



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 11:20 PM UTC

PDB ID : 7RL0 / pdb_00007r10
EMDB ID : EMD-24512
Title : Yeast CTP Synthase (URA8) Filament bound to ATP/UTP at low pH
Authors : Hansen, J.M.; Lynch, E.M.; Farrell, D.P.; DiMaio, F.; Quispe, J.; Kollman, J.M.
Deposited on : 2021-07-22
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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:

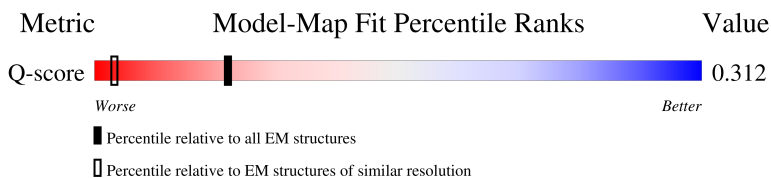
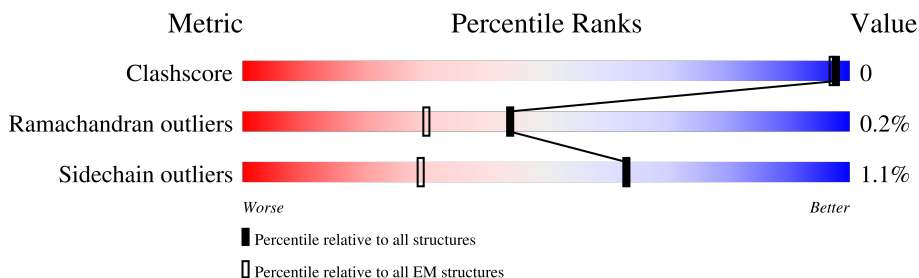
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



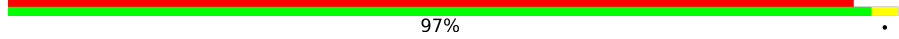
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	100% 97% .
1	B	559	94% 97% .
1	C	559	96% 97% .
1	D	559	100% 97% .

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Mol	Chain	Length	Quality of chain
1	E	559	 20% 97%
1	F	559	 19% 97%
1	G	559	 22% 97%
1	H	559	 23% 97%
1	W	559	 94% 97%
1	X	559	 100% 97%
1	Y	559	 100% 97%
1	Z	559	 95% 97%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 106308 atoms, of which 52944 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CTP synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	559	8778	2775	4393	757	833	20	0	0
1	B	559	8778	2775	4393	757	833	20	0	0
1	C	559	8778	2775	4393	757	833	20	0	0
1	D	559	8778	2775	4393	757	833	20	0	0
1	E	559	8778	2775	4393	757	833	20	0	0
1	F	559	8778	2775	4393	757	833	20	0	0
1	G	559	8778	2775	4393	757	833	20	0	0
1	H	559	8778	2775	4393	757	833	20	0	0
1	W	559	8778	2775	4393	757	833	20	0	0
1	X	559	8778	2775	4393	757	833	20	0	0
1	Y	559	8778	2775	4393	757	833	20	0	0
1	Z	559	8778	2775	4393	757	833	20	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A6A5PYW3
A	?	-	MET	deletion	UNP A0A6A5PYW3
A	?	-	PRO	deletion	UNP A0A6A5PYW3
A	?	-	GLU	deletion	UNP A0A6A5PYW3
A	?	-	ILE	deletion	UNP A0A6A5PYW3
A	?	-	ASP	deletion	UNP A0A6A5PYW3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP A0A6A5PYW3
A	?	-	GLU	deletion	UNP A0A6A5PYW3
A	?	-	HIS	deletion	UNP A0A6A5PYW3
A	?	-	MET	deletion	UNP A0A6A5PYW3
A	?	-	GLY	deletion	UNP A0A6A5PYW3
A	?	-	GLY	deletion	UNP A0A6A5PYW3
B	?	-	TYR	deletion	UNP A0A6A5PYW3
B	?	-	MET	deletion	UNP A0A6A5PYW3
B	?	-	PRO	deletion	UNP A0A6A5PYW3
B	?	-	GLU	deletion	UNP A0A6A5PYW3
B	?	-	ILE	deletion	UNP A0A6A5PYW3
B	?	-	ASP	deletion	UNP A0A6A5PYW3
B	?	-	LYS	deletion	UNP A0A6A5PYW3
B	?	-	GLU	deletion	UNP A0A6A5PYW3
B	?	-	HIS	deletion	UNP A0A6A5PYW3
B	?	-	MET	deletion	UNP A0A6A5PYW3
B	?	-	GLY	deletion	UNP A0A6A5PYW3
B	?	-	GLY	deletion	UNP A0A6A5PYW3
C	?	-	TYR	deletion	UNP A0A6A5PYW3
C	?	-	MET	deletion	UNP A0A6A5PYW3
C	?	-	PRO	deletion	UNP A0A6A5PYW3
C	?	-	GLU	deletion	UNP A0A6A5PYW3
C	?	-	ILE	deletion	UNP A0A6A5PYW3
C	?	-	ASP	deletion	UNP A0A6A5PYW3
C	?	-	LYS	deletion	UNP A0A6A5PYW3
C	?	-	GLU	deletion	UNP A0A6A5PYW3
C	?	-	HIS	deletion	UNP A0A6A5PYW3
C	?	-	MET	deletion	UNP A0A6A5PYW3
C	?	-	GLY	deletion	UNP A0A6A5PYW3
C	?	-	GLY	deletion	UNP A0A6A5PYW3
D	?	-	TYR	deletion	UNP A0A6A5PYW3
D	?	-	MET	deletion	UNP A0A6A5PYW3
D	?	-	PRO	deletion	UNP A0A6A5PYW3
D	?	-	GLU	deletion	UNP A0A6A5PYW3
D	?	-	ILE	deletion	UNP A0A6A5PYW3
D	?	-	ASP	deletion	UNP A0A6A5PYW3
D	?	-	LYS	deletion	UNP A0A6A5PYW3
D	?	-	GLU	deletion	UNP A0A6A5PYW3
D	?	-	HIS	deletion	UNP A0A6A5PYW3
D	?	-	MET	deletion	UNP A0A6A5PYW3
D	?	-	GLY	deletion	UNP A0A6A5PYW3
D	?	-	GLY	deletion	UNP A0A6A5PYW3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	TYR	deletion	UNP A0A6A5PYW3
E	?	-	MET	deletion	UNP A0A6A5PYW3
E	?	-	PRO	deletion	UNP A0A6A5PYW3
E	?	-	GLU	deletion	UNP A0A6A5PYW3
E	?	-	ILE	deletion	UNP A0A6A5PYW3
E	?	-	ASP	deletion	UNP A0A6A5PYW3
E	?	-	LYS	deletion	UNP A0A6A5PYW3
E	?	-	GLU	deletion	UNP A0A6A5PYW3
E	?	-	HIS	deletion	UNP A0A6A5PYW3
E	?	-	MET	deletion	UNP A0A6A5PYW3
E	?	-	GLY	deletion	UNP A0A6A5PYW3
E	?	-	GLY	deletion	UNP A0A6A5PYW3
F	?	-	TYR	deletion	UNP A0A6A5PYW3
F	?	-	MET	deletion	UNP A0A6A5PYW3
F	?	-	PRO	deletion	UNP A0A6A5PYW3
F	?	-	GLU	deletion	UNP A0A6A5PYW3
F	?	-	ILE	deletion	UNP A0A6A5PYW3
F	?	-	ASP	deletion	UNP A0A6A5PYW3
F	?	-	LYS	deletion	UNP A0A6A5PYW3
F	?	-	GLU	deletion	UNP A0A6A5PYW3
F	?	-	HIS	deletion	UNP A0A6A5PYW3
F	?	-	MET	deletion	UNP A0A6A5PYW3
F	?	-	GLY	deletion	UNP A0A6A5PYW3
F	?	-	GLY	deletion	UNP A0A6A5PYW3
G	?	-	TYR	deletion	UNP A0A6A5PYW3
G	?	-	MET	deletion	UNP A0A6A5PYW3
G	?	-	PRO	deletion	UNP A0A6A5PYW3
G	?	-	GLU	deletion	UNP A0A6A5PYW3
G	?	-	ILE	deletion	UNP A0A6A5PYW3
G	?	-	ASP	deletion	UNP A0A6A5PYW3
G	?	-	LYS	deletion	UNP A0A6A5PYW3
G	?	-	GLU	deletion	UNP A0A6A5PYW3
G	?	-	HIS	deletion	UNP A0A6A5PYW3
G	?	-	MET	deletion	UNP A0A6A5PYW3
G	?	-	GLY	deletion	UNP A0A6A5PYW3
G	?	-	GLY	deletion	UNP A0A6A5PYW3
H	?	-	TYR	deletion	UNP A0A6A5PYW3
H	?	-	MET	deletion	UNP A0A6A5PYW3
H	?	-	PRO	deletion	UNP A0A6A5PYW3
H	?	-	GLU	deletion	UNP A0A6A5PYW3
H	?	-	ILE	deletion	UNP A0A6A5PYW3
H	?	-	ASP	deletion	UNP A0A6A5PYW3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LYS	deletion	UNP A0A6A5PYW3
H	?	-	GLU	deletion	UNP A0A6A5PYW3
H	?	-	HIS	deletion	UNP A0A6A5PYW3
H	?	-	MET	deletion	UNP A0A6A5PYW3
H	?	-	GLY	deletion	UNP A0A6A5PYW3
H	?	-	GLY	deletion	UNP A0A6A5PYW3
W	?	-	TYR	deletion	UNP A0A6A5PYW3
W	?	-	MET	deletion	UNP A0A6A5PYW3
W	?	-	PRO	deletion	UNP A0A6A5PYW3
W	?	-	GLU	deletion	UNP A0A6A5PYW3
W	?	-	ILE	deletion	UNP A0A6A5PYW3
W	?	-	ASP	deletion	UNP A0A6A5PYW3
W	?	-	LYS	deletion	UNP A0A6A5PYW3
W	?	-	GLU	deletion	UNP A0A6A5PYW3
W	?	-	HIS	deletion	UNP A0A6A5PYW3
W	?	-	MET	deletion	UNP A0A6A5PYW3
W	?	-	GLY	deletion	UNP A0A6A5PYW3
W	?	-	GLY	deletion	UNP A0A6A5PYW3
X	?	-	TYR	deletion	UNP A0A6A5PYW3
X	?	-	MET	deletion	UNP A0A6A5PYW3
X	?	-	PRO	deletion	UNP A0A6A5PYW3
X	?	-	GLU	deletion	UNP A0A6A5PYW3
X	?	-	ILE	deletion	UNP A0A6A5PYW3
X	?	-	ASP	deletion	UNP A0A6A5PYW3
X	?	-	LYS	deletion	UNP A0A6A5PYW3
X	?	-	GLU	deletion	UNP A0A6A5PYW3
X	?	-	HIS	deletion	UNP A0A6A5PYW3
X	?	-	MET	deletion	UNP A0A6A5PYW3
X	?	-	GLY	deletion	UNP A0A6A5PYW3
X	?	-	GLY	deletion	UNP A0A6A5PYW3
Y	?	-	TYR	deletion	UNP A0A6A5PYW3
Y	?	-	MET	deletion	UNP A0A6A5PYW3
Y	?	-	PRO	deletion	UNP A0A6A5PYW3
Y	?	-	GLU	deletion	UNP A0A6A5PYW3
Y	?	-	ILE	deletion	UNP A0A6A5PYW3
Y	?	-	ASP	deletion	UNP A0A6A5PYW3
Y	?	-	LYS	deletion	UNP A0A6A5PYW3
Y	?	-	GLU	deletion	UNP A0A6A5PYW3
Y	?	-	HIS	deletion	UNP A0A6A5PYW3
Y	?	-	MET	deletion	UNP A0A6A5PYW3
Y	?	-	GLY	deletion	UNP A0A6A5PYW3
Y	?	-	GLY	deletion	UNP A0A6A5PYW3

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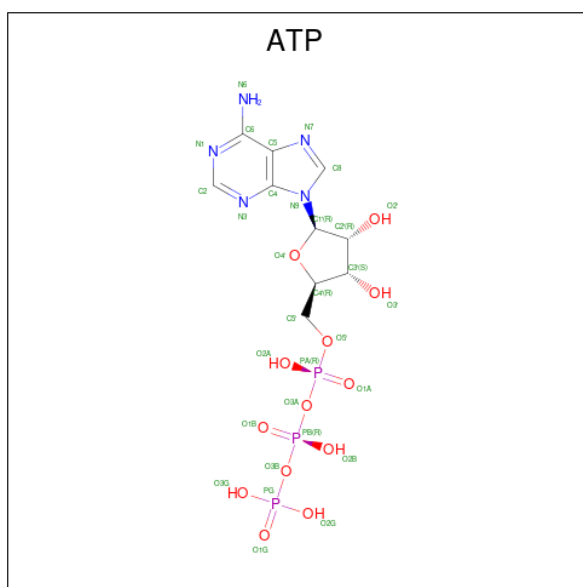
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Chain	Residue	Modelled	Actual	Comment	Reference
Z	?	-	TYR	deletion	UNP A0A6A5PYW3
Z	?	-	MET	deletion	UNP A0A6A5PYW3
Z	?	-	PRO	deletion	UNP A0A6A5PYW3
Z	?	-	GLU	deletion	UNP A0A6A5PYW3
Z	?	-	ILE	deletion	UNP A0A6A5PYW3
Z	?	-	ASP	deletion	UNP A0A6A5PYW3
Z	?	-	LYS	deletion	UNP A0A6A5PYW3
Z	?	-	GLU	deletion	UNP A0A6A5PYW3
Z	?	-	HIS	deletion	UNP A0A6A5PYW3
Z	?	-	MET	deletion	UNP A0A6A5PYW3
Z	?	-	GLY	deletion	UNP A0A6A5PYW3
Z	?	-	GLY	deletion	UNP A0A6A5PYW3

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

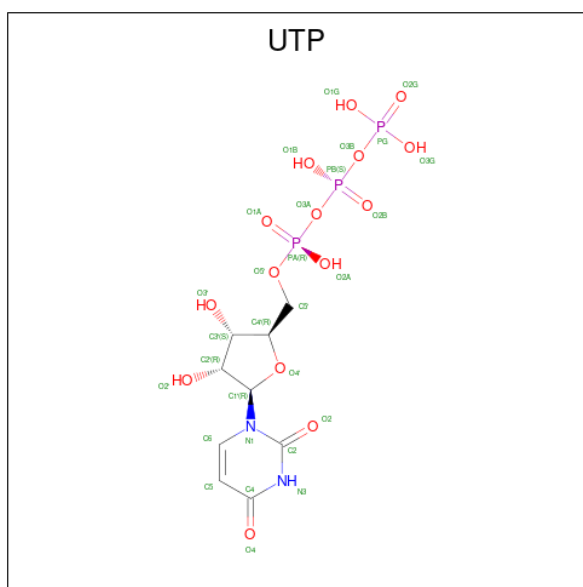
Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Mg 2 2	0
2	B	2	Total Mg 2 2	0
2	C	2	Total Mg 2 2	0
2	D	2	Total Mg 2 2	0
2	E	2	Total Mg 2 2	0
2	F	2	Total Mg 2 2	0
2	G	2	Total Mg 2 2	0
2	H	2	Total Mg 2 2	0
2	W	2	Total Mg 2 2	0
2	X	2	Total Mg 2 2	0
2	Y	2	Total Mg 2 2	0
2	Z	2	Total Mg 2 2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
3	A	1	Total 43	10	12	5	13	3	0
3	B	1	Total 43	10	12	5	13	3	0
3	C	1	Total 43	10	12	5	13	3	0
3	D	1	Total 43	10	12	5	13	3	0
3	E	1	Total 43	10	12	5	13	3	0
3	F	1	Total 43	10	12	5	13	3	0
3	G	1	Total 43	10	12	5	13	3	0
3	H	1	Total 43	10	12	5	13	3	0
3	W	1	Total 43	10	12	5	13	3	0
3	X	1	Total 43	10	12	5	13	3	0
3	Y	1	Total 43	10	12	5	13	3	0
3	Z	1	Total 43	10	12	5	13	3	0

- Molecule 4 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).

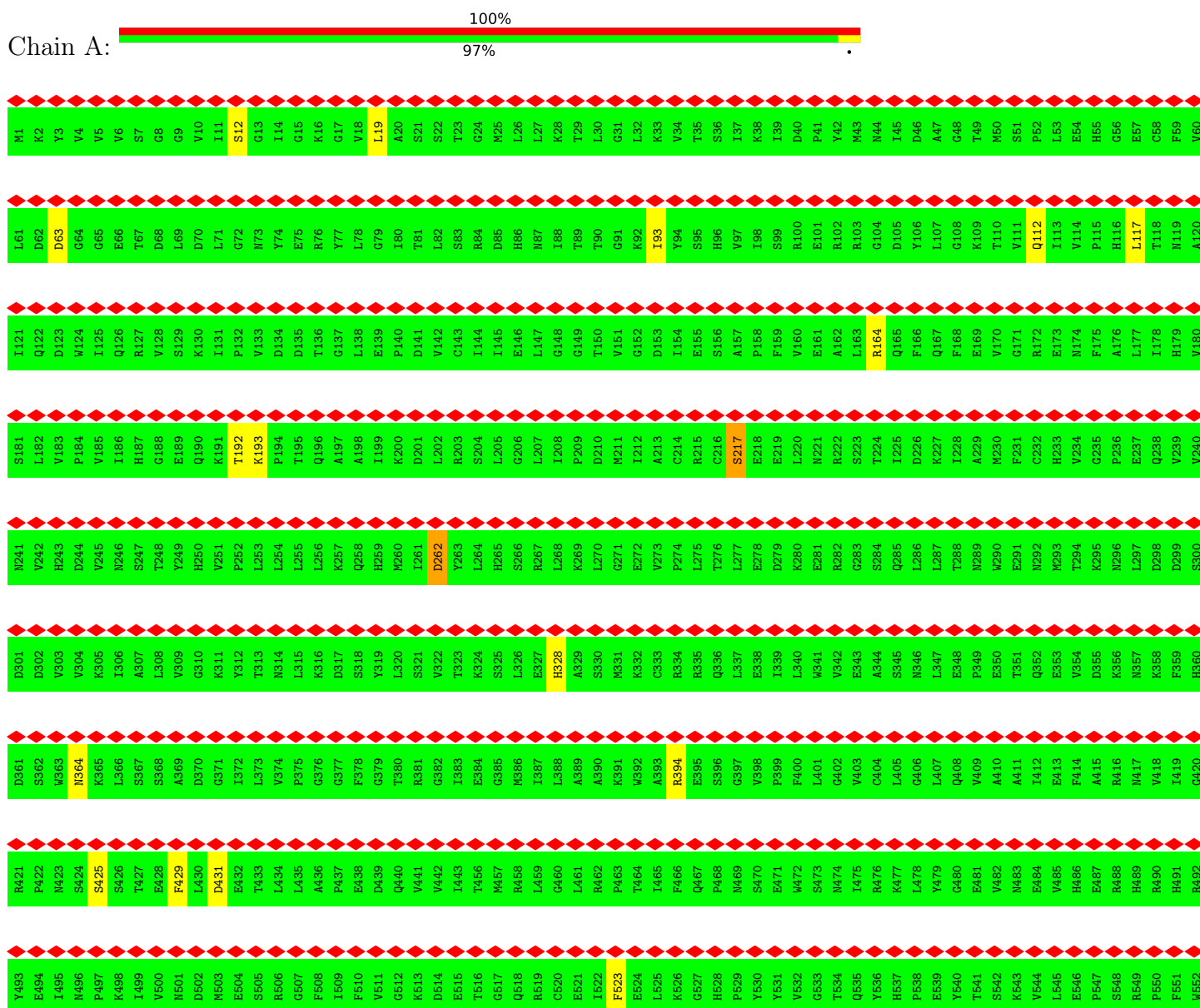


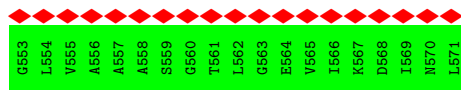
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
4	A	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	B	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	C	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	D	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	E	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	F	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	G	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	H	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	W	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	X	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	Y	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	
4	Z	1	Total	C	H	N	O	P	0
			36	9	7	2	15	3	

3 Residue-property plots

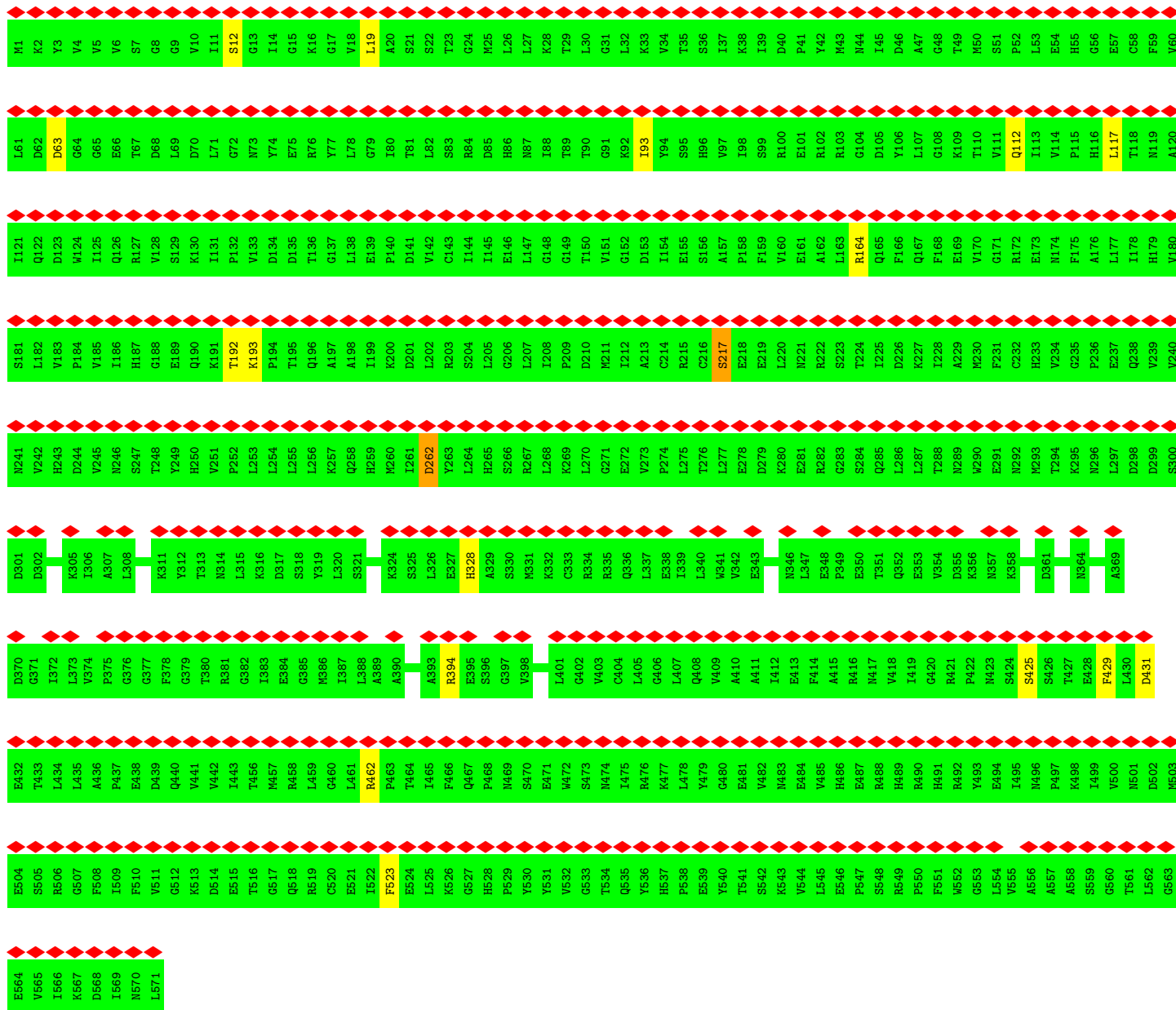
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: CTP synthase

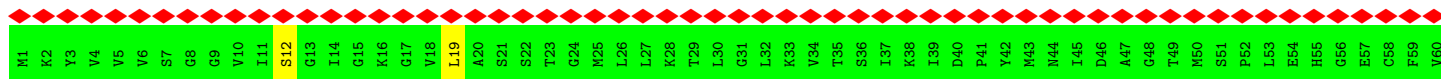




• Molecule 1: CTP synthase



• Molecule 1: CTP synthase

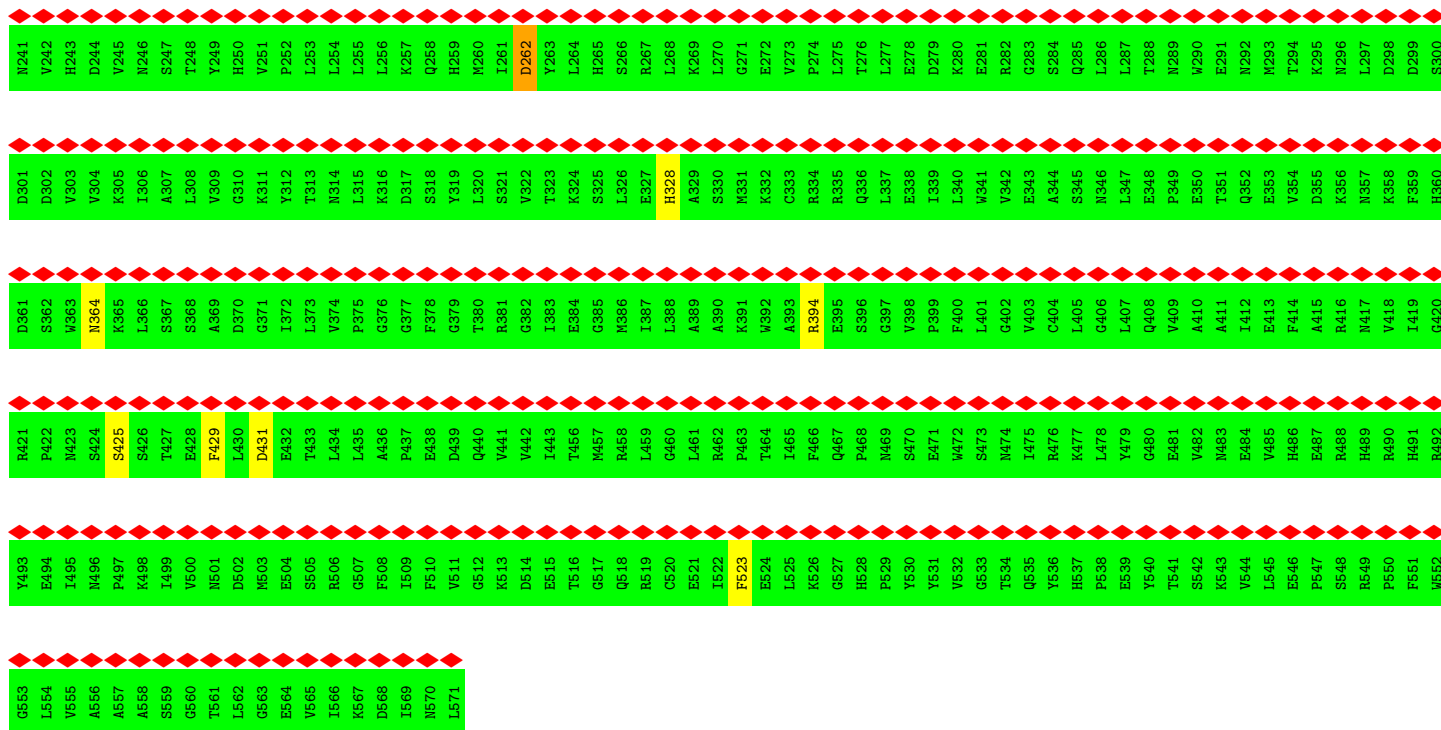


L61	D62	D63	G64	G65	E66	T67	D68	L69	D70	L71	G72	N73	Y74	E75	R76	Y77	L78	G79	I80	T81	L82	S83	R84	D85	H86	N87	I88	T89	T90	G91	K92	I93	Y94	S95	H96	V97	I98	S99	R100	E101	R102	R103	G104	D105	Y106	L107	G108	K109	T110	V111	Q112	I113	V114	P115	H116	L117	T118	N119	A120	
I121	Q122	D123	W124	I125	Q126	V128	L129	K130	I131	P132	V133	D134	D135	T136	G137	L138	E139	P140	D141	V142	C143	I144	I145	E146	L147	G148	P149	T150	V151	G152	D153	I154	E155	S156	A157	P158	F159	V160	E161	A162	L163	R164	Q165	F166	Q167	F168	E169	A229	M230	F231	C232	H233	V234	F175	G235	P236	E237	L178	H179	V180
S181	L182	V183	P184	V185	I186	H187	G188	E189	Q190	K191	T192	K193	P194	T195	Q196	A198	I199	K200	D201	L202	R203	S204	L205	G206	L207	I208	P209	D210	M211	I212	A213	C214	R215	C216	S217	E218	E219	L220	N221	R222	S223	T224	I225	D226	K227	I228	A229	M230	F231	C232	H233	V234	F175	G235	P236	E237	L178	H179	V180	
M241	V242	H243	D244	V245	N246	S247	T248	Y249	H250	V251	P252	L253	L254	L255	L256	Q258	H259	M260	D261	D262	Y263	L264	H265	S266	R267	L268	K269	L270	G271	E272	V273	P274	L275	T276	L277	E278	D279	K280	R281	E282	G283	S284	Q285	D286	L287	T288	N289	M290	E291	N292	M293	T294	K295	N296	L297	D298	D299	S300		
D301	D302	V303	K305	I306	A307	L308	V309	G310	K311	Y312	T313	N314	L315	K316	D317	S318	Y319	L320	S321	V322	T323	K324	S325	L326	E327	H328	A329	S330	M331	K332	C333	R334	R335	Q336	L337	E338	I339	L340	E343	A344	S345	N346	L347	L348	P349	E350	T351	Q352	E353	V354	D355	K356	N357	K358	D361					
K364	K365	L366	S367	S368	A369	D370	G371	I372	L373	V374	P375	G376	G377	F378	G379	T380	R381	G382	I383	E384	G385	M386	I387	A390	K391	V392	A393	E395	S396	G397	V398	L401	G402	V403	C404	L405	G406	L407	Q408	V409	A410	A411	I412	E413	F414	A415	R416	N417	V418	I419	G420	R421	P422	N423	S424	S425				
S426	T427	E428	F429	L430	D431	E432	T433	L434	L435	A436	P437	E438	D439	Q440	V441	V442	L443	T446	L446	R447	L448	L449	G460	L461	R462	T464	L465	F466	Q467	P468	N469	S470	E471	W472	S473	N474	L475	R476	K477	L478	V479	G480	E481	W482	N483	E484	V485	H486	P487	R488	H489	R490	H491	R492	Y493	E494	L495	N496	P497	
K498	L499	V500	N501	D502	M503	E504	S505	R506	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	G517	H518	S519	C520	E521	I522	F523	E524	L525	K526	G527	H528	P529	Y530	Y531	V532	G533	T534	O535	V536	H537	P538	E539	Y540	T541	S542	K543	V544	L545	E546	P547	S548	R549	P550	F551	M552	G553	L554	V555	A556	A557	
A558	S559	G560	T561	L562	G563	E564	V565	I566	K567	D568	V569	N570	L571																																															

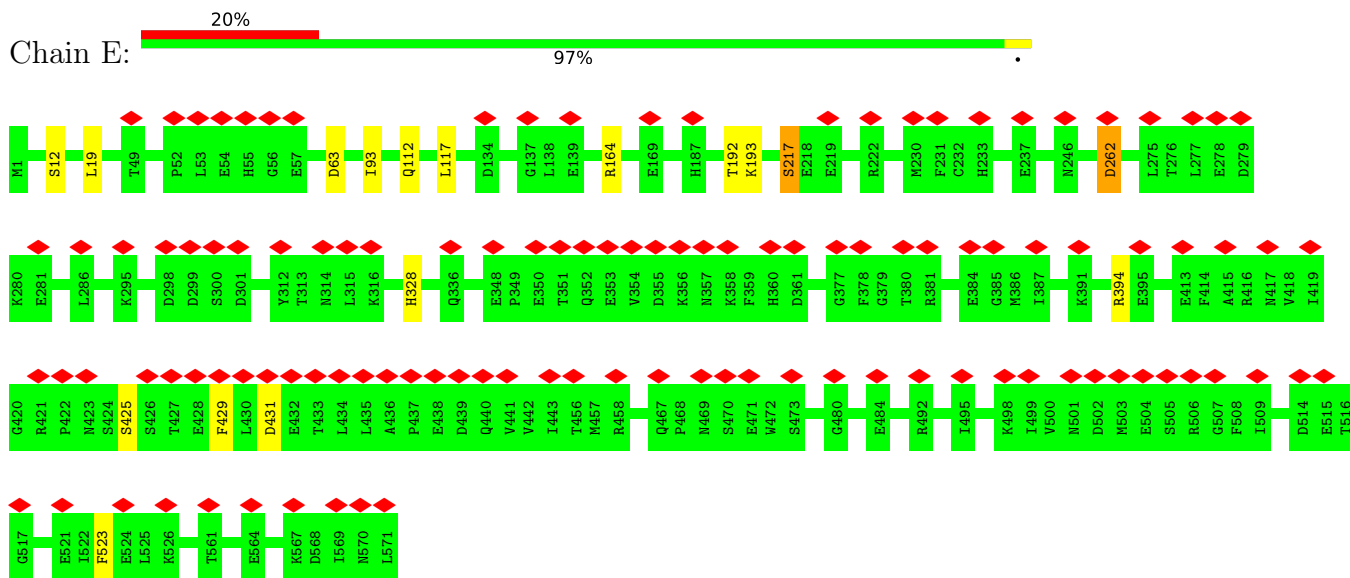
• Molecule 1: CTP synthase



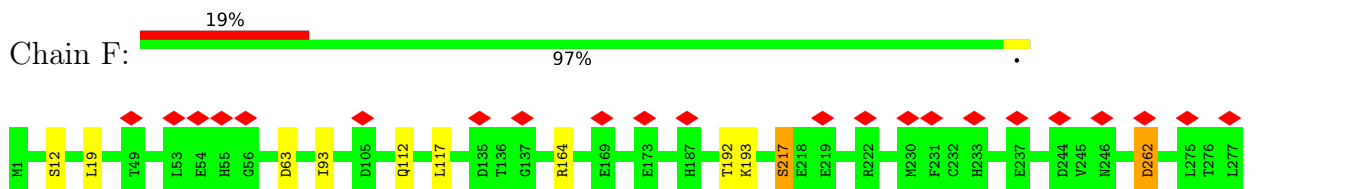
M1	K2	Y3	V4	V5	V6	S7	G8	G9	V10	I11	S12	G13	I14	G15	K16	G17	V18	L19	A20	S21	S22	T23	Q24	M25	L26	L27	K28	T29	L30	G31	L32	K33	V34	T35	S36	I37	K38	I39	D40	P41	Y42	M43	M44	I45	D46	A47	C48	T49	M50	S51	P52	L53	E54	H55	M56	G57	C58	F59	V60	
L61	D62	D63	G64	G65	E66	T67	D68	L69	D70	L71	G72	N73	Y74	E75	R76	Y77	L78	G79	I80	T81	L82	S83	R84	D85	H86	N87	I88	T89	T90	G91	K92	I93	Y94	S95	H96	V97	I98	S99	R100	E101	R102	R103	G104	D105	Y106	L107	G108	K109	T110	V111	Q112	I113	V114	P115	H116	L117	T118	N119	A120	
I121	Q122	D123	W124	I125	Q126	V128	L129	K130	I131	P132	V133	D134	D135	T136	G137	L138	E139	P140	D141	V142	C143	I144	I145	E146	L147	G148	P149	T150	V151	G152	D153	I154	E155	S156	A157	P158	F159	V160	E161	A162	L163	R164	Q165	F166	Q167	F168	E169	A229	M230	F231	C232	H233	V234	F175	G235	P236	E237	L178	H179	V180
S181	L182	V183	P184	V185	I186	H187	G188	E189	Q190	K191	T192	K193	P194	T195	Q196	A198	I199	K200	D201	L202	R203	S204	L205	G206	L207	I208	P209	D210	M211	I212	A213	C214	R215	C216	S217	E218	E219	L220	N221	R222	S223	T224	I225	D226	K227	I228	A229	M230	F231	C232	H233	V234	F175	G235	P236	E237	L178	H179	V180	

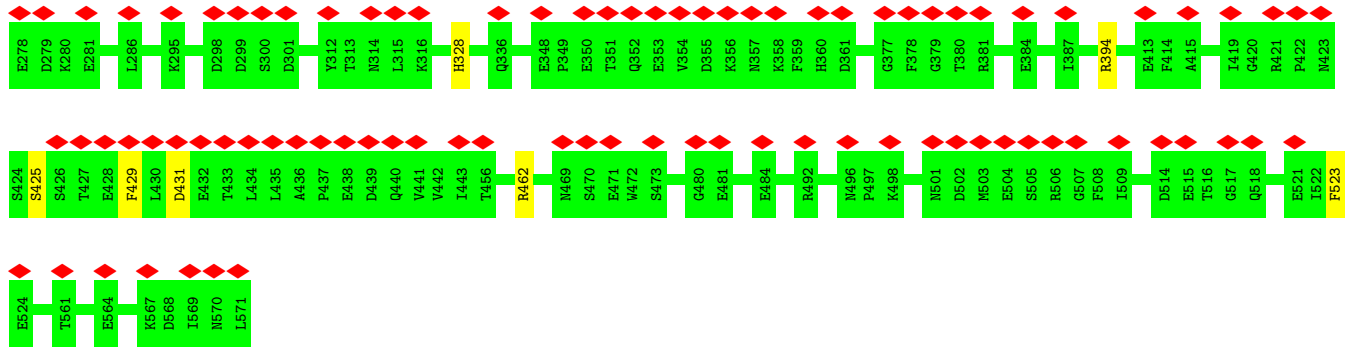


• Molecule 1: CTP synthase

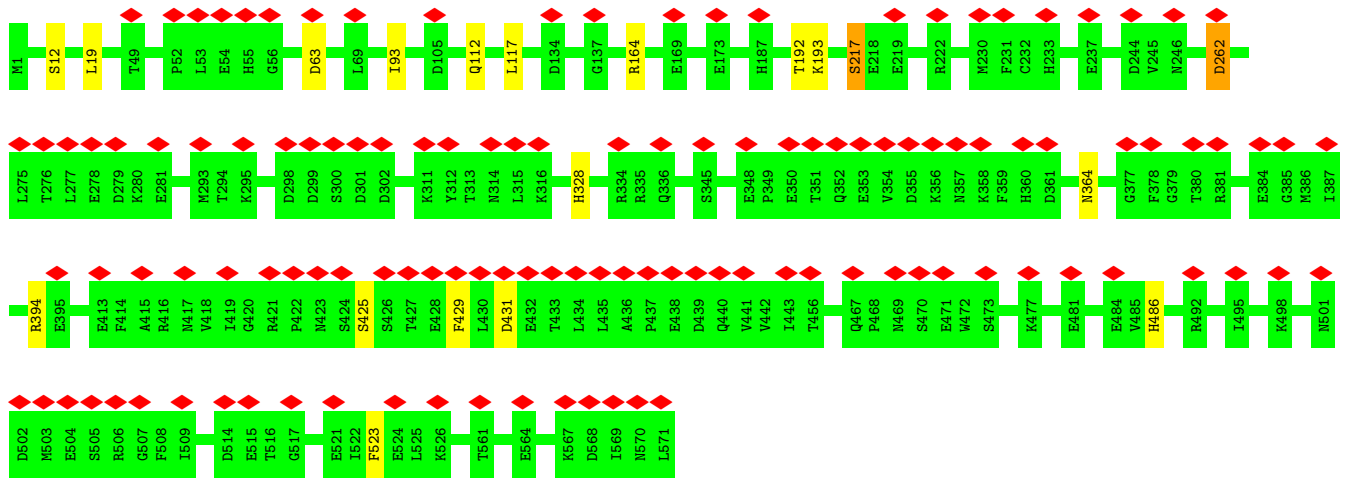


• Molecule 1: CTP synthase

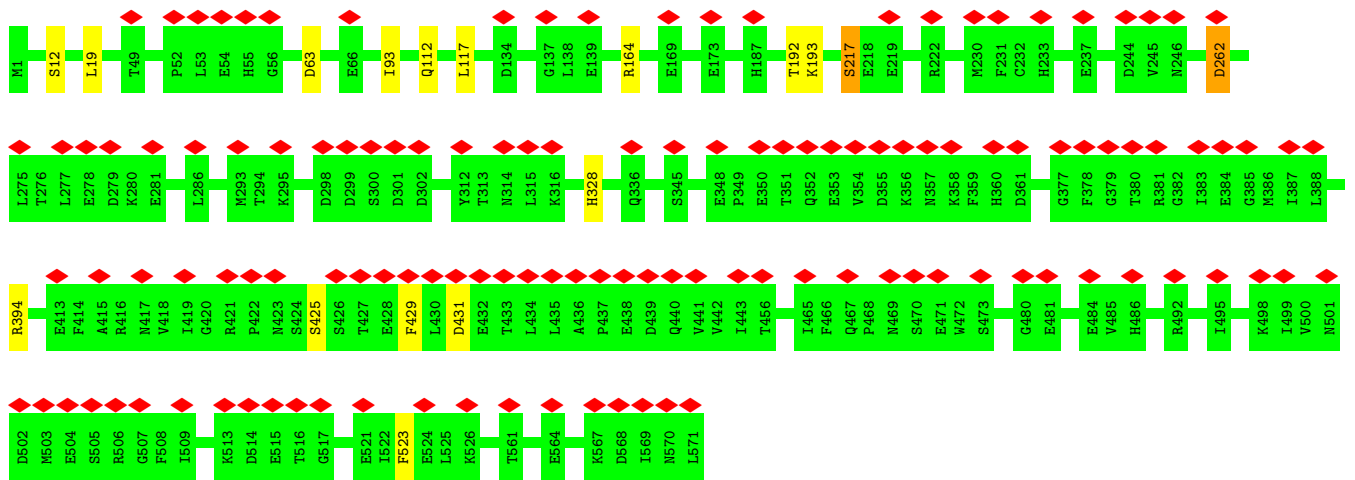




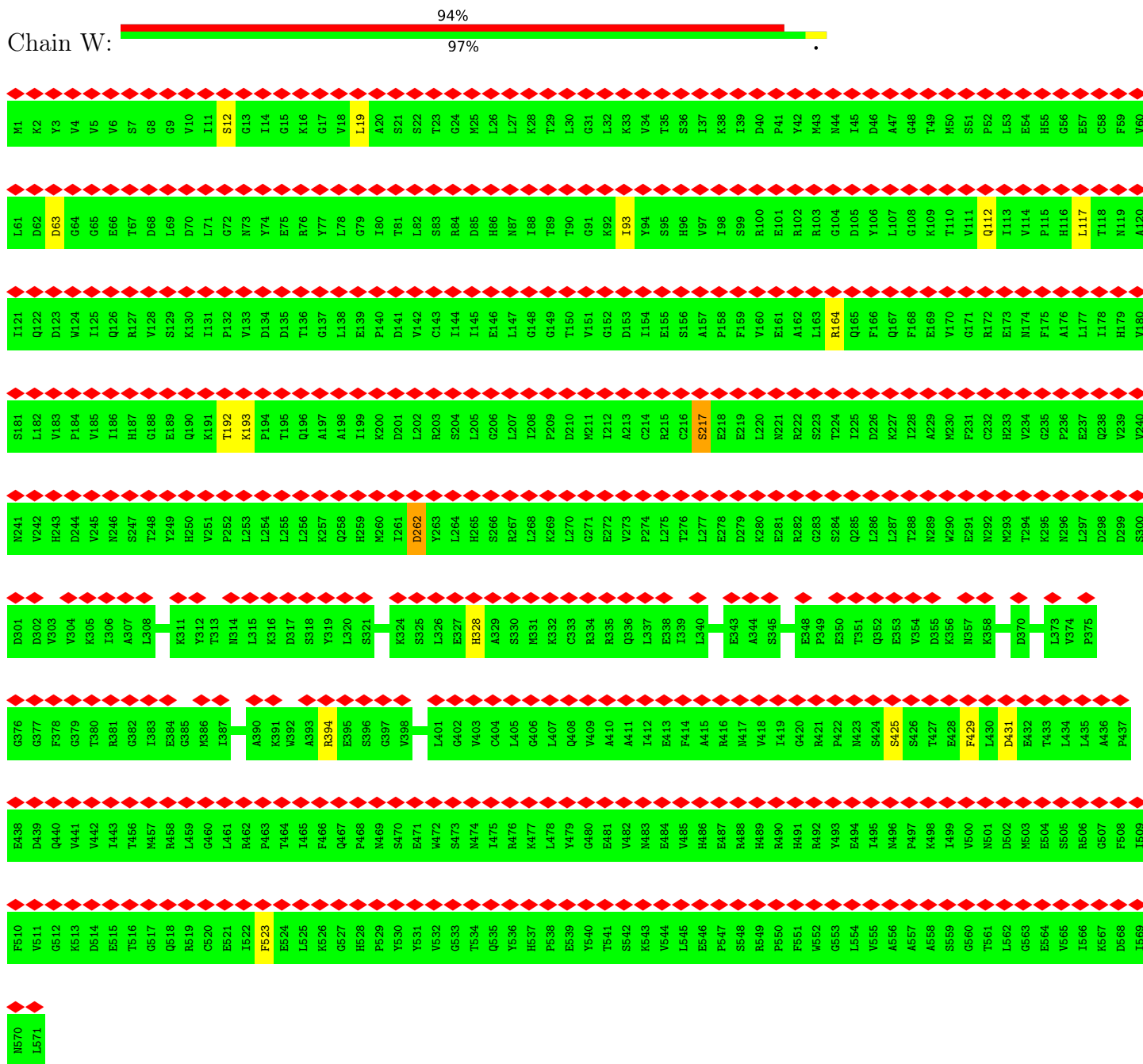
• Molecule 1: CTP synthase



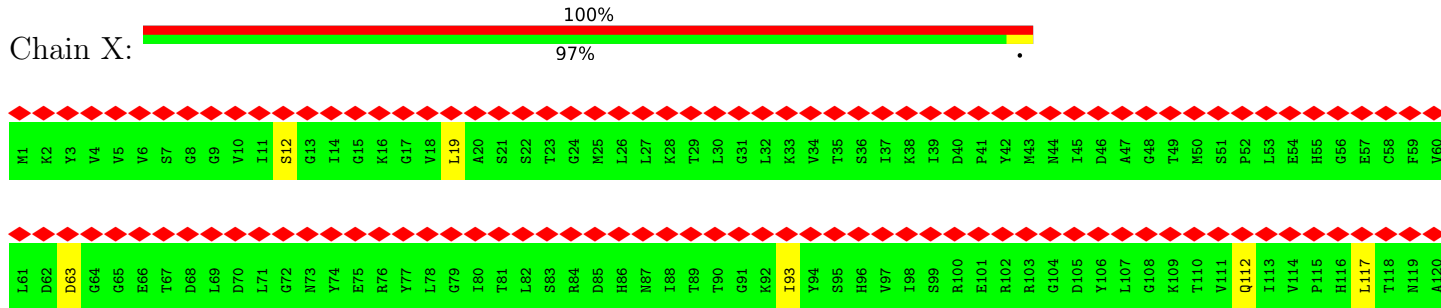
• Molecule 1: CTP synthase



• Molecule 1: CTP synthase



• Molecule 1: CTP synthase



M503	E504	S505	R506	G507	F508	I509	F510	V511	G512	K513	D514	E515	T516	G517	Q518	R519	C520	E521	I522	F523	E524	L525	K526	G527	H528	P529	Y530	Y531	V532	G533	T534	Q535	Y536	H537	P538	E539	Y540	T541	S542	K543	V544	L545	E546	P547	S548	R549	P550	F551	W552	G553	L554	V555	A556	A557	A558	S559	G560	T561	L562
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G563	E564	V565	I566	K567	D568	I569	N570	L571
------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	40474	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	19.614	Depositor
Minimum map value	-14.688	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.343	Depositor
Recommended contour level	2.9	Depositor
Map size (\AA)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, UTP

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	0.80	0/4471	1.40	9/6056 (0.1%)
1	B	0.80	0/4471	1.40	8/6056 (0.1%)
1	C	0.80	0/4471	1.40	9/6056 (0.1%)
1	D	0.80	0/4471	1.40	9/6056 (0.1%)
1	E	0.80	0/4471	1.40	8/6056 (0.1%)
1	F	0.80	0/4471	1.40	8/6056 (0.1%)
1	G	0.80	0/4471	1.40	10/6056 (0.2%)
1	H	0.80	0/4471	1.40	8/6056 (0.1%)
1	W	0.80	0/4471	1.40	8/6056 (0.1%)
1	X	0.80	0/4471	1.40	8/6056 (0.1%)
1	Y	0.80	0/4471	1.40	8/6056 (0.1%)
1	Z	0.80	0/4471	1.40	9/6056 (0.1%)
All	All	0.80	0/53652	1.40	102/72672 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	W	0	1
1	X	0	1
1	Y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Z	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	217	SER	N-CA-C	7.33	121.91	113.19
1	F	217	SER	N-CA-C	7.32	121.91	113.19
1	W	217	SER	N-CA-C	7.32	121.90	113.19
1	E	217	SER	N-CA-C	7.32	121.90	113.19
1	A	217	SER	N-CA-C	7.32	121.90	113.19

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ARG	Sidechain
1	B	164	ARG	Sidechain
1	C	164	ARG	Sidechain
1	D	164	ARG	Sidechain
1	E	164	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4385	4393	4392	4	0
1	B	4385	4393	4392	4	0
1	C	4385	4393	4392	5	0
1	D	4385	4393	4392	4	0
1	E	4385	4393	4392	4	0
1	F	4385	4393	4392	4	0
1	G	4385	4393	4392	4	0
1	H	4385	4393	4392	4	0
1	W	4385	4393	4392	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	4385	4393	4392	4	0
1	Y	4385	4393	4392	4	0
1	Z	4385	4393	4392	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	W	2	0	0	0	0
2	X	2	0	0	0	0
2	Y	2	0	0	0	0
2	Z	2	0	0	0	0
3	A	31	12	12	0	0
3	B	31	12	12	0	0
3	C	31	12	12	0	0
3	D	31	12	12	0	0
3	E	31	12	12	0	0
3	F	31	12	12	0	0
3	G	31	12	12	0	0
3	H	31	12	12	0	0
3	W	31	12	12	0	0
3	X	31	12	12	0	0
3	Y	31	12	12	0	0
3	Z	31	12	12	0	0
4	A	29	7	11	4	0
4	B	29	7	11	5	0
4	C	29	7	11	4	0
4	D	29	7	11	4	0
4	E	29	7	11	4	0
4	F	29	7	11	4	0
4	G	29	7	11	4	0
4	H	29	7	11	4	0
4	W	29	7	11	5	0
4	X	29	7	11	4	0
4	Y	29	7	11	4	0
4	Z	29	7	11	4	0
All	All	53364	52944	52980	50	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 0.

The worst 5 of 50 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:Y:193:LYS:HE3	4:Y:602:UTP:O2B	1.67	0.94
1:C:193:LYS:HE3	4:C:603:UTP:O2B	1.67	0.93
1:G:193:LYS:HE3	4:G:602:UTP:O2B	1.67	0.93
1:X:193:LYS:HE3	4:X:604:UTP:O2B	1.69	0.93
1:W:193:LYS:HE3	4:W:604:UTP:O1B	1.70	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	B	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	C	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	D	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	E	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	F	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	G	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	H	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	W	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	X	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	Y	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
1	Z	555/559 (99%)	540 (97%)	14 (2%)	1 (0%)	43 72
All	All	6660/6708 (99%)	6480 (97%)	168 (2%)	12 (0%)	44 72

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	ASP
1	B	431	ASP
1	C	431	ASP
1	D	431	ASP
1	E	431	ASP

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	B	488/488 (100%)	482 (99%)	6 (1%)	63	87
1	C	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	D	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	E	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	F	488/488 (100%)	482 (99%)	6 (1%)	63	87
1	G	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	H	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	W	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	X	488/488 (100%)	482 (99%)	6 (1%)	63	87
1	Y	488/488 (100%)	483 (99%)	5 (1%)	68	88
1	Z	488/488 (100%)	483 (99%)	5 (1%)	68	88
All	All	5856/5856 (100%)	5793 (99%)	63 (1%)	63	87

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	117	LEU
1	Y	117	LEU
1	G	217	SER
1	Y	93	ILE
1	Z	93	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	165	GLN
1	Y	165	GLN
1	Z	167	GLN
1	Y	167	GLN
1	E	165	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	$\# Z > 2$
4	UTP	A	604	2	29,30,30	0.76	1 (3%)	43,47,47	0.80	1 (2%)
3	ATP	Y	603	2	32,33,33	0.64	0	48,52,52	0.55	0
4	UTP	W	604	2	29,30,30	0.75	1 (3%)	43,47,47	0.80	1 (2%)
3	ATP	X	601	2	32,33,33	0.63	0	48,52,52	0.55	0
3	ATP	F	601	2	32,33,33	0.63	0	48,52,52	0.55	0
3	ATP	E	602	2	32,33,33	0.64	0	48,52,52	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UTP	E	604	2	29,30,30	0.76	1 (3%)	43,47,47	0.80	1 (2%)
4	UTP	C	603	2	29,30,30	0.75	1 (3%)	43,47,47	0.95	2 (4%)
3	ATP	Z	603	2	32,33,33	0.63	0	48,52,52	0.55	0
4	UTP	Y	602	2	29,30,30	0.75	1 (3%)	43,47,47	0.95	2 (4%)
3	ATP	G	603	2	32,33,33	0.63	0	48,52,52	0.55	0
4	UTP	G	602	2	29,30,30	0.75	1 (3%)	43,47,47	0.95	2 (4%)
3	ATP	H	603	2	32,33,33	0.64	0	48,52,52	0.55	0
3	ATP	B	602	2	32,33,33	0.64	0	48,52,52	0.55	0
4	UTP	X	604	2	29,30,30	0.74	1 (3%)	43,47,47	0.95	2 (4%)
3	ATP	D	603	2	32,33,33	0.63	0	48,52,52	0.55	0
4	UTP	Z	602	2	29,30,30	0.76	1 (3%)	43,47,47	0.80	1 (2%)
4	UTP	H	602	2	29,30,30	0.76	1 (3%)	43,47,47	0.80	1 (2%)
4	UTP	B	604	2	29,30,30	0.76	1 (3%)	43,47,47	0.95	2 (4%)
3	ATP	W	602	2	32,33,33	0.64	0	48,52,52	0.55	0
3	ATP	A	602	2	32,33,33	0.63	0	48,52,52	0.55	0
4	UTP	F	604	2	29,30,30	0.75	1 (3%)	43,47,47	0.95	2 (4%)
3	ATP	C	604	2	32,33,33	0.63	0	48,52,52	0.55	0
4	UTP	D	602	2	29,30,30	0.76	1 (3%)	43,47,47	0.80	1 (2%)

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
4	UTP	A	604	2	-	7/22/38/38	0/2/2/2
3	ATP	Y	603	2	-	3/22/38/38	0/3/3/3
4	UTP	W	604	2	-	7/22/38/38	0/2/2/2
3	ATP	X	601	2	-	3/22/38/38	0/3/3/3
3	ATP	F	601	2	-	3/22/38/38	0/3/3/3
3	ATP	E	602	2	-	3/22/38/38	0/3/3/3
4	UTP	E	604	2	-	7/22/38/38	0/2/2/2
4	UTP	C	603	2	-	7/22/38/38	0/2/2/2
3	ATP	Z	603	2	-	3/22/38/38	0/3/3/3
4	UTP	Y	602	2	-	7/22/38/38	0/2/2/2
3	ATP	G	603	2	-	3/22/38/38	0/3/3/3
4	UTP	G	602	2	-	7/22/38/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	H	603	2	-	3/22/38/38	0/3/3/3
3	ATP	B	602	2	-	3/22/38/38	0/3/3/3
4	UTP	X	604	2	-	7/22/38/38	0/2/2/2
3	ATP	D	603	2	-	3/22/38/38	0/3/3/3
4	UTP	Z	602	2	-	7/22/38/38	0/2/2/2
4	UTP	H	602	2	-	7/22/38/38	0/2/2/2
4	UTP	B	604	2	-	7/22/38/38	0/2/2/2
3	ATP	W	602	2	-	3/22/38/38	0/3/3/3
3	ATP	A	602	2	-	3/22/38/38	0/3/3/3
4	UTP	F	604	2	-	7/22/38/38	0/2/2/2
3	ATP	C	604	2	-	3/22/38/38	0/3/3/3
4	UTP	D	602	2	-	7/22/38/38	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	604	UTP	PA-O3A	2.21	1.61	1.59
4	Z	602	UTP	PA-O3A	2.18	1.61	1.59
4	A	604	UTP	PA-O3A	2.16	1.61	1.59
4	H	602	UTP	PA-O3A	2.15	1.61	1.59
4	D	602	UTP	PA-O3A	2.15	1.61	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	UTP	O2A-PA-O1A	3.73	129.78	112.44
4	H	602	UTP	O2A-PA-O1A	3.72	129.76	112.44
4	D	602	UTP	O2A-PA-O1A	3.72	129.75	112.44
4	E	604	UTP	O2A-PA-O1A	3.72	129.74	112.44
4	F	604	UTP	O2A-PA-O1A	3.72	129.74	112.44

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	UTP	PB-O3A-PA-O5'
4	A	604	UTP	C5'-O5'-PA-O1A
4	A	604	UTP	C5'-O5'-PA-O3A
4	B	604	UTP	PB-O3A-PA-O5'

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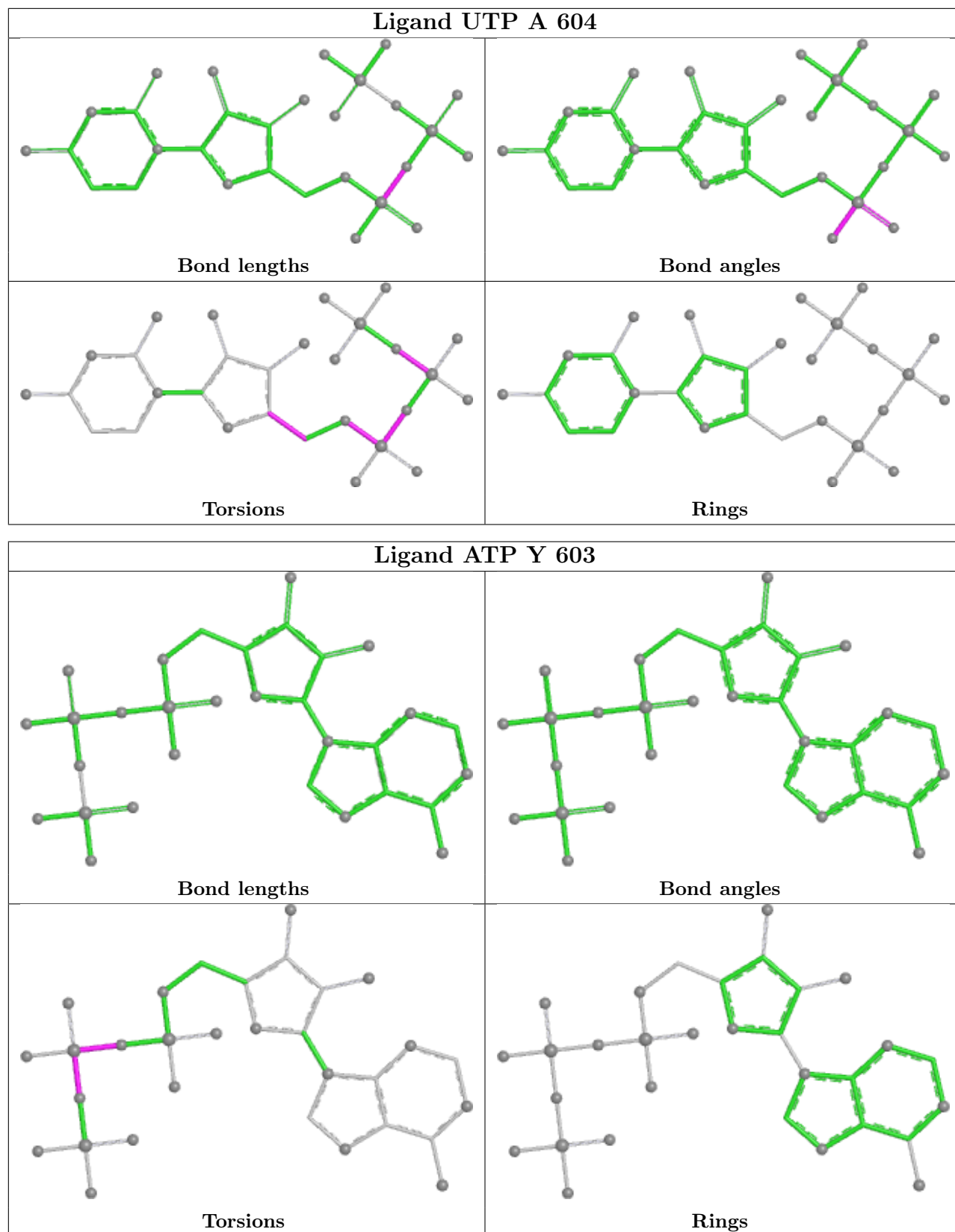
Mol	Chain	Res	Type	Atoms
4	B	604	UTP	C5'-O5'-PA-O1A

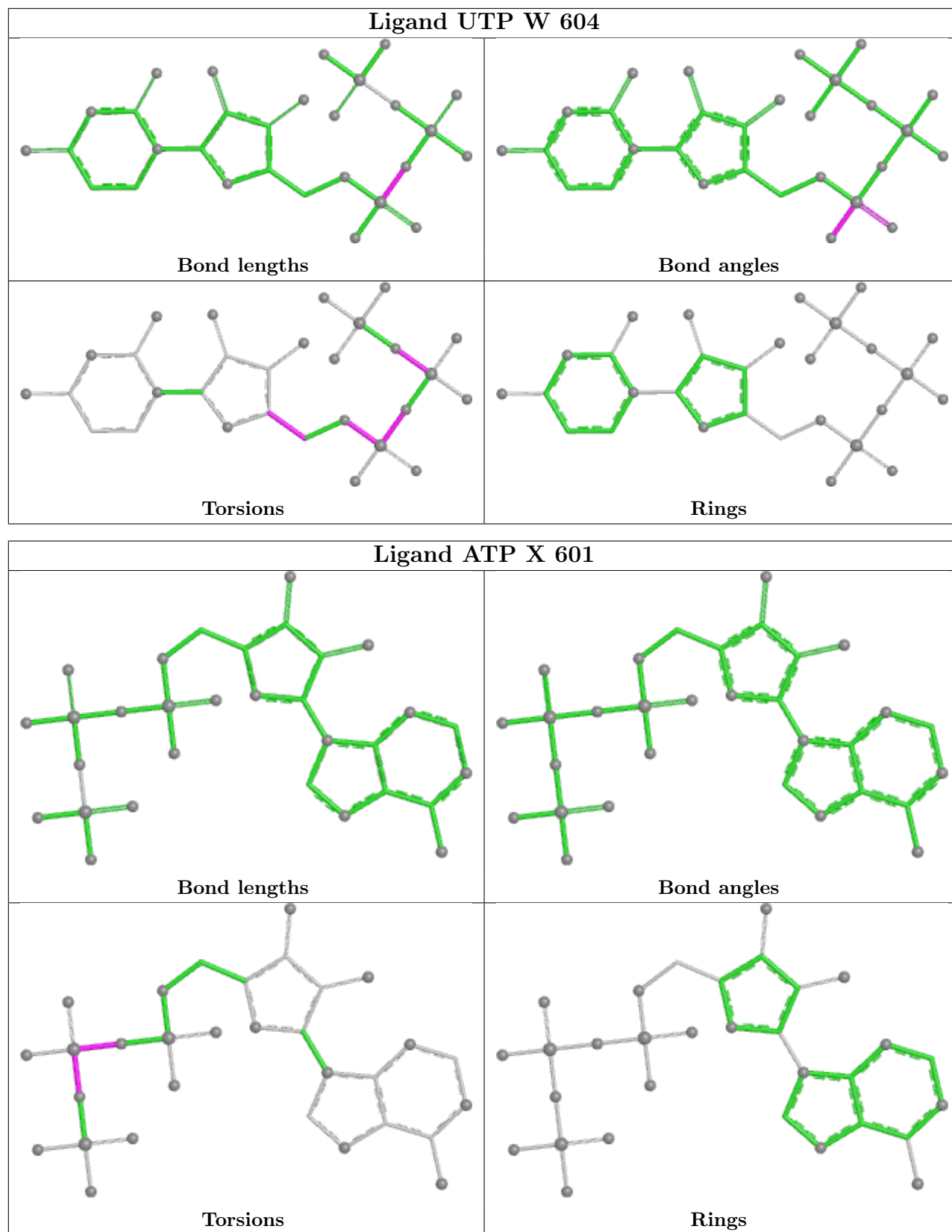
There are no ring outliers.

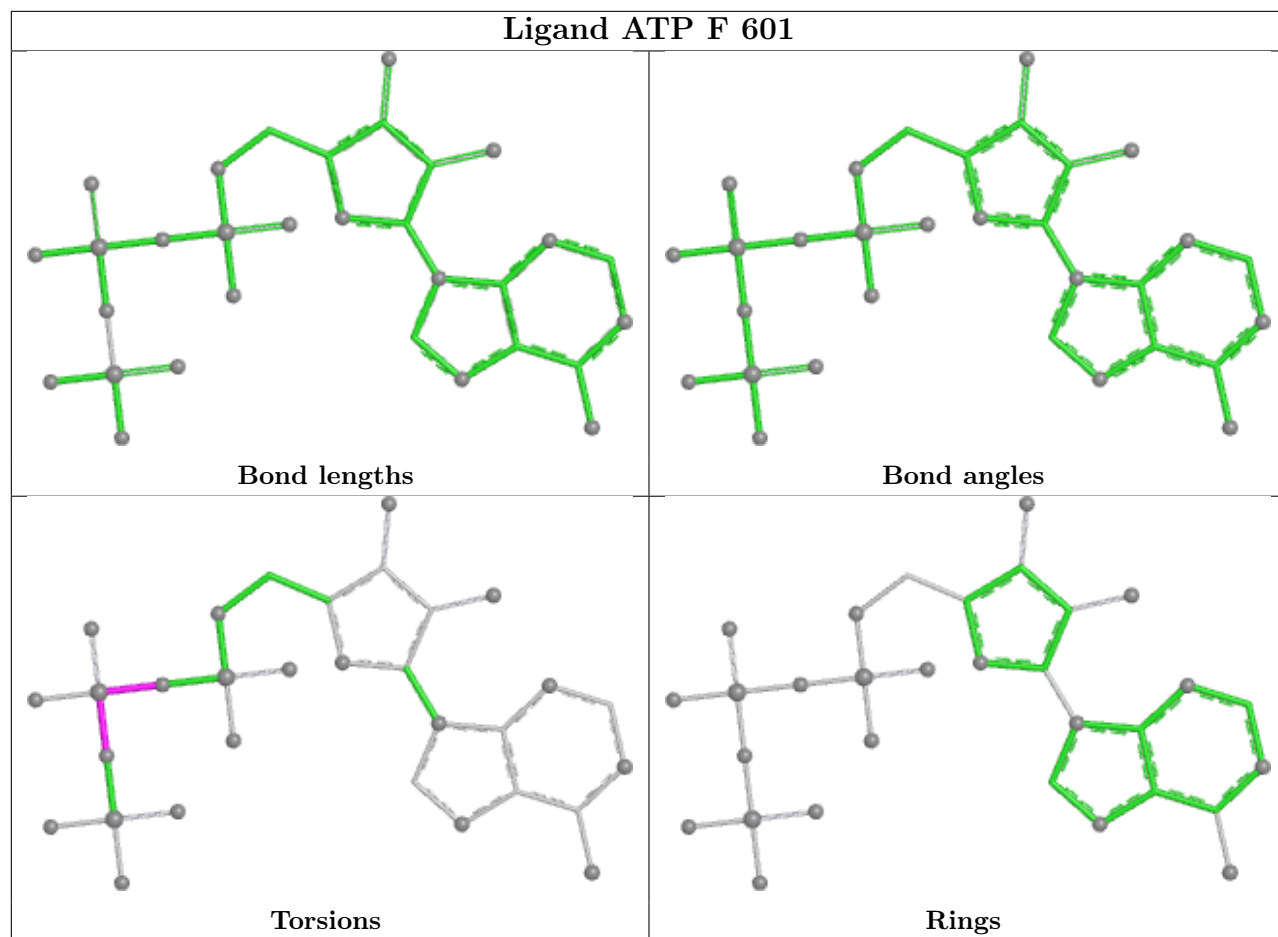
12 monomers are involved in 50 short contacts:

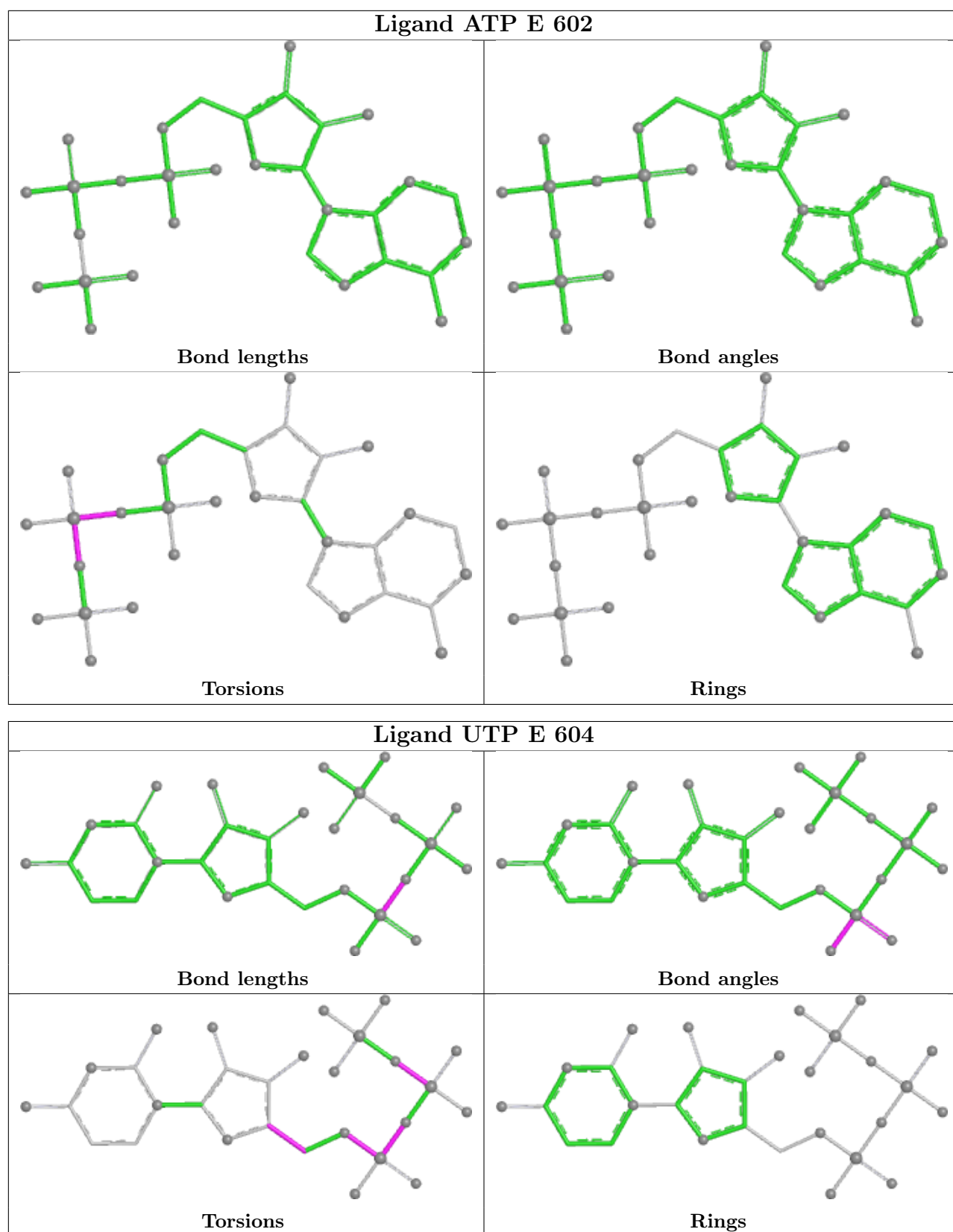
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	UTP	4	0
4	W	604	UTP	5	0
4	E	604	UTP	4	0
4	C	603	UTP	4	0
4	Y	602	UTP	4	0
4	G	602	UTP	4	0
4	X	604	UTP	4	0
4	Z	602	UTP	4	0
4	H	602	UTP	4	0
4	B	604	UTP	5	0
4	F	604	UTP	4	0
4	D	602	UTP	4	0

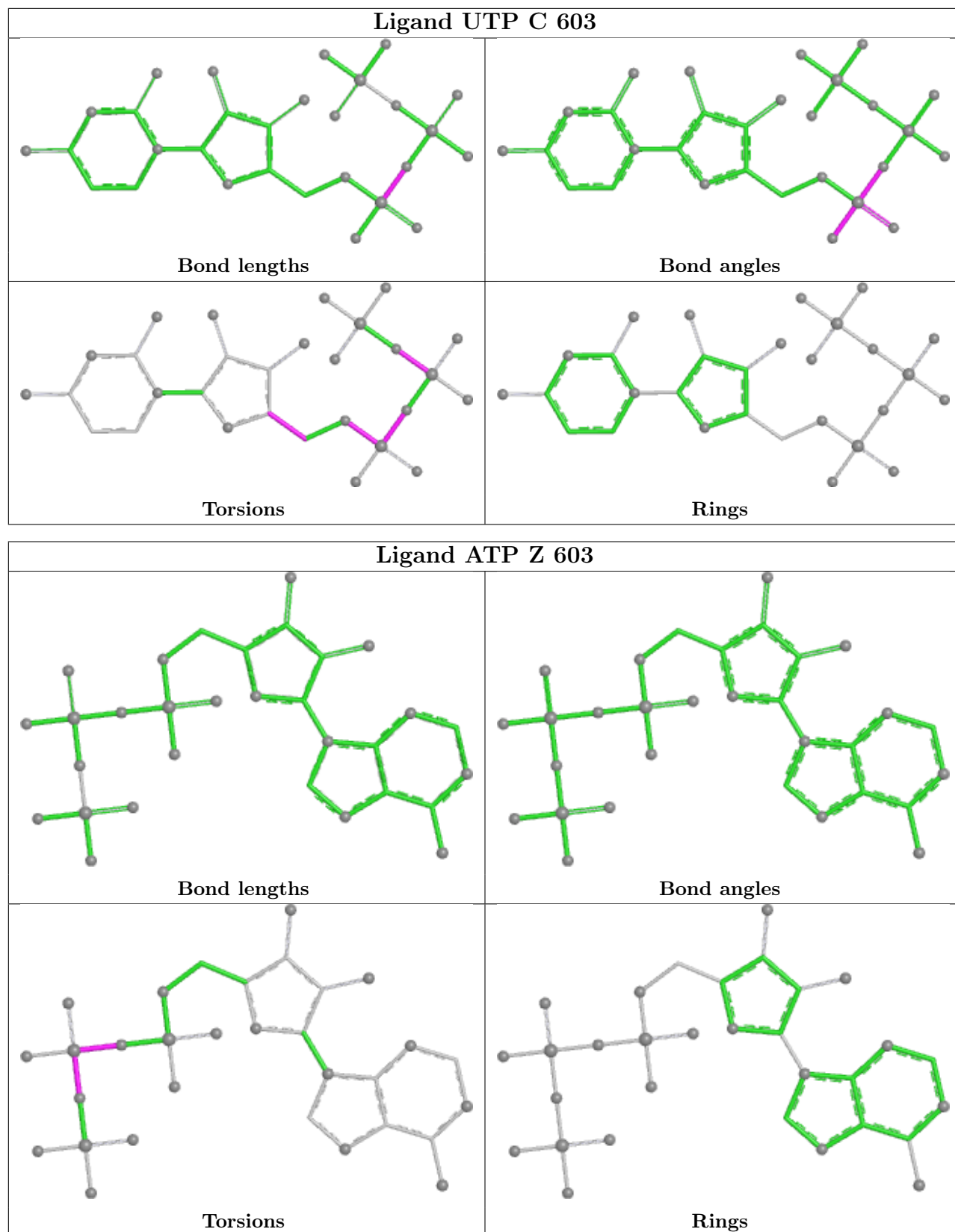
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

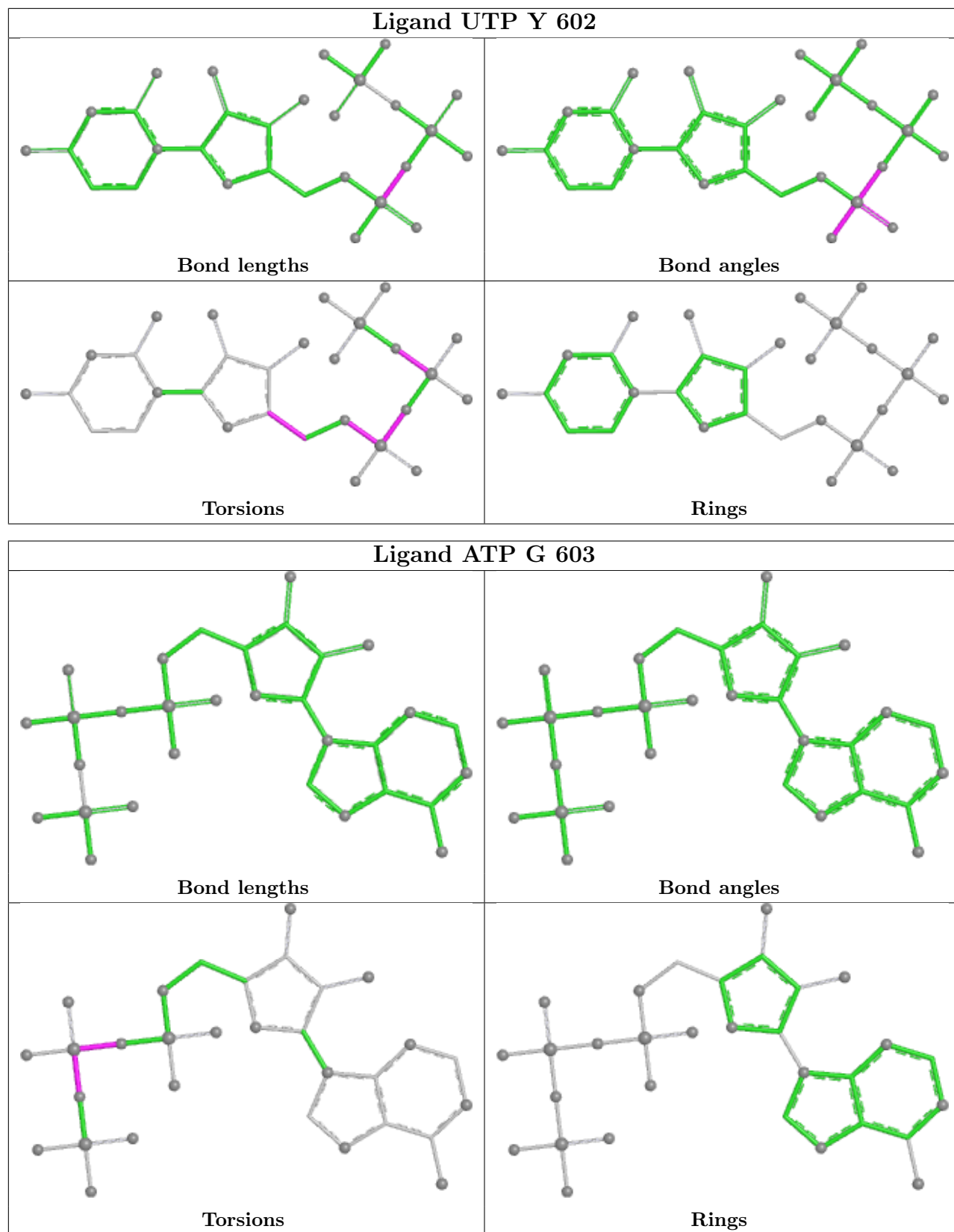


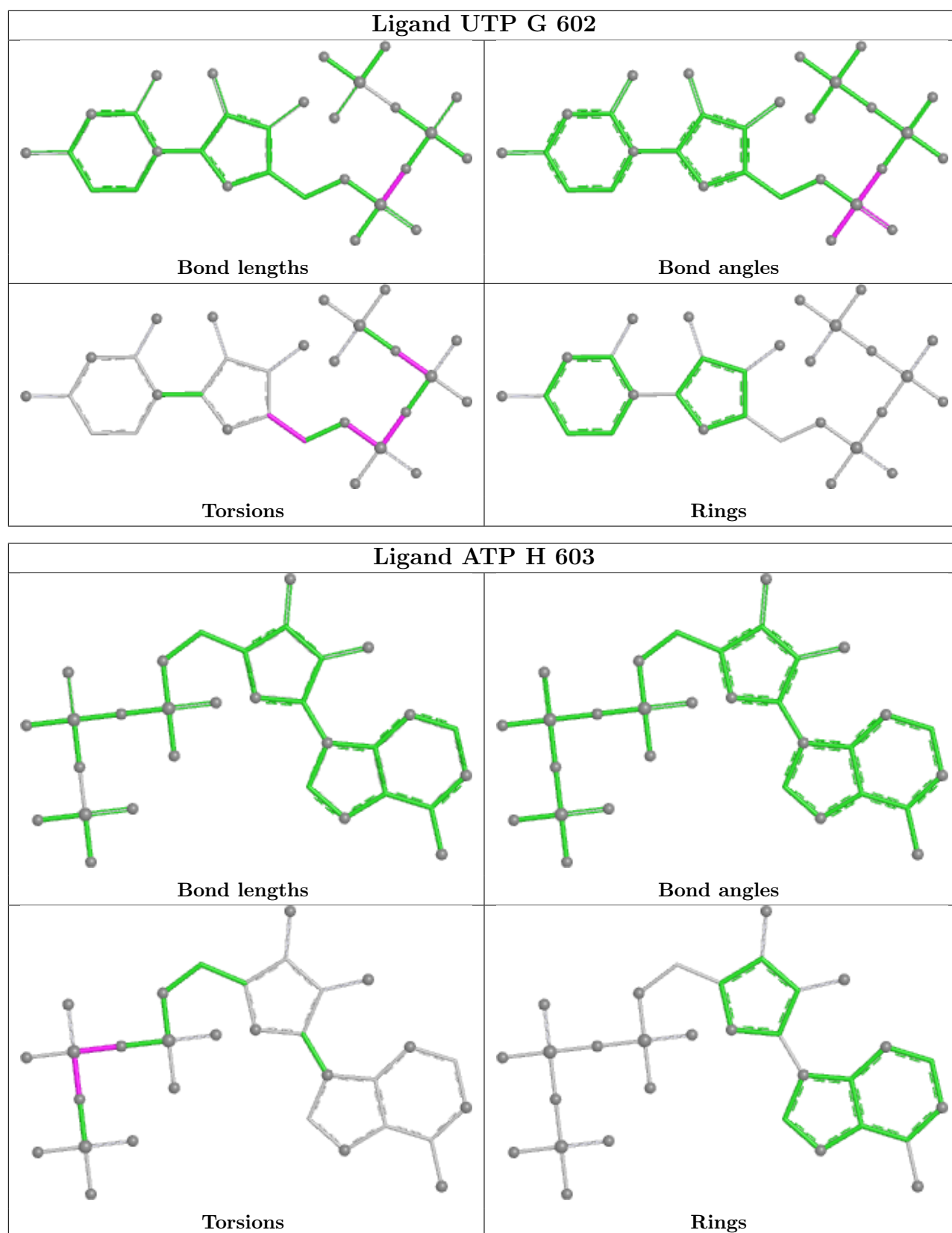


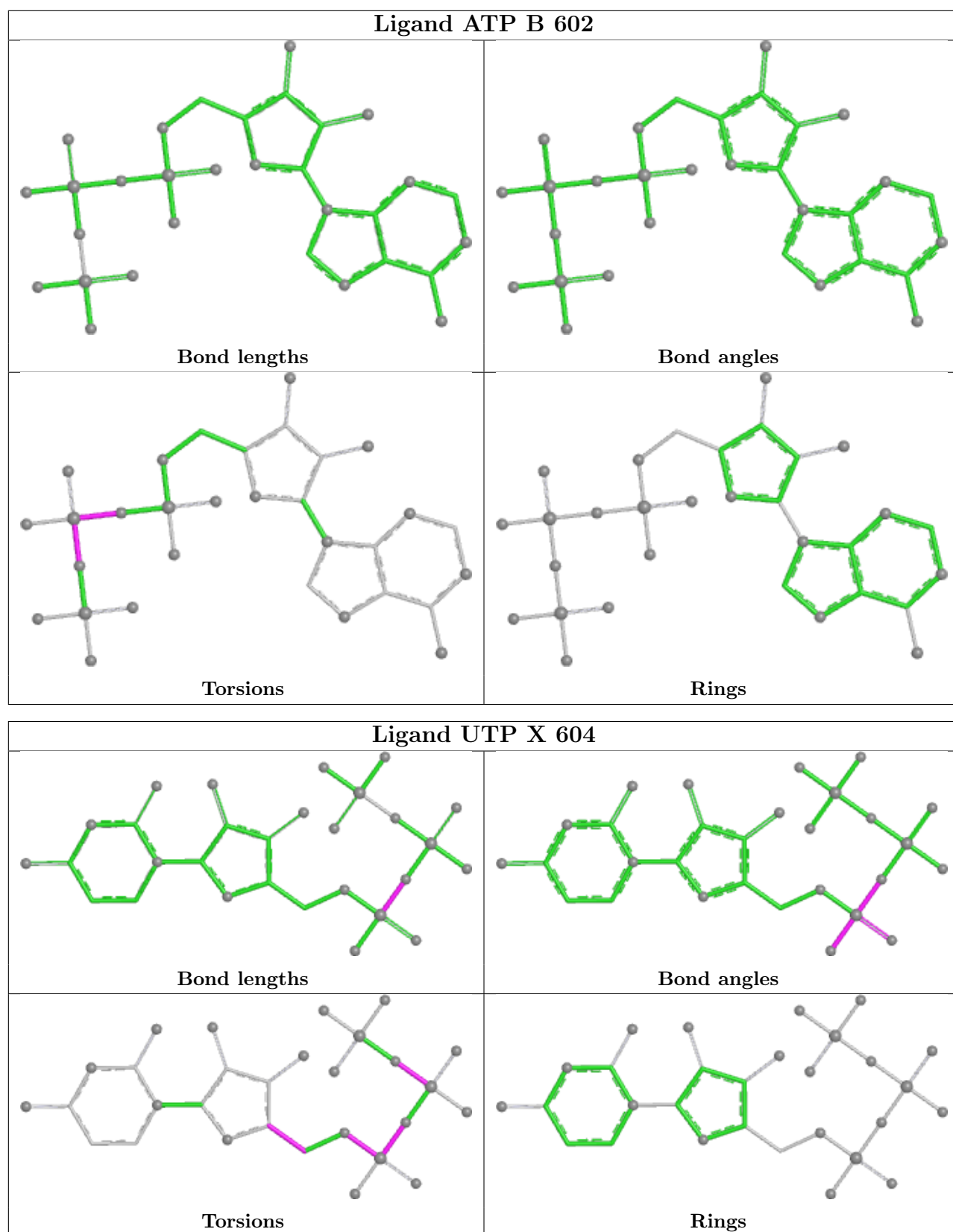


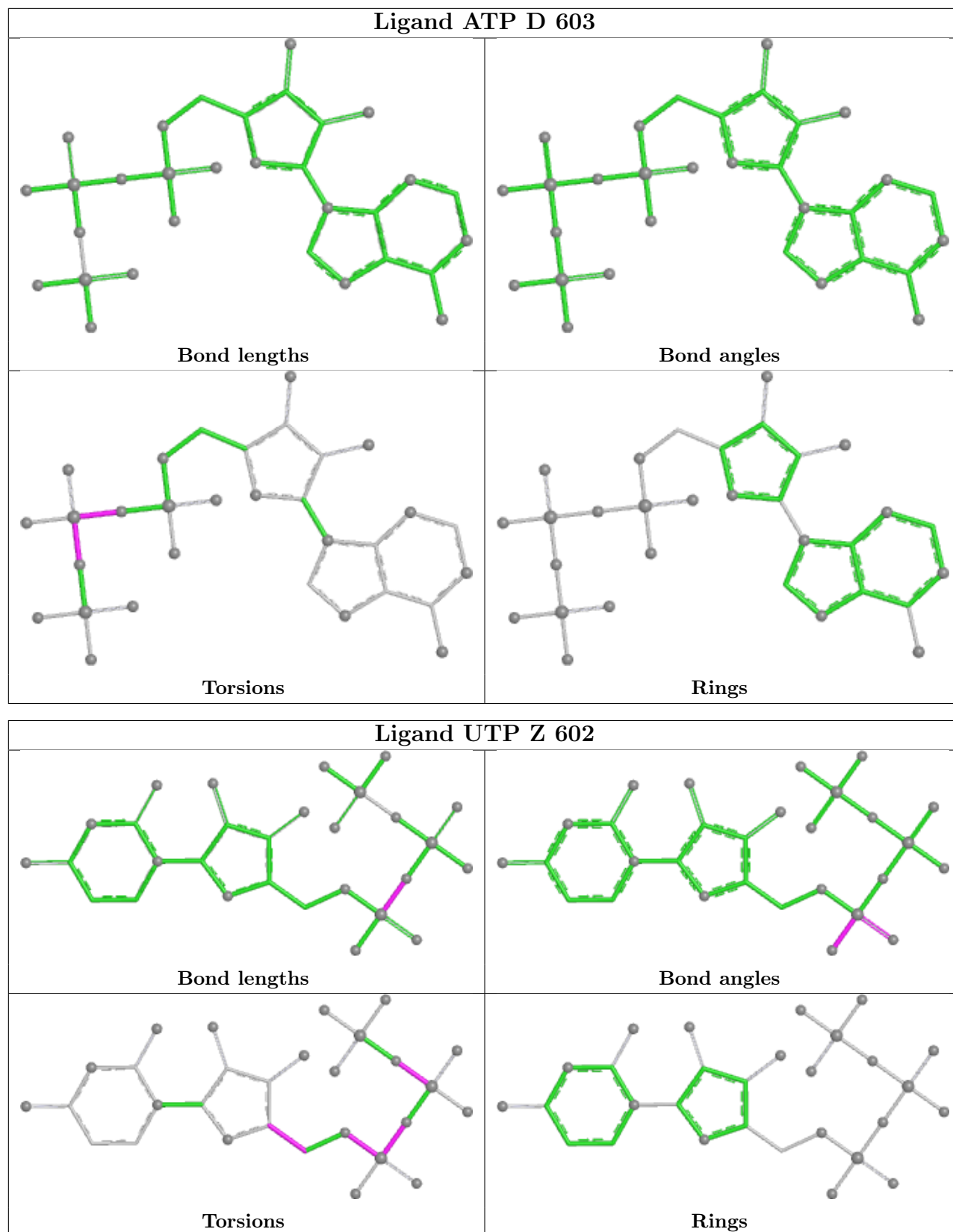


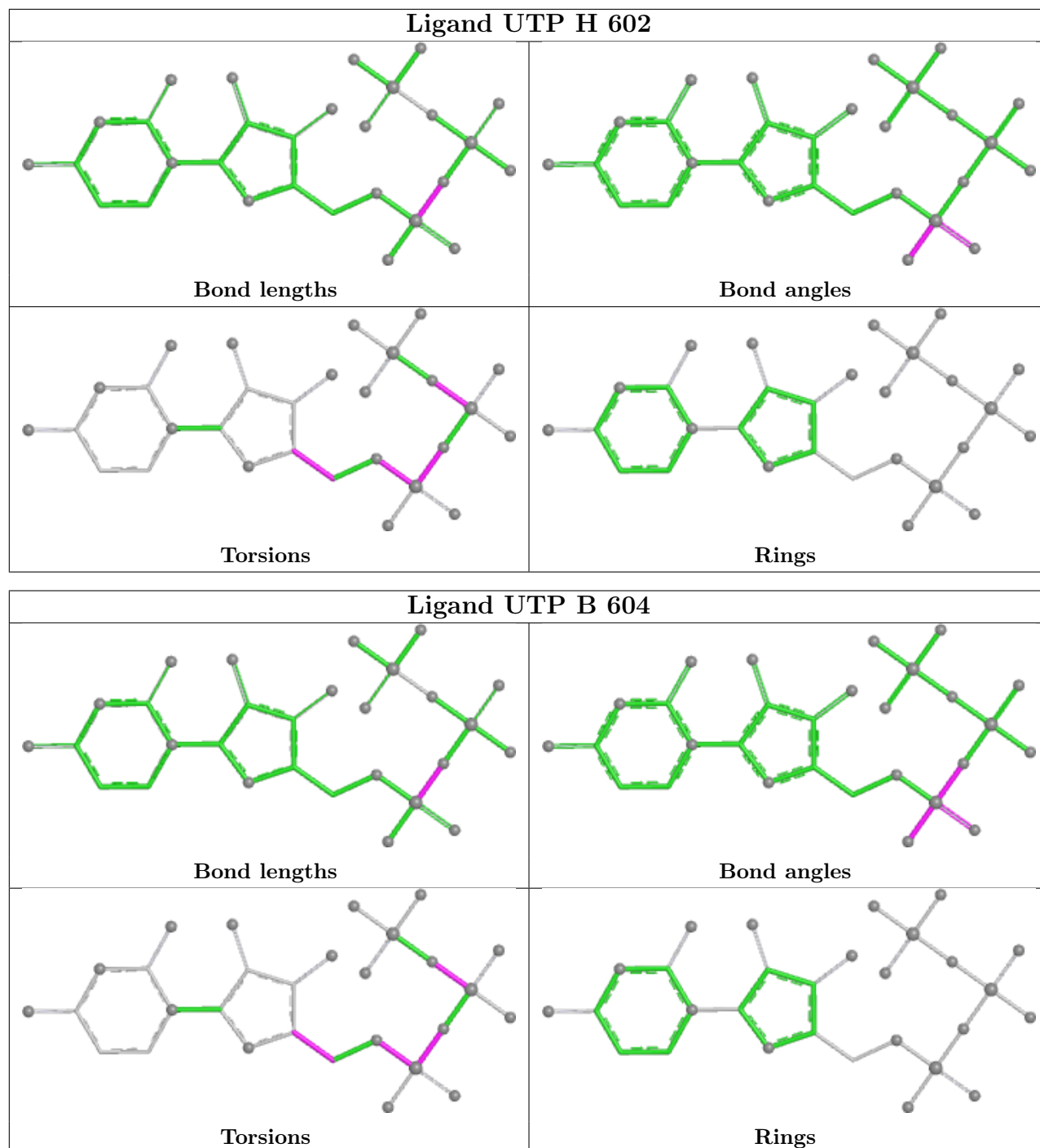


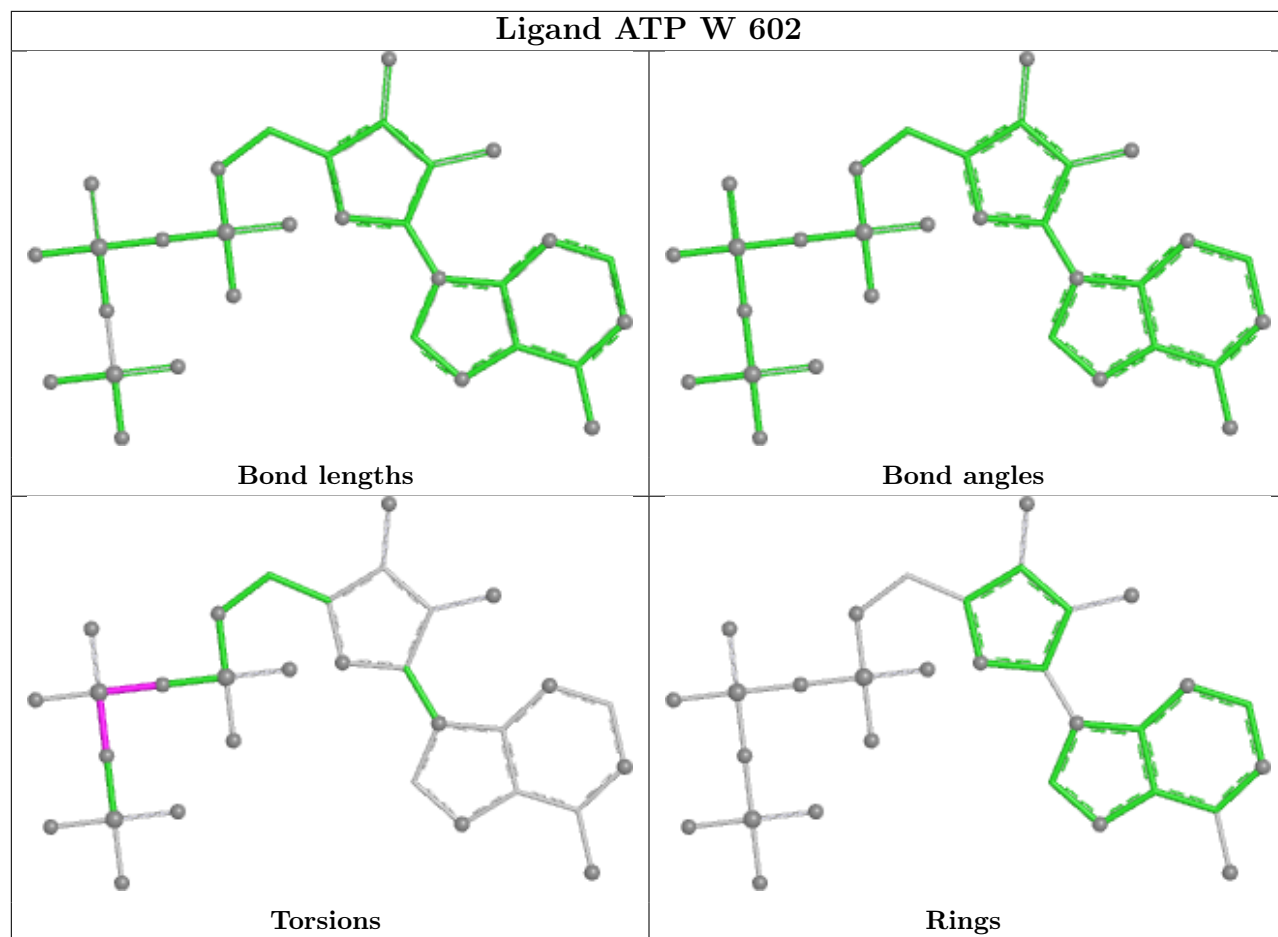


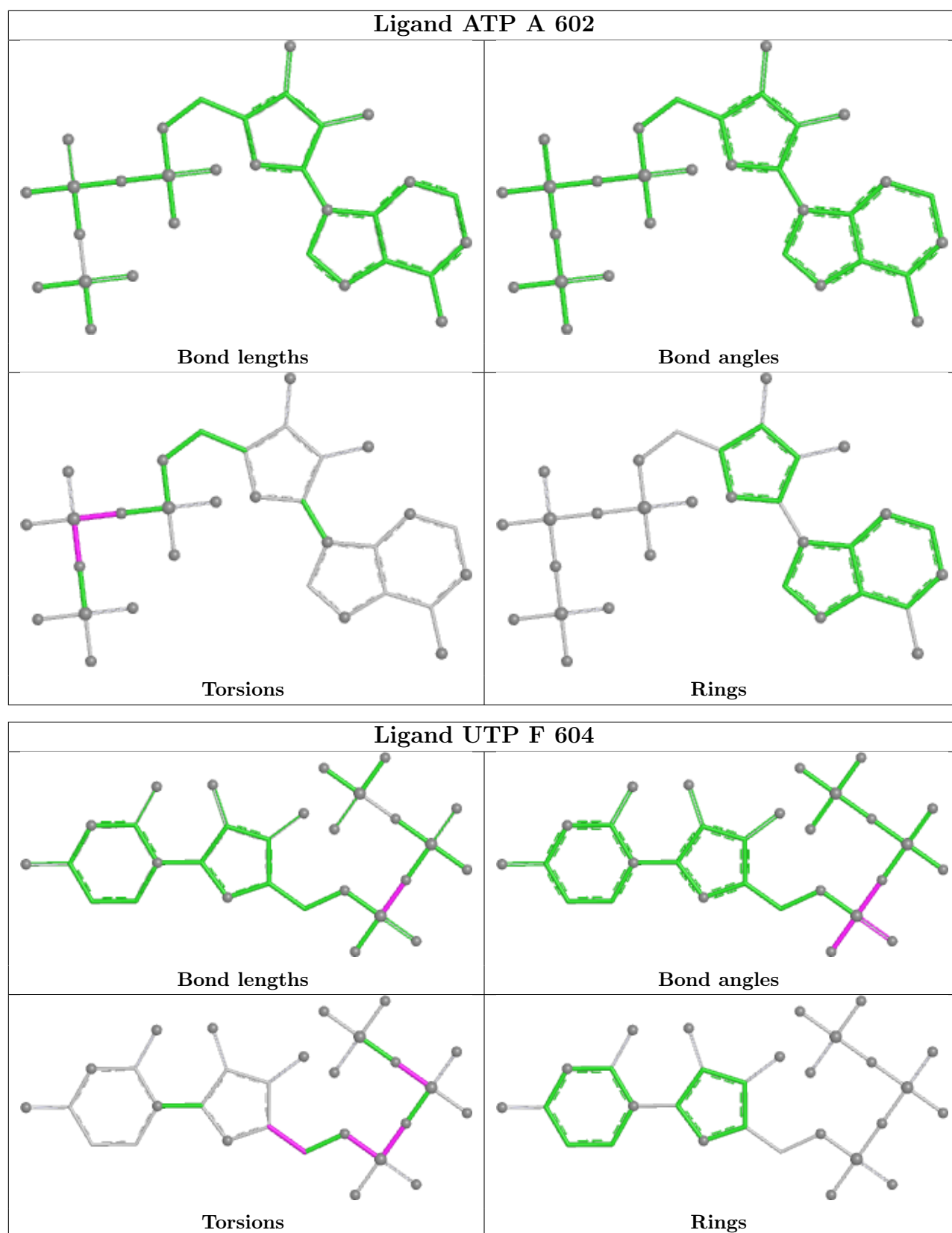


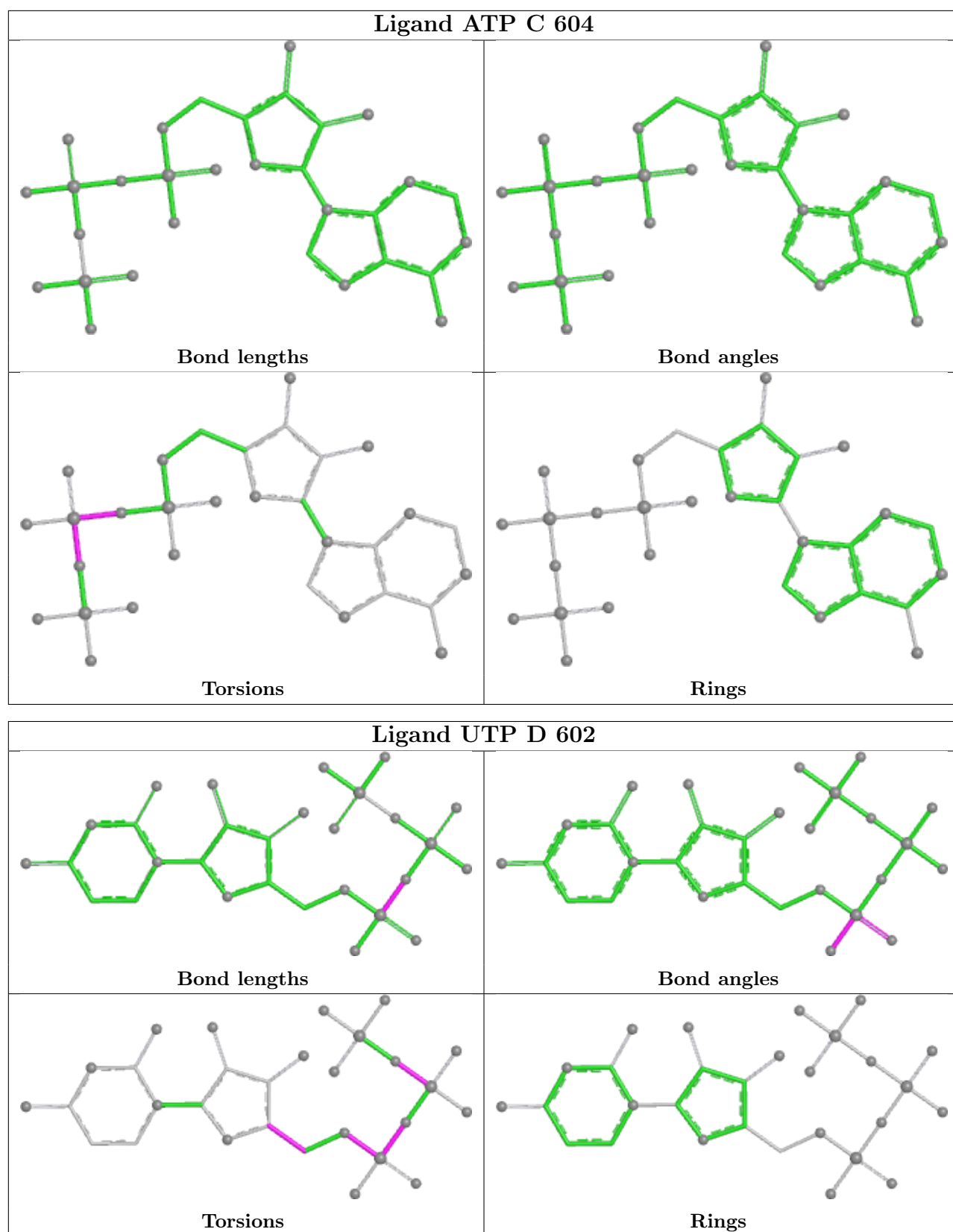












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1
1	E	1
1	F	1
1	G	1
1	H	1
1	W	1
1	X	1
1	Y	1
1	Z	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	443:ILE	C	456:THR	N	8.92
1	B	443:ILE	C	456:THR	N	8.92
1	C	443:ILE	C	456:THR	N	8.92
1	D	443:ILE	C	456:THR	N	8.92
1	E	443:ILE	C	456:THR	N	8.92

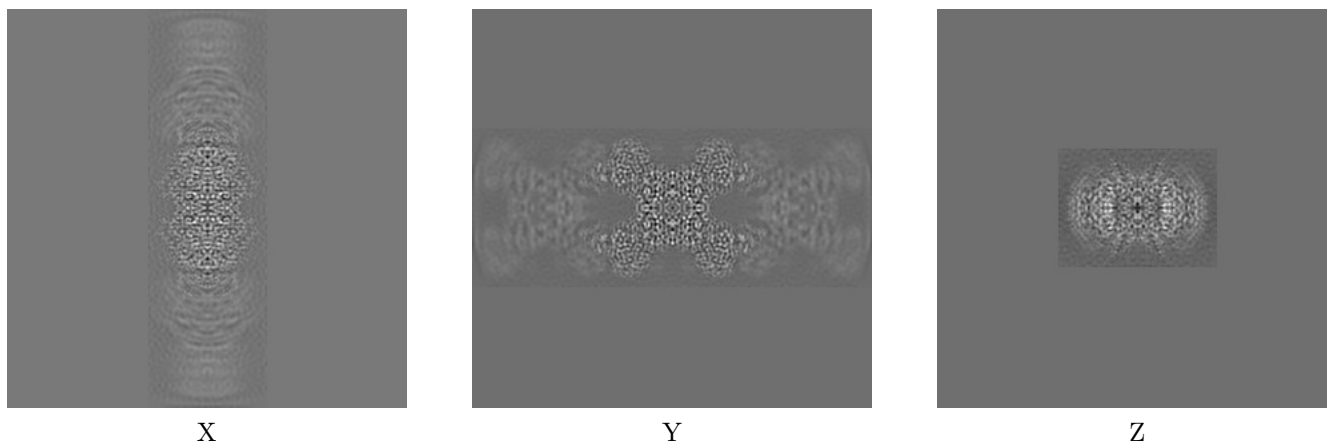
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24512. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

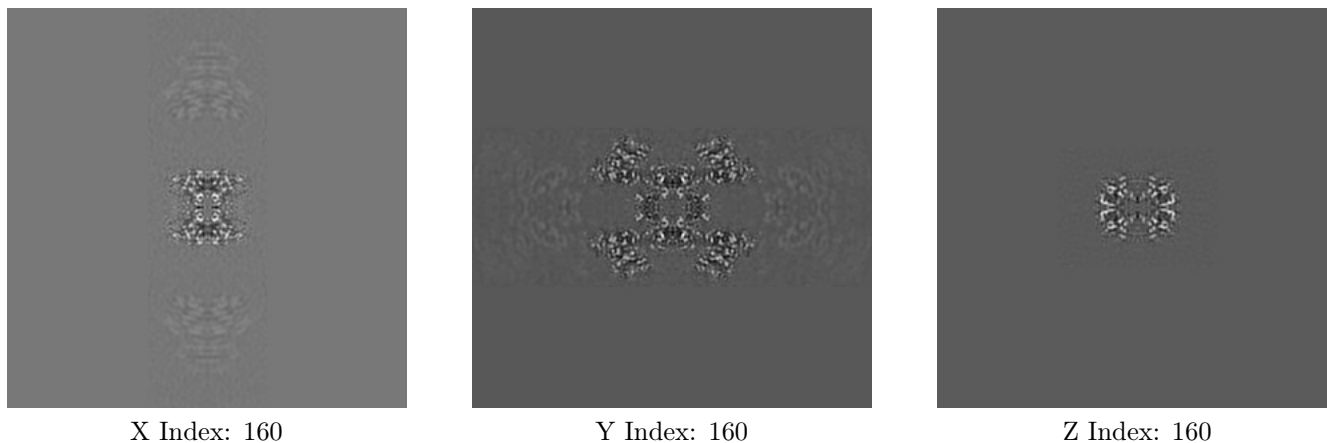
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

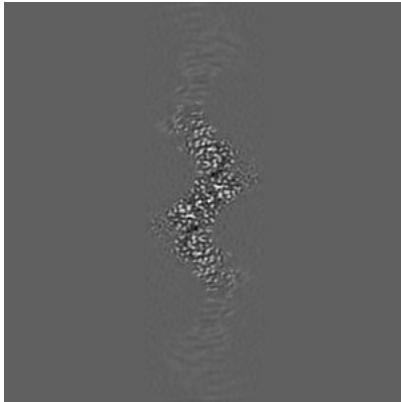
6.2.1 Primary map



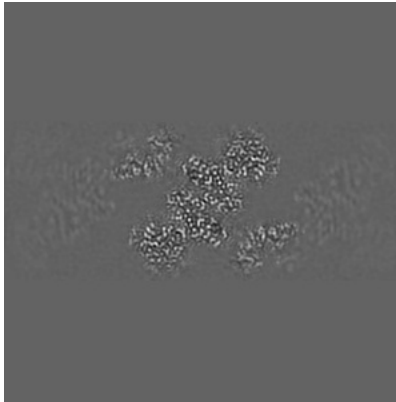
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

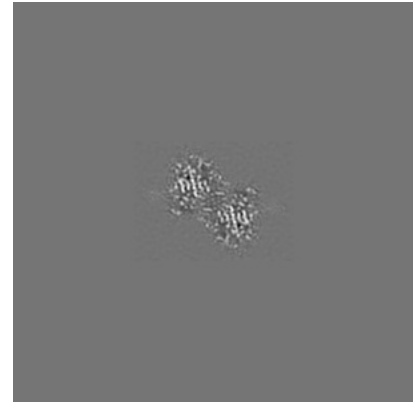
6.3.1 Primary map



X Index: 135



Y Index: 153

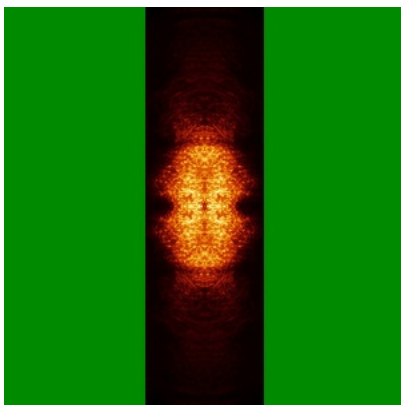


Z Index: 172

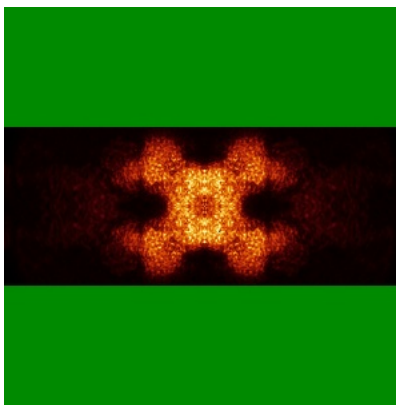
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

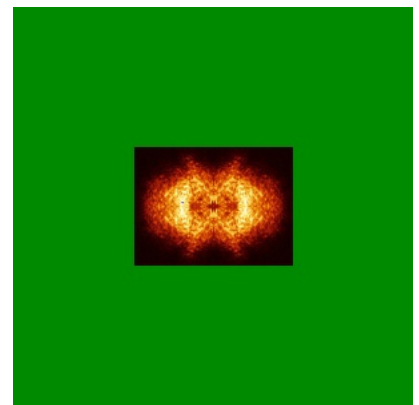
6.4.1 Primary map



X



Y

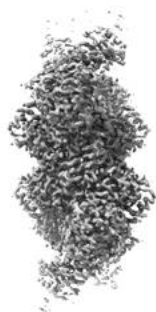


Z

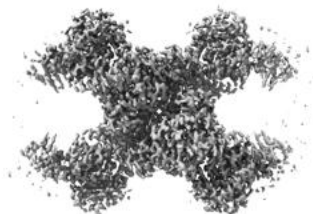
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

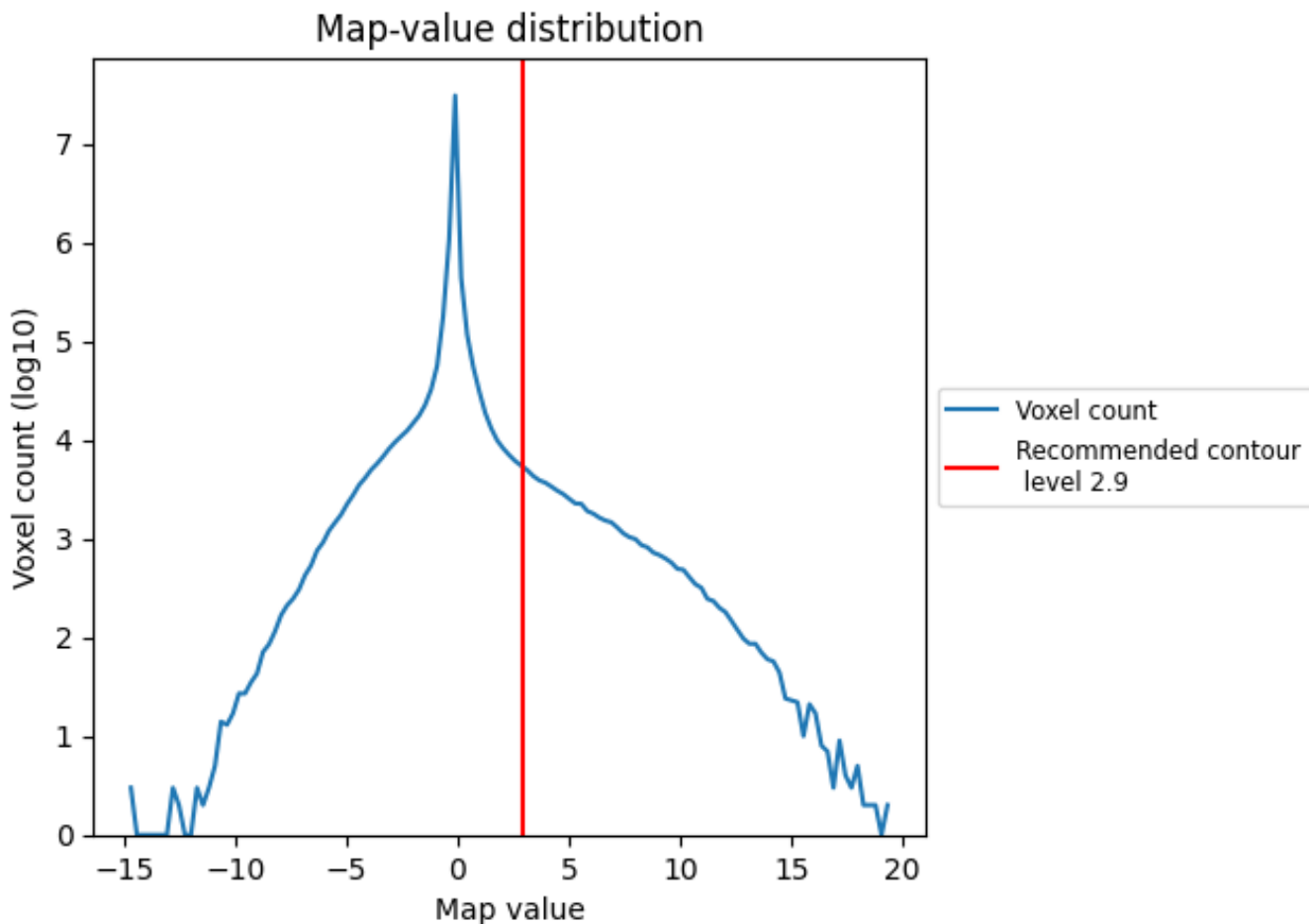
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

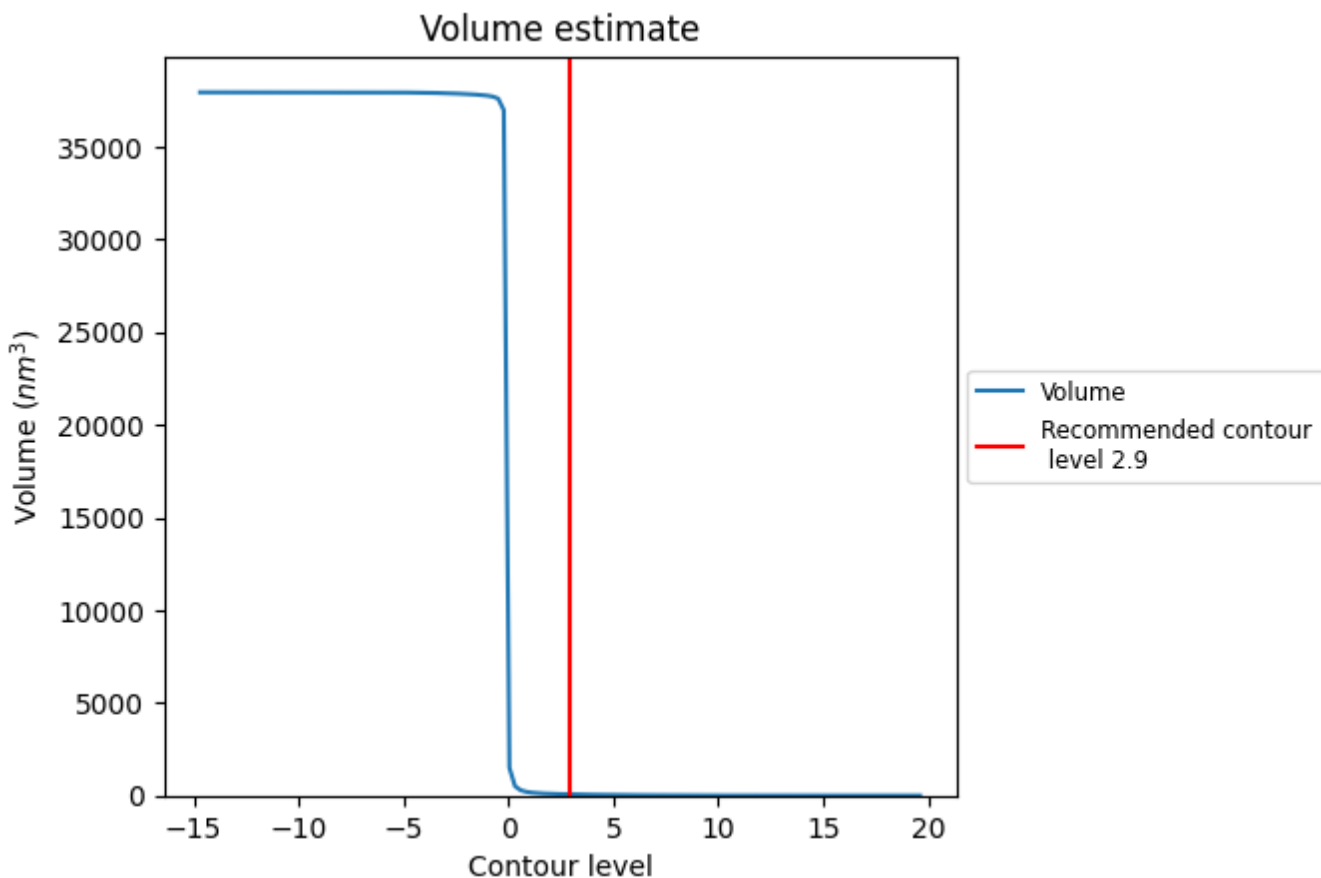
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

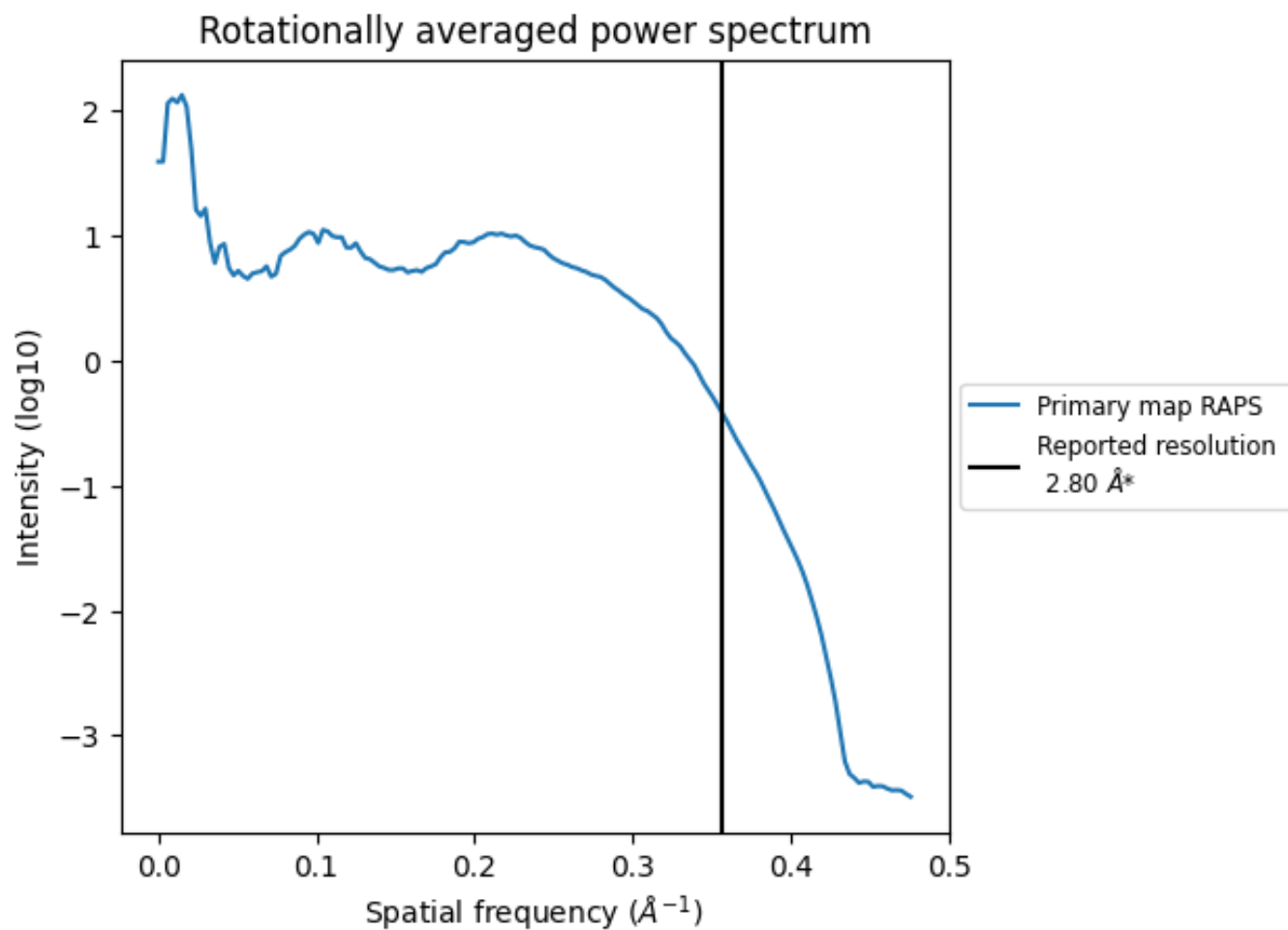
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68 nm^3 ; this corresponds to an approximate mass of 61 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

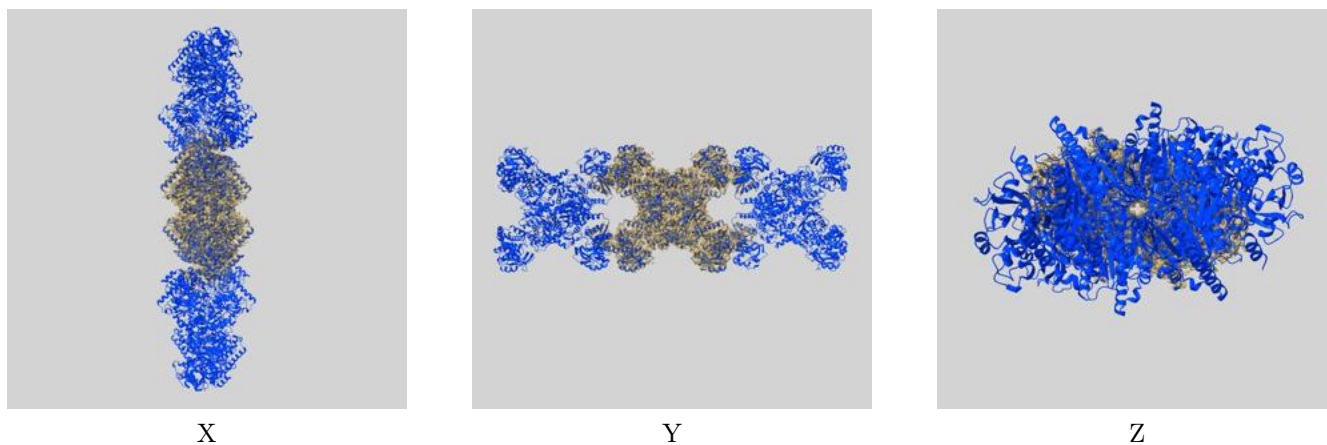
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

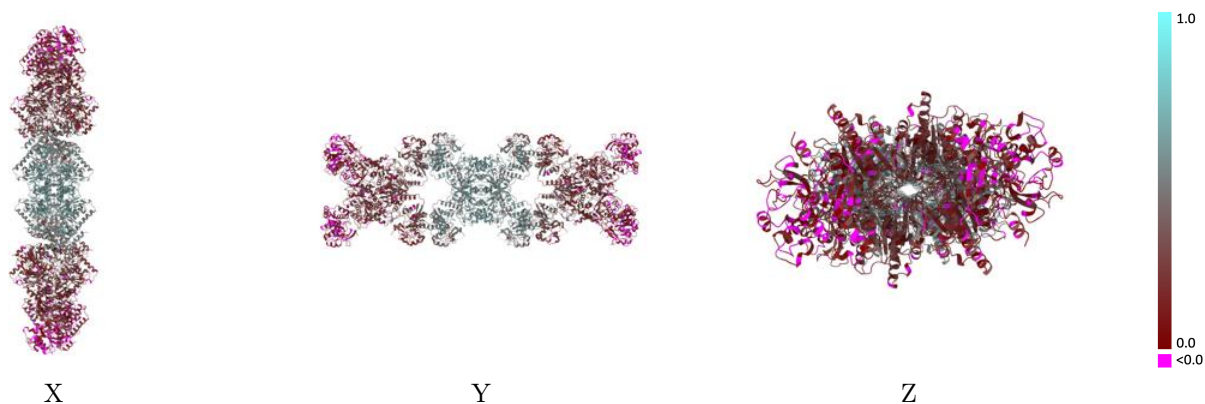
This section contains information regarding the fit between EMDB map EMD-24512 and PDB model 7RL0. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



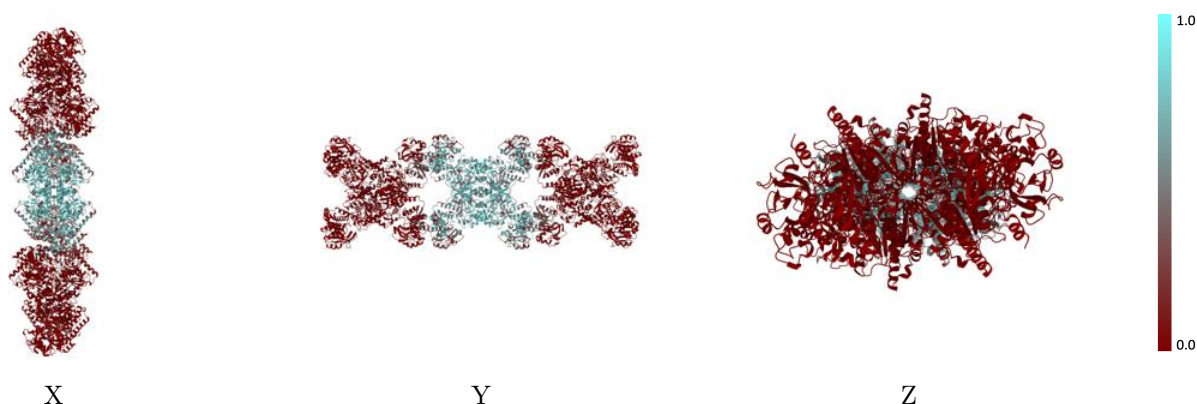
The images above show the 3D surface view of the map at the recommended contour level 2.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



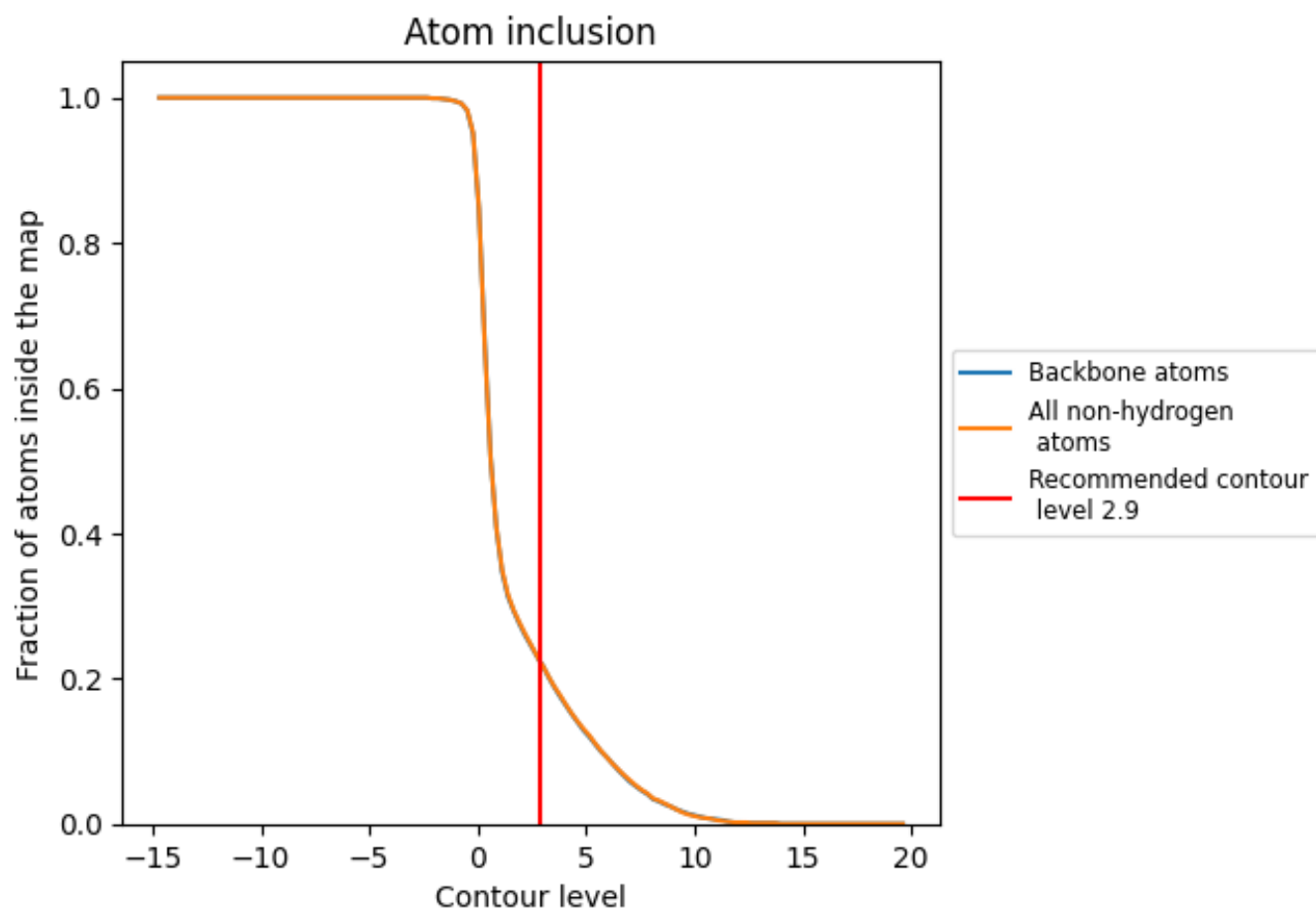
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.9).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 22% of all backbone atoms, 22% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2220	 0.3120
A	 0.0000	 0.1330
B	 0.0510	 0.2700
C	 0.0430	 0.2580
D	 0.0000	 0.1260
E	 0.6260	 0.5350
F	 0.6330	 0.5350
G	 0.6200	 0.5330
H	 0.6220	 0.5350
W	 0.0570	 0.2730
X	 0.0000	 0.1290
Y	 0.0000	 0.1400
Z	 0.0520	 0.2740

