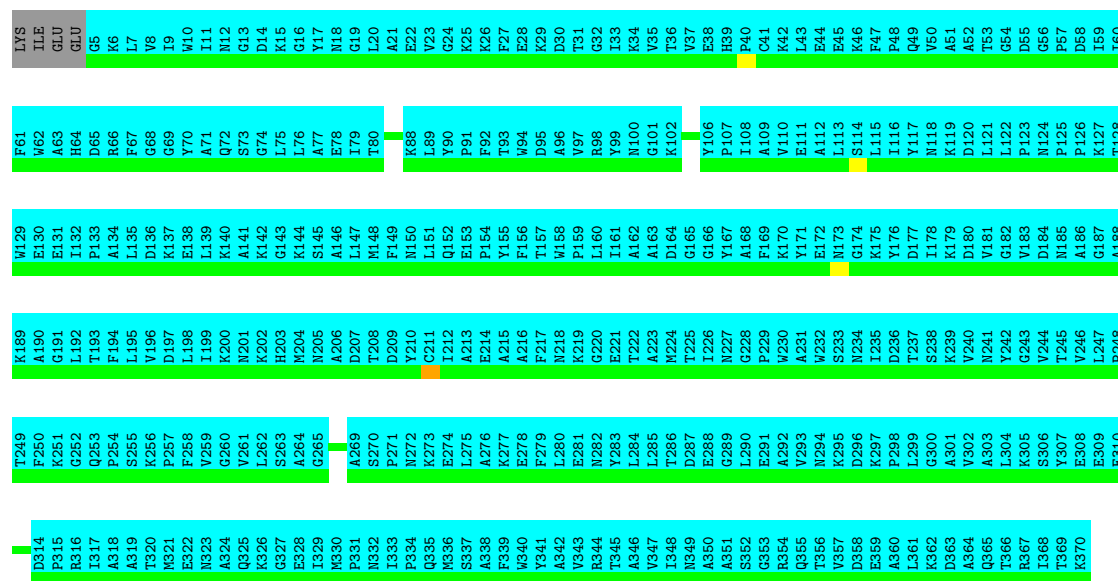




4.2.12 Score per residue for model 12

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

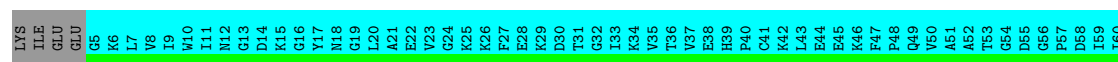
Chain A: . 95%

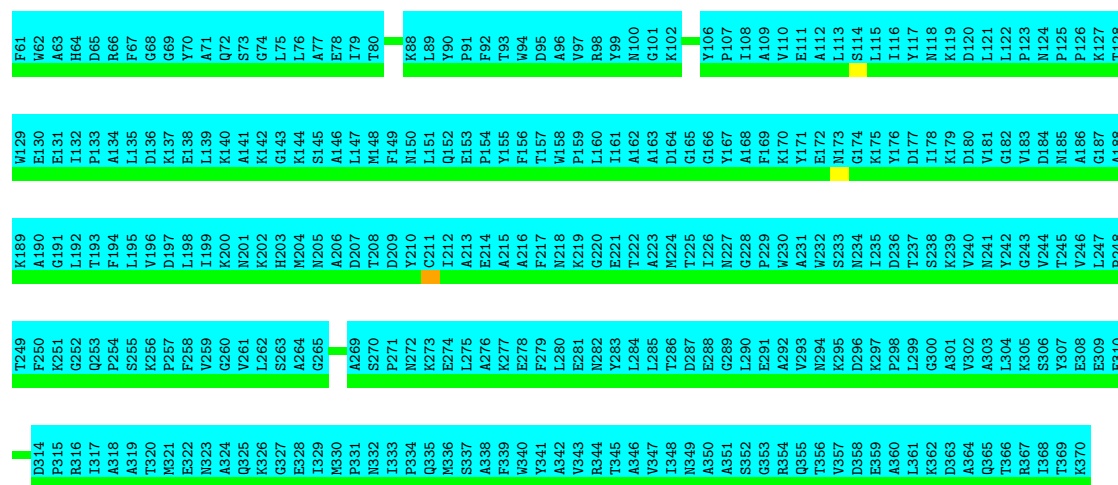


4.2.13 Score per residue for model 13

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

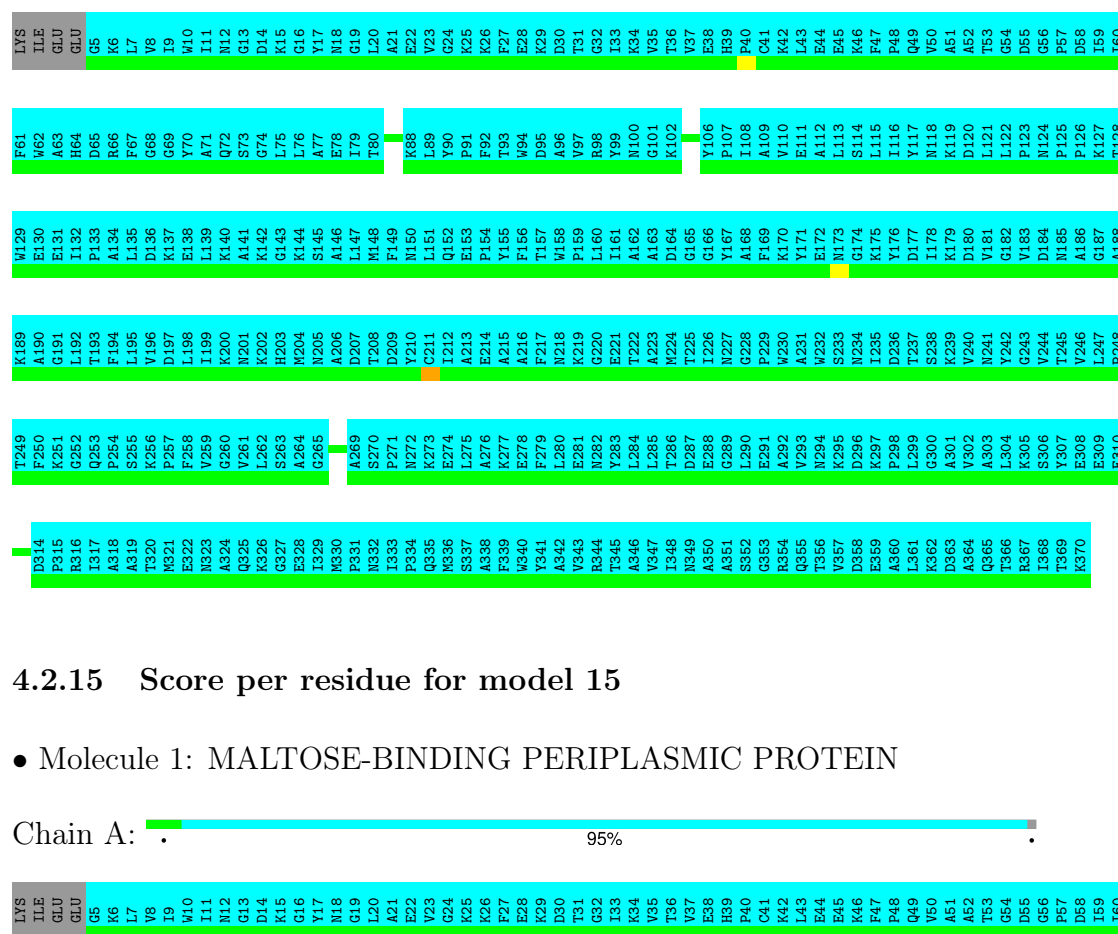




4.2.14 Score per residue for model 14

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

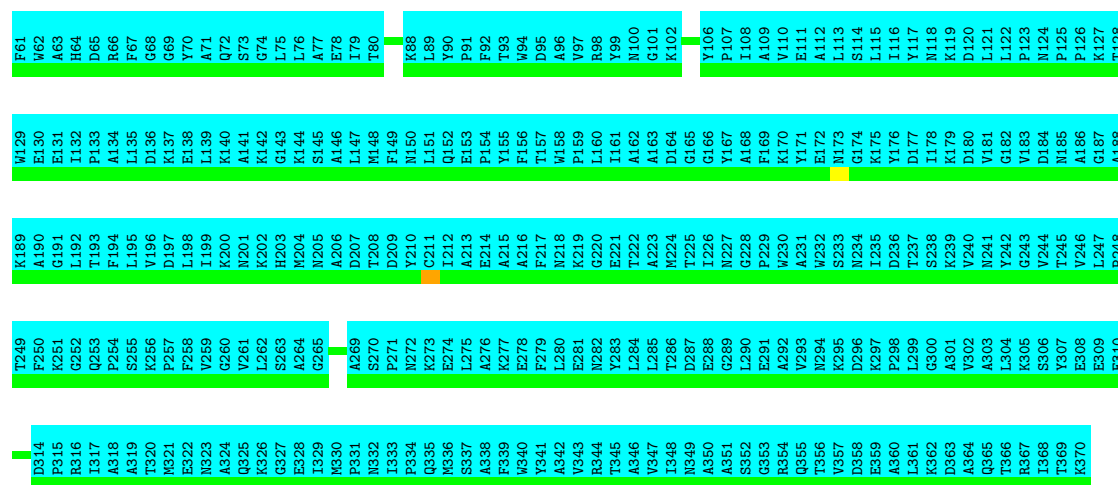
Chain A: . 95%



4.2.15 Score per residue for model 15

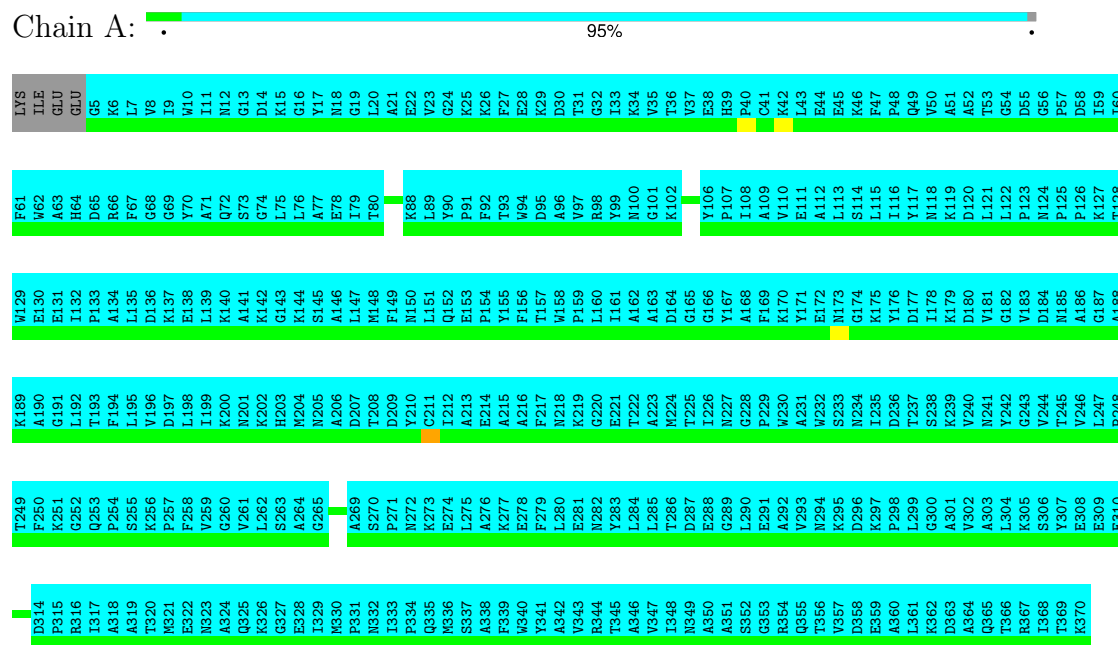
- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%



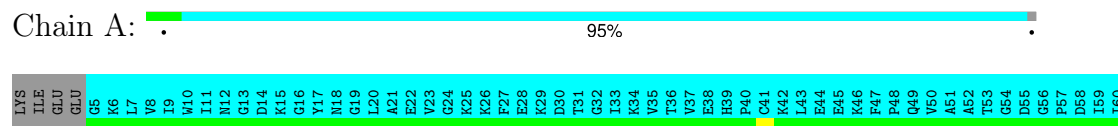
4.2.16 Score per residue for model 16

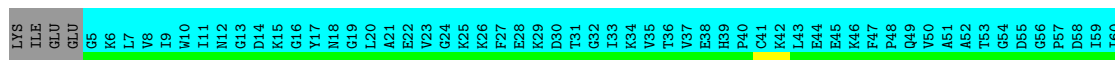
- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

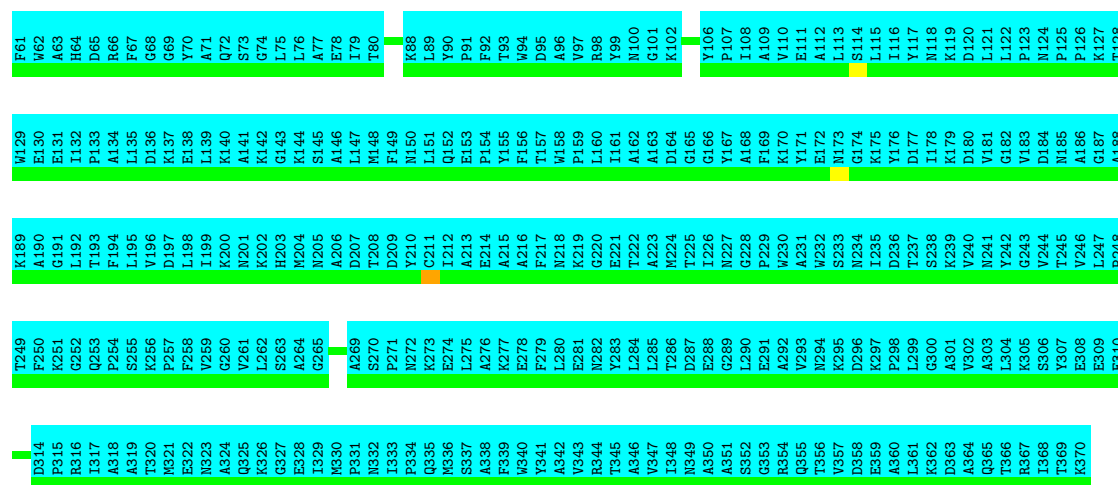


4.2.17 Score per residue for model 17

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN



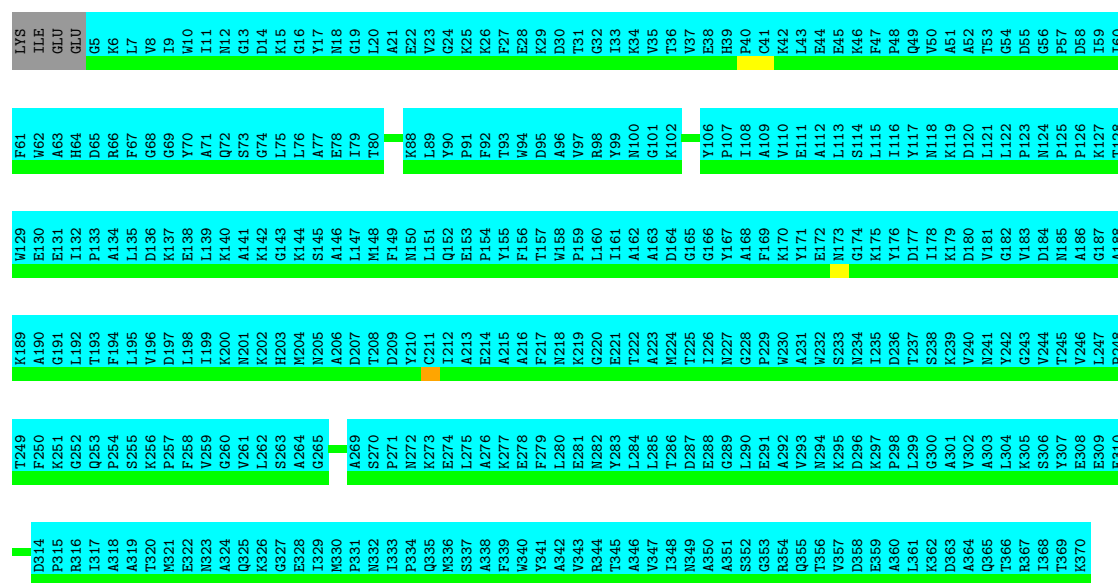




4.2.20 Score per residue for model 20

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

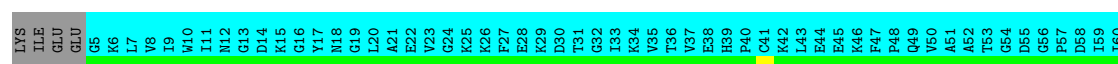
Chain A: .

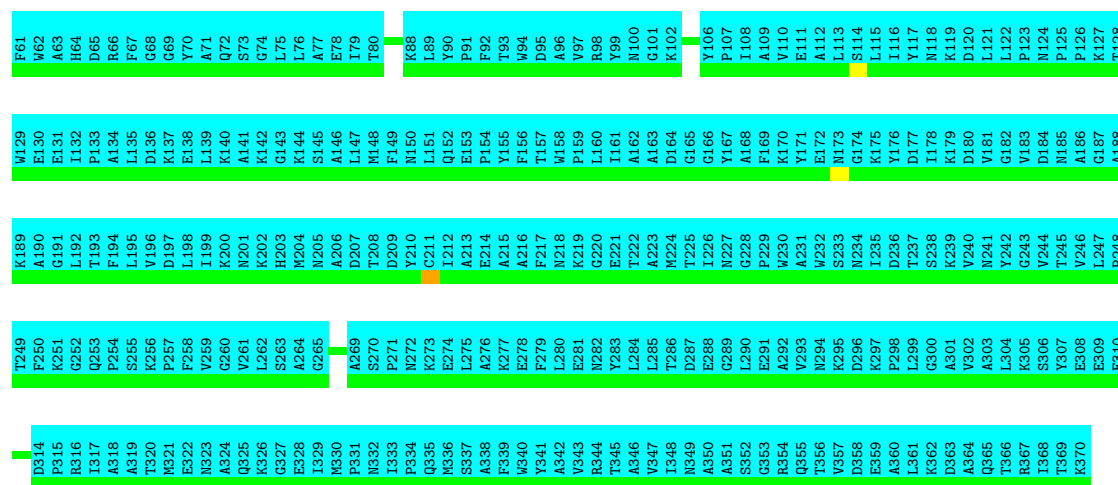


4.2.21 Score per residue for model 21

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: .

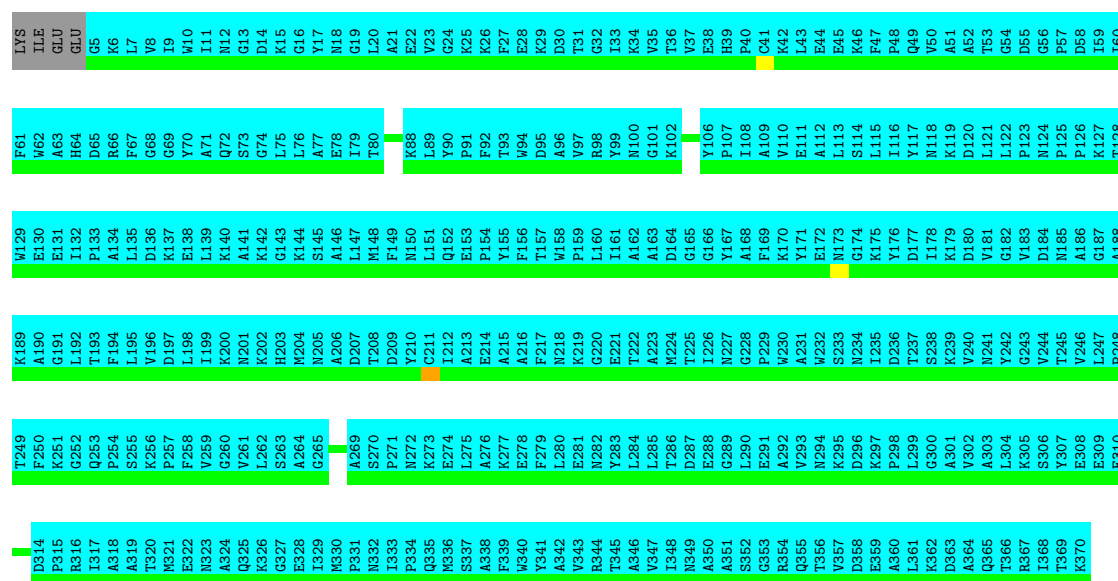




4.2.22 Score per residue for model 22

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

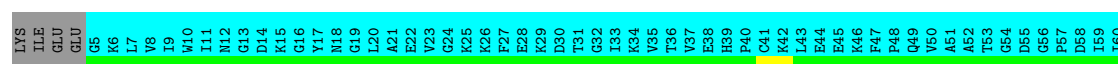
Chain A: . 95%

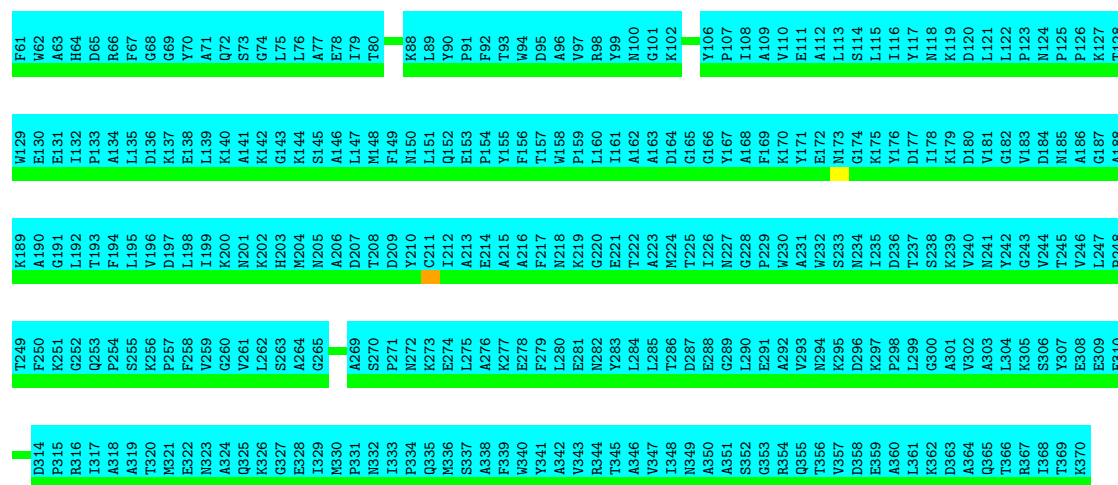


4.2.23 Score per residue for model 23

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

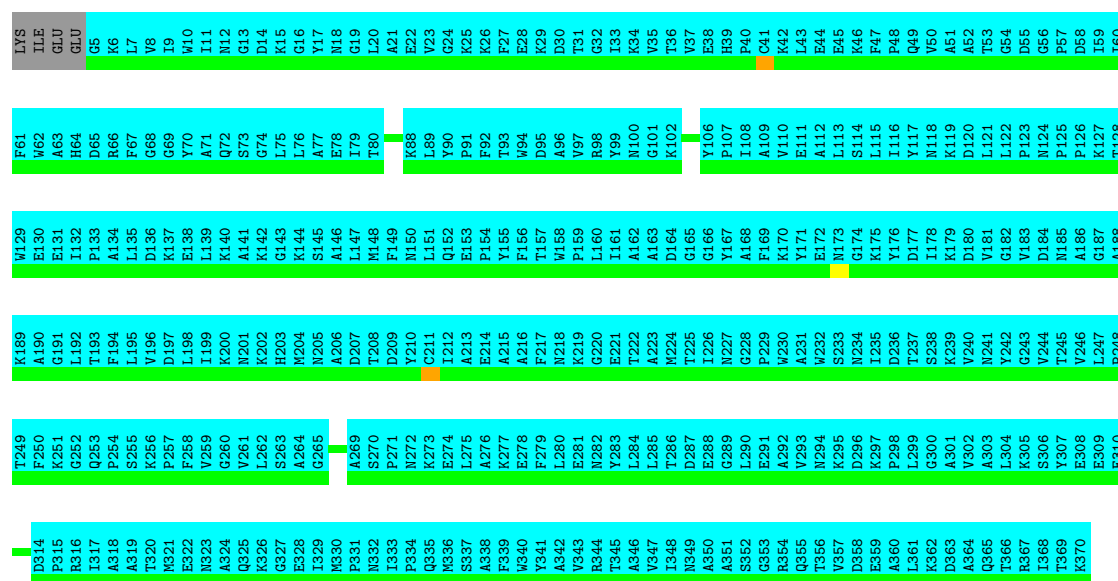




4.2.24 Score per residue for model 24

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

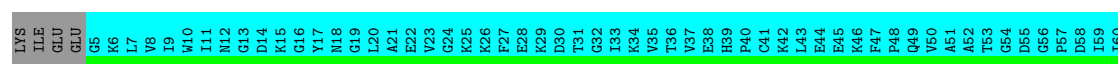
Chain A: . 95%

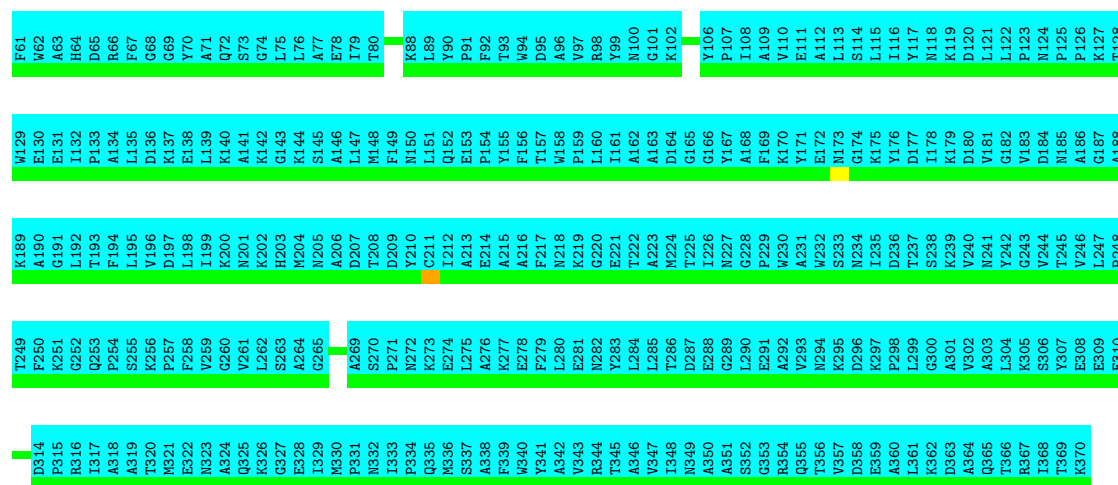


4.2.25 Score per residue for model 25

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

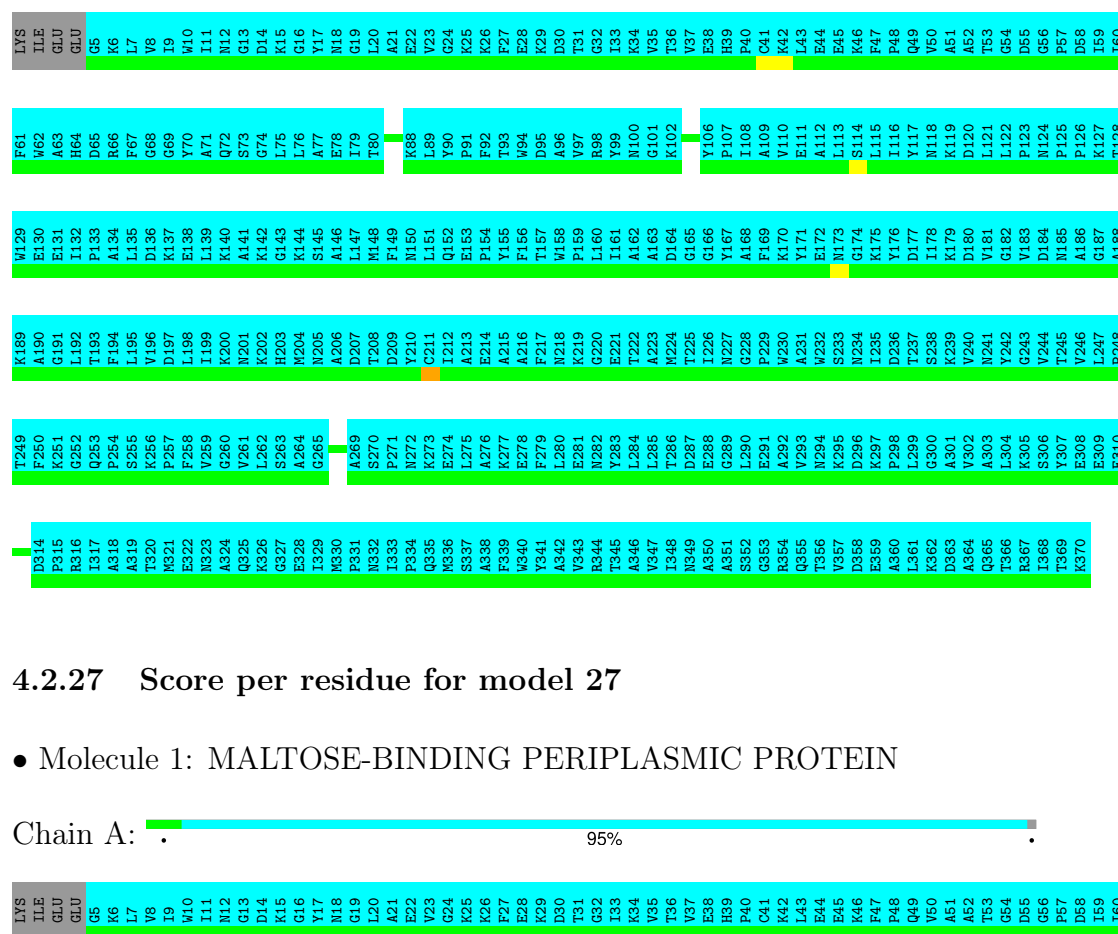




4.2.26 Score per residue for model 26

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

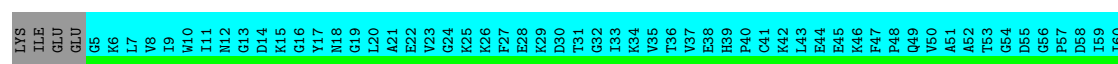
Chain A: . 95%

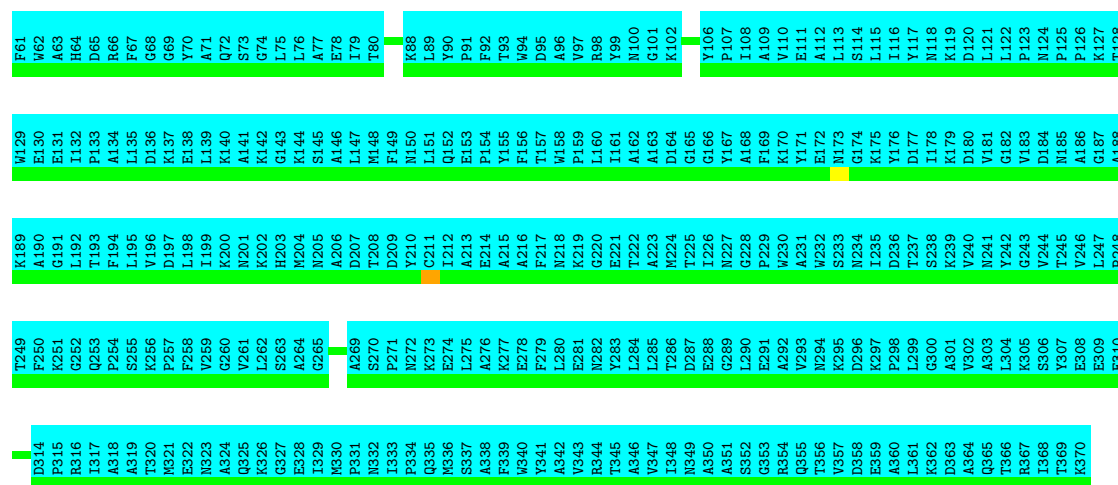


4.2.27 Score per residue for model 27

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

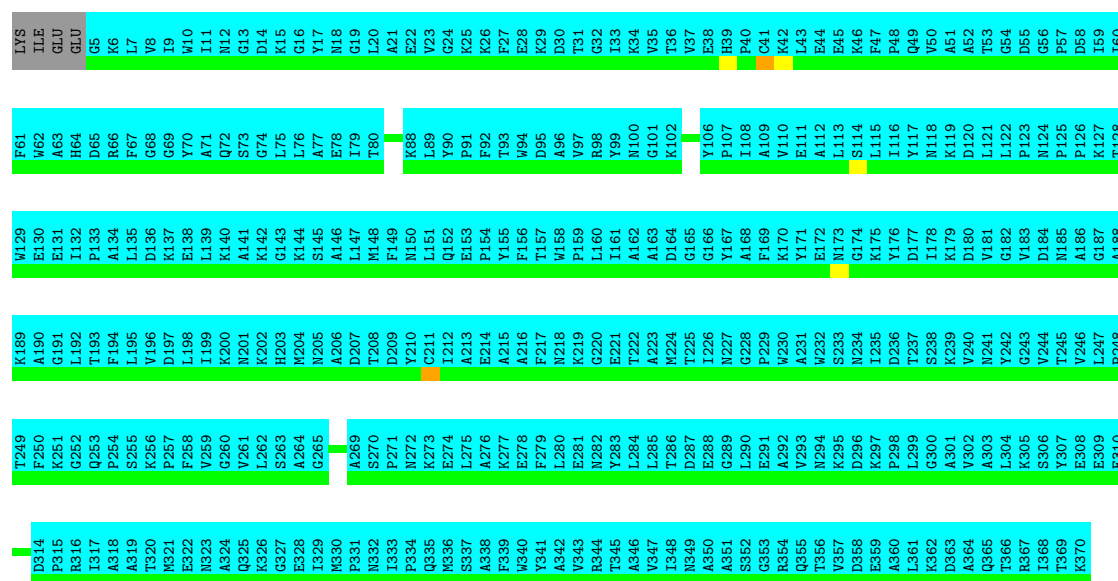




4.2.28 Score per residue for model 28

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

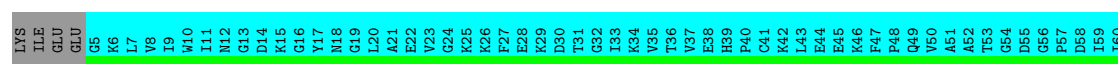
Chain A: . 95%

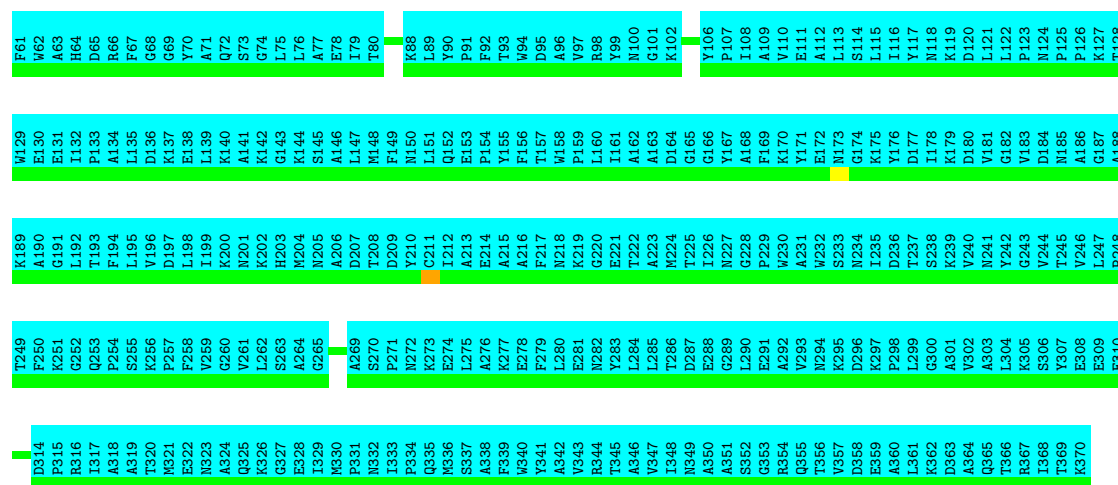


4.2.29 Score per residue for model 29

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

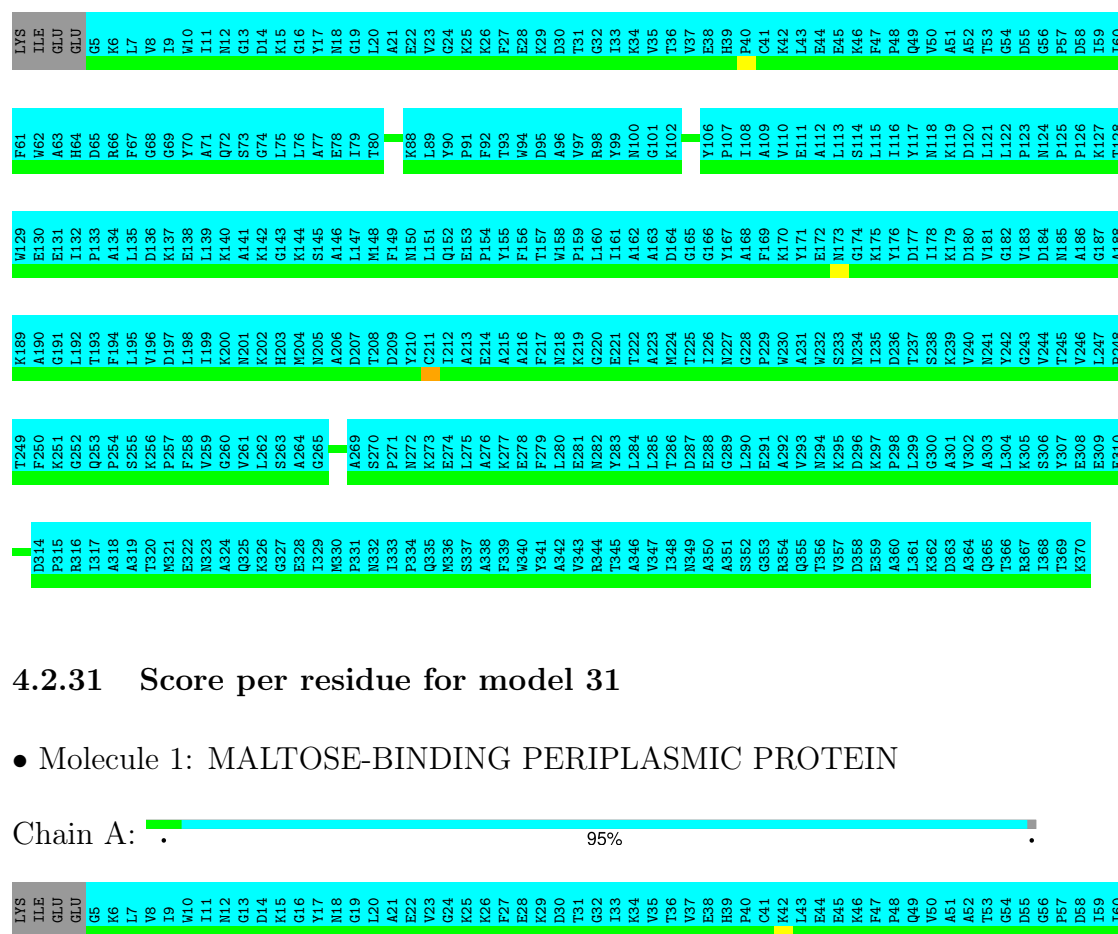




4.2.30 Score per residue for model 30

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

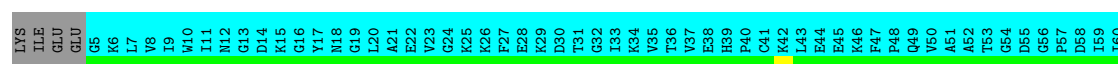
Chain A: . 95%

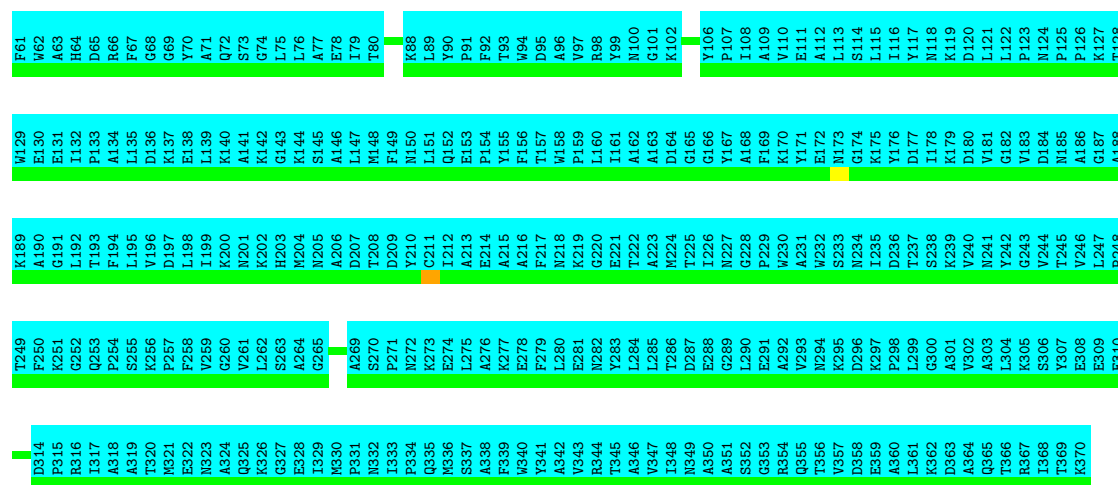


4.2.31 Score per residue for model 31

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

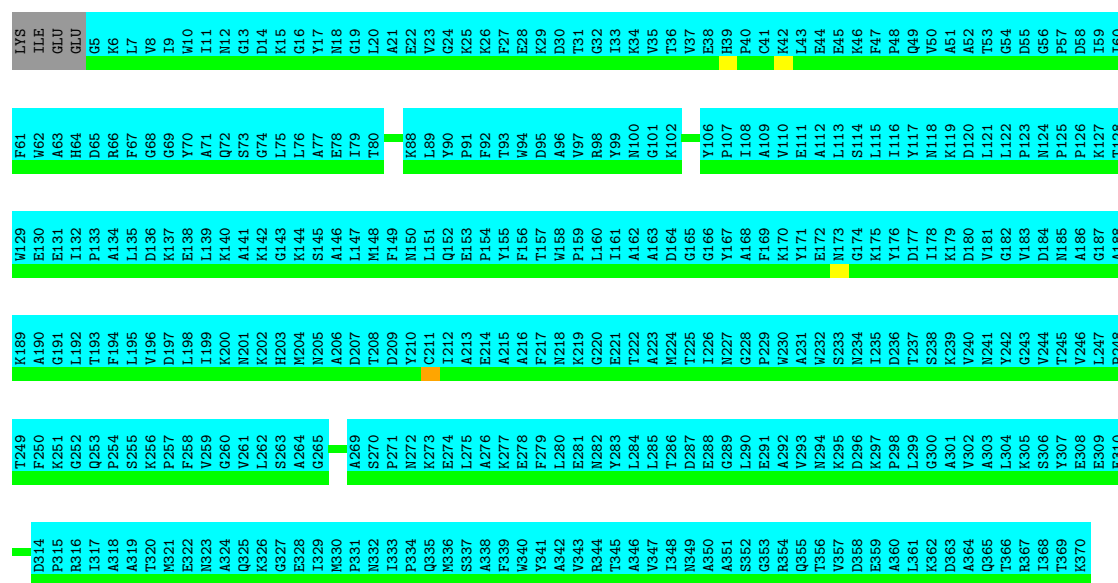




4.2.32 Score per residue for model 32

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

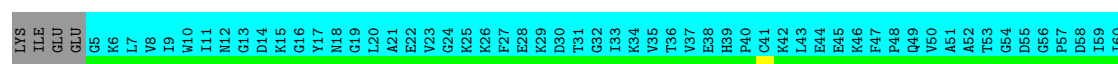
Chain A: .

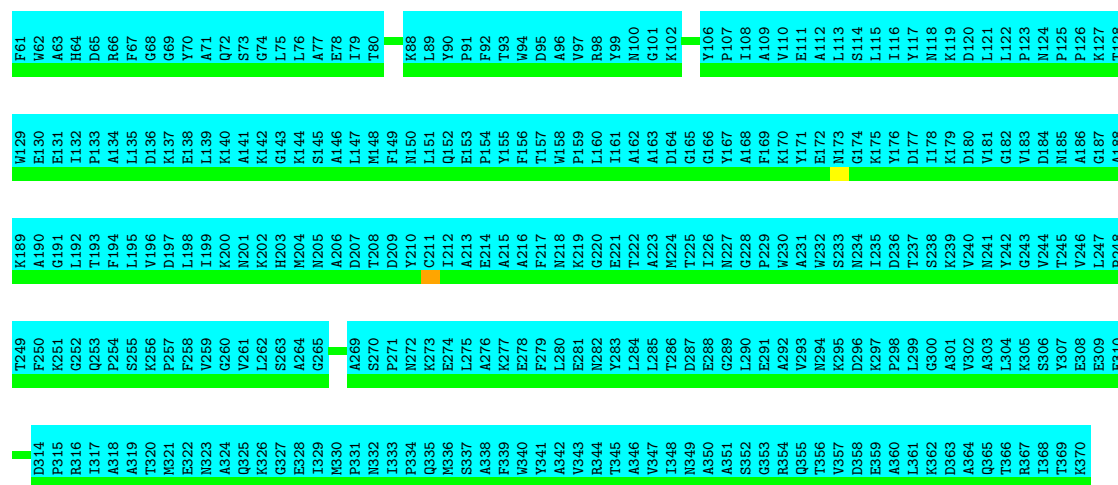


4.2.33 Score per residue for model 33

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: .

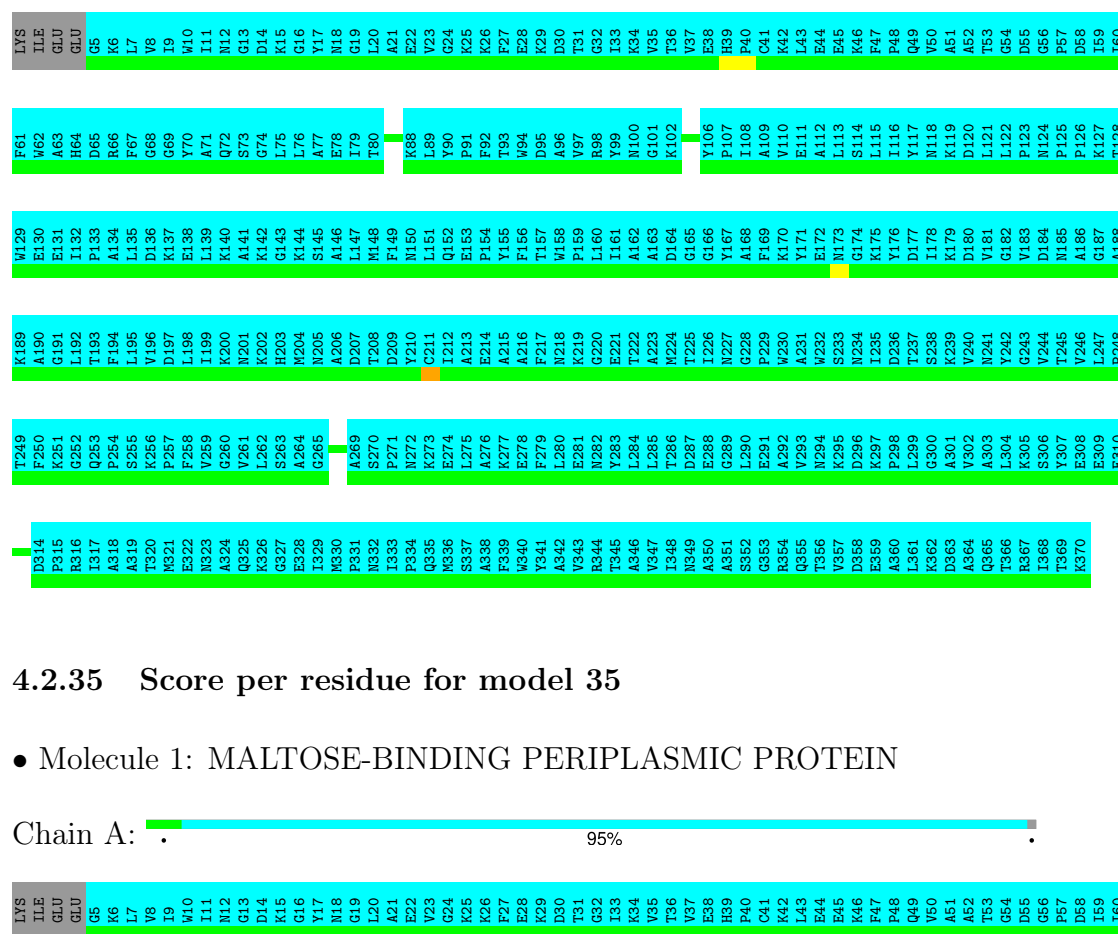




4.2.34 Score per residue for model 34

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

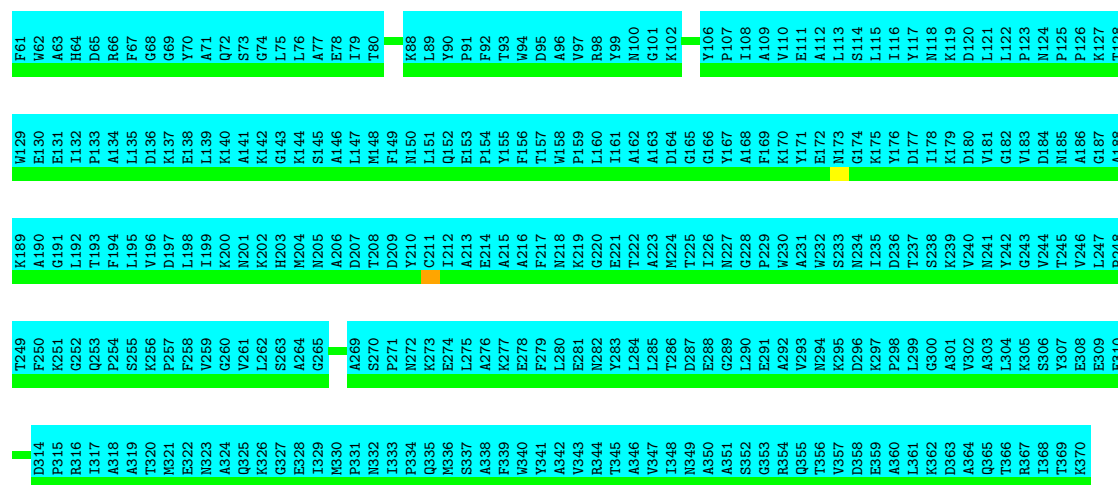
Chain A: . 95%



4.2.35 Score per residue for model 35

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

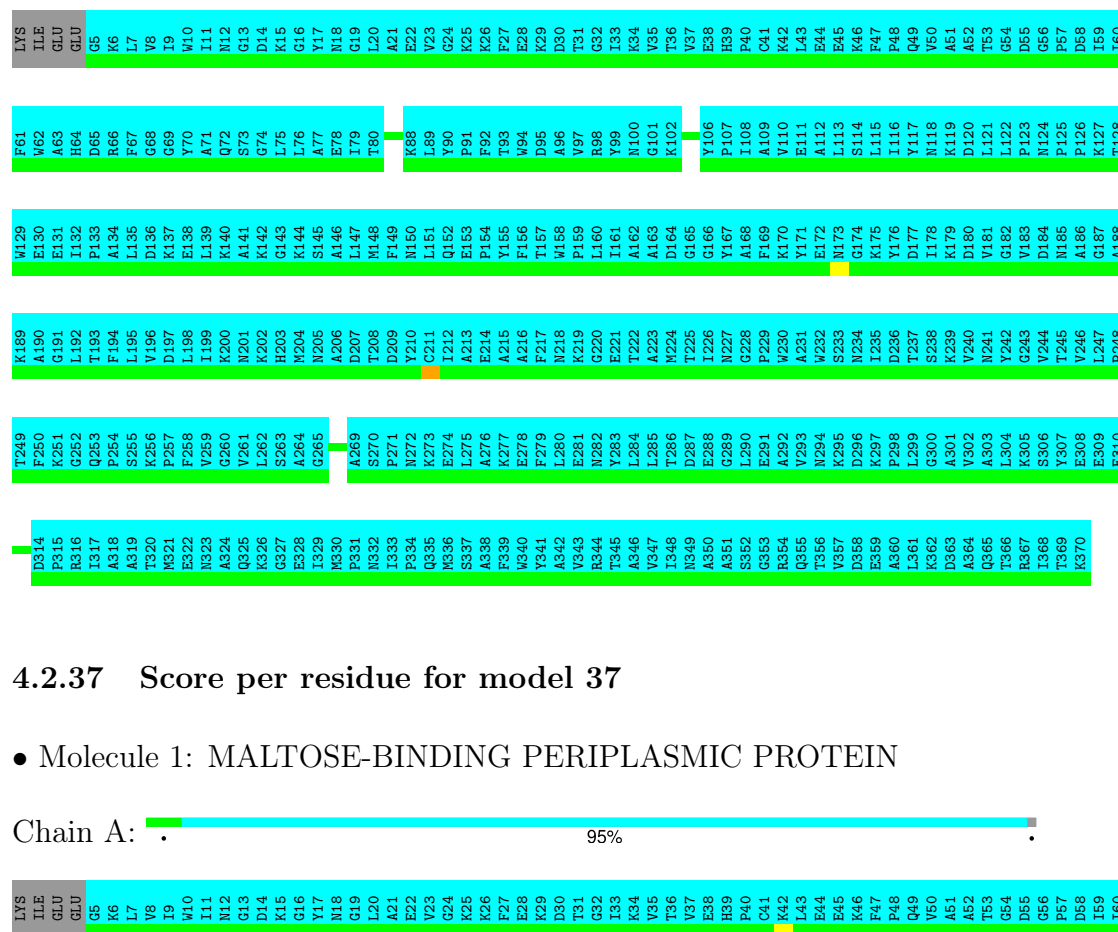
Chain A: . 95%



4.2.36 Score per residue for model 36

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

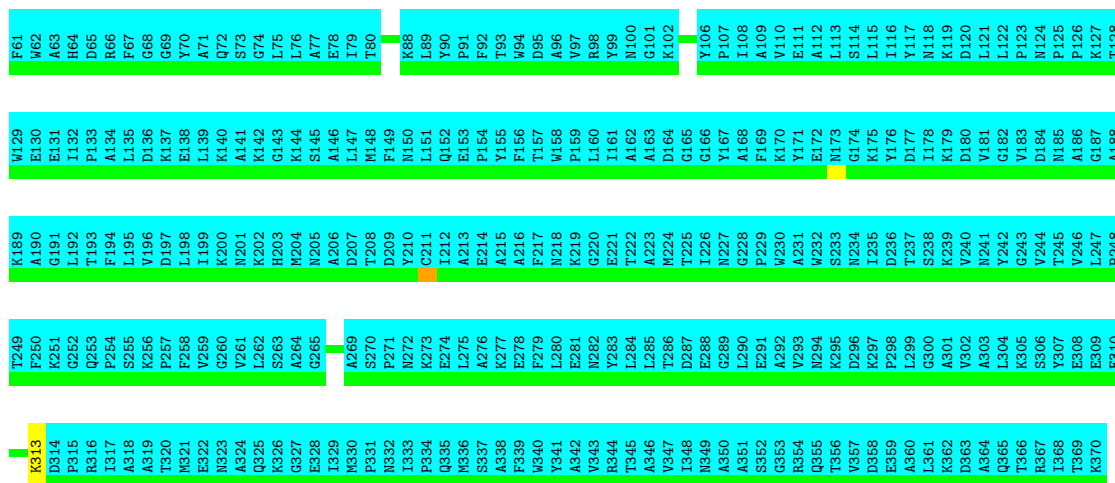
Chain A: . 95%



4.2.37 Score per residue for model 37

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

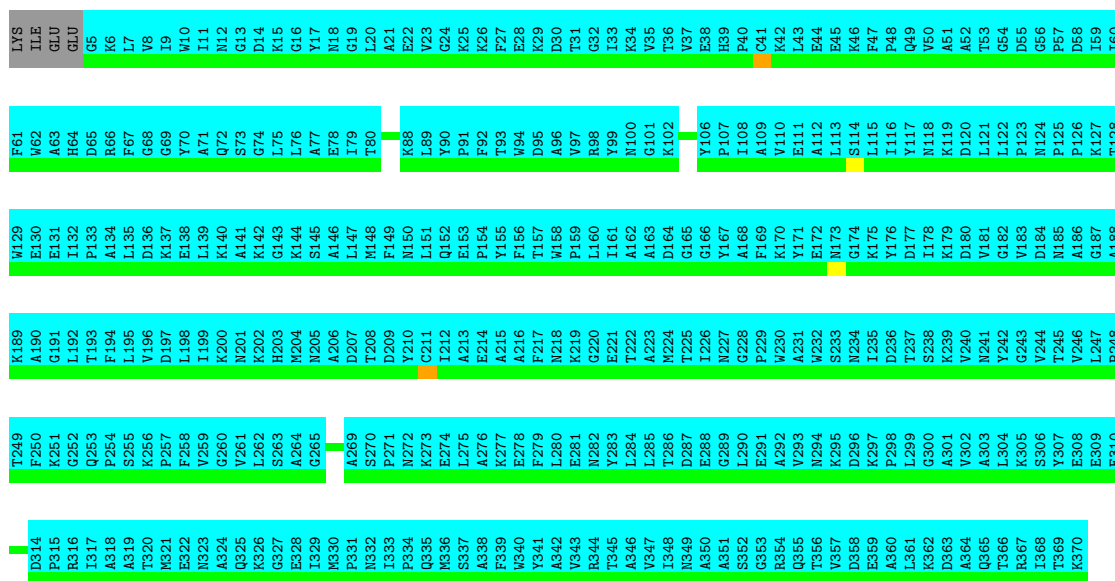
Chain A: . 95%



4.2.38 Score per residue for model 38

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

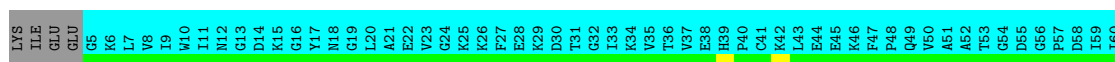
Chain A:  95%

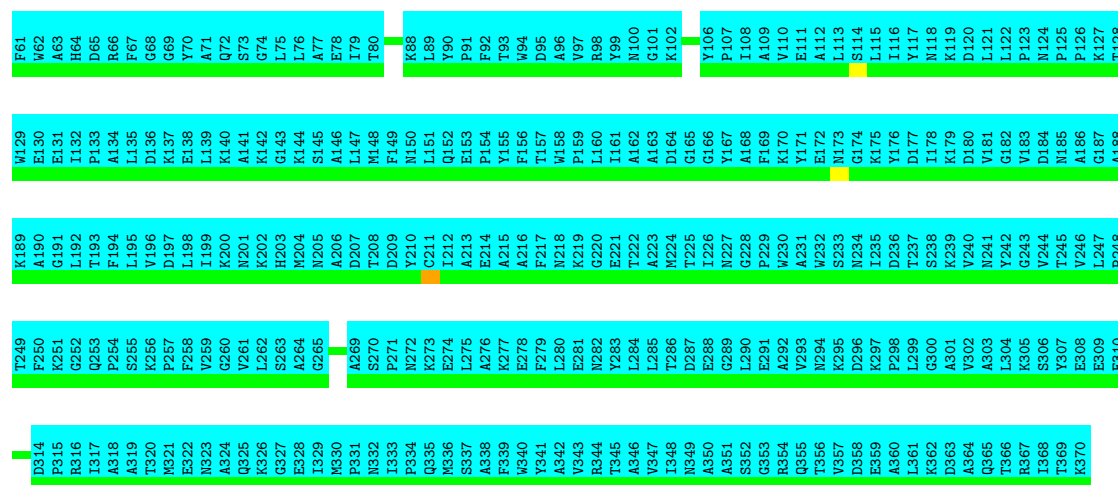


4.2.39 Score per residue for model 39

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: 95%

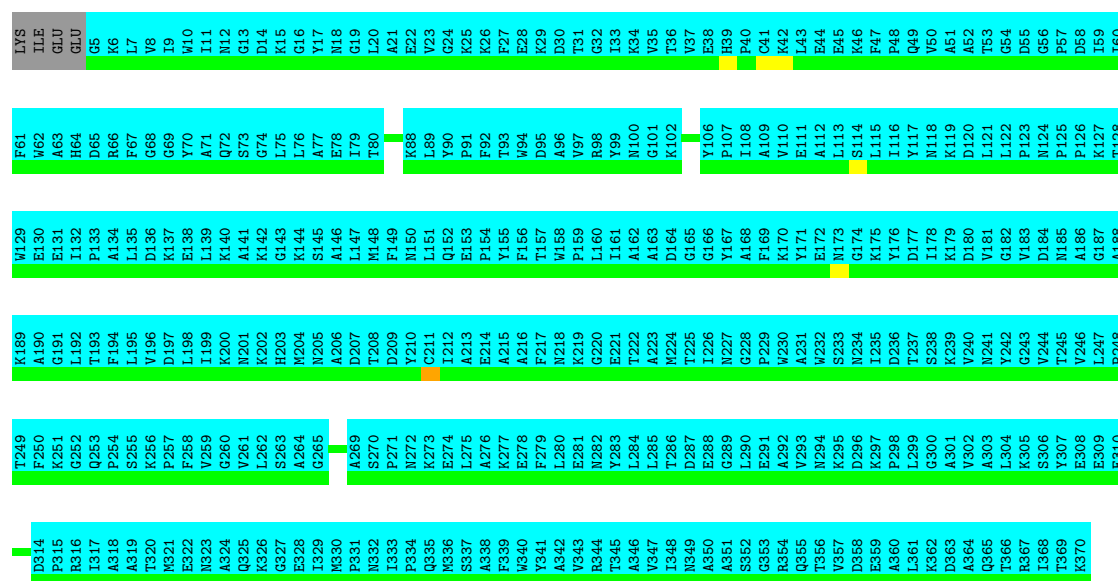




4.2.40 Score per residue for model 40

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

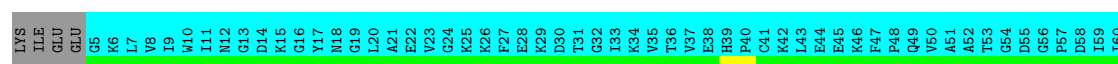
Chain A: . 95%

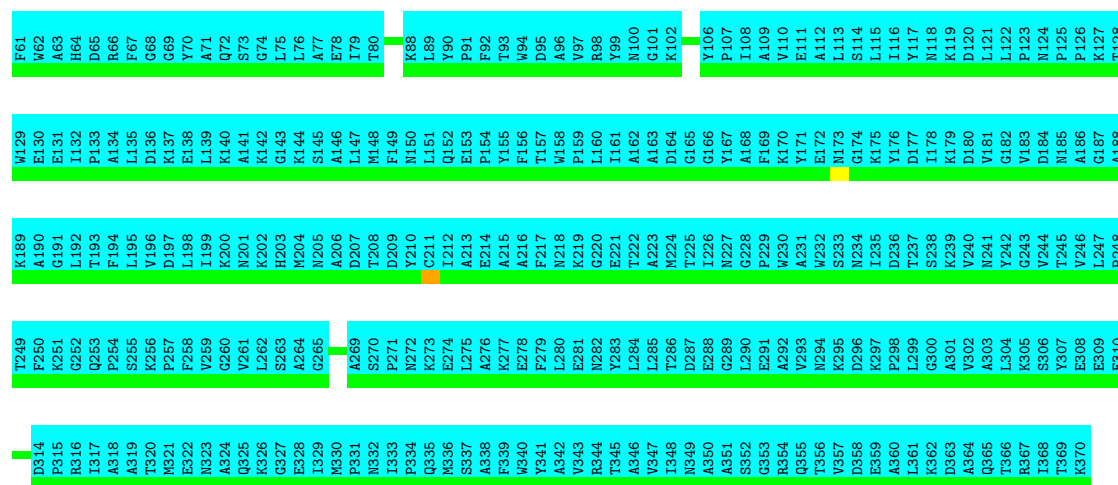


4.2.41 Score per residue for model 41

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

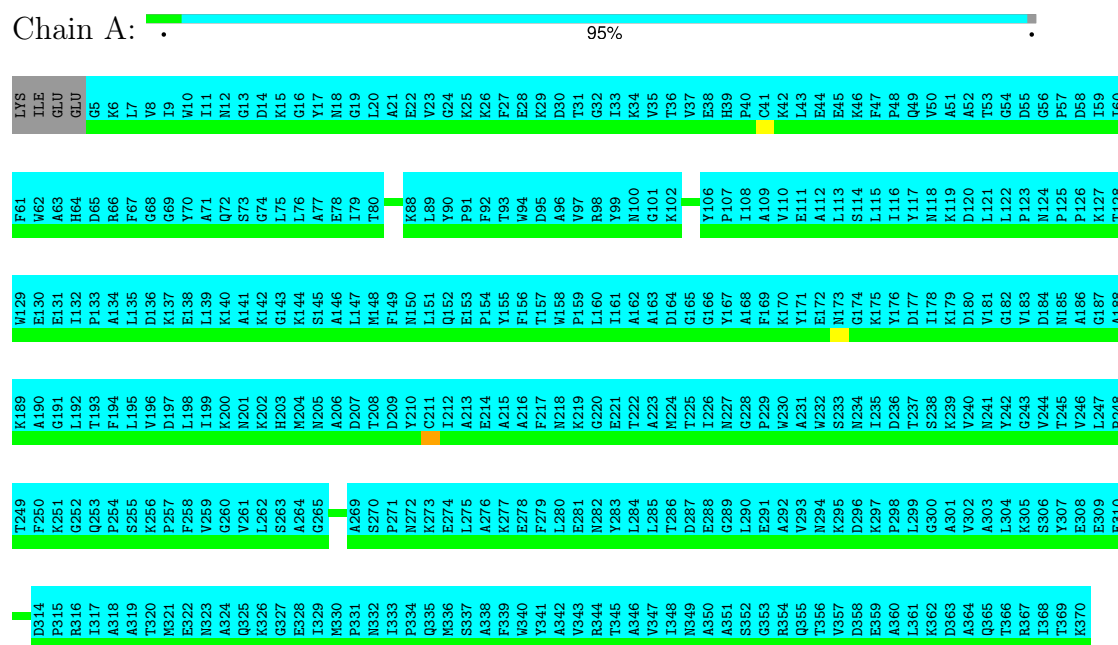
Chain A: . 95%





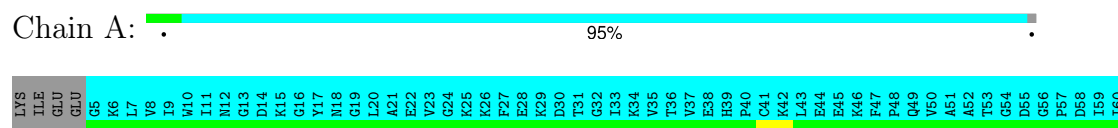
4.2.42 Score per residue for model 42

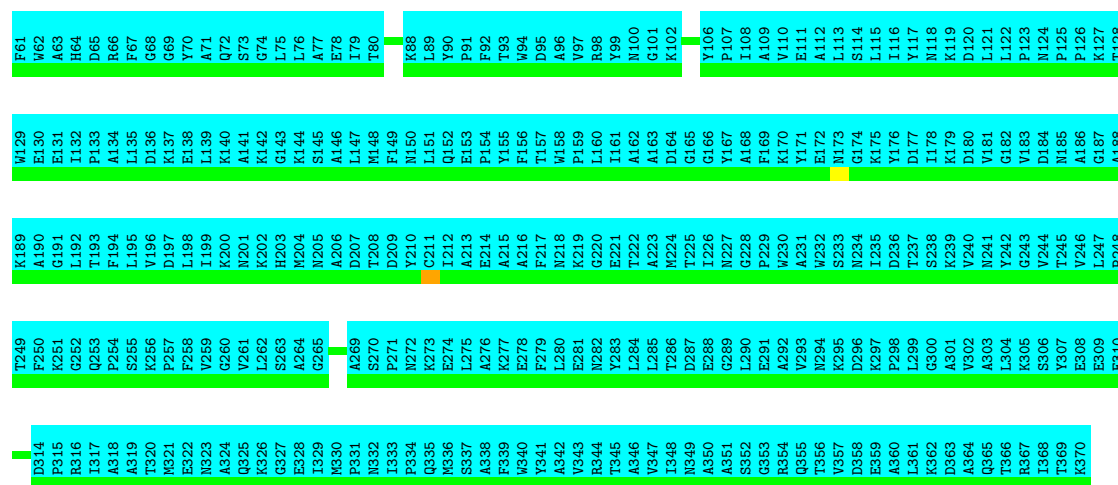
- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN



4.2.43 Score per residue for model 43

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

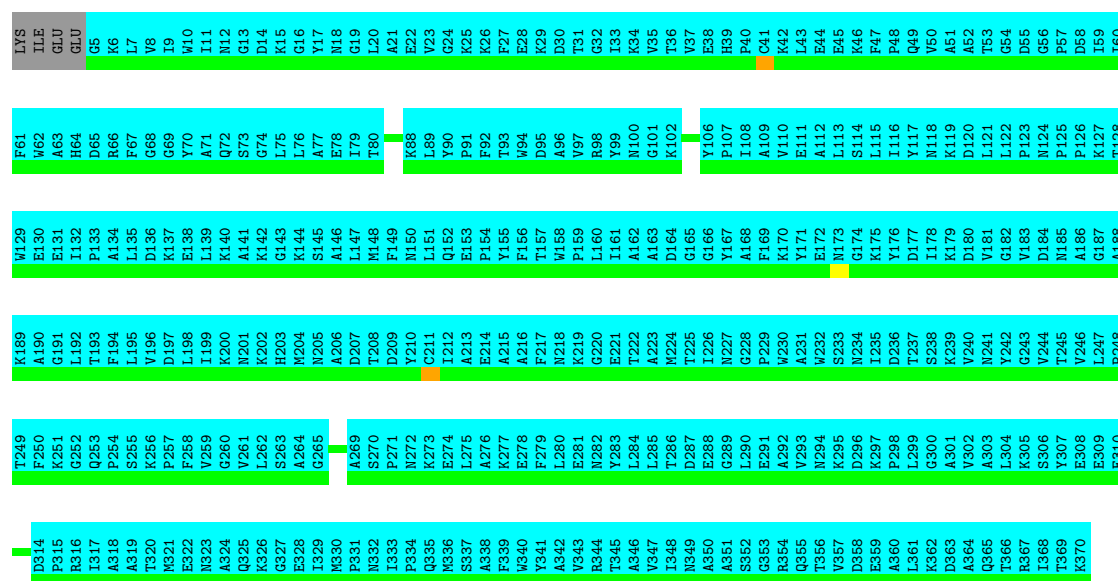




4.2.44 Score per residue for model 44

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

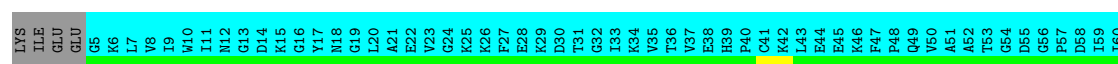
Chain A: . 95%

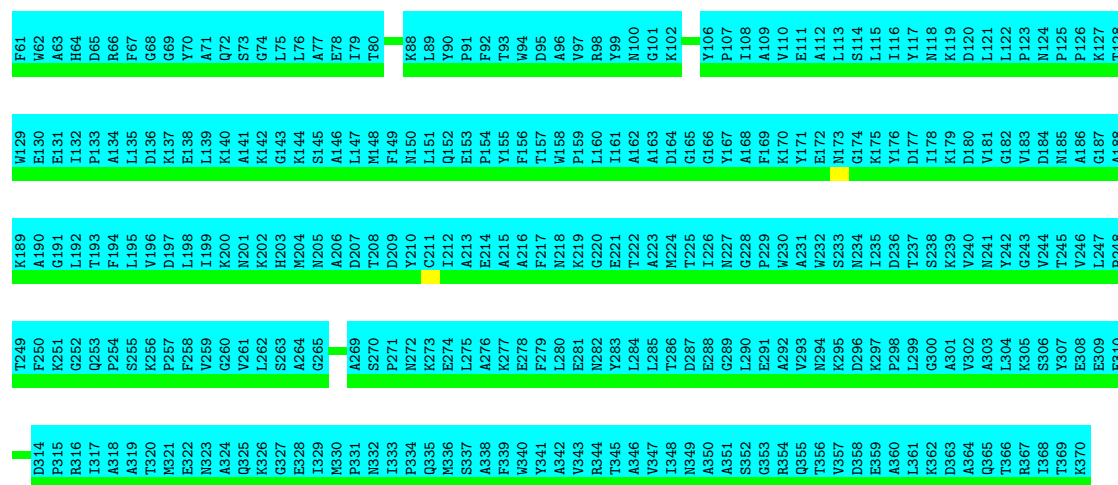


4.2.45 Score per residue for model 45

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

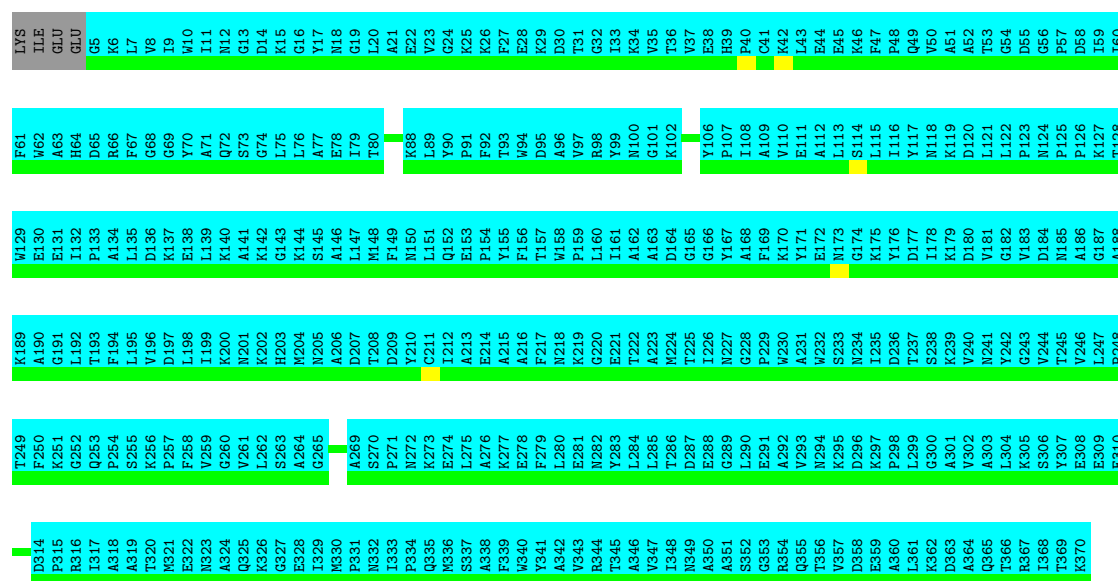




4.2.46 Score per residue for model 46

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

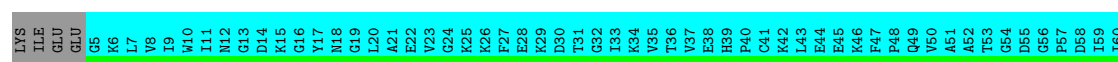
Chain A: . 95%

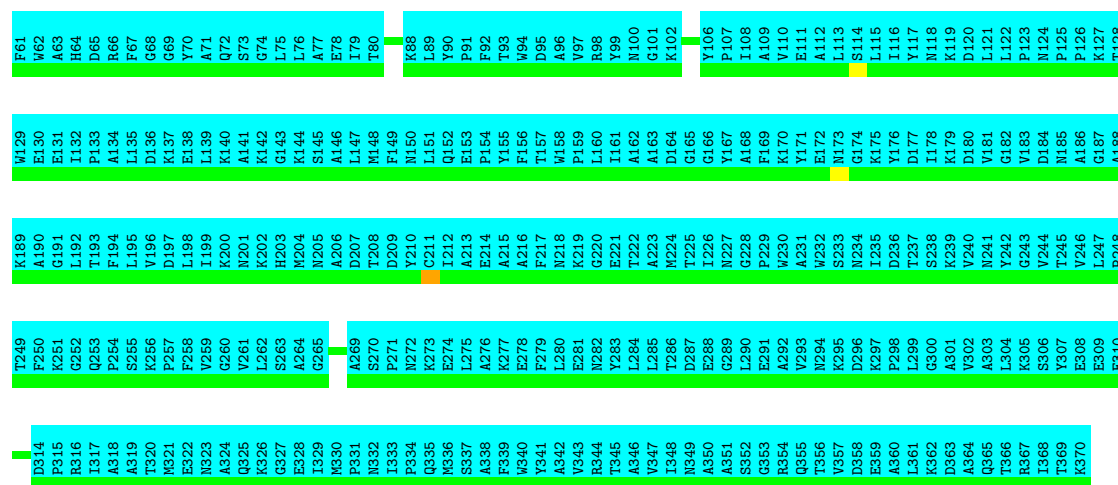


4.2.47 Score per residue for model 47

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

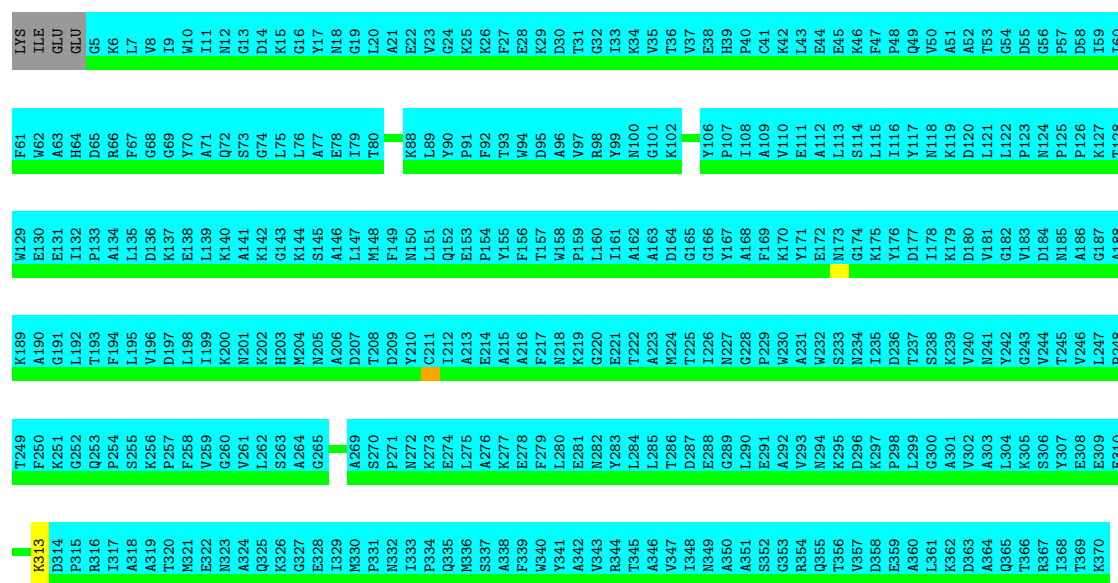




4.2.48 Score per residue for model 48

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

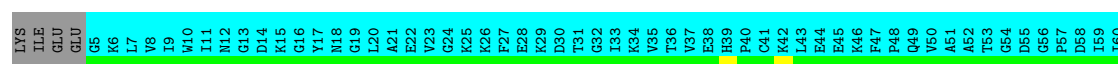
Chain A: . 95%

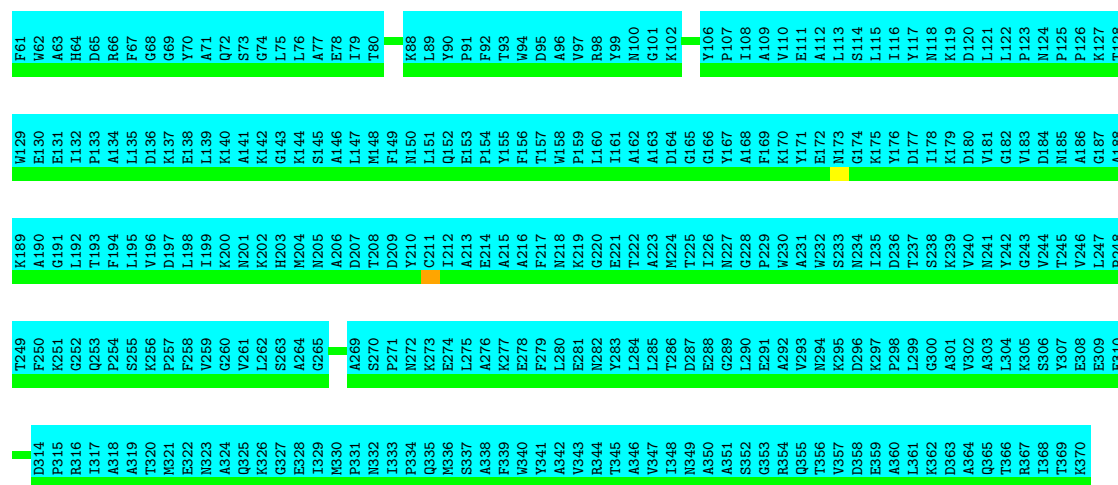


4.2.49 Score per residue for model 49

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

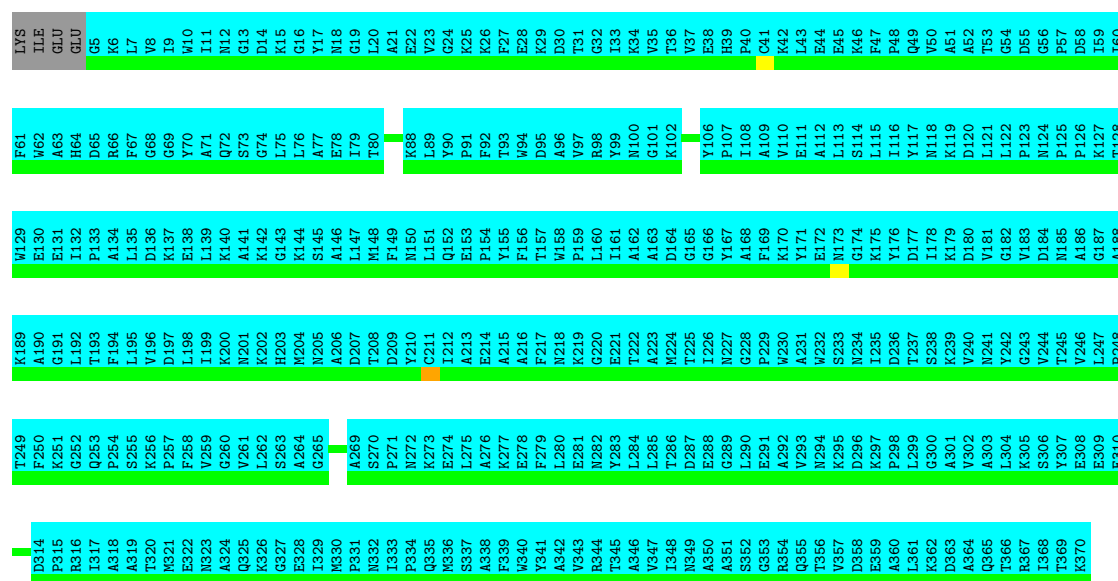




4.2.50 Score per residue for model 50

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY/TORSION ANGLE SIMULATED ANNEALING DYNAMICS*.

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *PRE AND VDW ENERGIES*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
NIH	refinement	
XPLOR-NIH	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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 (average) 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	1.00±0.01	0±0/64 (0.0± 0.0%)	1.17±0.04	0±0/80 (0.1± 0.2%)
All	All	1.00	0/3200 (0.0%)	1.17	2/4000 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	313	LYS	O-C-N	-5.74	113.51	122.70	48	2

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	-2113	-424	14	0±0
2	A	432	456	500	14±4
All	All	-84050	1600	25660	695

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:H231	0.83	1.73	29	11
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:H231	0.83	1.73	46	12
2:A:500[F]:MXT:H231	2:A:500[F]:MXT:O11	0.83	1.73	24	12
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:H231	0.83	1.73	10	14
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:H231	0.82	1.75	24	6
2:A:500[C]:MXT:H231	2:A:500[C]:MXT:O11	0.81	1.75	2	14
2:A:500[B]:MXT:H231	2:A:500[B]:MXT:O11	0.81	1.73	13	5
2:A:600[D]:MXT:H231	2:A:600[D]:MXT:O11	0.81	1.74	5	10
2:A:500[E]:MXT:O11	2:A:500[E]:MXT:H231	0.80	1.73	50	24
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:H231	0.80	1.74	32	4
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:H231	0.78	1.77	34	2
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:H231	0.69	1.86	17	4
2:A:600[D]:MXT:O12	2:A:600[D]:MXT:H231	0.68	1.89	14	9
2:A:500[B]:MXT:O12	2:A:500[B]:MXT:H231	0.68	1.88	45	10
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:H231	0.68	1.89	3	7
2:A:600[E]:MXT:O12	2:A:600[E]:MXT:H231	0.67	1.89	45	24
2:A:600[F]:MXT:O12	2:A:600[F]:MXT:H231	0.67	1.88	32	18
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:H231	0.66	1.89	40	11
2:A:600[C]:MXT:O11	2:A:600[C]:MXT:H231	0.66	1.90	37	2
2:A:600[C]:MXT:H231	2:A:600[C]:MXT:O12	0.66	1.89	3	9
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:H231	0.64	1.91	31	1
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:H231	0.63	1.92	44	4
2:A:600[D]:MXT:H231	2:A:600[D]:MXT:O12	0.61	1.94	18	4
2:A:500[D]:MXT:O12	2:A:500[D]:MXT:H231	0.61	1.94	16	6
2:A:600[B]:MXT:H231	2:A:600[B]:MXT:O12	0.61	1.94	34	2
2:A:600[C]:MXT:O12	2:A:600[C]:MXT:H231	0.59	1.97	46	1
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:C23	0.58	2.52	49	5
2:A:500[E]:MXT:O11	2:A:500[E]:MXT:C23	0.57	2.52	19	7
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:C23	0.57	2.53	33	3
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:C22	0.57	2.52	37	7
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:C22	0.57	2.53	16	15
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:C23	0.57	2.52	33	5
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:C23	0.57	2.52	34	8
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:C22	0.57	2.53	32	4
2:A:500[D]:MXT:C22	2:A:500[D]:MXT:O11	0.57	2.52	13	5
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:C23	0.57	2.52	4	11
2:A:600[C]:MXT:C22	2:A:600[C]:MXT:O11	0.57	2.53	24	4
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:H221	0.56	2.00	26	15
2:A:500[E]:MXT:O12	2:A:500[E]:MXT:H231	0.56	2.00	27	2
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:H221	0.56	2.00	36	3
2:A:600[D]:MXT:H221	2:A:600[D]:MXT:O11	0.56	2.00	49	2
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:H221	0.56	2.00	41	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:500[F]:MXT:H231	2:A:500[F]:MXT:O12	0.56	1.98	22	1
2:A:500[E]:MXT:O11	2:A:500[E]:MXT:H221	0.56	2.00	42	2
2:A:500[C]:MXT:C22	2:A:500[C]:MXT:O11	0.55	2.54	19	4
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:C23	0.55	2.53	7	10
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:H221	0.55	2.01	18	6
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:C23	0.55	2.52	17	7
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:H221	0.55	2.00	40	2
2:A:600[D]:MXT:C22	2:A:600[D]:MXT:O11	0.54	2.55	1	1
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:H221	0.54	2.03	47	5
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:C23	0.54	2.55	9	5
2:A:600[C]:MXT:O11	2:A:600[C]:MXT:C22	0.53	2.56	18	2
2:A:500[C]:MXT:H231	2:A:500[C]:MXT:O12	0.52	2.02	31	1
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:C22	0.52	2.57	47	5
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:C22	0.52	2.57	41	1
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:C22	0.52	2.58	48	7
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:C22	0.51	2.58	22	4
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:C22	0.51	2.59	4	4
2:A:600[C]:MXT:O11	2:A:600[C]:MXT:H221	0.51	2.05	28	2
2:A:600[F]:MXT:C22	2:A:600[F]:MXT:O11	0.51	2.58	46	2
2:A:500[F]:MXT:C22	2:A:500[F]:MXT:O11	0.51	2.59	1	2
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:H221	0.49	2.05	32	1
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:C22	0.49	2.60	49	2
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:H221	0.49	2.07	11	3
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:H221	0.48	2.07	4	1
2:A:500[E]:MXT:O11	2:A:500[E]:MXT:C22	0.48	2.61	42	2
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:C23	0.47	2.62	45	1
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:C22	0.47	2.62	42	1
2:A:500[B]:MXT:O11	2:A:500[B]:MXT:H222	0.47	2.10	29	3
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:H222	0.46	2.10	43	9
2:A:500[D]:MXT:O11	2:A:500[D]:MXT:H222	0.46	2.10	42	3
2:A:600[F]:MXT:H222	2:A:600[F]:MXT:O11	0.46	2.10	19	2
2:A:600[B]:MXT:H222	2:A:600[B]:MXT:O11	0.46	2.11	30	1
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:H221	0.46	2.09	30	1
2:A:600[F]:MXT:O11	2:A:600[F]:MXT:H222	0.46	2.10	49	7
2:A:600[D]:MXT:H222	2:A:600[D]:MXT:O11	0.46	2.10	10	1
2:A:500[A]:MXT:O11	2:A:500[A]:MXT:H222	0.46	2.11	34	2
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:H222	0.46	2.11	4	1
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:H222	0.46	2.11	1	7
2:A:500[B]:MXT:H222	2:A:500[B]:MXT:O11	0.46	2.11	44	3
2:A:600[E]:MXT:O11	2:A:600[E]:MXT:C23	0.46	2.63	42	1
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:H222	0.46	2.11	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:500[C]:MXT:H222	2:A:500[C]:MXT:O11	0.45	2.11	9	1
2:A:600[C]:MXT:H222	2:A:600[C]:MXT:O11	0.45	2.11	49	1
2:A:500[F]:MXT:O11	2:A:500[F]:MXT:H222	0.45	2.11	1	2
2:A:600[D]:MXT:O11	2:A:600[D]:MXT:H222	0.45	2.11	22	2
2:A:500[E]:MXT:H222	2:A:500[E]:MXT:O11	0.45	2.12	11	2
2:A:600[C]:MXT:O11	2:A:600[C]:MXT:H222	0.44	2.12	15	2
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:C22	0.44	2.66	38	8
2:A:600[C]:MXT:C22	2:A:600[C]:MXT:O12	0.44	2.66	31	1
2:A:500[E]:MXT:C22	2:A:500[E]:MXT:O12	0.43	2.66	38	1
2:A:500[E]:MXT:O12	2:A:500[E]:MXT:C22	0.43	2.66	6	3
2:A:600[F]:MXT:O12	2:A:600[F]:MXT:C23	0.43	2.67	6	3
2:A:500[B]:MXT:O12	2:A:500[B]:MXT:C23	0.43	2.67	17	4
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:C23	0.43	2.67	43	1
2:A:500[D]:MXT:O12	2:A:500[D]:MXT:C23	0.43	2.66	16	3
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:C22	0.43	2.66	20	2
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:C22	0.43	2.67	23	2
2:A:500[B]:MXT:O12	2:A:500[B]:MXT:C22	0.43	2.66	32	4
2:A:500[F]:MXT:O12	2:A:500[F]:MXT:C22	0.43	2.66	40	7
2:A:500[B]:MXT:C22	2:A:500[B]:MXT:O12	0.43	2.66	36	2
2:A:600[A]:MXT:C22	2:A:600[A]:MXT:O12	0.43	2.66	16	1
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:C23	0.43	2.66	43	2
2:A:600[C]:MXT:O12	2:A:600[C]:MXT:C23	0.43	2.67	6	3
2:A:600[B]:MXT:C22	2:A:600[B]:MXT:O12	0.43	2.66	15	1
2:A:600[F]:MXT:O12	2:A:600[F]:MXT:C22	0.43	2.66	5	3
2:A:600[E]:MXT:O12	2:A:600[E]:MXT:C23	0.43	2.66	41	8
2:A:600[E]:MXT:O12	2:A:600[E]:MXT:C22	0.43	2.67	21	2
2:A:600[C]:MXT:O12	2:A:600[C]:MXT:C22	0.42	2.66	36	5
2:A:600[D]:MXT:O12	2:A:600[D]:MXT:C23	0.42	2.67	28	4
2:A:500[A]:MXT:C22	2:A:500[A]:MXT:O12	0.42	2.67	17	1
2:A:500[C]:MXT:O11	2:A:500[C]:MXT:H231	0.42	2.13	27	2
2:A:500[F]:MXT:O12	2:A:500[F]:MXT:H231	0.42	2.13	29	1
2:A:500[D]:MXT:O12	2:A:500[D]:MXT:C22	0.42	2.68	27	1
2:A:500[F]:MXT:H221	2:A:500[F]:MXT:O12	0.42	2.15	3	1
2:A:500[C]:MXT:O12	2:A:500[C]:MXT:C22	0.41	2.66	28	1
2:A:600[A]:MXT:O12	2:A:600[A]:MXT:H221	0.41	2.16	23	3
2:A:500[D]:MXT:O12	2:A:500[D]:MXT:H221	0.41	2.16	46	1
2:A:600[D]:MXT:O12	2:A:600[D]:MXT:C22	0.41	2.68	15	1
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:C23	0.41	2.70	10	2
2:A:500[F]:MXT:O12	2:A:500[F]:MXT:H221	0.41	2.15	45	2
2:A:600[A]:MXT:H221	2:A:600[A]:MXT:O12	0.41	2.16	44	1
2:A:500[A]:MXT:O12	2:A:500[A]:MXT:H221	0.40	2.16	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:600[B]:MXT:O12	2:A:600[B]:MXT:H221	0.40	2.16	13	1
2:A:500[E]:MXT:O12	2:A:500[E]:MXT:H221	0.40	2.15	17	1
2:A:600[B]:MXT:H221	2:A:600[B]:MXT:O12	0.40	2.16	39	1

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	A	16/370 (4%)	15±0 (94±0%)	1±0 (6±0%)	0±0 (0±0%)	100	100
All	All	800/18500 (4%)	750 (94%)	50 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 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 PDB entries followed by that with respect to all NMR 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	A	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MXT	A	600[F]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	600[U]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	500[W]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	500[E]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	500[Z]	1	19,19,19	1.84±0.00	5±0 (26±0%)
2	MXT	A	500[X]	1	19,19,19	1.81±0.00	5±0 (26±0%)
2	MXT	A	500[U]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	600[W]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	600[A]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	500[A]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	500[F]	1	19,19,19	1.84±0.00	5±0 (26±0%)
2	MXT	A	600[D]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	500[V]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	600[E]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	500[B]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	600[V]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	600[C]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	600[B]	1	19,19,19	1.82±0.00	5±0 (26±0%)

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
2	MXT	A	600[Z]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	600[Y]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	500[C]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	600[X]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	500[Y]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	500[D]	1	19,19,19	1.81±0.00	5±0 (26±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
2	MXT	A	600[F]	1	27,31,31	1.21±0.01	3±1 (10±2%)
2	MXT	A	600[U]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	500[W]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	500[E]	1	27,31,31	1.22±0.01	3±1 (11±1%)
2	MXT	A	500[Z]	1	27,31,31	1.24±0.01	4±0 (14±1%)
2	MXT	A	500[X]	1	27,31,31	1.22±0.01	4±0 (13±1%)
2	MXT	A	500[U]	1	27,31,31	1.23±0.01	3±0 (11±1%)
2	MXT	A	600[W]	1	27,31,31	1.24±0.01	4±0 (14±1%)
2	MXT	A	600[A]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	500[A]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	500[F]	1	27,31,31	1.24±0.01	4±0 (13±1%)
2	MXT	A	600[D]	1	27,31,31	1.25±0.01	4±0 (13±1%)
2	MXT	A	500[V]	1	27,31,31	1.23±0.01	3±0 (12±1%)
2	MXT	A	600[E]	1	27,31,31	1.25±0.01	4±0 (14±1%)
2	MXT	A	500[B]	1	27,31,31	1.23±0.01	3±0 (12±1%)
2	MXT	A	600[V]	1	27,31,31	1.21±0.01	3±1 (11±2%)
2	MXT	A	600[C]	1	27,31,31	1.24±0.01	4±0 (14±0%)
2	MXT	A	600[B]	1	27,31,31	1.21±0.01	3±0 (11±1%)
2	MXT	A	600[Z]	1	27,31,31	1.21±0.01	3±1 (11±2%)
2	MXT	A	600[Y]	1	27,31,31	1.25±0.01	4±0 (14±1%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
2	MXT	A	500[C]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	600[X]	1	27,31,31	1.25±0.01	4±0 (13±1%)
2	MXT	A	500[Y]	1	27,31,31	1.22±0.01	3±1 (10±2%)
2	MXT	A	500[D]	1	27,31,31	1.22±0.01	4±0 (13±1%)

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
2	MXT	A	500[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[U]	1	-	0±0,4,39,39	0±0,2,2,2

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	500[A]	MXT	O2-N2	3.84	1.22	1.43	24	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	600[D]	MXT	O2-N2	3.84	1.22	1.43	49	50
2	A	500[U]	MXT	O2-N2	3.84	1.22	1.43	17	50
2	A	600[C]	MXT	O2-N2	3.84	1.22	1.43	21	50
2	A	600[U]	MXT	O2-N2	3.84	1.22	1.43	9	50
2	A	500[E]	MXT	O2-N2	3.84	1.22	1.43	36	50
2	A	500[Z]	MXT	O2-N2	3.84	1.22	1.43	29	50
2	A	600[A]	MXT	O2-N2	3.84	1.22	1.43	6	50
2	A	600[X]	MXT	O2-N2	3.84	1.22	1.43	5	50
2	A	600[Y]	MXT	O2-N2	3.84	1.22	1.43	35	50
2	A	600[Z]	MXT	O2-N2	3.84	1.22	1.43	45	50
2	A	500[Y]	MXT	O2-N2	3.84	1.22	1.43	6	50
2	A	600[F]	MXT	O2-N2	3.84	1.22	1.43	46	50
2	A	500[F]	MXT	O2-N2	3.83	1.22	1.43	43	50
2	A	600[E]	MXT	O2-N2	3.83	1.22	1.43	19	50
2	A	600[W]	MXT	O2-N2	3.83	1.22	1.43	48	50
2	A	600[B]	MXT	O2-N2	3.83	1.22	1.43	20	50
2	A	600[V]	MXT	O2-N2	3.83	1.22	1.43	46	50
2	A	500[V]	MXT	O2-N2	3.82	1.22	1.43	40	50
2	A	500[D]	MXT	O2-N2	3.82	1.22	1.43	42	50
2	A	500[B]	MXT	O2-N2	3.82	1.22	1.43	23	50
2	A	500[C]	MXT	O2-N2	3.82	1.22	1.43	9	50
2	A	500[W]	MXT	O2-N2	3.82	1.23	1.43	11	50
2	A	500[X]	MXT	O2-N2	3.82	1.23	1.43	48	50
2	A	500[F]	MXT	C24-N2	3.26	1.53	1.48	8	50
2	A	500[Z]	MXT	C24-N2	3.25	1.53	1.48	48	50
2	A	600[B]	MXT	C24-N2	3.24	1.53	1.48	10	50
2	A	600[E]	MXT	C24-N2	3.24	1.53	1.48	16	50
2	A	600[Y]	MXT	C24-N2	3.24	1.53	1.48	21	50
2	A	600[V]	MXT	C24-N2	3.23	1.53	1.48	29	50
2	A	500[V]	MXT	C24-N2	3.22	1.53	1.48	49	50
2	A	600[X]	MXT	C24-N2	3.22	1.53	1.48	30	50
2	A	500[F]	MXT	C27-N2	3.22	1.53	1.48	32	50
2	A	500[U]	MXT	C27-N2	3.22	1.53	1.48	31	50
2	A	500[B]	MXT	C24-N2	3.21	1.53	1.48	44	50
2	A	600[F]	MXT	C24-N2	3.21	1.53	1.48	25	50
2	A	500[Y]	MXT	C24-N2	3.21	1.53	1.48	7	50
2	A	600[D]	MXT	C24-N2	3.20	1.53	1.48	39	50
2	A	600[C]	MXT	C24-N2	3.20	1.53	1.48	47	50
2	A	500[C]	MXT	C24-N2	3.19	1.53	1.48	2	50
2	A	500[Z]	MXT	C27-N2	3.20	1.53	1.48	31	50
2	A	600[Z]	MXT	C24-N2	3.19	1.53	1.48	10	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	600[W]	MXT	C24-N2	3.18	1.53	1.48	21	50
2	A	500[E]	MXT	C24-N2	3.18	1.53	1.48	1	50
2	A	600[U]	MXT	C27-N2	3.18	1.53	1.48	7	50
2	A	600[A]	MXT	C24-N2	3.17	1.53	1.48	9	50
2	A	500[A]	MXT	C27-N2	3.17	1.53	1.48	2	50
2	A	600[A]	MXT	C27-N2	3.17	1.53	1.48	1	50
2	A	500[U]	MXT	C24-N2	3.17	1.53	1.48	10	50
2	A	500[W]	MXT	C24-N2	3.16	1.53	1.48	18	50
2	A	600[W]	MXT	C27-N2	3.16	1.53	1.48	6	50
2	A	500[A]	MXT	C24-N2	3.16	1.53	1.48	21	50
2	A	600[C]	MXT	C27-N2	3.16	1.53	1.48	6	50
2	A	600[Z]	MXT	C27-N2	3.16	1.53	1.48	36	50
2	A	500[D]	MXT	C27-N2	3.15	1.52	1.48	22	50
2	A	500[E]	MXT	C27-N2	3.14	1.52	1.48	5	50
2	A	500[X]	MXT	C27-N2	3.14	1.52	1.48	33	50
2	A	600[U]	MXT	C24-N2	3.14	1.52	1.48	18	50
2	A	500[Y]	MXT	C27-N2	3.13	1.52	1.48	6	50
2	A	500[W]	MXT	C27-N2	3.12	1.52	1.48	30	50
2	A	600[F]	MXT	C27-N2	3.13	1.52	1.48	12	50
2	A	500[V]	MXT	C27-N2	3.12	1.52	1.48	15	50
2	A	500[B]	MXT	C27-N2	3.11	1.52	1.48	9	50
2	A	600[X]	MXT	C27-N2	3.11	1.52	1.48	41	50
2	A	600[B]	MXT	C27-N2	3.11	1.52	1.48	48	50
2	A	600[D]	MXT	C27-N2	3.10	1.52	1.48	28	50
2	A	600[V]	MXT	C27-N2	3.10	1.52	1.48	31	50
2	A	500[C]	MXT	C27-N2	3.09	1.52	1.48	38	50
2	A	600[E]	MXT	C27-N2	3.09	1.52	1.48	50	50
2	A	500[X]	MXT	C24-N2	3.08	1.52	1.48	27	50
2	A	500[D]	MXT	C24-N2	3.08	1.52	1.48	45	50
2	A	600[Y]	MXT	C27-N2	3.07	1.52	1.48	12	50
2	A	500[A]	MXT	C14-N1	2.47	1.44	1.39	23	50
2	A	600[E]	MXT	C14-N1	2.45	1.44	1.39	22	50
2	A	500[C]	MXT	C14-N1	2.45	1.44	1.39	21	50
2	A	600[Y]	MXT	C14-N1	2.44	1.44	1.39	18	50
2	A	500[U]	MXT	C14-N1	2.44	1.44	1.39	27	50
2	A	500[W]	MXT	C14-N1	2.43	1.44	1.39	38	50
2	A	600[D]	MXT	C14-N1	2.42	1.43	1.39	35	50
2	A	600[X]	MXT	C14-N1	2.41	1.43	1.39	32	50
2	A	500[B]	MXT	C14-N1	2.41	1.43	1.39	24	50
2	A	500[X]	MXT	C14-N1	2.41	1.43	1.39	14	50
2	A	600[C]	MXT	C14-N1	2.41	1.43	1.39	46	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	600[V]	MXT	C14-N1	2.40	1.43	1.39	50	50
2	A	500[D]	MXT	C14-N1	2.40	1.43	1.39	45	50
2	A	500[V]	MXT	C14-N1	2.40	1.43	1.39	33	50
2	A	600[A]	MXT	C14-N1	2.39	1.43	1.39	49	50
2	A	600[W]	MXT	C14-N1	2.39	1.43	1.39	5	50
2	A	600[B]	MXT	C14-N1	2.38	1.43	1.39	41	50
2	A	500[Z]	MXT	C14-N1	2.38	1.43	1.39	16	50
2	A	600[U]	MXT	C14-N1	2.37	1.43	1.39	26	50
2	A	500[F]	MXT	C14-N1	2.36	1.43	1.39	39	50
2	A	600[F]	MXT	C14-N1	2.34	1.43	1.39	7	50
2	A	600[Z]	MXT	C14-N1	2.34	1.43	1.39	1	50
2	A	500[Y]	MXT	C14-N1	2.33	1.43	1.39	12	50
2	A	500[E]	MXT	C14-N1	2.31	1.43	1.39	21	50
2	A	600[Y]	MXT	C13-N1	2.22	1.43	1.39	7	50
2	A	500[F]	MXT	C13-N1	2.21	1.43	1.39	9	50
2	A	500[Z]	MXT	C13-N1	2.21	1.43	1.39	6	50
2	A	600[E]	MXT	C13-N1	2.20	1.43	1.39	2	50
2	A	600[D]	MXT	C13-N1	2.19	1.43	1.39	50	50
2	A	500[Y]	MXT	C13-N1	2.19	1.43	1.39	31	50
2	A	600[C]	MXT	C13-N1	2.18	1.43	1.39	46	50
2	A	500[E]	MXT	C13-N1	2.18	1.43	1.39	30	50
2	A	600[W]	MXT	C13-N1	2.18	1.43	1.39	48	50
2	A	600[X]	MXT	C13-N1	2.17	1.43	1.39	21	50
2	A	600[A]	MXT	C13-N1	2.16	1.43	1.39	19	50
2	A	600[U]	MXT	C13-N1	2.16	1.43	1.39	15	50
2	A	500[X]	MXT	C13-N1	2.14	1.43	1.39	17	50
2	A	500[C]	MXT	C13-N1	2.14	1.43	1.39	40	50
2	A	500[V]	MXT	C13-N1	2.14	1.43	1.39	14	50
2	A	500[D]	MXT	C13-N1	2.13	1.43	1.39	30	50
2	A	600[Z]	MXT	C13-N1	2.13	1.43	1.39	26	50
2	A	600[V]	MXT	C13-N1	2.13	1.43	1.39	5	50
2	A	600[B]	MXT	C13-N1	2.13	1.43	1.39	48	50
2	A	600[F]	MXT	C13-N1	2.13	1.43	1.39	45	50
2	A	500[A]	MXT	C13-N1	2.13	1.43	1.39	40	50
2	A	500[W]	MXT	C13-N1	2.12	1.43	1.39	42	50
2	A	500[B]	MXT	C13-N1	2.12	1.43	1.39	50	50
2	A	500[U]	MXT	C13-N1	2.11	1.43	1.39	38	50

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	600[X]	MXT	C13-N1-C14	3.73	110.14	112.48	31	50
2	A	600[D]	MXT	C13-N1-C14	3.68	110.17	112.48	1	50
2	A	600[E]	MXT	C13-N1-C14	3.67	110.17	112.48	45	50
2	A	600[Y]	MXT	C13-N1-C14	3.66	110.18	112.48	38	50
2	A	500[F]	MXT	C13-N1-C14	3.63	110.20	112.48	33	50
2	A	500[Z]	MXT	C13-N1-C14	3.63	110.20	112.48	10	50
2	A	500[C]	MXT	C13-N1-C14	3.61	110.21	112.48	7	50
2	A	600[W]	MXT	C13-N1-C14	3.61	110.22	112.48	16	50
2	A	600[U]	MXT	C13-N1-C14	3.59	110.22	112.48	39	50
2	A	600[A]	MXT	C13-N1-C14	3.59	110.22	112.48	21	50
2	A	500[W]	MXT	C13-N1-C14	3.59	110.23	112.48	38	50
2	A	500[B]	MXT	C13-N1-C14	3.59	110.23	112.48	2	50
2	A	600[C]	MXT	C13-N1-C14	3.58	110.23	112.48	46	50
2	A	500[V]	MXT	C13-N1-C14	3.57	110.23	112.48	10	50
2	A	500[A]	MXT	C13-N1-C14	3.54	110.26	112.48	17	50
2	A	500[Y]	MXT	C13-N1-C14	3.54	110.26	112.48	27	50
2	A	500[U]	MXT	C13-N1-C14	3.53	110.26	112.48	5	50
2	A	500[E]	MXT	C13-N1-C14	3.51	110.27	112.48	30	50
2	A	600[B]	MXT	C13-N1-C14	3.50	110.28	112.48	15	50
2	A	600[V]	MXT	C13-N1-C14	3.49	110.29	112.48	47	50
2	A	500[D]	MXT	C13-N1-C14	3.49	110.29	112.48	3	50
2	A	500[X]	MXT	C13-N1-C14	3.48	110.30	112.48	11	50
2	A	600[F]	MXT	C13-N1-C14	3.45	110.31	112.48	42	50
2	A	600[Z]	MXT	C13-N1-C14	3.42	110.33	112.48	43	50
2	A	500[A]	MXT	C11-C13-N1	2.22	109.88	107.98	17	50
2	A	500[U]	MXT	C11-C13-N1	2.22	109.88	107.98	27	50
2	A	600[W]	MXT	C11-C13-N1	2.20	109.86	107.98	38	50
2	A	600[X]	MXT	C11-C13-N1	2.20	109.86	107.98	31	50
2	A	500[B]	MXT	C11-C13-N1	2.20	109.86	107.98	42	50
2	A	500[V]	MXT	C11-C13-N1	2.19	109.86	107.98	42	50
2	A	600[Y]	MXT	C11-C13-N1	2.18	109.85	107.98	3	50
2	A	500[F]	MXT	C11-C13-N1	2.18	109.84	107.98	12	50
2	A	600[D]	MXT	C11-C13-N1	2.18	109.84	107.98	31	50
2	A	500[Z]	MXT	C11-C13-N1	2.18	109.84	107.98	41	50
2	A	600[E]	MXT	C11-C13-N1	2.18	109.84	107.98	20	50
2	A	600[C]	MXT	C11-C13-N1	2.17	109.84	107.98	35	50
2	A	600[A]	MXT	C11-C13-N1	2.16	109.83	107.98	21	50
2	A	500[W]	MXT	C11-C13-N1	2.14	109.81	107.98	15	50
2	A	600[U]	MXT	C11-C13-N1	2.14	109.81	107.98	4	50
2	A	500[C]	MXT	C11-C13-N1	2.13	109.80	107.98	34	49
2	A	600[B]	MXT	C11-C13-N1	2.12	109.79	107.98	4	45
2	A	500[U]	MXT	C27-C23-C21	2.11	117.82	113.50	3	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	600[V]	MXT	C11-C13-N1	2.10	109.78	107.98	38	43
2	A	500[A]	MXT	C27-C23-C21	2.10	117.79	113.50	42	50
2	A	600[A]	MXT	C27-C23-C21	2.10	117.79	113.50	28	50
2	A	600[F]	MXT	C27-C23-C21	2.10	117.79	113.50	9	50
2	A	600[U]	MXT	C27-C23-C21	2.10	117.79	113.50	10	50
2	A	600[D]	MXT	C27-C23-C21	2.10	117.78	113.50	17	50
2	A	600[Z]	MXT	C27-C23-C21	2.10	117.78	113.50	11	50
2	A	500[C]	MXT	C27-C23-C21	2.09	117.78	113.50	49	50
2	A	500[W]	MXT	C27-C23-C21	2.09	117.77	113.50	27	50
2	A	500[Y]	MXT	C27-C23-C21	2.09	117.77	113.50	41	50
2	A	500[B]	MXT	C27-C23-C21	2.09	117.77	113.50	49	50
2	A	500[D]	MXT	C23-C27-N2	2.09	111.30	108.66	1	50
2	A	500[V]	MXT	C27-C23-C21	2.09	117.77	113.50	7	50
2	A	500[Y]	MXT	C11-C13-N1	2.09	109.77	107.98	2	38
2	A	500[E]	MXT	C11-C13-N1	2.08	109.76	107.98	6	41
2	A	500[X]	MXT	C23-C27-N2	2.08	111.30	108.66	45	50
2	A	600[B]	MXT	C27-C23-C21	2.08	117.76	113.50	28	50
2	A	600[X]	MXT	C27-C23-C21	2.08	117.76	113.50	29	50
2	A	600[F]	MXT	C11-C13-N1	2.08	109.76	107.98	47	35
2	A	500[Z]	MXT	C27-C23-C21	2.08	117.75	113.50	3	50
2	A	500[E]	MXT	C27-C23-C21	2.08	117.75	113.50	16	50
2	A	600[V]	MXT	C27-C23-C21	2.08	117.75	113.50	13	50
2	A	600[Z]	MXT	C11-C13-N1	2.08	109.76	107.98	13	35
2	A	500[F]	MXT	C27-C23-C21	2.08	117.75	113.50	27	50
2	A	500[X]	MXT	C11-C13-N1	2.08	109.76	107.98	50	33
2	A	500[D]	MXT	C11-C13-N1	2.08	109.76	107.98	25	26
2	A	600[Y]	MXT	C27-C23-C21	2.07	117.73	113.50	5	50
2	A	600[E]	MXT	C27-C23-C21	2.07	117.73	113.50	15	50
2	A	600[C]	MXT	C27-C23-C21	2.07	117.73	113.50	25	50
2	A	600[Y]	MXT	C23-C27-N2	2.06	111.27	108.66	49	42
2	A	600[W]	MXT	C27-C23-C21	2.06	117.71	113.50	7	50
2	A	600[W]	MXT	C23-C27-N2	2.06	111.27	108.66	37	44
2	A	500[D]	MXT	C27-C23-C21	2.06	117.71	113.50	39	50
2	A	500[X]	MXT	C27-C23-C21	2.06	117.70	113.50	8	50
2	A	600[E]	MXT	C23-C27-N2	2.06	111.27	108.66	19	42
2	A	600[C]	MXT	C23-C27-N2	2.05	111.26	108.66	27	47
2	A	500[F]	MXT	C23-C27-N2	2.05	111.26	108.66	38	33
2	A	500[Z]	MXT	C23-C27-N2	2.05	111.25	108.66	27	41
2	A	600[D]	MXT	C23-C27-N2	2.05	111.25	108.66	10	31
2	A	500[B]	MXT	C23-C27-N2	2.04	111.24	108.66	44	24
2	A	500[E]	MXT	C23-C27-N2	2.04	111.24	108.66	2	11

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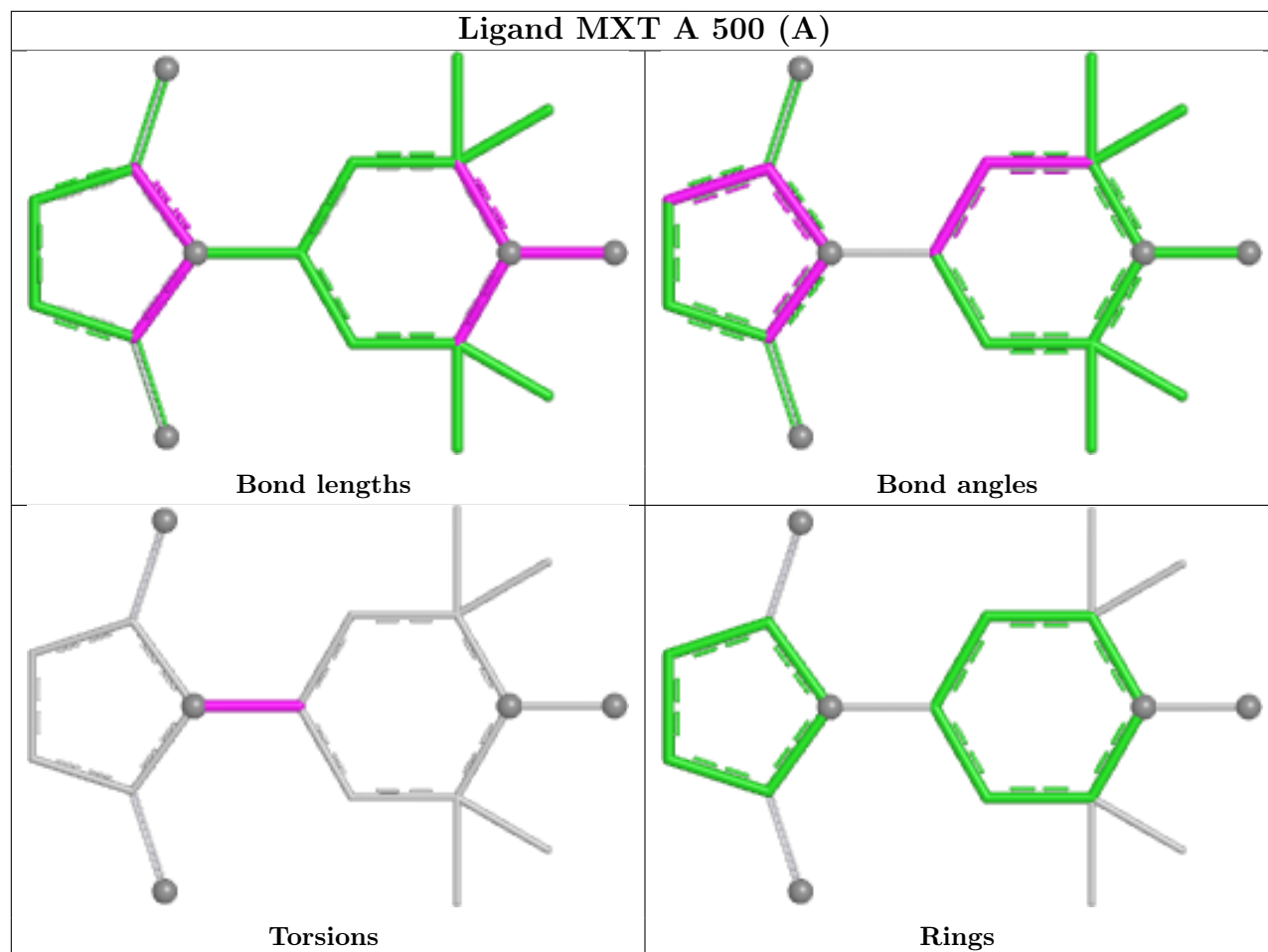
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	500[Y]	MXT	C23-C27-N2	2.04	111.24	108.66	11	10
2	A	600[X]	MXT	C23-C27-N2	2.04	111.24	108.66	1	34
2	A	500[V]	MXT	C23-C27-N2	2.03	111.23	108.66	25	24
2	A	600[Z]	MXT	C23-C27-N2	2.03	111.23	108.66	13	17
2	A	600[F]	MXT	C23-C27-N2	2.03	111.22	108.66	42	13
2	A	600[V]	MXT	C23-C27-N2	2.02	111.22	108.66	49	9
2	A	600[B]	MXT	C23-C27-N2	2.02	111.22	108.66	12	8
2	A	500[A]	MXT	C23-C27-N2	2.01	111.21	108.66	21	3
2	A	500[U]	MXT	C23-C27-N2	2.01	111.20	108.66	1	4
2	A	600[A]	MXT	C23-C27-N2	2.00	111.20	108.66	47	1
2	A	600[U]	MXT	C23-C27-N2	2.00	111.20	108.66	48	1

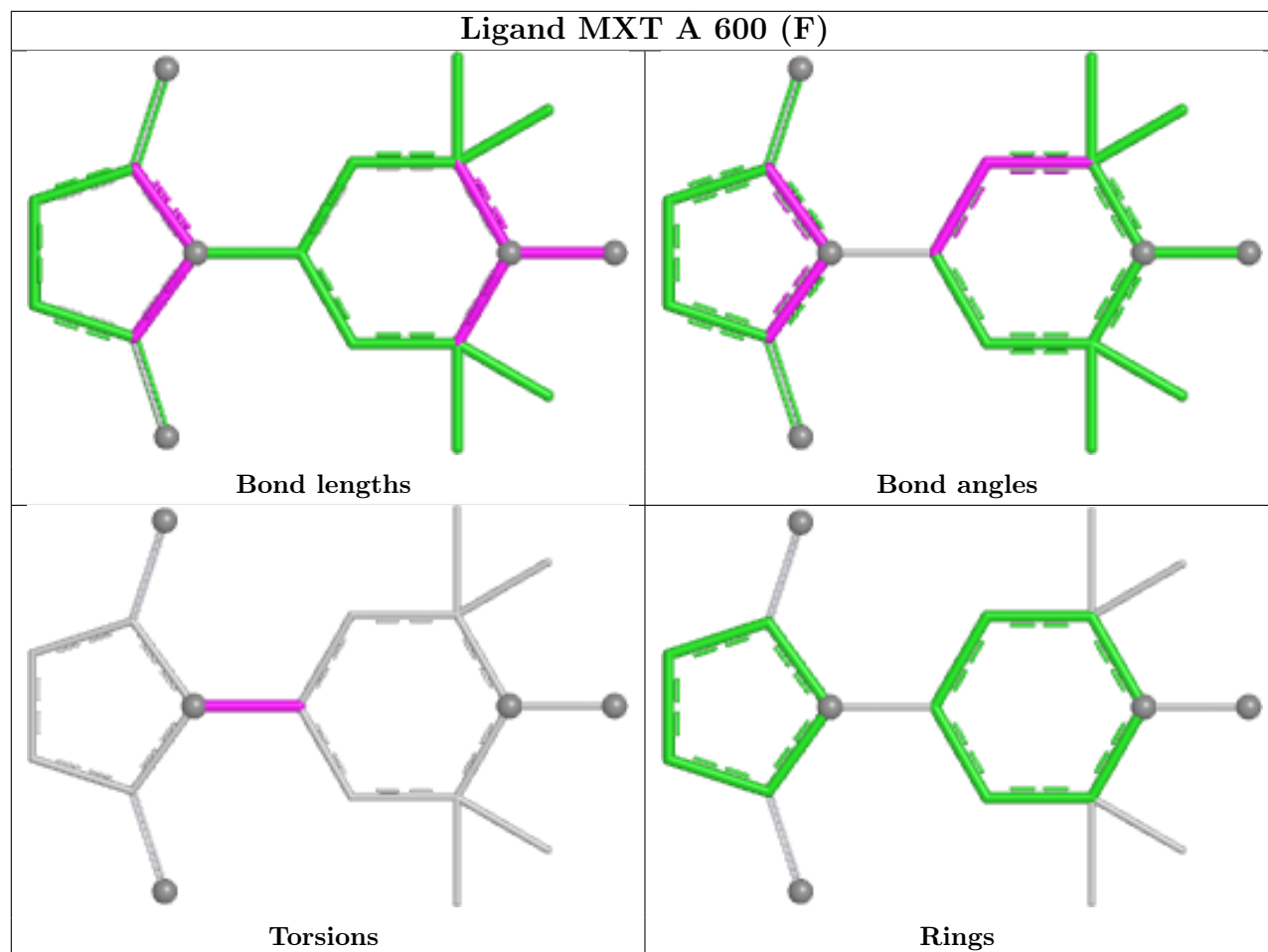
There are no chirality outliers.

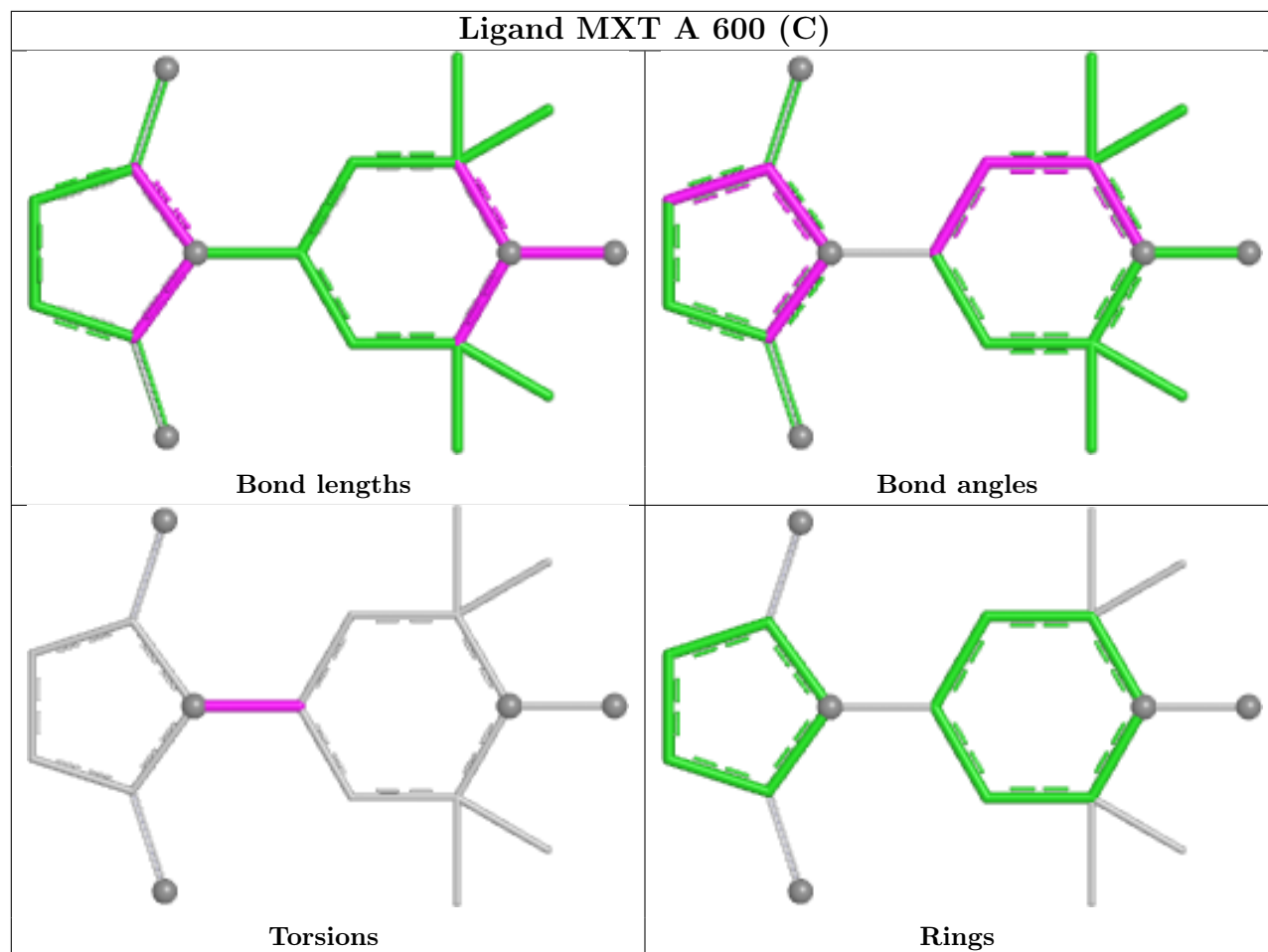
There are no torsion outliers.

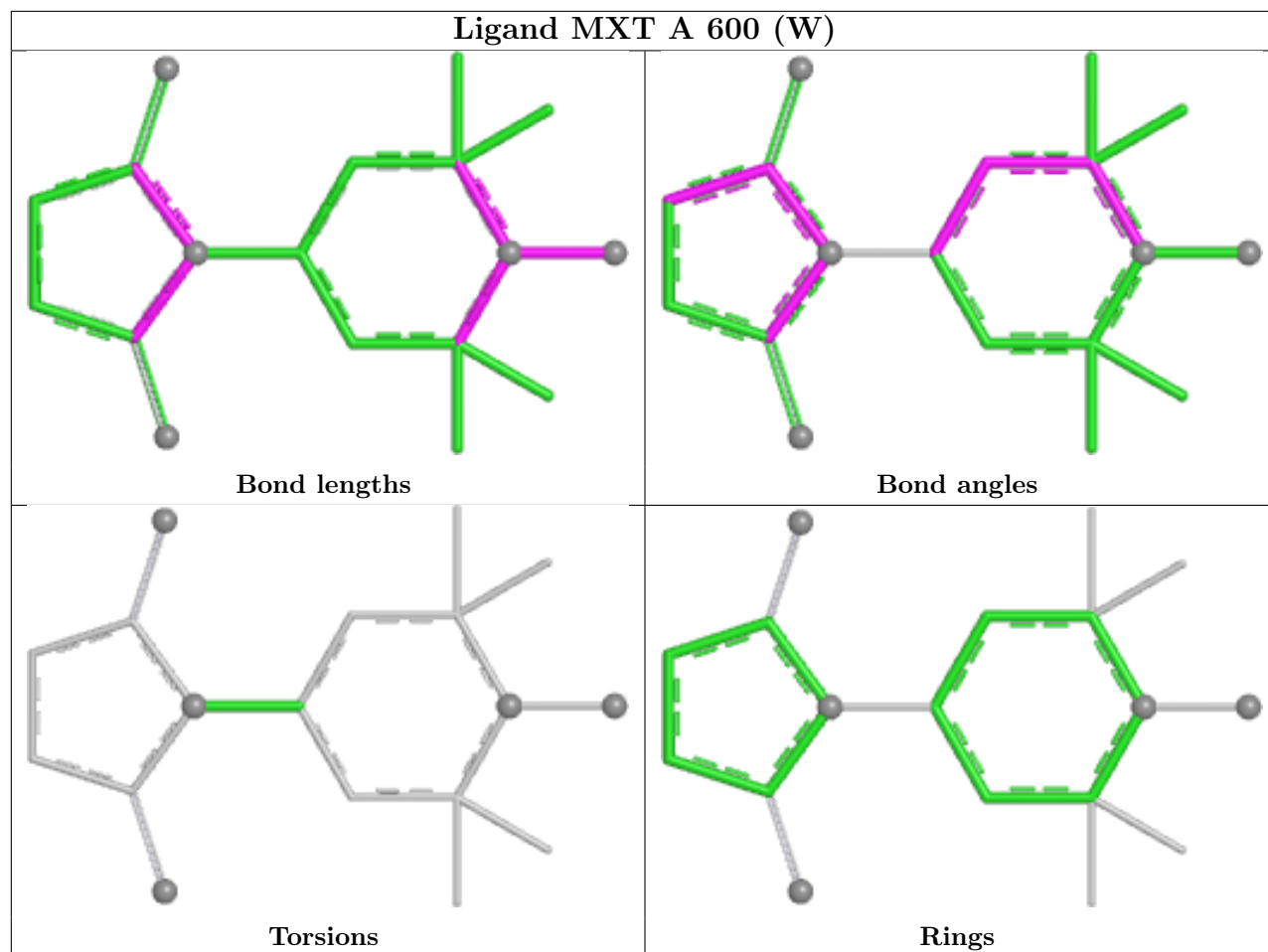
There are no ring outliers.

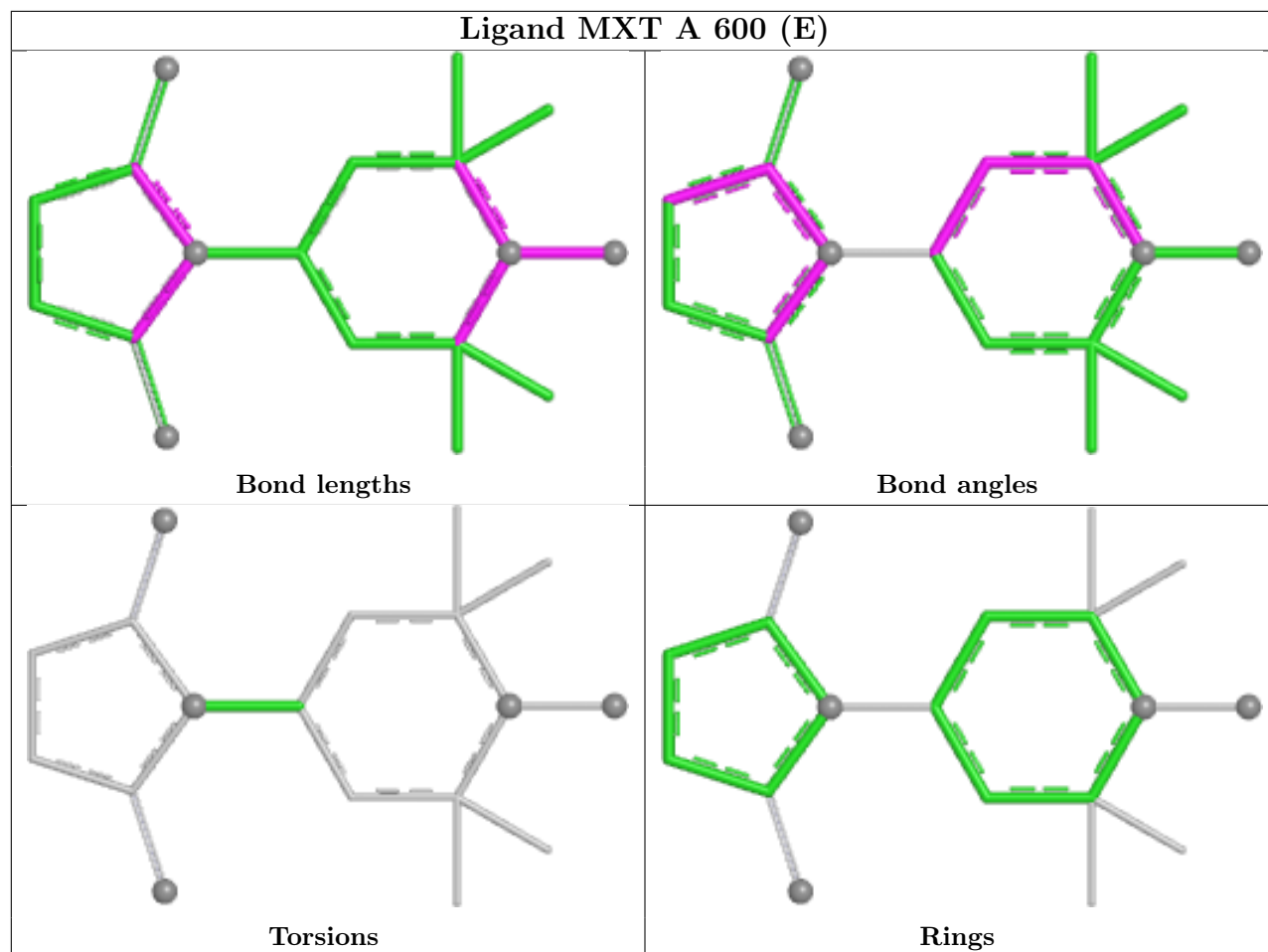
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

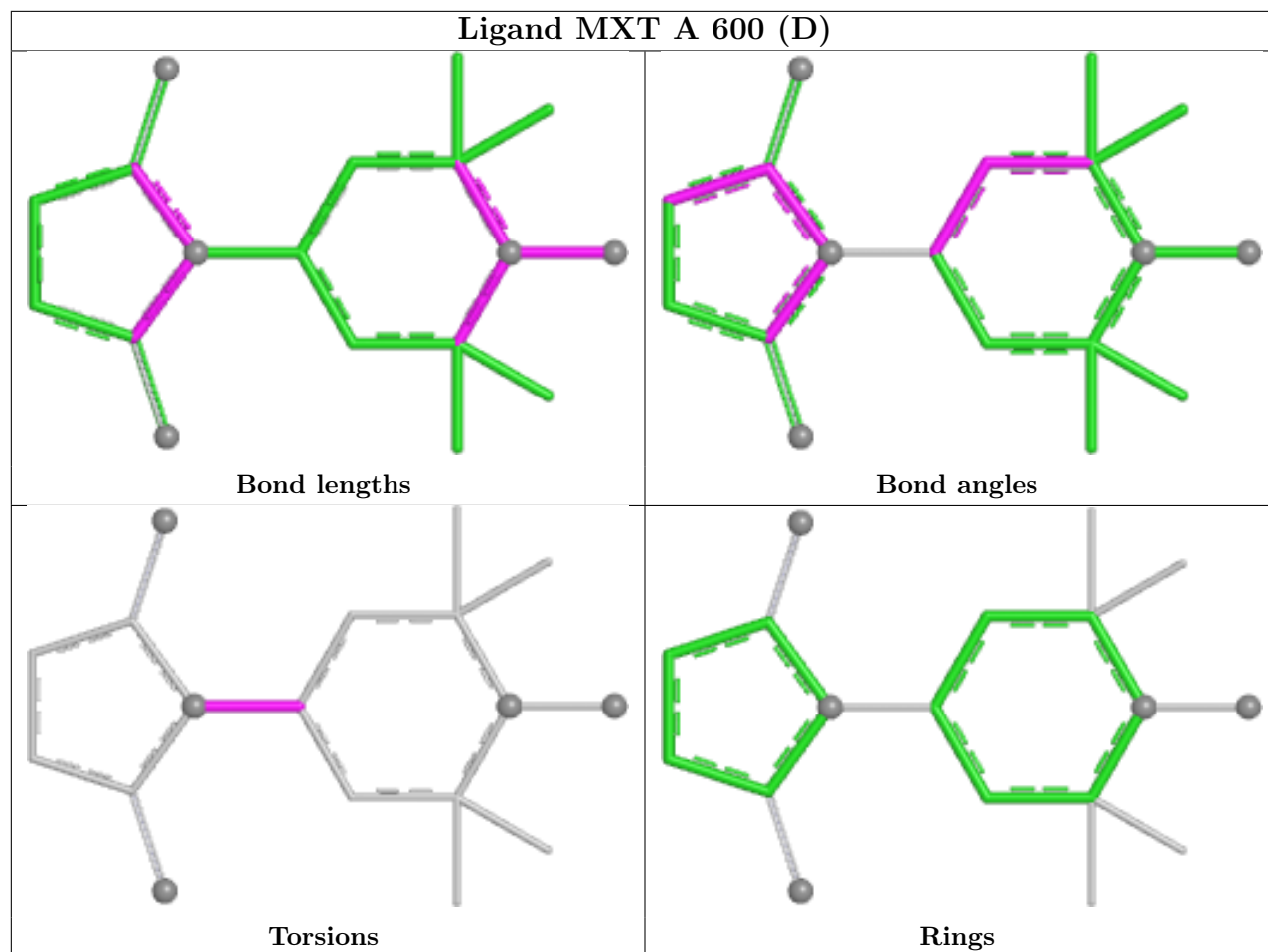


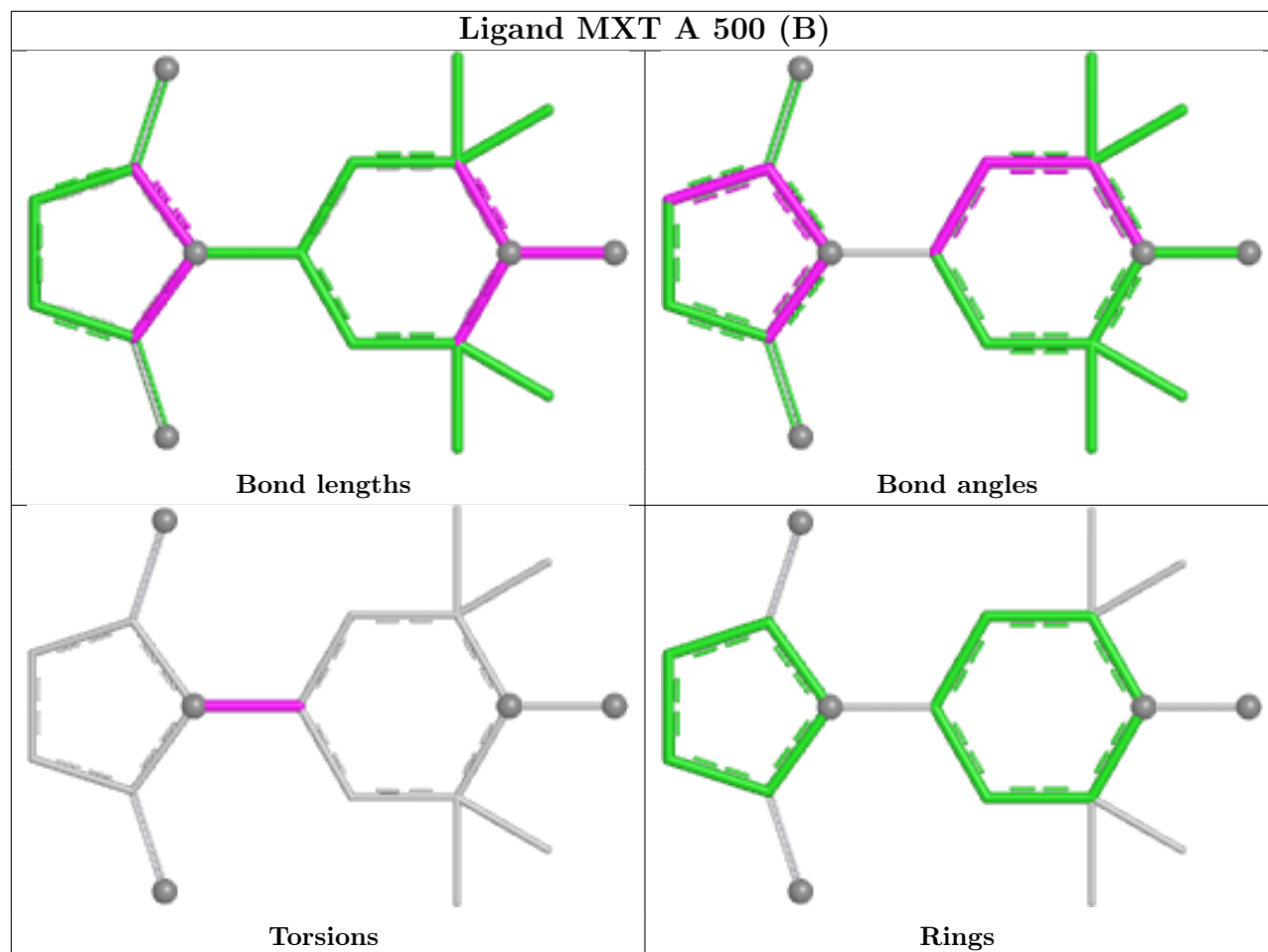


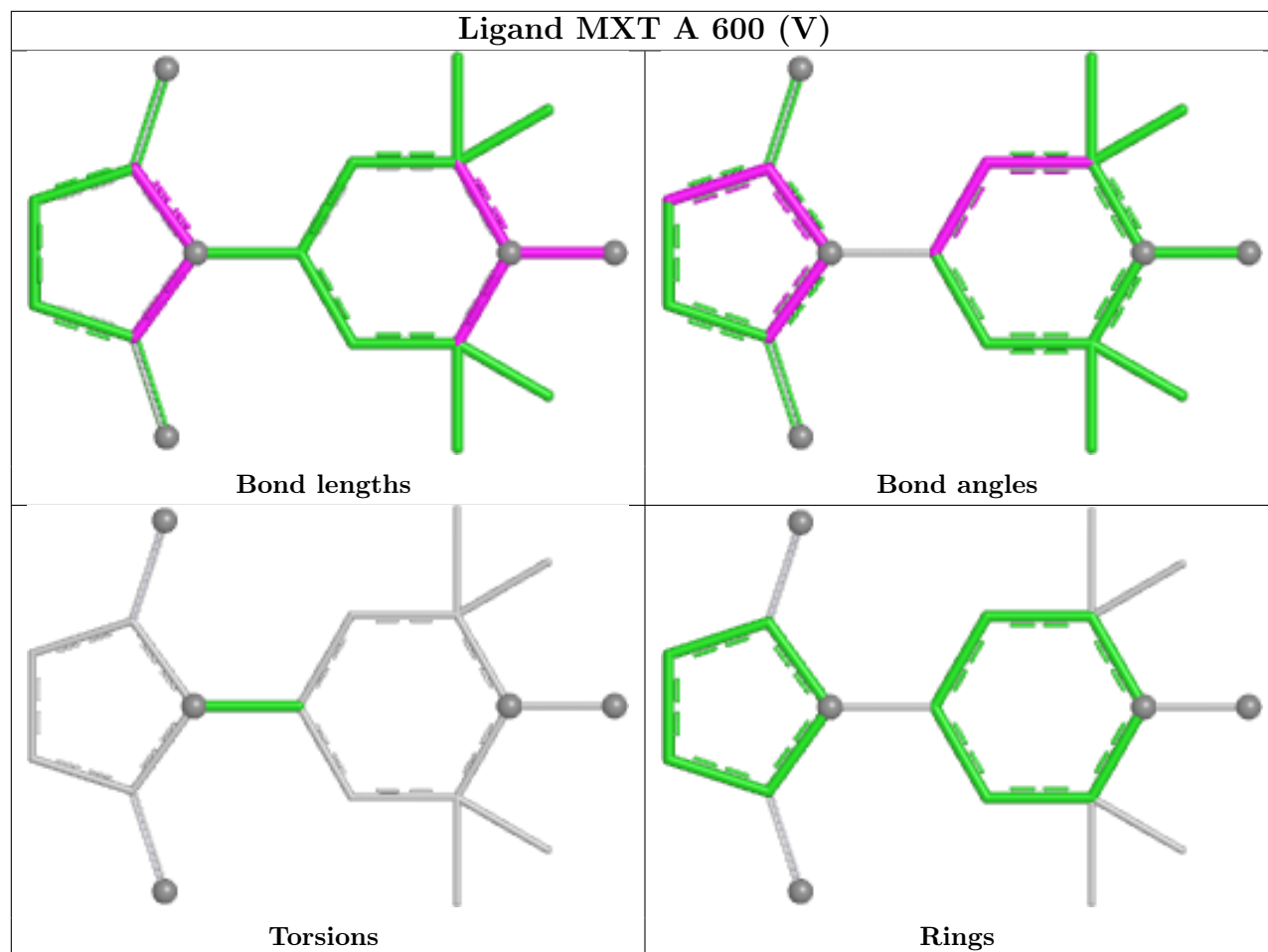


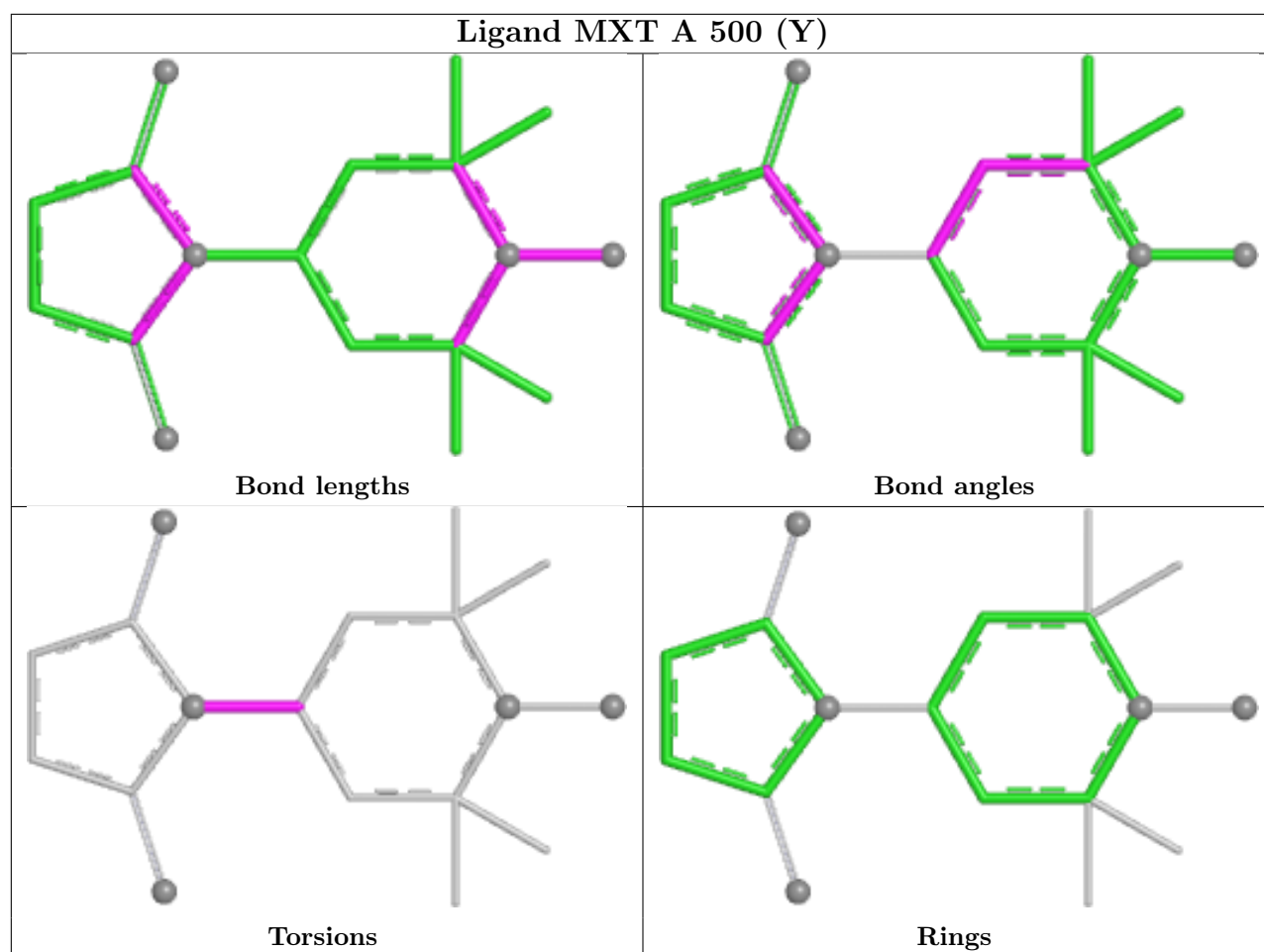


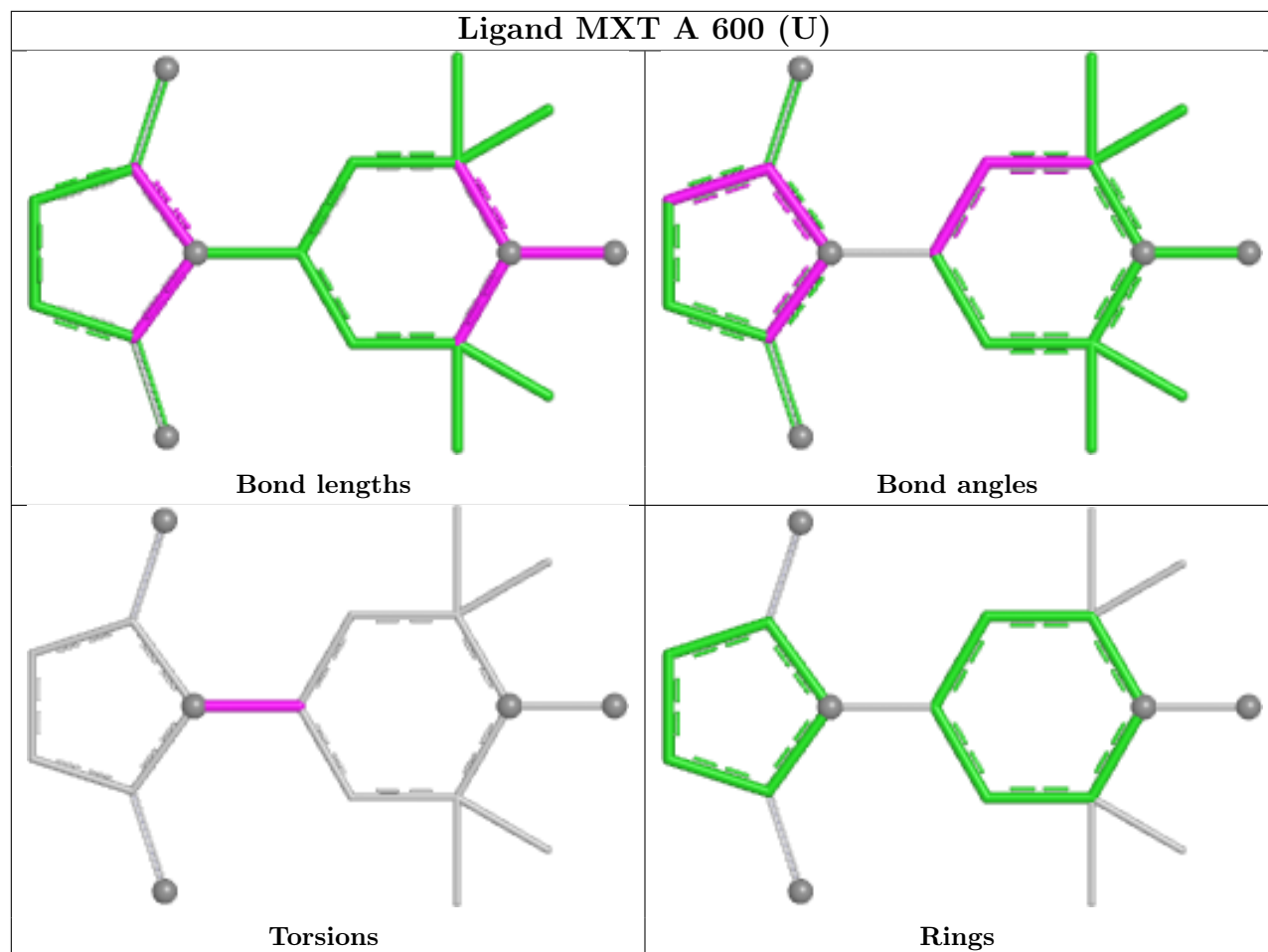


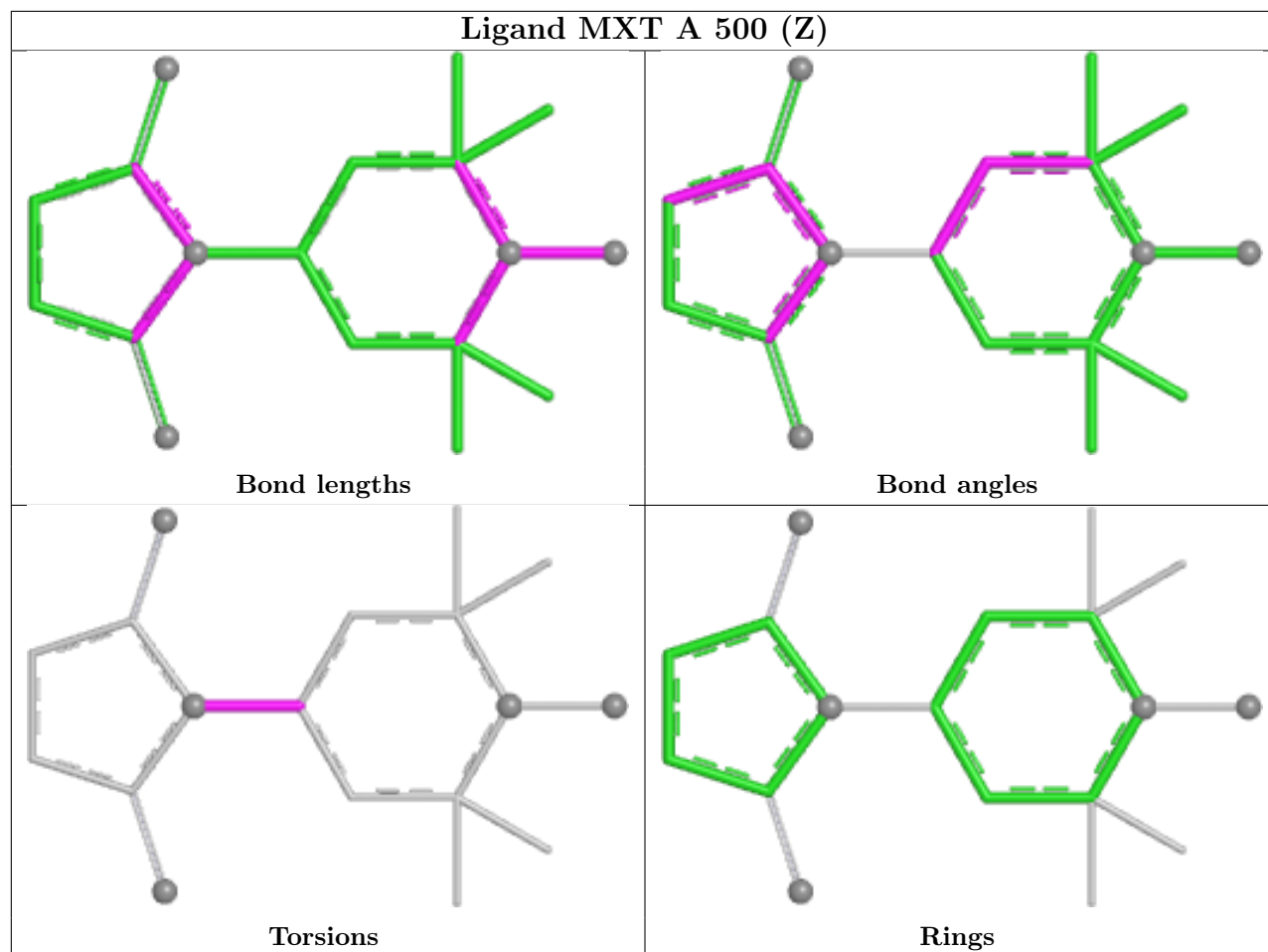


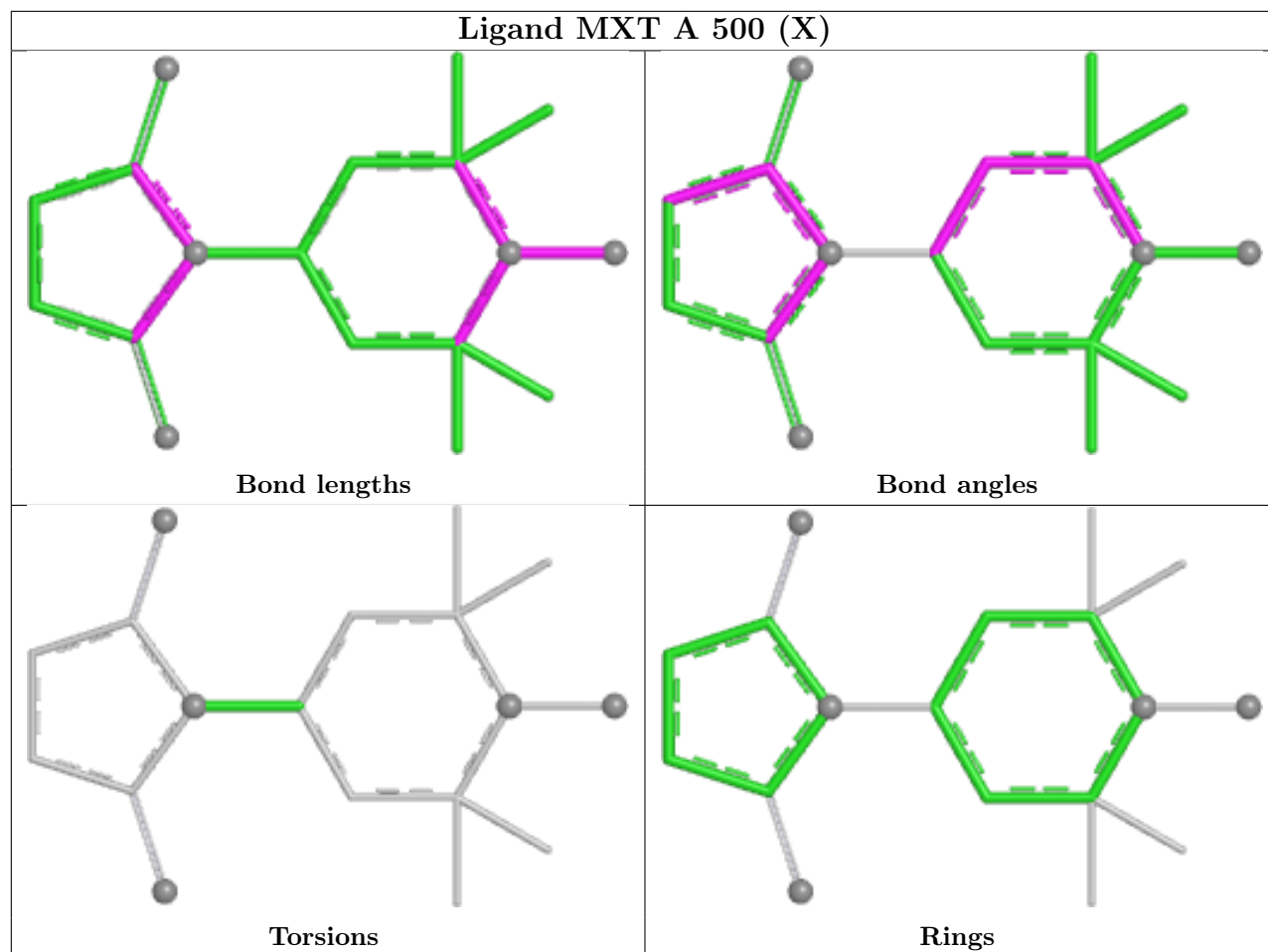


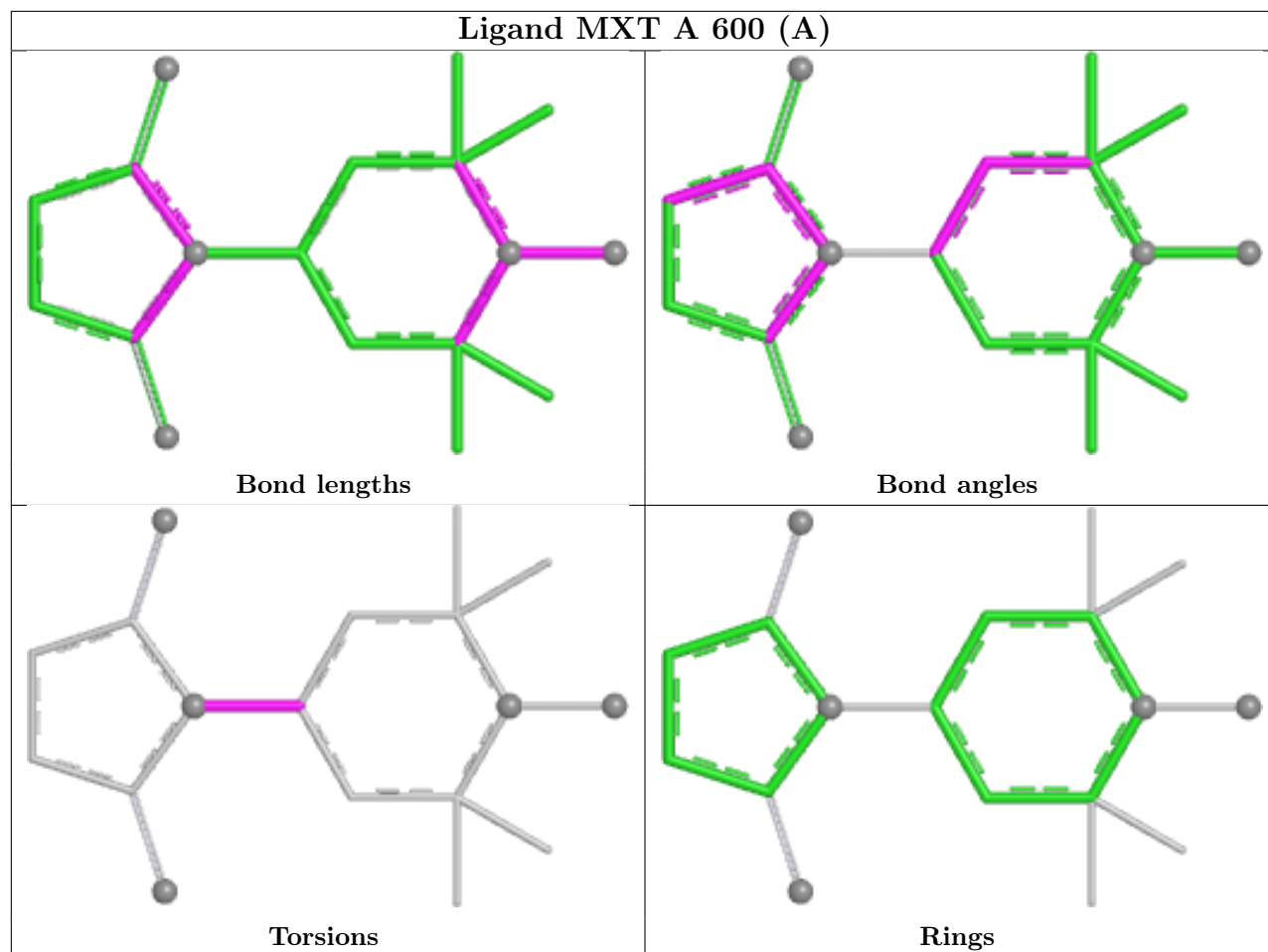


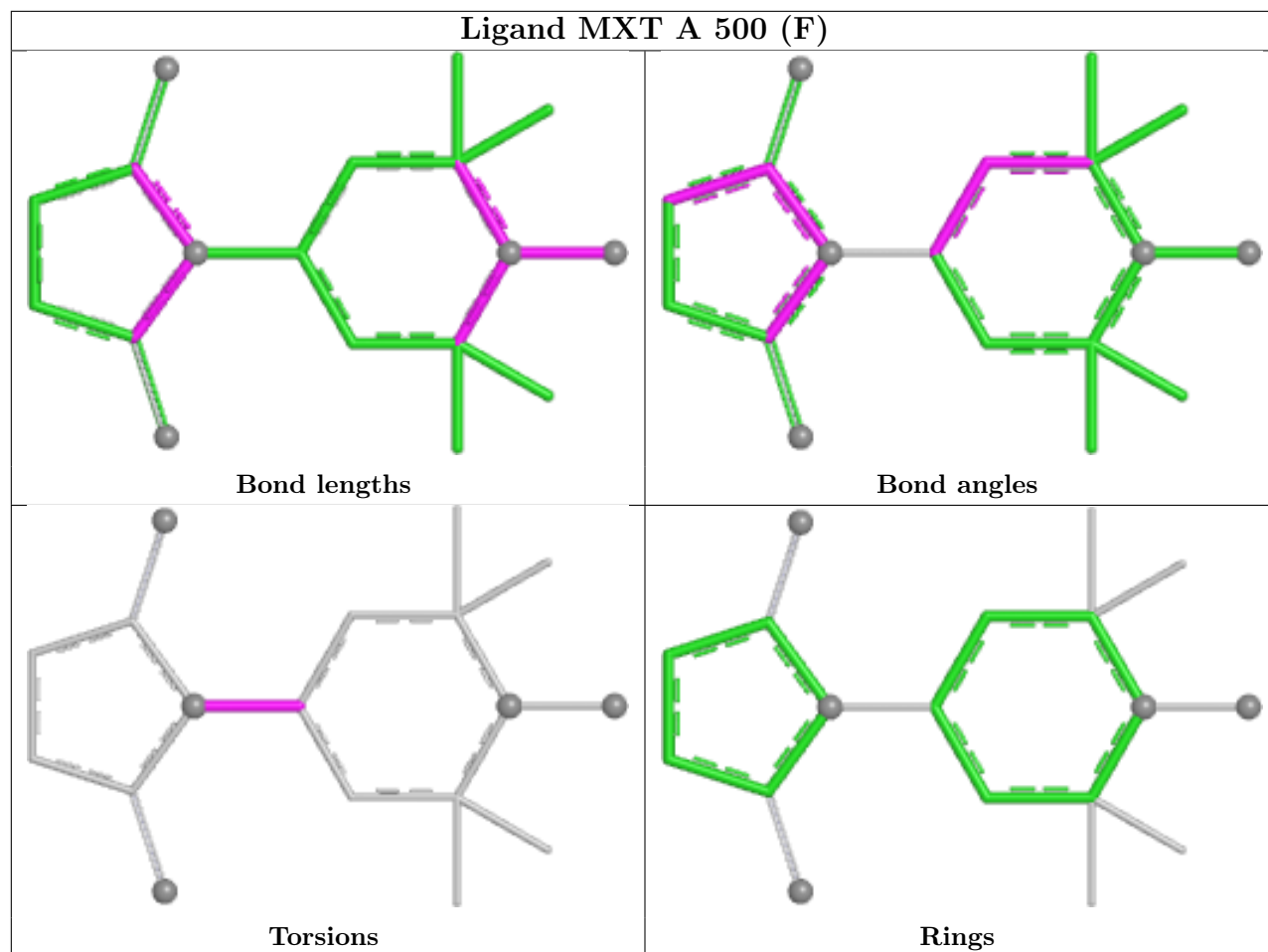


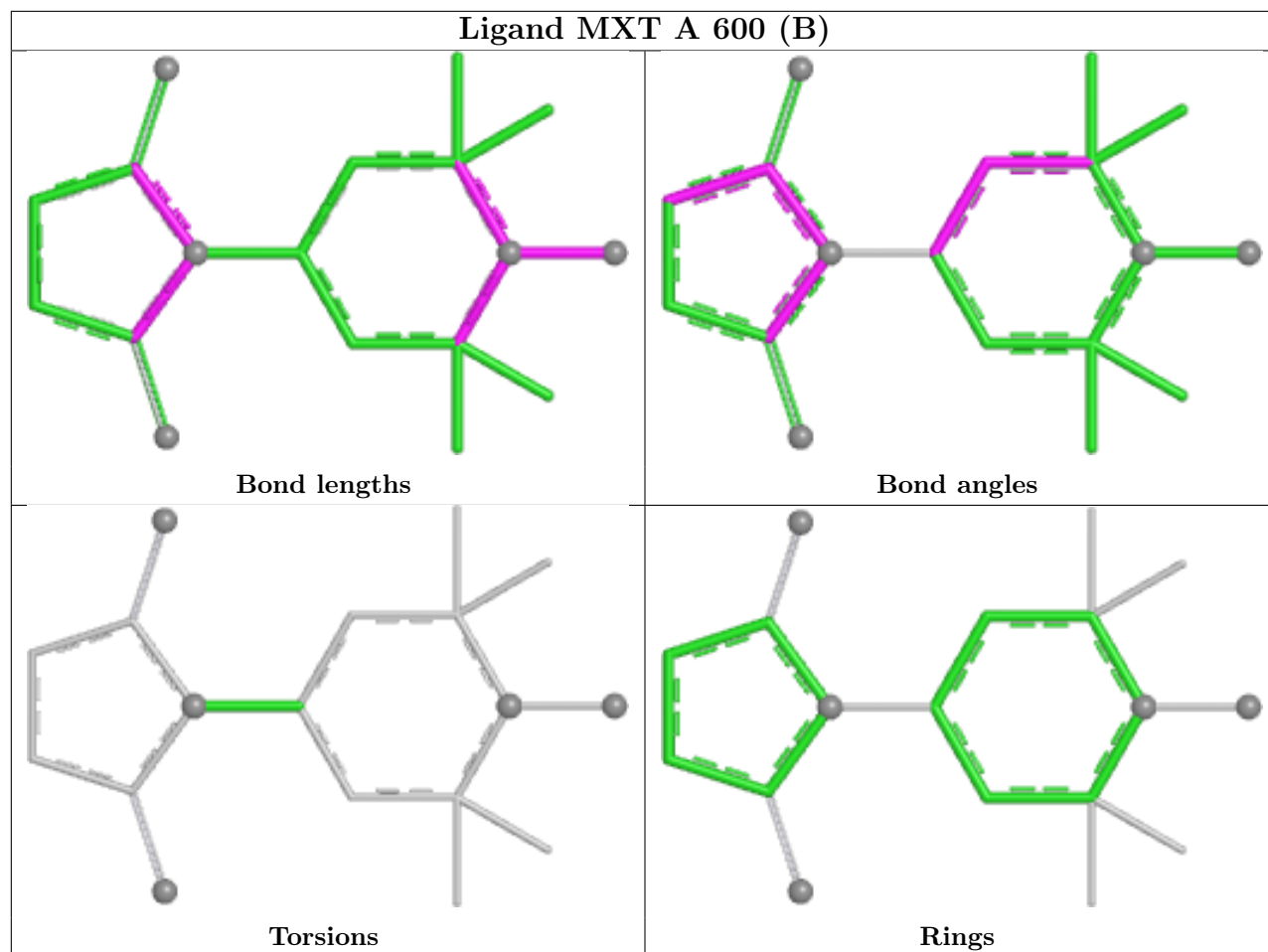


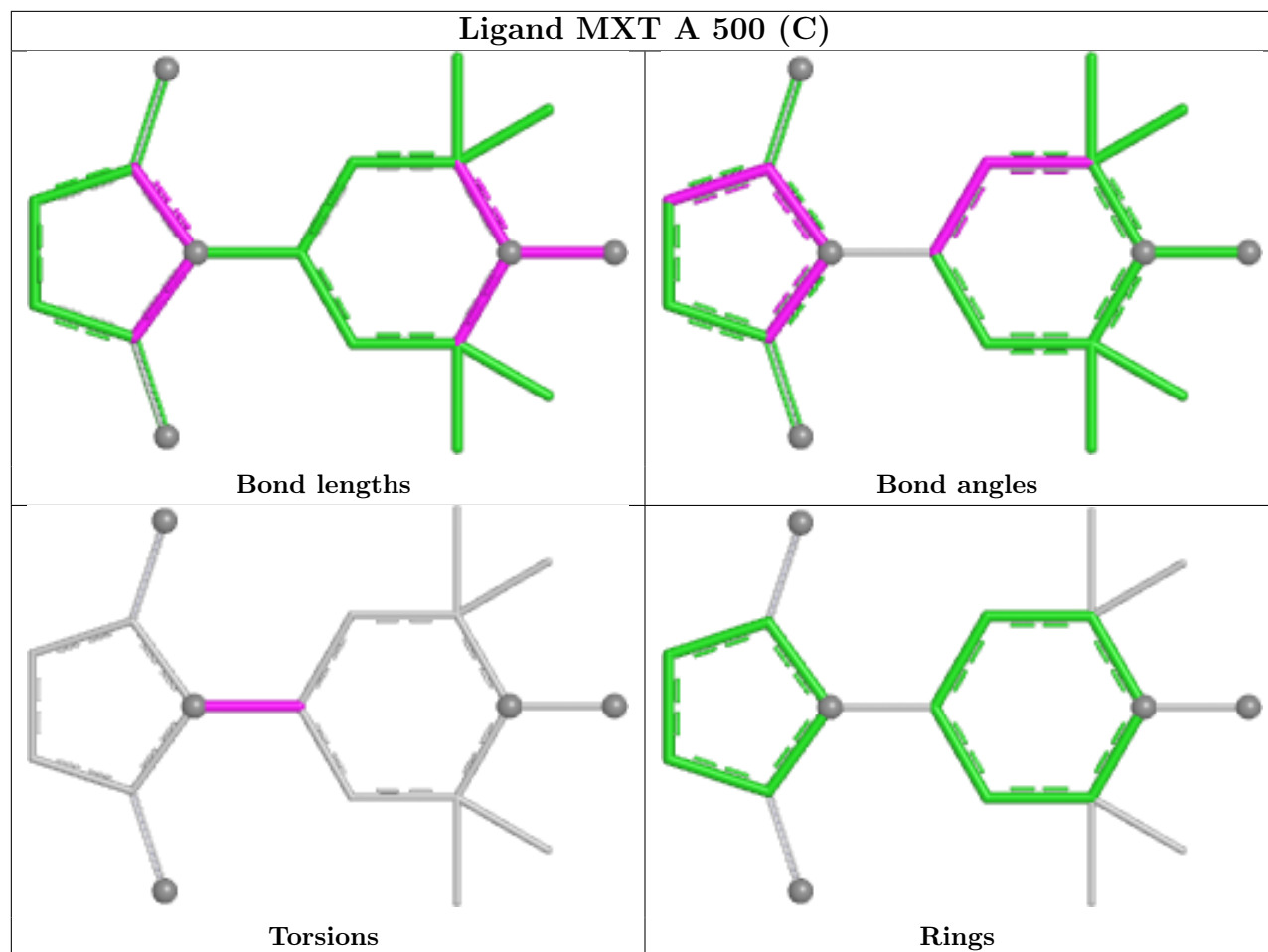


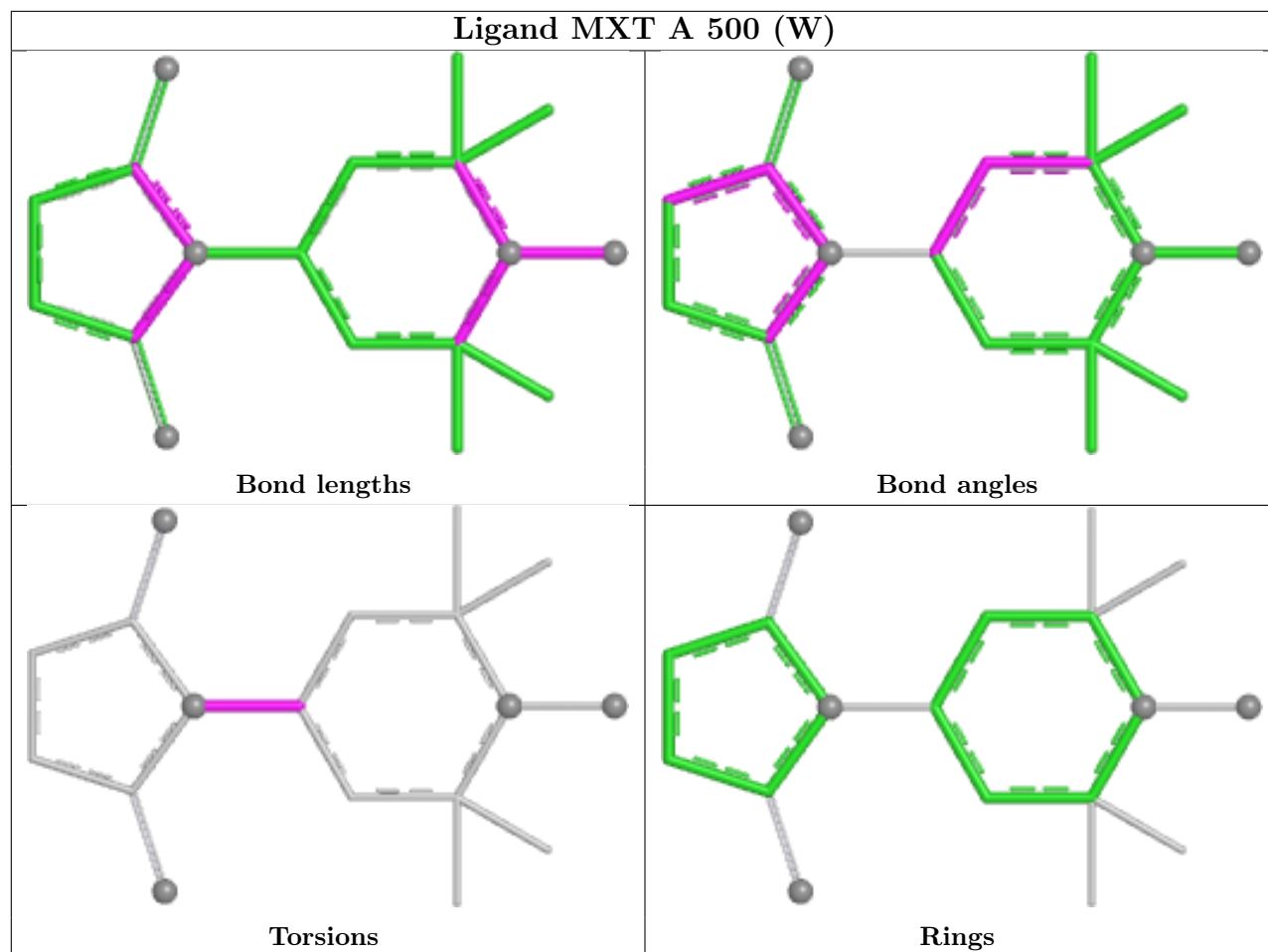


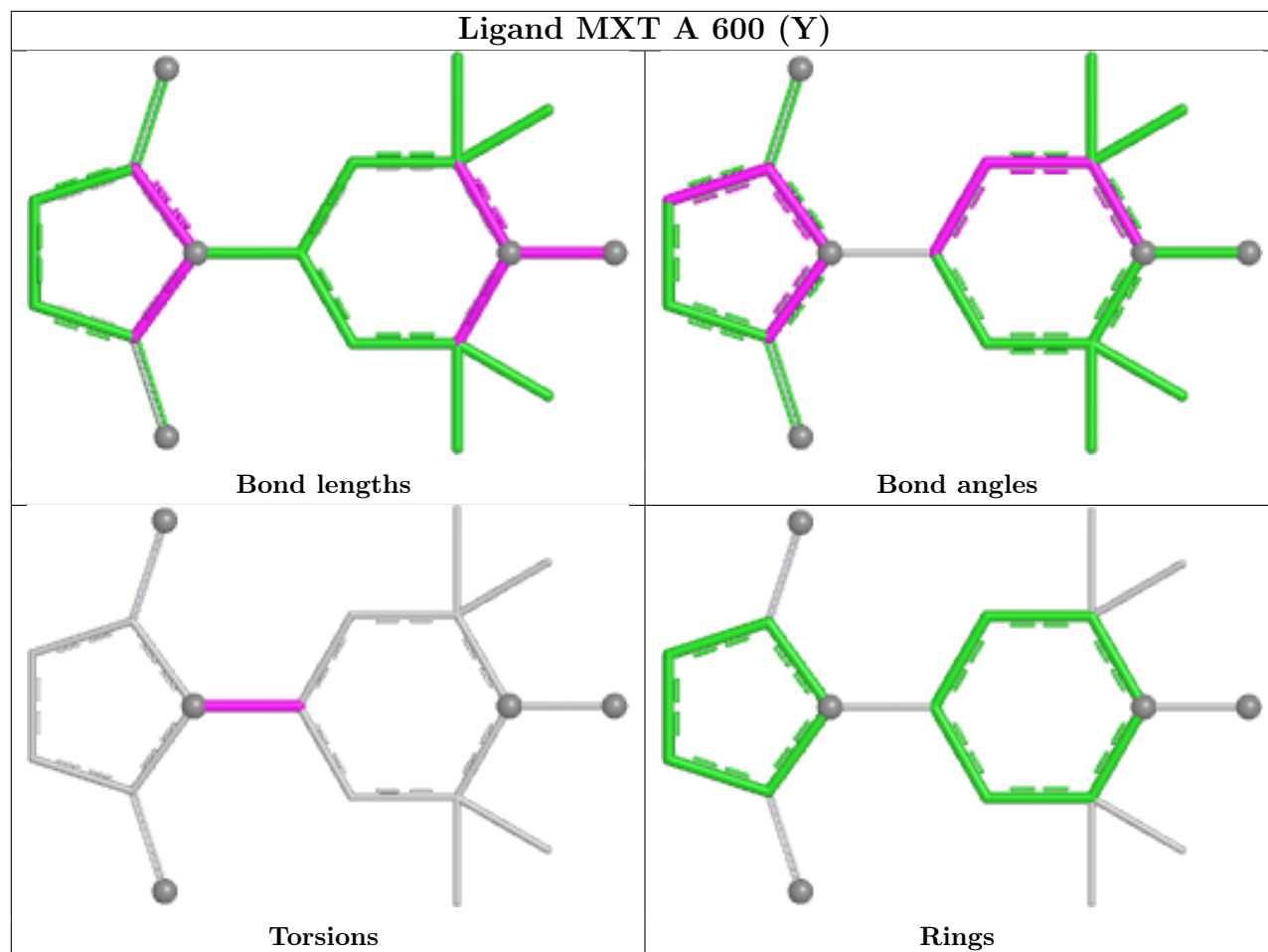


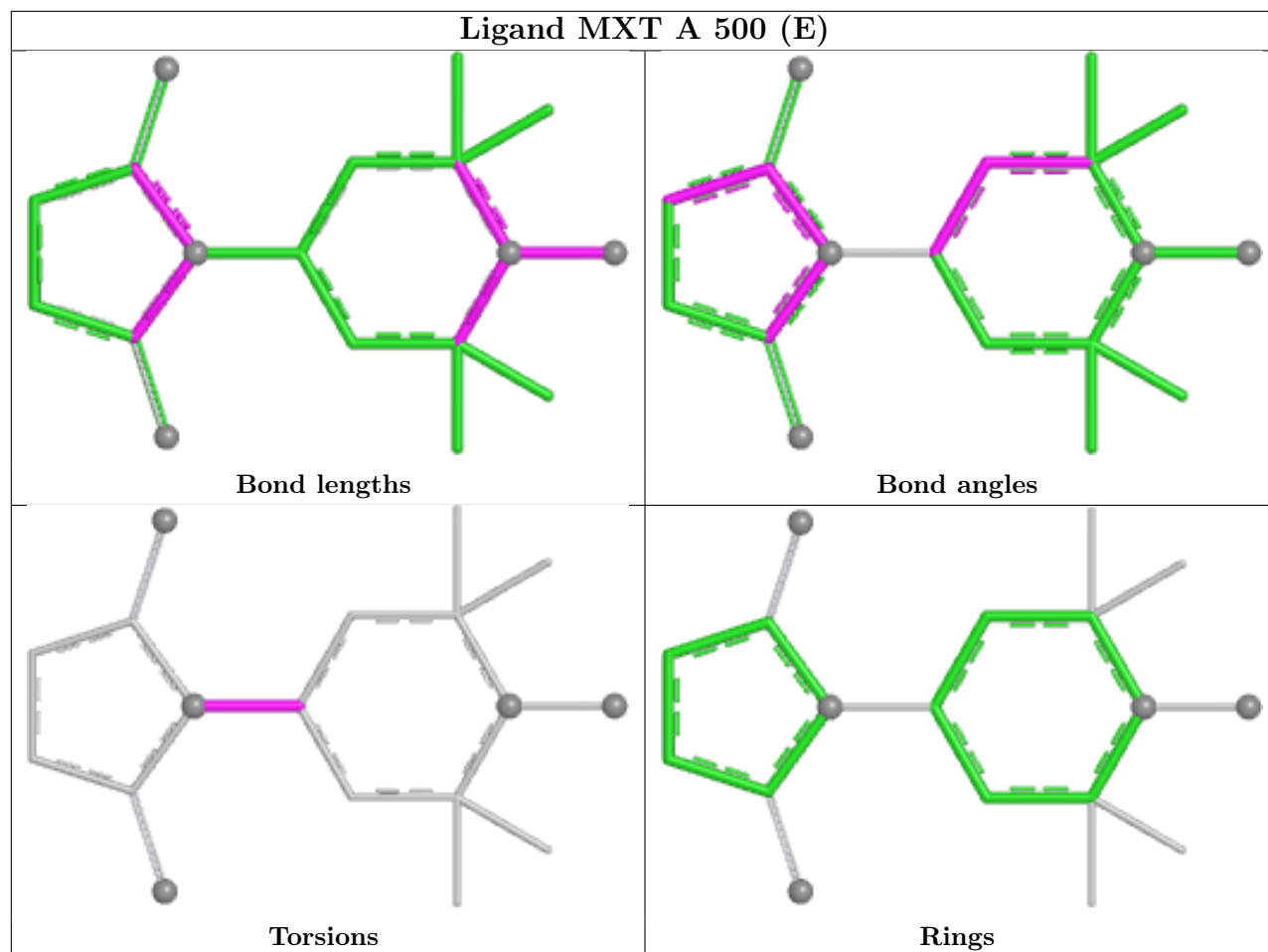


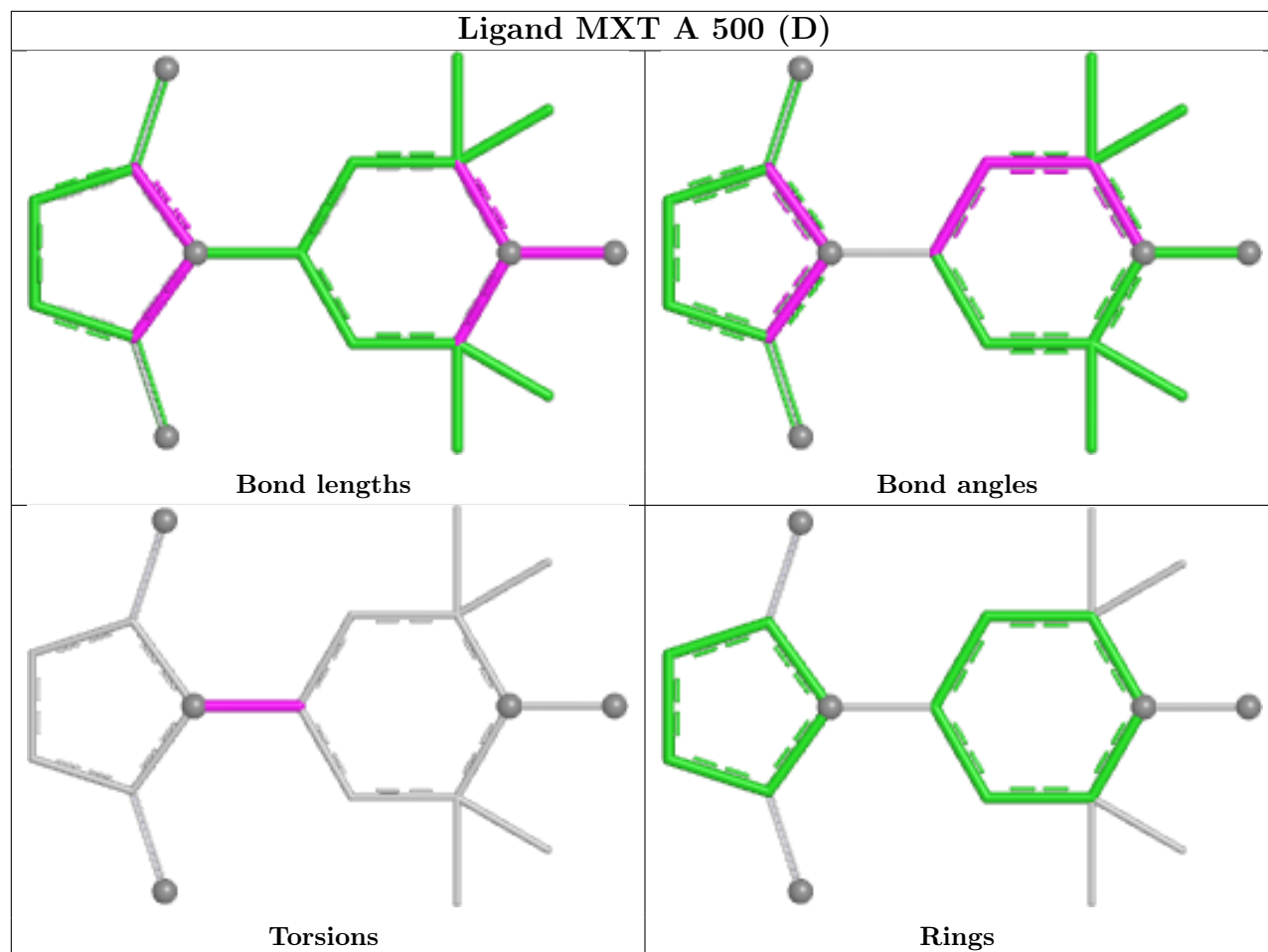


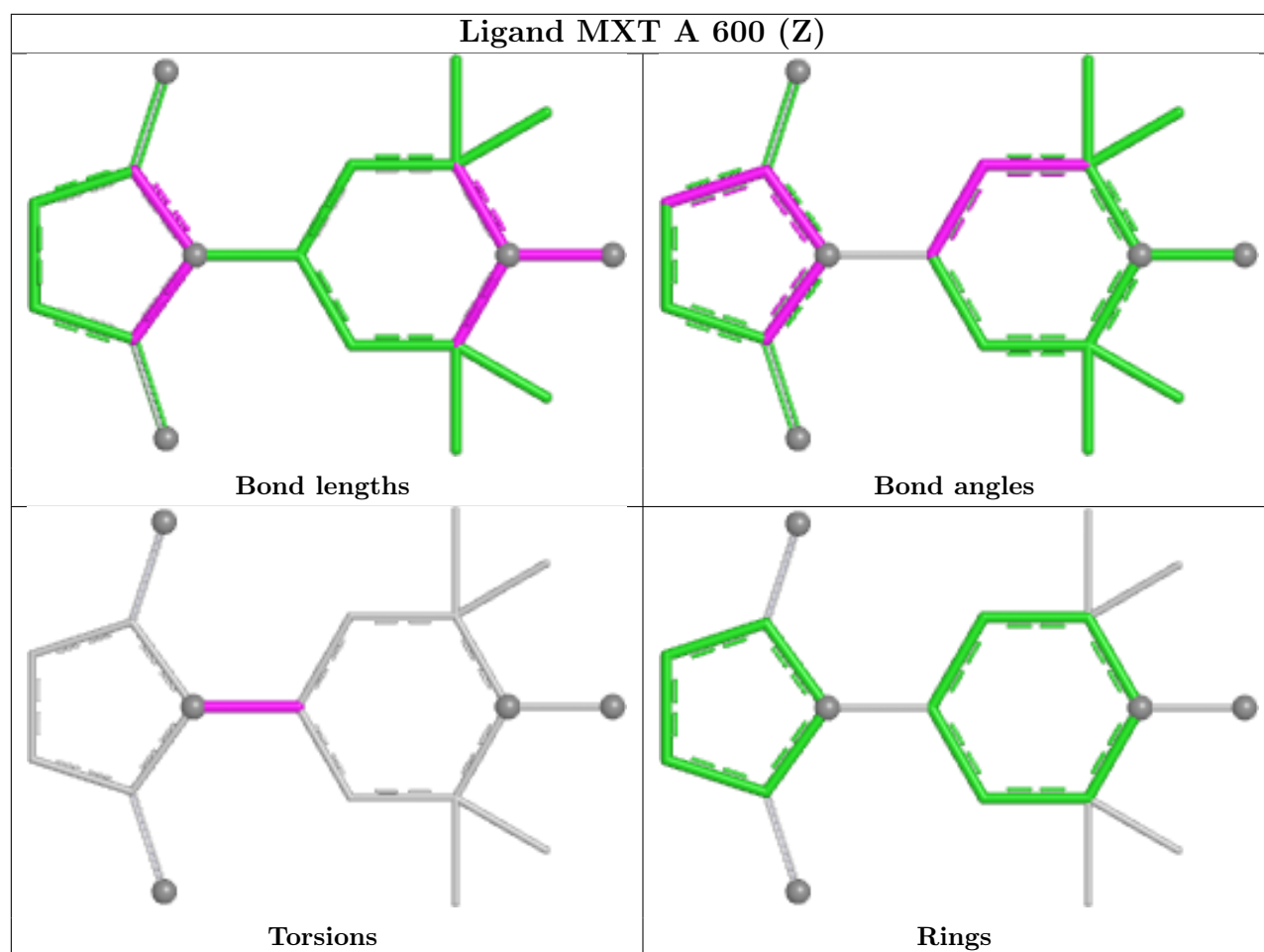


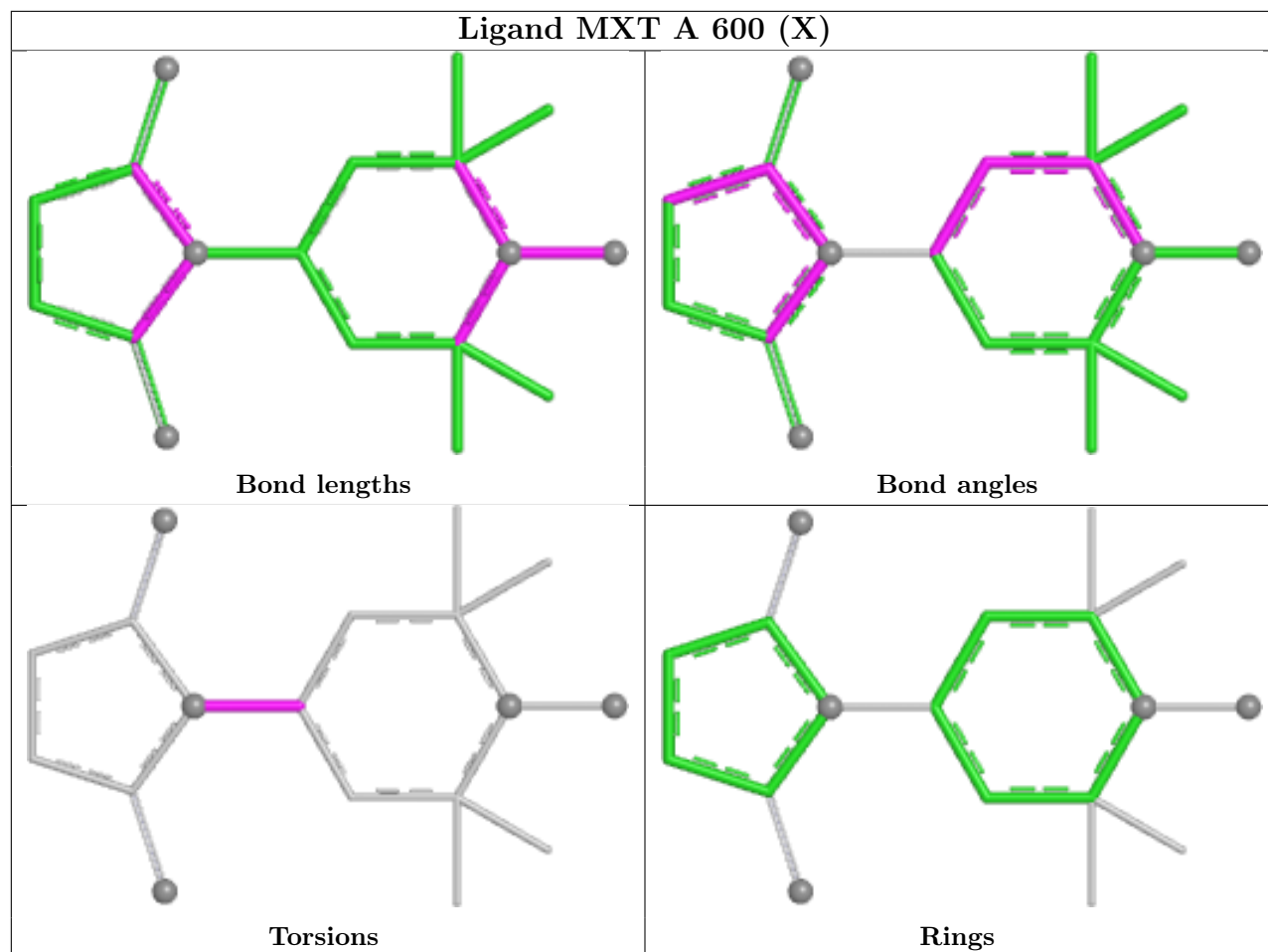


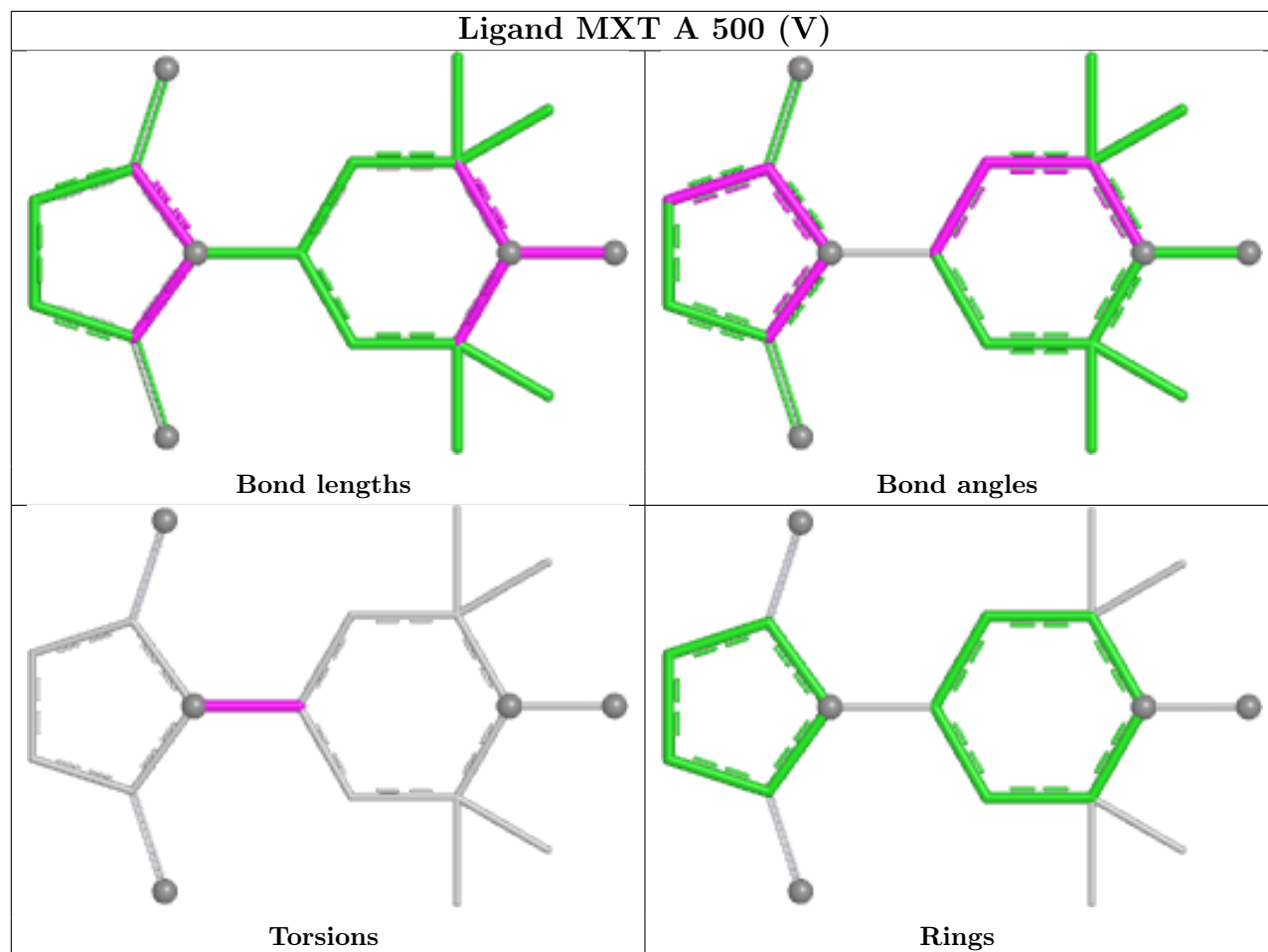


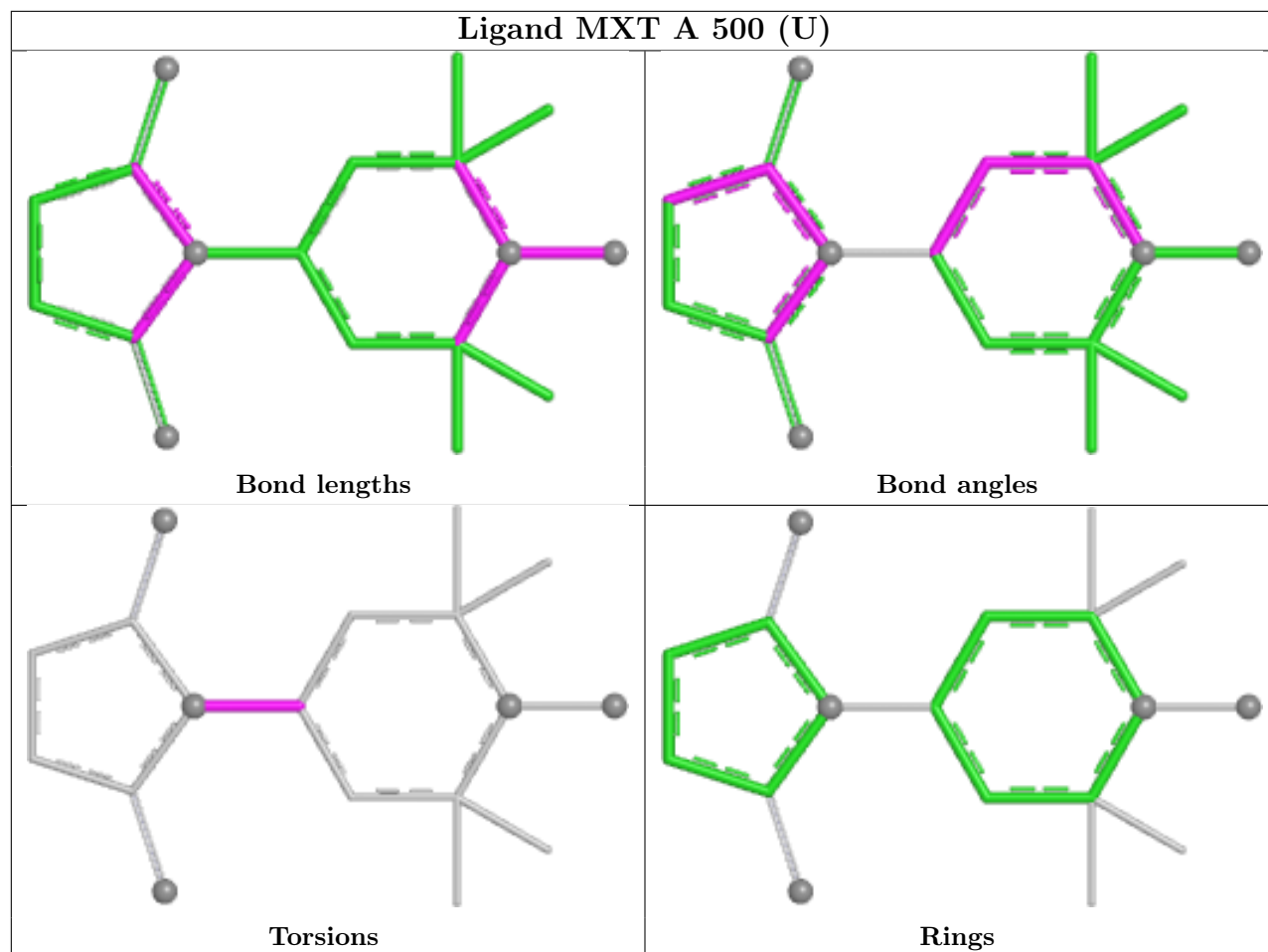












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided