



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 11:21 PM UTC

PDB ID : 7RL0 / pdb_00007rl0
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 Full wwPDB EM 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/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:

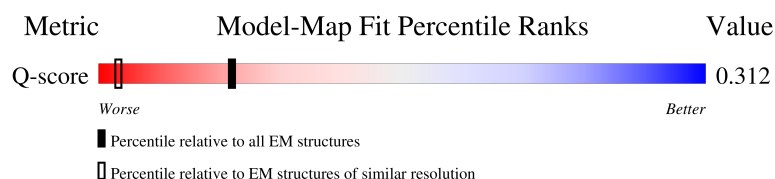
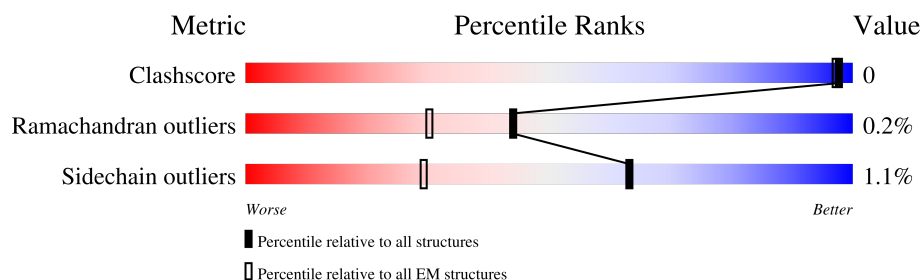
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

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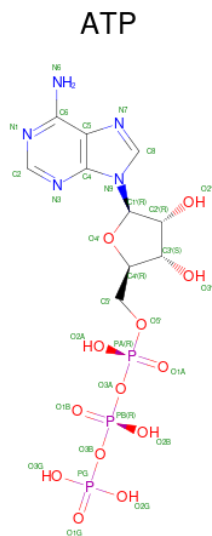
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Chain	Residue	Modelled	Actual	Comment	Reference
Z	?	-	TYR	deletion	UNP A0A6A5PYW3
Z	?	-	MET	deletion	UNP A0A6A5PYW3
Z	?	-	PRO	deletion	UNP A0A6A5PYW3
Z	?	-	GLU	deletion	UNP A0A6A5PYW3
Z	?	-	ILE	deletion	UNP A0A6A5PYW3
Z	?	-	ASP	deletion	UNP A0A6A5PYW3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



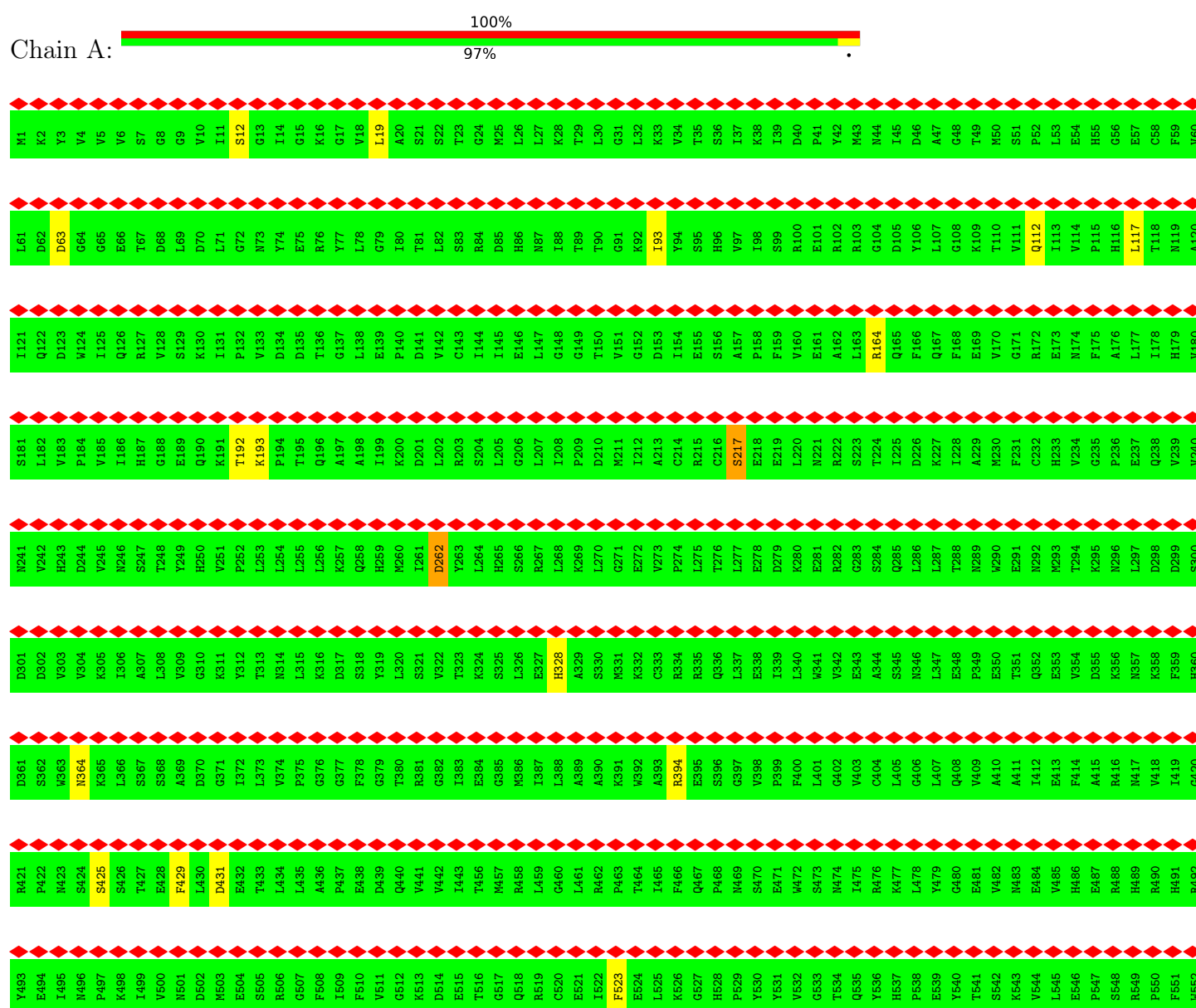
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
3	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
3	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
3	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
3	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
3	F	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
3	G	1	Total 43	C 10	H 12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

- Molecule 4 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $\text{C}_9\text{H}_{15}\text{N}_2\text{O}_{15}\text{P}_3$).

3 Residue-property plots

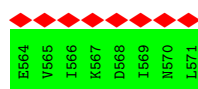
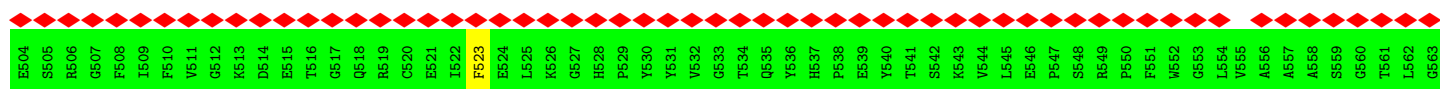
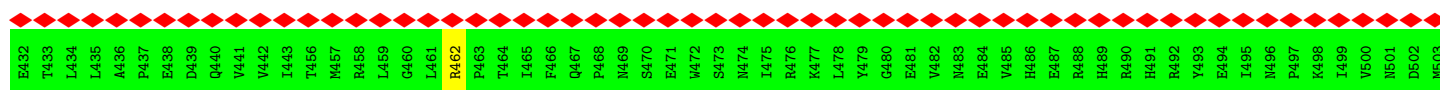
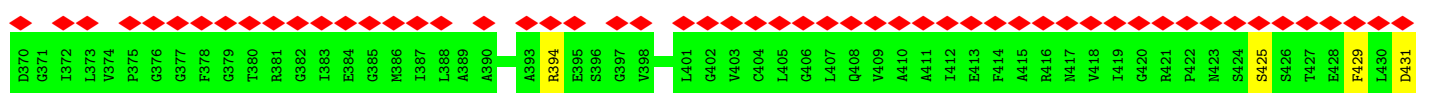
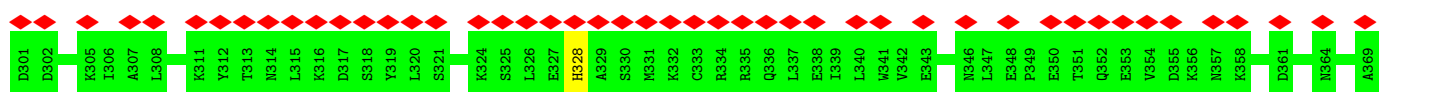
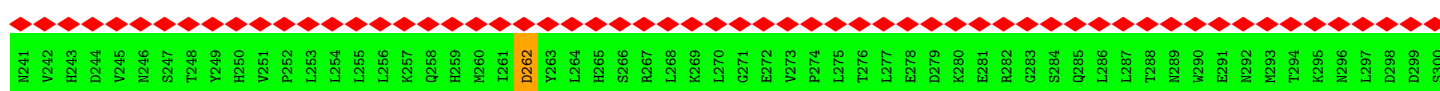
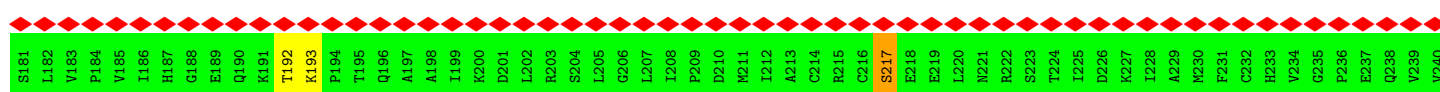
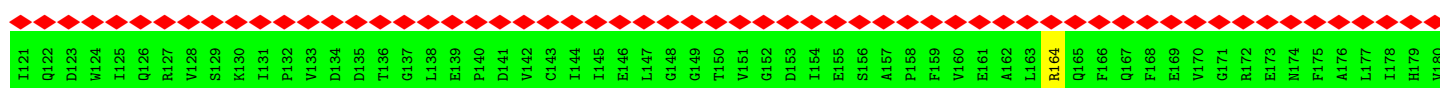
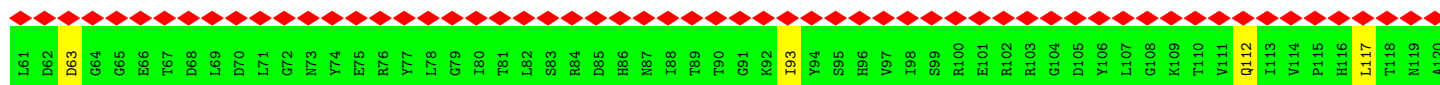
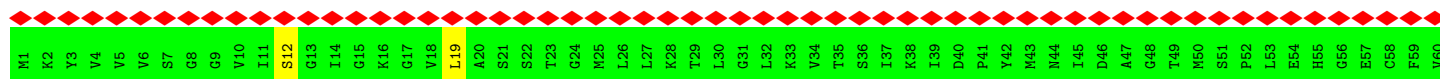
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

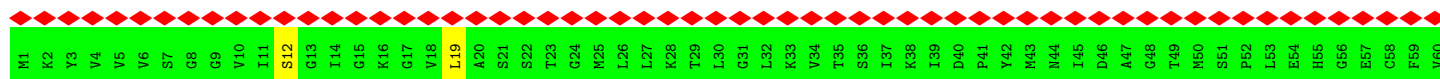


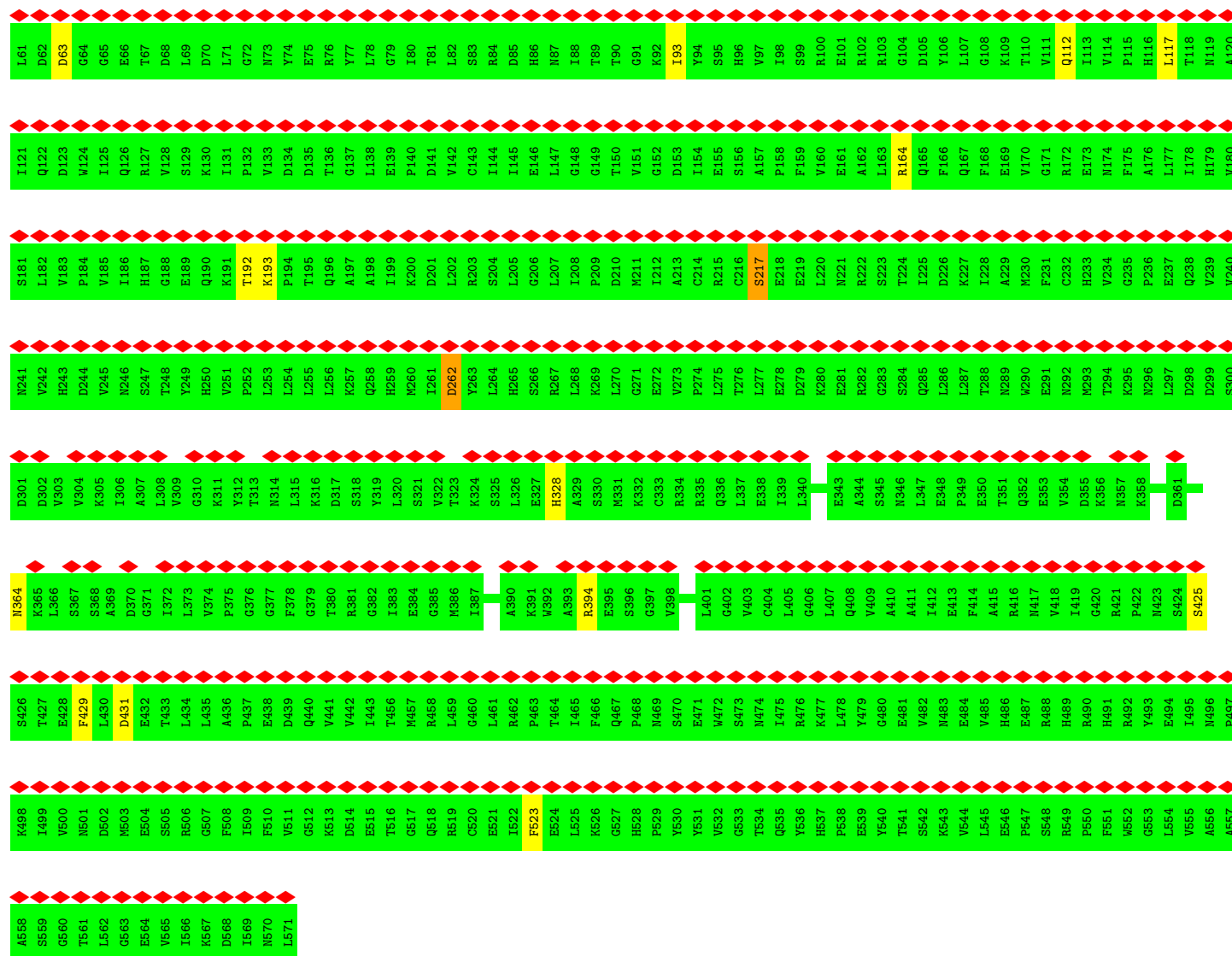


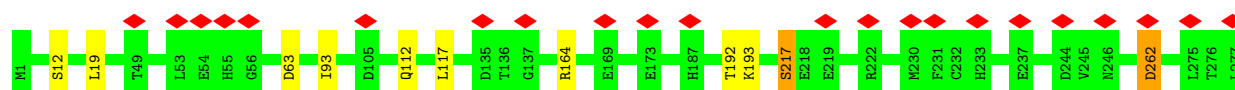
• Molecule 1: CTP synthase

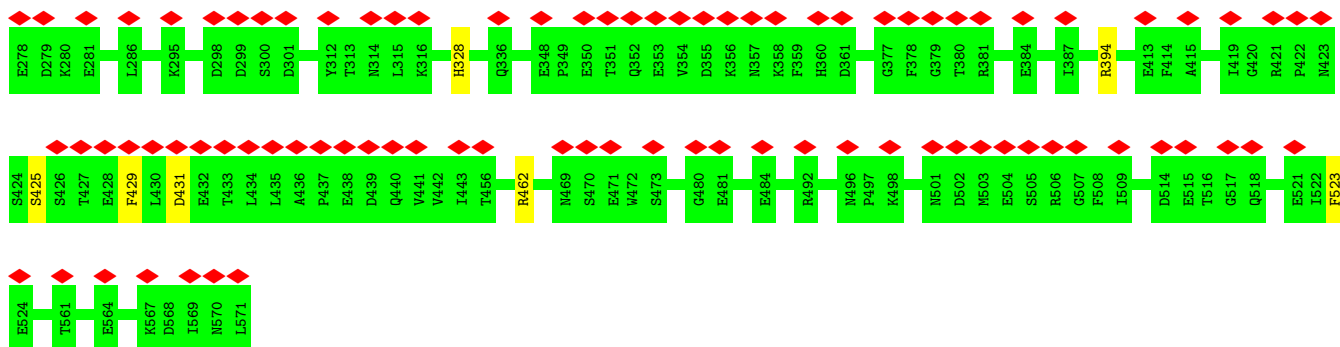


• Molecule 1: CTP synthase

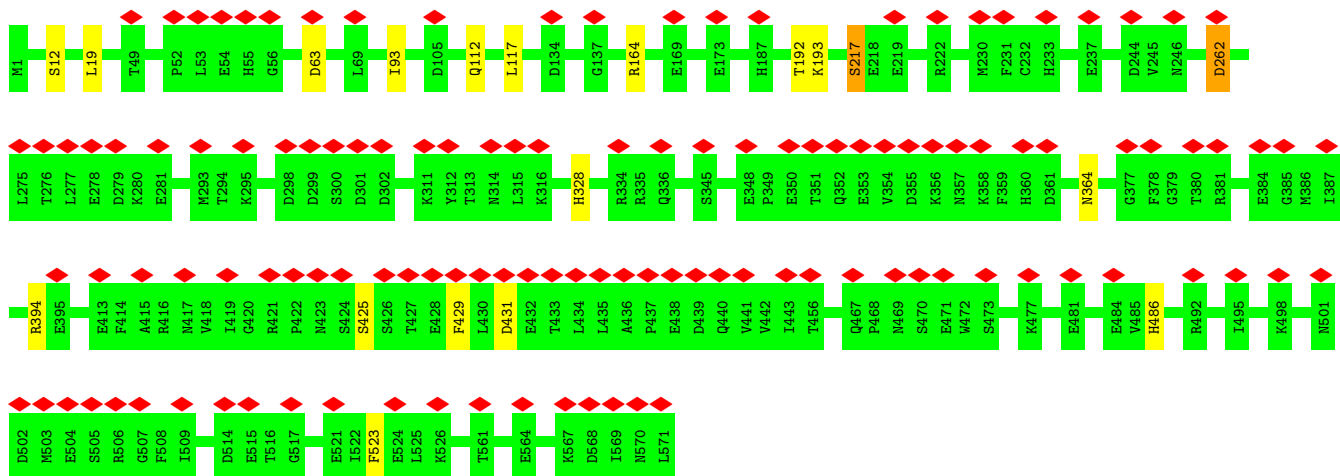




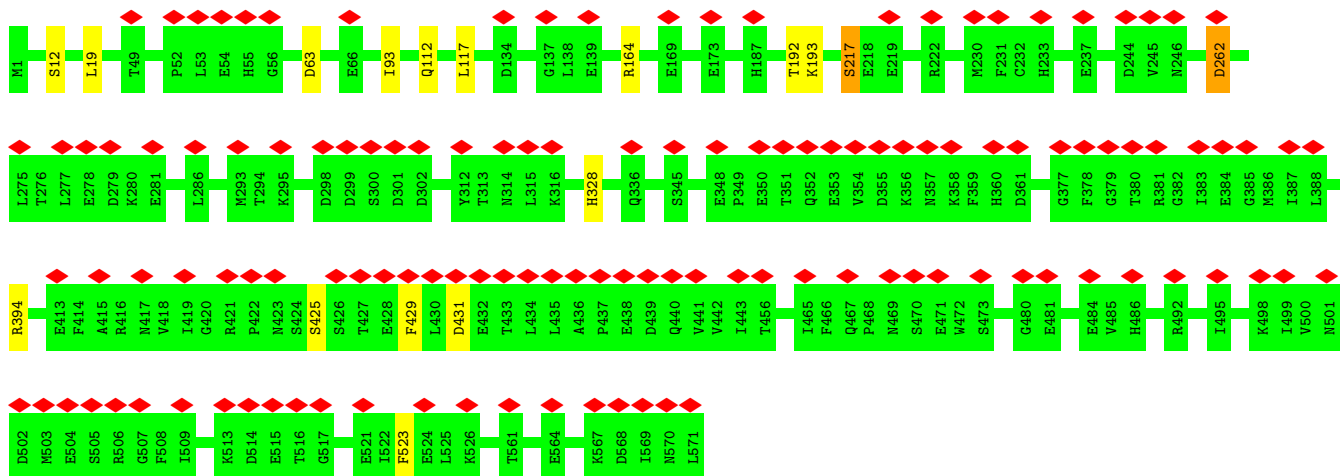




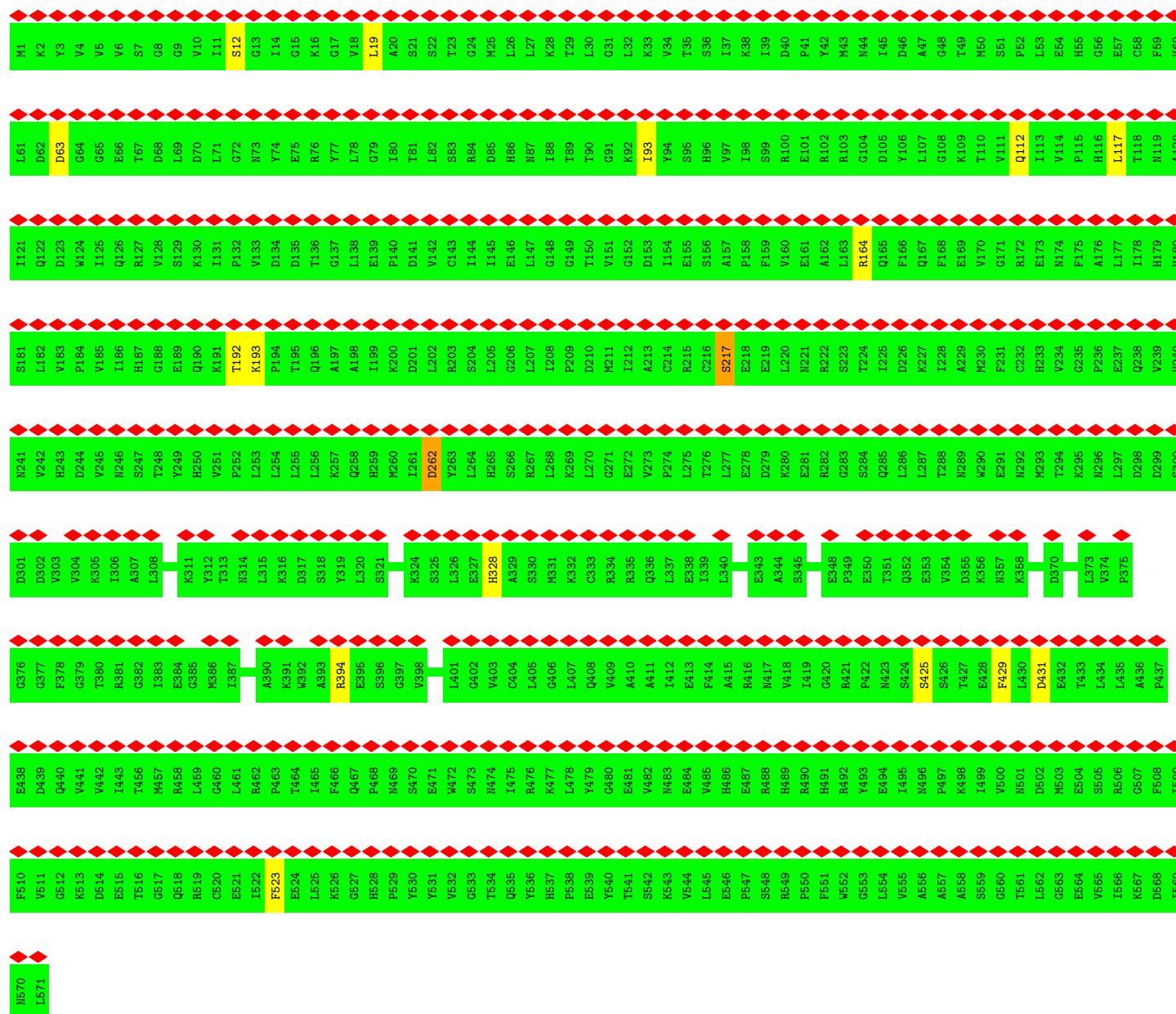
• Molecule 1: CTP synthase



• Molecule 1: CTP synthase



• Molecule 1: CTP synthase



● Molecule 1: CTP synthase

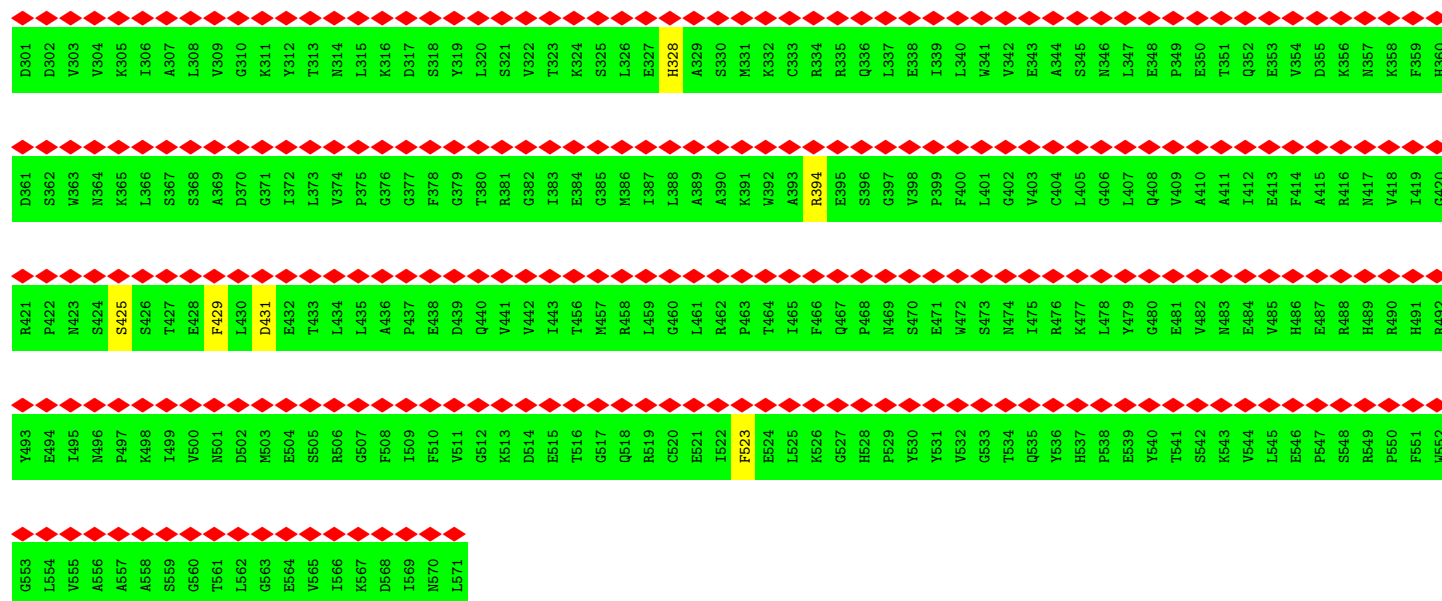


I121	S181	N241	D301	D361	R421	Y493	G553
Q122	L182	V242	D302	S362	P422	E494	L554
D123	V183	H243	V303	W363	M423	I495	V555
W124	P184	D244	V304	N364	S424	N496	A556
I125	V185	V245	I306	K366	S425	K497	A557
Q126	I186	N246	I307	K367	S426	K498	A558
R127	H187	S247	L308	S368	T427	I499	S559
V128	G188	T248	V309	A369	E428	M501	G560
V129	E189	S249	G310	A370	F429	D502	L562
K130	Q190	H250	K311	G371	L430	M503	G563
I131	K191	V251	Y312	I372	D431	E504	E564
P132	T192	P252	Y313	L373	E432	S505	V565
V133	K193	L253	N314	V374	T433	R506	L566
D134	P194	L254	L315	F375	L434	G507	K567
D135	T195	L255	K316	G376	L435	F508	D568
T136	Q196	L256	D317	G377	A436	I509	L569
G137	A197	K257	S318	F378	P437	F510	N570
L138	A198	Q258	Y319	G379	E438	V511	L571
E139	I199	H259	L320	T380	D439	G512	
P140	K200	M260	S321	R381	Q440	K513	
D141	D201	I261	V322	G382	V441	D514	
V142	L202	D262	T323	I383	I443	E515	
C143	R203	Y263	K324	E384	T456	T516	
I144	S204	L264	S325	G385	M457	G517	
I145	L205	H265	L326	K386	L458	R518	
I146	G206	S266	E227	I387	G460	C520	
E147	L207	R267	H328	L388	L461	E521	
L147	I208	L268	A329	A389	R462	I522	
G148	P209	K269	S330	A390	P463	F523	
G149	T210	L270	M331	K391	T464	E524	
T150	M211	G271	K332	W392	I465	L525	
V151	I212	E272	C333	A393	F466	K526	
G152	A213	V273	R334	R394	Q467	G527	
D153	C214	P274	R335	E395	P468	H528	
I154	R215	L275	Q336	S396	M469	P529	
E155	R216	T276	L337	G397	E470	Y530	
S156	C217	L277	E338	V398	E471	Y531	
A157	E218	E278	I339	F399	W472	V532	
P158	E219	D279	L340	F400	S473	G533	
F159	L220	K280	W341	G402	N474	T534	
V160	N221	E281	V342	W403	I475	Q535	
E161	R222	R282	E343	C404	R476	Y536	
A162	S223	G283	A344	L405	K477	H537	
L163	T224	S284	S345	G406	L478	P538	
R164	I225	Q285	N346	L407	Y479	E539	
Q165	D226	L286	L347	Q408	G480	Y540	
F166	K227	T287	E348	V409	E481	T541	
Q167	I228	T288	P349	A410	M482	S542	
F168	A229	N289	E291	T351	M483	K543	
E169	M230	W290	N292	Q352	E484	V544	
V170	F231	E291	E353	E413	H486	L545	
G171	C232	M293	T294	F414	E487	E546	
R172	H273	V234	K295	A415	R488	P547	
E173	N174	F175	N296	R416	H489	S548	
N174	F175	A176	N297	M417	R490	R549	
F175	A176	E177	K357	V418	H491	F551	
A176	E177	L178	K358	I419	R492	M552	
L178	E178	D298	F359	G420			
H179	H179	D299	H360				
V180	V240	S300					

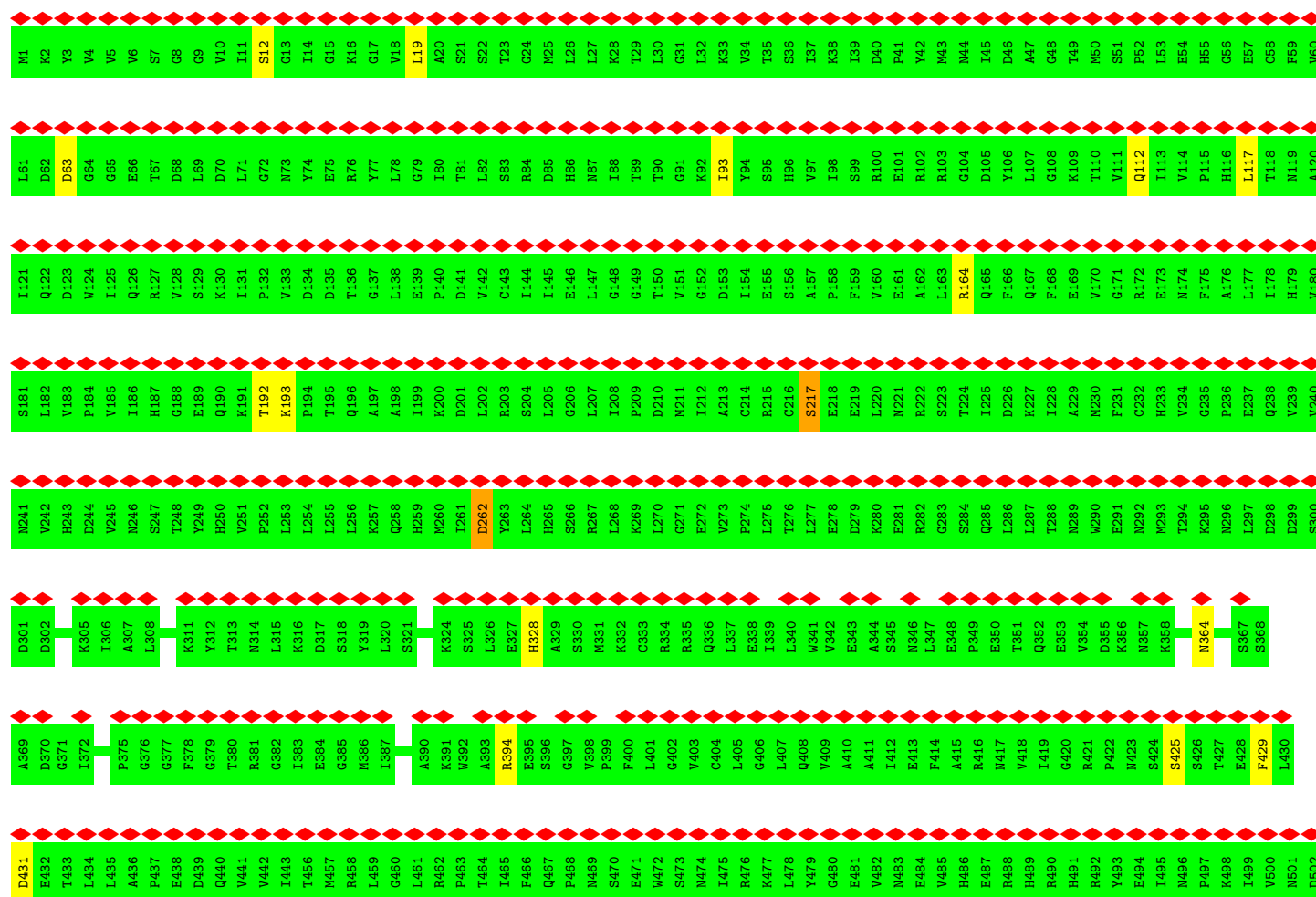
• Molecule 1: CTP synthase



M1	L61	I121	S181	N241
K2	D62	Q122	L182	V242
Y3	D63	D123	V183	H243
V4	G64	W124	P184	D244
V5	G65	I125	V185	V245
V6	E66	Q126	I186	N246
S7	T67	R127	H187	S247
G8	D68	V128	G188	T248
G9	L69	S129	E189	S249
V10	D70	K130	Q190	H250
I11	L71	I131	K191	V251
S12	G72	P132	T192	P252
G13	M73	V133	K193	L253
I14	Y74	D134	P194	L254
G15	E75	D135	T195	L255
K16	R76	T136	Q196	L256
G17	Y77	G137	A197	K257
V18	L78	L138	A198	Q258
L19	G79	E139	I199	H259
A20	T80	P140	K200	M260
S21	T81	D141	D201	I261
S22	L82	V142	L202	D262
T23	S83	C143	R203	Y263
Q24	R84	I144	S204	L264
M25	D85	I145	L205	H265
L26	H86	E146	G206	S266
L27	N87	L147	L207	R267
K28	T88	G148	I208	L268
T29	T89	G149	P209	K269
L30	T90	T150	D210	L270
G31	G91	V151	M211	G271
L32	K92	G152	I212	E272
K33	I93	D153	A213	V273
V34	Y94	I154	C214	P274
T35	S95	E155	R215	L275
S36	H96	S156	C216	T276
I37	Y97	A157	S217	L277
K38	T98	P158	E218	E278
I39	S99	F159	E219	D279
D40	R100	V160	L220	K280
P41	E101	E161	N221	E281
Y42	R102	A162	R222	E282
M43	R103	L163	S223	G283
N44	G104	R164	T224	S284
I45	D105	Q165	I225	Q285
D46	Y106	F166	D226	L286
A47	L107	Q167	K227	T287
C48	G108	F168	I228	T288
T49	K109	E169	A229	N289
M50	V110	V170	M230	W290
S51	V111	G171	F231	E291
P52	Q112	R172	C232	E291
L53	I113	E173	H233	N292
E54	V114	M174	V234	T294
H55	P115	F175	G235	K295
O56	H116	A176	P236	N296
E57	L117	L177	E237	L297
C58	T118	I178	Q238	D298
F59	M119	H179	V239	D299
V60	A120	V180	S300	



• Molecule 1: CTP synthase



WORLDWIDE
 **PDB**
PROTEIN DATA BANK

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 (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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.

All (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
1	H	217	SER	N-CA-C	7.31	121.89	113.19
1	D	217	SER	N-CA-C	7.30	121.88	113.19
1	B	217	SER	N-CA-C	7.30	121.87	113.19
1	Z	217	SER	N-CA-C	7.30	121.87	113.19
1	Y	217	SER	N-CA-C	7.28	121.86	113.19
1	C	217	SER	N-CA-C	7.28	121.85	113.19
1	G	217	SER	N-CA-C	7.24	121.80	113.19
1	F	63	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	63	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	63	ASP	CA-CB-CG	5.96	118.56	112.60
1	X	262	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	63	ASP	CA-CB-CG	5.95	118.55	112.60
1	F	262	ASP	CA-CB-CG	5.95	118.55	112.60
1	X	63	ASP	CA-CB-CG	5.95	118.55	112.60
1	W	63	ASP	CA-CB-CG	5.95	118.55	112.60
1	H	63	ASP	CA-CB-CG	5.93	118.53	112.60
1	E	63	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	262	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	262	ASP	CA-CB-CG	5.92	118.52	112.60
1	E	262	ASP	CA-CB-CG	5.92	118.52	112.60
1	C	262	ASP	CA-CB-CG	5.91	118.51	112.60
1	H	262	ASP	CA-CB-CG	5.91	118.51	112.60
1	D	262	ASP	CA-CB-CG	5.91	118.50	112.60
1	G	63	ASP	CA-CB-CG	5.91	118.51	112.60
1	Y	63	ASP	CA-CB-CG	5.90	118.50	112.60
1	Z	262	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	63	ASP	CA-CB-CG	5.89	118.49	112.60
1	Z	63	ASP	CA-CB-CG	5.89	118.49	112.60
1	W	262	ASP	CA-CB-CG	5.89	118.49	112.60
1	Y	262	ASP	CA-CB-CG	5.88	118.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	262	ASP	CA-CB-CG	5.88	118.47	112.60
1	C	429	PHE	CA-CB-CG	5.82	119.61	113.80
1	G	429	PHE	CA-CB-CG	5.79	119.59	113.80
1	Y	429	PHE	CA-CB-CG	5.78	119.58	113.80
1	E	429	PHE	CA-CB-CG	5.77	119.57	113.80
1	H	429	PHE	CA-CB-CG	5.76	119.56	113.80
1	W	429	PHE	CA-CB-CG	5.76	119.56	113.80
1	Z	429	PHE	CA-CB-CG	5.75	119.55	113.80
1	D	429	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	429	PHE	CA-CB-CG	5.75	119.55	113.80
1	F	429	PHE	CA-CB-CG	5.73	119.53	113.80
1	A	429	PHE	CA-CB-CG	5.71	119.51	113.80
1	X	429	PHE	CA-CB-CG	5.71	119.51	113.80
1	B	394	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	D	394	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	Z	394	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	C	394	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	G	394	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	Y	394	ARG	NE-CZ-NH2	5.62	124.25	119.20
1	A	394	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	H	394	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	F	394	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	X	394	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	W	394	ARG	NE-CZ-NH2	5.58	124.23	119.20
1	E	394	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	C	523	PHE	CA-CB-CG	5.26	119.06	113.80
1	E	523	PHE	CA-CB-CG	5.24	119.04	113.80
1	Y	328	HIS	CA-CB-CG	5.23	119.03	113.80
1	Y	523	PHE	CA-CB-CG	5.22	119.02	113.80
1	Z	523	PHE	CA-CB-CG	5.22	119.02	113.80
1	G	523	PHE	CA-CB-CG	5.22	119.02	113.80
1	D	523	PHE	CA-CB-CG	5.21	119.01	113.80
1	Z	328	HIS	CA-CB-CG	5.21	119.01	113.80
1	C	328	HIS	CA-CB-CG	5.21	119.01	113.80
1	X	523	PHE	CA-CB-CG	5.21	119.01	113.80
1	F	523	PHE	CA-CB-CG	5.20	119.00	113.80
1	G	328	HIS	CA-CB-CG	5.20	119.00	113.80
1	H	523	PHE	CA-CB-CG	5.20	119.00	113.80
1	E	328	HIS	CA-CB-CG	5.19	118.99	113.80
1	F	328	HIS	CA-CB-CG	5.19	118.99	113.80
1	B	328	HIS	CA-CB-CG	5.19	118.99	113.80
1	W	523	PHE	CA-CB-CG	5.18	118.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	328	HIS	CA-CB-CG	5.18	118.98	113.80
1	A	523	PHE	CA-CB-CG	5.17	118.97	113.80
1	D	328	HIS	CA-CB-CG	5.17	118.97	113.80
1	A	328	HIS	CA-CB-CG	5.17	118.97	113.80
1	X	328	HIS	CA-CB-CG	5.17	118.97	113.80
1	B	523	PHE	CA-CB-CG	5.14	118.94	113.80
1	W	328	HIS	CA-CB-CG	5.13	118.93	113.80
1	D	425	SER	N-CA-C	5.12	116.86	109.07
1	Z	425	SER	N-CA-C	5.12	116.86	109.07
1	Y	425	SER	N-CA-C	5.11	116.84	109.07
1	G	425	SER	N-CA-C	5.11	116.84	109.07
1	E	425	SER	N-CA-C	5.10	116.83	109.07
1	C	425	SER	N-CA-C	5.10	116.82	109.07
1	H	425	SER	N-CA-C	5.10	116.82	109.07
1	A	425	SER	N-CA-C	5.09	116.81	109.07
1	F	425	SER	N-CA-C	5.08	116.79	109.07
1	X	425	SER	N-CA-C	5.08	116.79	109.07
1	B	425	SER	N-CA-C	5.07	116.78	109.07
1	W	425	SER	N-CA-C	5.06	116.76	109.07
1	A	364	ASN	CA-CB-CG	5.03	117.63	112.60
1	G	486	HIS	CA-CB-CG	5.02	118.82	113.80
1	D	364	ASN	CA-CB-CG	5.01	117.61	112.60
1	C	364	ASN	CA-CB-CG	5.00	117.60	112.60
1	G	364	ASN	CA-CB-CG	5.00	117.60	112.60
1	Z	364	ASN	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (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
1	F	164	ARG	Sidechain
1	G	164	ARG	Sidechain
1	H	164	ARG	Sidechain
1	W	164	ARG	Sidechain
1	X	164	ARG	Sidechain
1	Y	164	ARG	Sidechain
1	Z	164	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:B:193:LYS:HE3	4:B:604:UTP:O2B	1.69	0.92
1:E:193:LYS:HE3	4:E:604:UTP:O1B	1.70	0.91
1:D:193:LYS:HE3	4:D:602:UTP:O1B	1.69	0.91
1:F:193:LYS:HE3	4:F:604:UTP:O2B	1.69	0.91
1:Z:193:LYS:HE3	4:Z:602:UTP:O1B	1.69	0.91
1:A:193:LYS:HE3	4:A:604:UTP:O1B	1.70	0.90
1:H:193:LYS:HE3	4:H:602:UTP:O1B	1.69	0.90
1:W:192:THR:N	4:W:604:UTP:O1G	2.09	0.86
1:A:192:THR:N	4:A:604:UTP:O1G	2.08	0.86
1:D:192:THR:N	4:D:602:UTP:O1G	2.10	0.84
1:E:192:THR:N	4:E:604:UTP:O1G	2.08	0.83
1:H:192:THR:N	4:H:602:UTP:O1G	2.10	0.82
1:Z:192:THR:N	4:Z:602:UTP:O1G	2.10	0.80
1:B:192:THR:N	4:B:604:UTP:O1G	2.13	0.77
1:C:192:THR:N	4:C:603:UTP:O1G	2.14	0.76
1:X:192:THR:N	4:X:604:UTP:O1G	2.13	0.75
1:Y:192:THR:N	4:Y:602:UTP:O1G	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:THR:N	4:F:604:UTP:O1G	2.13	0.73
1:G:192:THR:N	4:G:602:UTP:O1G	2.14	0.71
4:B:604:UTP:H4'	1:D:112:GLN:NE2	2.24	0.52
4:F:604:UTP:H4'	1:H:112:GLN:NE2	2.24	0.52
1:W:112:GLN:NE2	4:Y:602:UTP:H4'	2.25	0.52
1:A:112:GLN:NE2	4:C:603:UTP:H4'	2.25	0.52
1:E:112:GLN:NE2	4:G:602:UTP:H4'	2.25	0.52
4:X:604:UTP:H4'	1:Z:112:GLN:NE2	2.24	0.51
1:B:112:GLN:NE2	4:D:602:UTP:H4'	2.27	0.50
1:X:112:GLN:NE2	4:Z:602:UTP:H4'	2.27	0.49
1:F:112:GLN:NE2	4:H:602:UTP:H4'	2.27	0.49
4:E:604:UTP:H4'	1:G:112:GLN:NE2	2.29	0.48
4:W:604:UTP:H4'	1:Y:112:GLN:NE2	2.29	0.48
4:A:604:UTP:H4'	1:C:112:GLN:NE2	2.29	0.47
4:X:604:UTP:PA	1:Y:12:SER:CB	3.05	0.45
4:A:604:UTP:PA	1:D:12:SER:CB	3.05	0.45
4:F:604:UTP:PA	1:G:12:SER:CB	3.05	0.45
4:E:604:UTP:PA	1:H:12:SER:CB	3.05	0.45
1:W:12:SER:CB	4:Z:602:UTP:PA	3.05	0.45
1:B:12:SER:CB	4:C:603:UTP:PA	3.05	0.45
4:B:604:UTP:PA	1:C:12:SER:CB	3.05	0.45
4:W:604:UTP:PA	1:Z:12:SER:CB	3.05	0.45
1:E:12:SER:CB	4:H:602:UTP:PA	3.05	0.44
1:F:12:SER:CB	4:G:602:UTP:PA	3.05	0.44
1:A:12:SER:CB	4:D:602:UTP:PA	3.05	0.44
1:X:12:SER:CB	4:Y:602:UTP:PA	3.05	0.44
4:B:604:UTP:O1A	1:C:12:SER:HB3	2.22	0.40
4:W:604:UTP:O2A	1:Z:12:SER:HB3	2.22	0.40

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

All (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
1	F	431	ASP
1	G	431	ASP
1	H	431	ASP
1	W	431	ASP
1	X	431	ASP
1	Y	431	ASP
1	Z	431	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	93	ILE
1	A	117	LEU
1	A	217	SER
1	A	262	ASP
1	B	19	LEU
1	B	93	ILE
1	B	117	LEU
1	B	217	SER
1	B	262	ASP
1	B	462	ARG
1	C	19	LEU
1	C	93	ILE
1	C	117	LEU
1	C	217	SER
1	C	262	ASP
1	D	19	LEU
1	D	93	ILE
1	D	117	LEU
1	D	217	SER
1	D	262	ASP
1	E	19	LEU

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Mol	Chain	Res	Type
1	E	93	ILE
1	E	117	LEU
1	E	217	SER
1	E	262	ASP
1	F	19	LEU
1	F	93	ILE
1	F	117	LEU
1	F	217	SER
1	F	262	ASP
1	F	462	ARG
1	G	19	LEU
1	G	93	ILE
1	G	117	LEU
1	G	217	SER
1	G	262	ASP
1	H	19	LEU
1	H	93	ILE
1	H	117	LEU
1	H	217	SER
1	H	262	ASP
1	W	19	LEU
1	W	93	ILE
1	W	117	LEU
1	W	217	SER
1	W	262	ASP
1	X	19	LEU
1	X	93	ILE
1	X	117	LEU
1	X	217	SER
1	X	262	ASP
1	X	462	ARG
1	Y	19	LEU
1	Y	93	ILE
1	Y	117	LEU
1	Y	217	SER
1	Y	262	ASP
1	Z	19	LEU
1	Z	93	ILE
1	Z	117	LEU
1	Z	217	SER
1	Z	262	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	B	165	GLN
1	B	167	GLN
1	C	167	GLN
1	D	165	GLN
1	D	167	GLN
1	E	165	GLN
1	E	167	GLN
1	F	165	GLN
1	F	167	GLN
1	G	165	GLN
1	G	167	GLN
1	H	165	GLN
1	H	167	GLN
1	W	165	GLN
1	W	167	GLN
1	X	167	GLN
1	Y	165	GLN
1	Y	167	GLN
1	Z	167	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
4	E	604	UTP	PA-O3A	2.14	1.61	1.59
4	F	604	UTP	PA-O3A	2.12	1.61	1.59
4	B	604	UTP	PA-O3A	2.11	1.61	1.59
4	G	602	UTP	PA-O3A	2.11	1.61	1.59
4	C	603	UTP	PA-O3A	2.09	1.61	1.59
4	Y	602	UTP	PA-O3A	2.08	1.61	1.59
4	X	604	UTP	PA-O3A	2.08	1.61	1.59

All (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
4	W	604	UTP	O2A-PA-O1A	3.72	129.73	112.44
4	C	603	UTP	O2A-PA-O1A	3.72	129.73	112.44
4	Z	602	UTP	O2A-PA-O1A	3.72	129.73	112.44
4	X	604	UTP	O2A-PA-O1A	3.71	129.72	112.44
4	B	604	UTP	O2A-PA-O1A	3.71	129.71	112.44
4	G	602	UTP	O2A-PA-O1A	3.71	129.70	112.44
4	Y	602	UTP	O2A-PA-O1A	3.71	129.69	112.44
4	B	604	UTP	O2A-PA-O3A	2.27	113.42	107.27
4	F	604	UTP	O2A-PA-O3A	2.26	113.38	107.27
4	C	603	UTP	O2A-PA-O3A	2.26	113.37	107.27
4	X	604	UTP	O2A-PA-O3A	2.25	113.36	107.27
4	G	602	UTP	O2A-PA-O3A	2.25	113.36	107.27
4	Y	602	UTP	O2A-PA-O3A	2.25	113.35	107.27

There are no chirality outliers.

All (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'
4	B	604	UTP	C5'-O5'-PA-O1A
4	B	604	UTP	C5'-O5'-PA-O2A
4	B	604	UTP	C5'-O5'-PA-O3A
4	C	603	UTP	PB-O3A-PA-O5'
4	C	603	UTP	C5'-O5'-PA-O1A
4	C	603	UTP	C5'-O5'-PA-O2A
4	C	603	UTP	C5'-O5'-PA-O3A
4	D	602	UTP	PB-O3A-PA-O5'
4	D	602	UTP	C5'-O5'-PA-O1A
4	D	602	UTP	C5'-O5'-PA-O3A
4	E	604	UTP	PB-O3A-PA-O5'
4	E	604	UTP	C5'-O5'-PA-O1A
4	E	604	UTP	C5'-O5'-PA-O3A
4	F	604	UTP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
4	F	604	UTP	C5'-O5'-PA-O1A
4	F	604	UTP	C5'-O5'-PA-O2A
4	F	604	UTP	C5'-O5'-PA-O3A
4	G	602	UTP	PB-O3A-PA-O5'
4	G	602	UTP	C5'-O5'-PA-O1A
4	G	602	UTP	C5'-O5'-PA-O2A
4	G	602	UTP	C5'-O5'-PA-O3A
4	H	602	UTP	PB-O3A-PA-O5'
4	H	602	UTP	C5'-O5'-PA-O1A
4	H	602	UTP	C5'-O5'-PA-O3A
4	W	604	UTP	PB-O3A-PA-O5'
4	W	604	UTP	C5'-O5'-PA-O1A
4	W	604	UTP	C5'-O5'-PA-O3A
4	X	604	UTP	PB-O3A-PA-O5'
4	X	604	UTP	C5'-O5'-PA-O1A
4	X	604	UTP	C5'-O5'-PA-O2A
4	X	604	UTP	C5'-O5'-PA-O3A
4	Y	602	UTP	PB-O3A-PA-O5'
4	Y	602	UTP	C5'-O5'-PA-O1A
4	Y	602	UTP	C5'-O5'-PA-O2A
4	Y	602	UTP	C5'-O5'-PA-O3A
4	Z	602	UTP	PB-O3A-PA-O5'
4	Z	602	UTP	C5'-O5'-PA-O1A
4	Z	602	UTP	C5'-O5'-PA-O3A
4	A	604	UTP	O4'-C4'-C5'-O5'
4	B	604	UTP	O4'-C4'-C5'-O5'
4	C	603	UTP	O4'-C4'-C5'-O5'
4	D	602	UTP	O4'-C4'-C5'-O5'
4	E	604	UTP	O4'-C4'-C5'-O5'
4	F	604	UTP	O4'-C4'-C5'-O5'
4	G	602	UTP	O4'-C4'-C5'-O5'
4	H	602	UTP	O4'-C4'-C5'-O5'
4	W	604	UTP	O4'-C4'-C5'-O5'
4	X	604	UTP	O4'-C4'-C5'-O5'
4	Y	602	UTP	O4'-C4'-C5'-O5'
4	Z	602	UTP	O4'-C4'-C5'-O5'
3	A	602	ATP	PA-O3A-PB-O1B
3	B	602	ATP	PA-O3A-PB-O1B
3	C	604	ATP	PA-O3A-PB-O1B
3	D	603	ATP	PA-O3A-PB-O1B
3	E	602	ATP	PA-O3A-PB-O1B
3	F	601	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	G	603	ATP	PA-O3A-PB-O1B
3	H	603	ATP	PA-O3A-PB-O1B
3	W	602	ATP	PA-O3A-PB-O1B
3	X	601	ATP	PA-O3A-PB-O1B
3	Y	603	ATP	PA-O3A-PB-O1B
3	Z	603	ATP	PA-O3A-PB-O1B
4	A	604	UTP	C5'-O5'-PA-O2A
4	D	602	UTP	C5'-O5'-PA-O2A
4	E	604	UTP	C5'-O5'-PA-O2A
4	H	602	UTP	C5'-O5'-PA-O2A
4	W	604	UTP	C5'-O5'-PA-O2A
4	Z	602	UTP	C5'-O5'-PA-O2A
4	A	604	UTP	PG-O3B-PB-O2B
4	D	602	UTP	PG-O3B-PB-O2B
4	E	604	UTP	PG-O3B-PB-O2B
4	H	602	UTP	PG-O3B-PB-O2B
4	W	604	UTP	PG-O3B-PB-O2B
4	Z	602	UTP	PG-O3B-PB-O2B
3	A	602	ATP	PA-O3A-PB-O2B
3	B	602	ATP	PA-O3A-PB-O2B
3	C	604	ATP	PA-O3A-PB-O2B
3	D	603	ATP	PA-O3A-PB-O2B
3	E	602	ATP	PA-O3A-PB-O2B
3	F	601	ATP	PA-O3A-PB-O2B
3	G	603	ATP	PA-O3A-PB-O2B
3	H	603	ATP	PA-O3A-PB-O2B
3	W	602	ATP	PA-O3A-PB-O2B
3	X	601	ATP	PA-O3A-PB-O2B
3	Y	603	ATP	PA-O3A-PB-O2B
3	Z	603	ATP	PA-O3A-PB-O2B
4	B	604	UTP	PG-O3B-PB-O1B
4	C	603	UTP	PG-O3B-PB-O1B
4	F	604	UTP	PG-O3B-PB-O1B
4	G	602	UTP	PG-O3B-PB-O1B
4	X	604	UTP	PG-O3B-PB-O1B
4	Y	602	UTP	PG-O3B-PB-O1B
3	A	602	ATP	PG-O3B-PB-O2B
3	B	602	ATP	PG-O3B-PB-O2B
3	C	604	ATP	PG-O3B-PB-O2B
3	D	603	ATP	PG-O3B-PB-O2B
3	E	602	ATP	PG-O3B-PB-O2B
3	F	601	ATP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	G	603	ATP	PG-O3B-PB-O2B
3	H	603	ATP	PG-O3B-PB-O2B
3	W	602	ATP	PG-O3B-PB-O2B
3	X	601	ATP	PG-O3B-PB-O2B
3	Y	603	ATP	PG-O3B-PB-O2B
3	Z	603	ATP	PG-O3B-PB-O2B
4	A	604	UTP	PG-O3B-PB-O3A
4	B	604	UTP	PG-O3B-PB-O3A
4	C	603	UTP	PG-O3B-PB-O3A
4	D	602	UTP	PG-O3B-PB-O3A
4	E	604	UTP	PG-O3B-PB-O3A
4	F	604	UTP	PG-O3B-PB-O3A
4	G	602	UTP	PG-O3B-PB-O3A
4	H	602	UTP	PG-O3B-PB-O3A
4	W	604	UTP	PG-O3B-PB-O3A
4	X	604	UTP	PG-O3B-PB-O3A
4	Y	602	UTP	PG-O3B-PB-O3A
4	Z	602	UTP	PG-O3B-PB-O3A

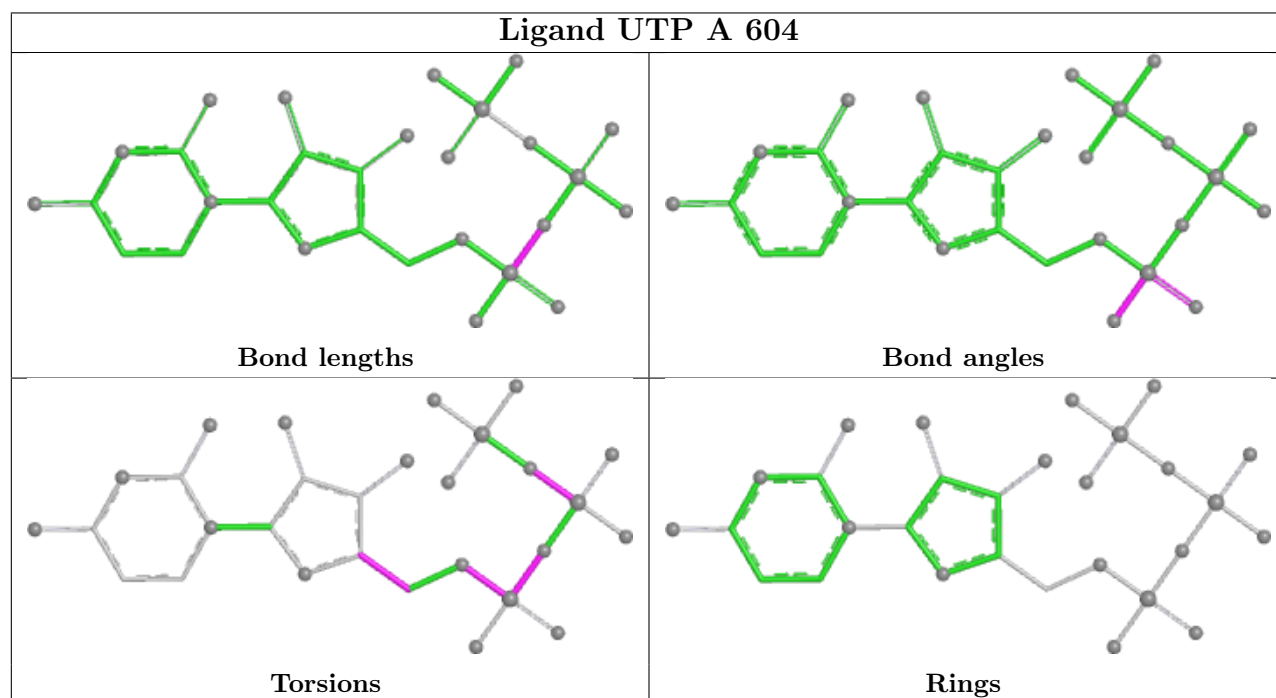
There are no ring outliers.

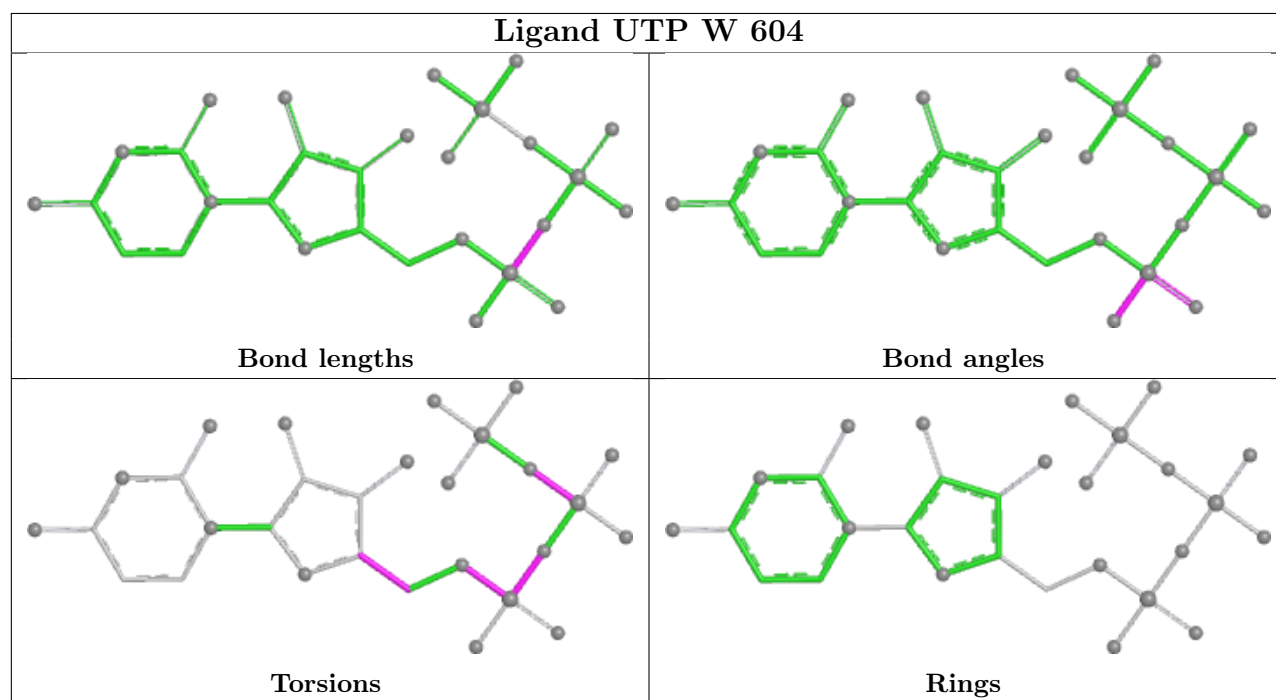
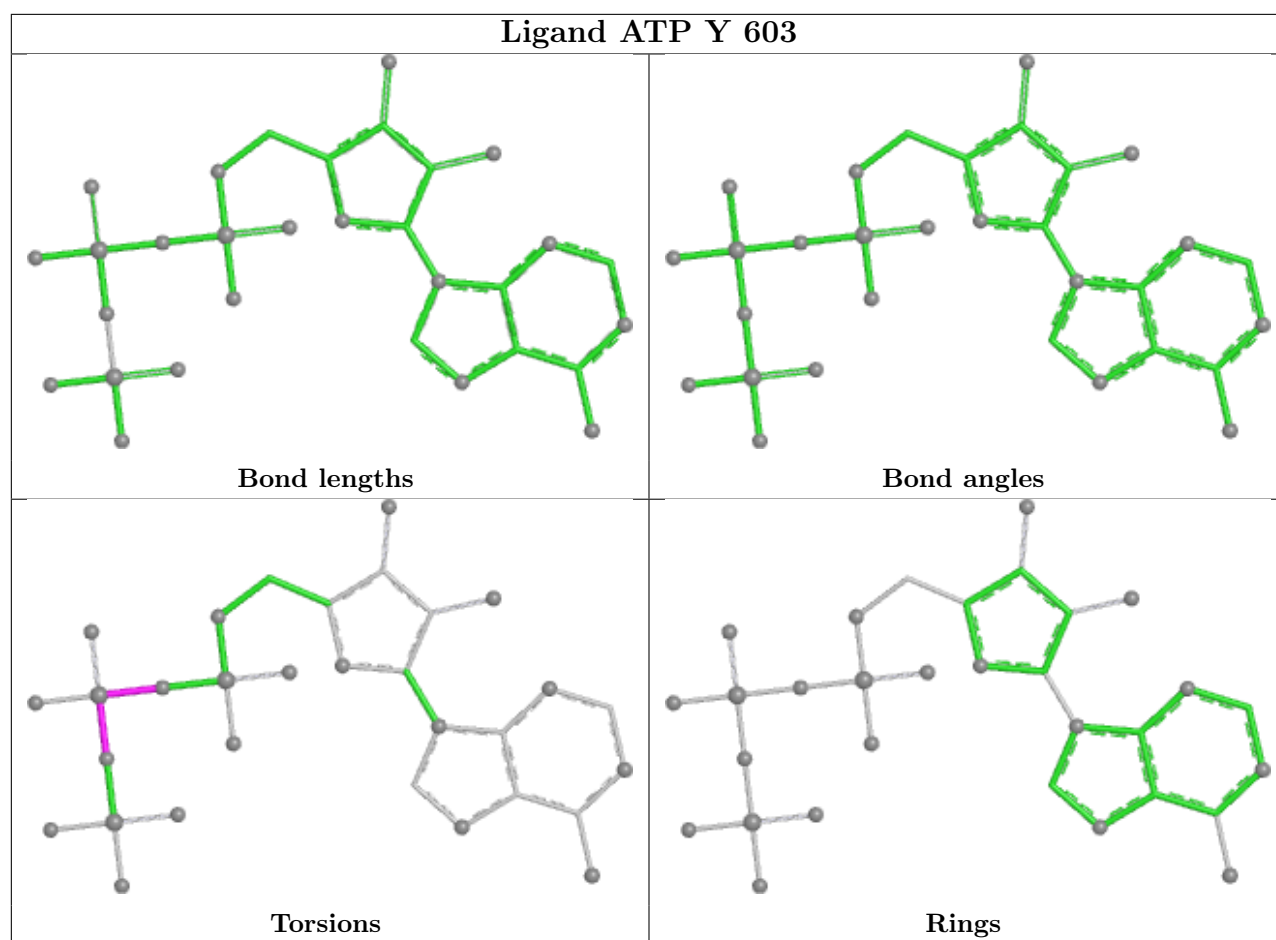
12 monomers are involved in 50 short contacts:

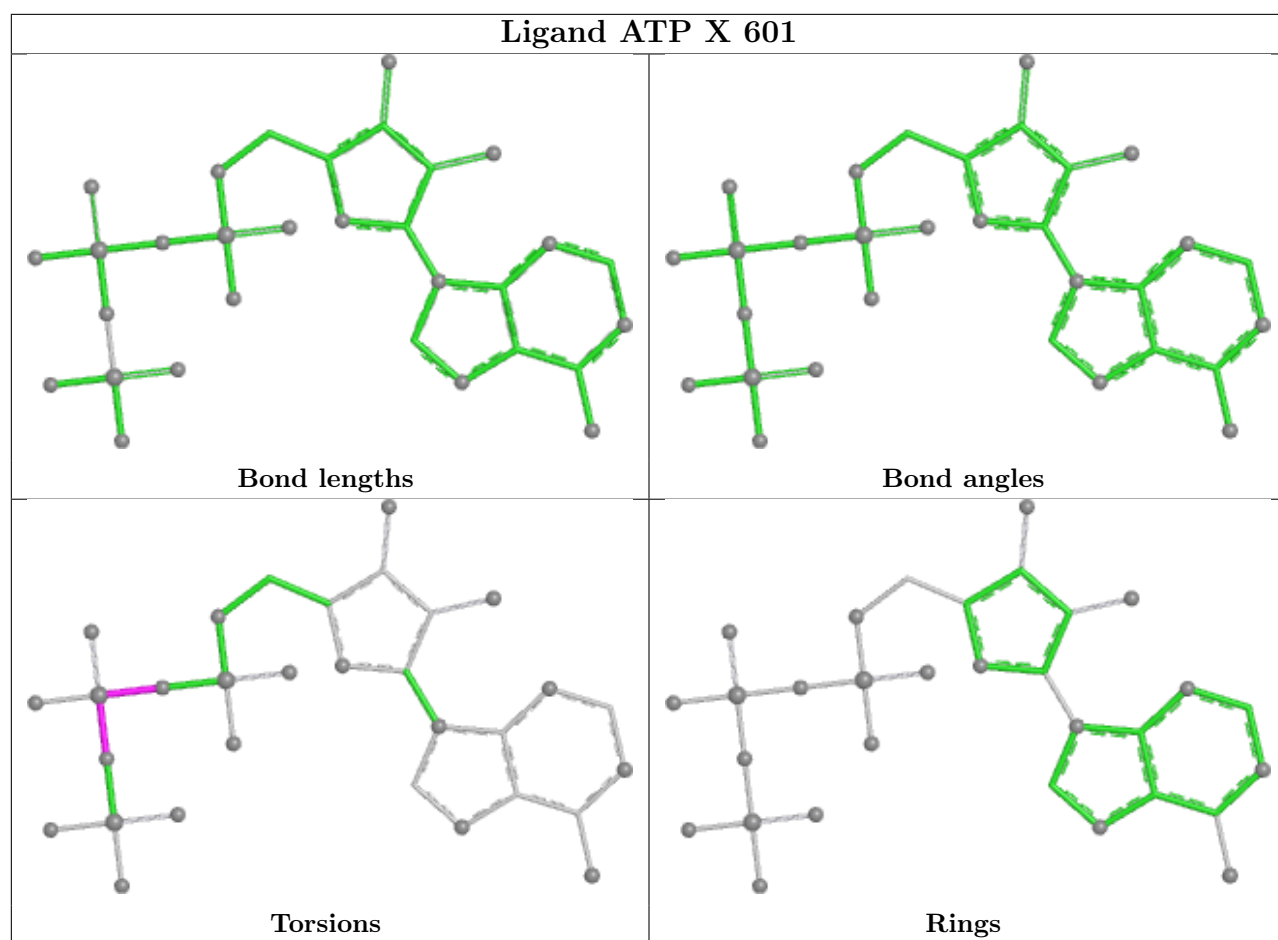
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	UTP	4	0
4	W	604	UTP	5	0
4	E	604	UTP	4	0
4	C	603	UTP	4	0
4	Y	602	UTP	4	0
4	G	602	UTP	4	0
4	X	604	UTP	4	0
4	Z	602	UTP	4	0
4	H	602	UTP	4	0
4	B	604	UTP	5	0
4	F	604	UTP	4	0
4	D	602	UTP	4	0

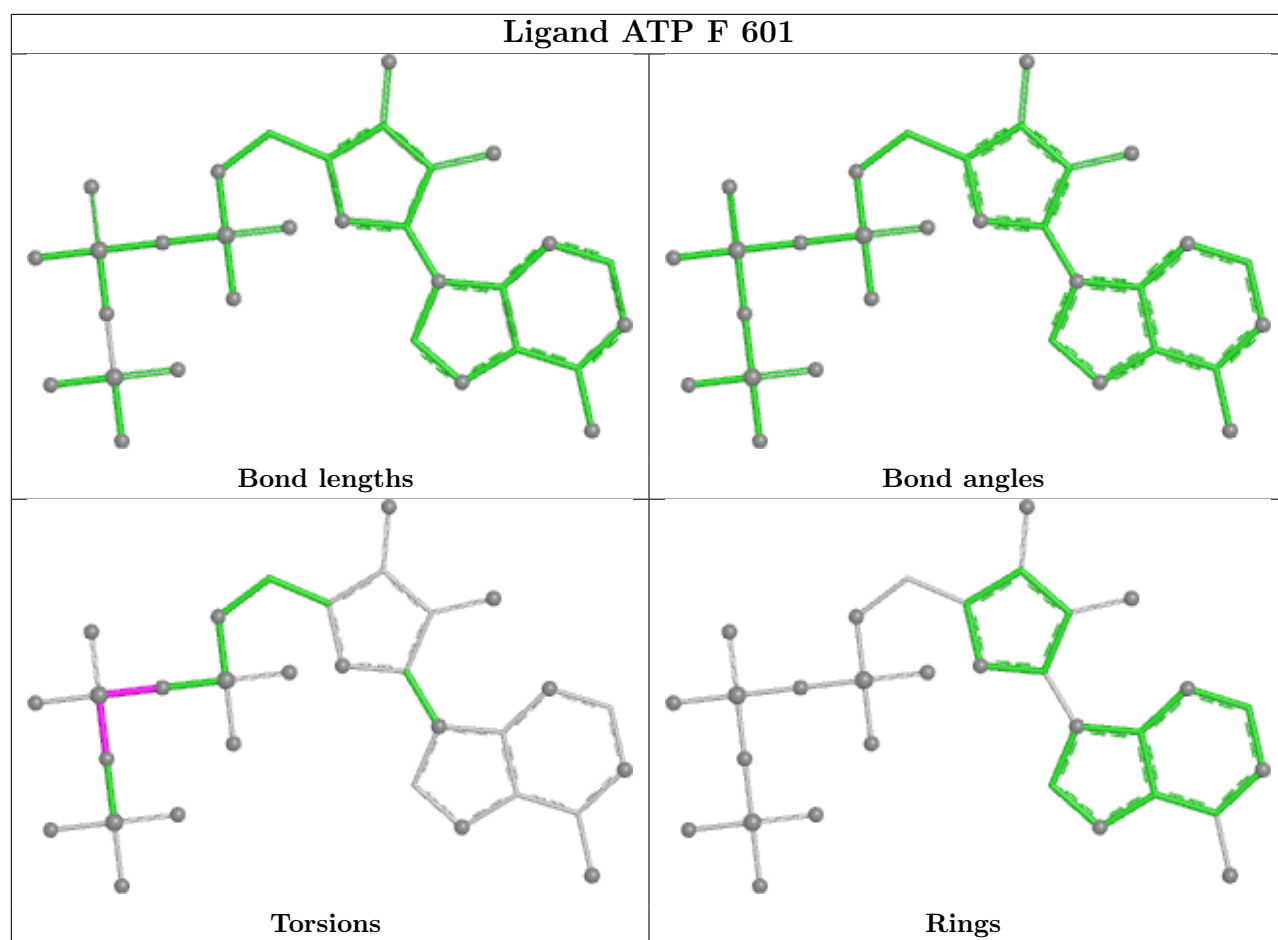
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

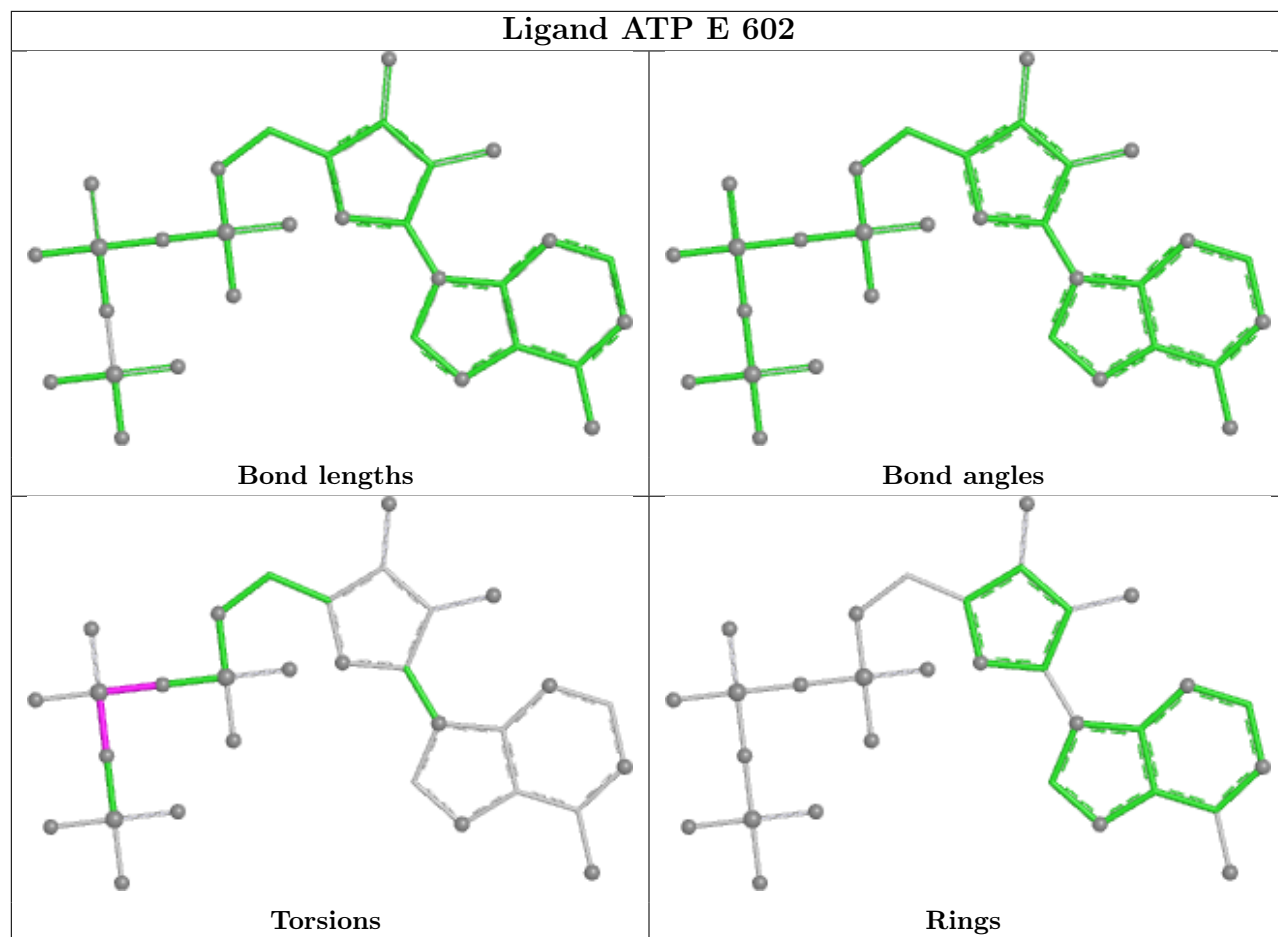




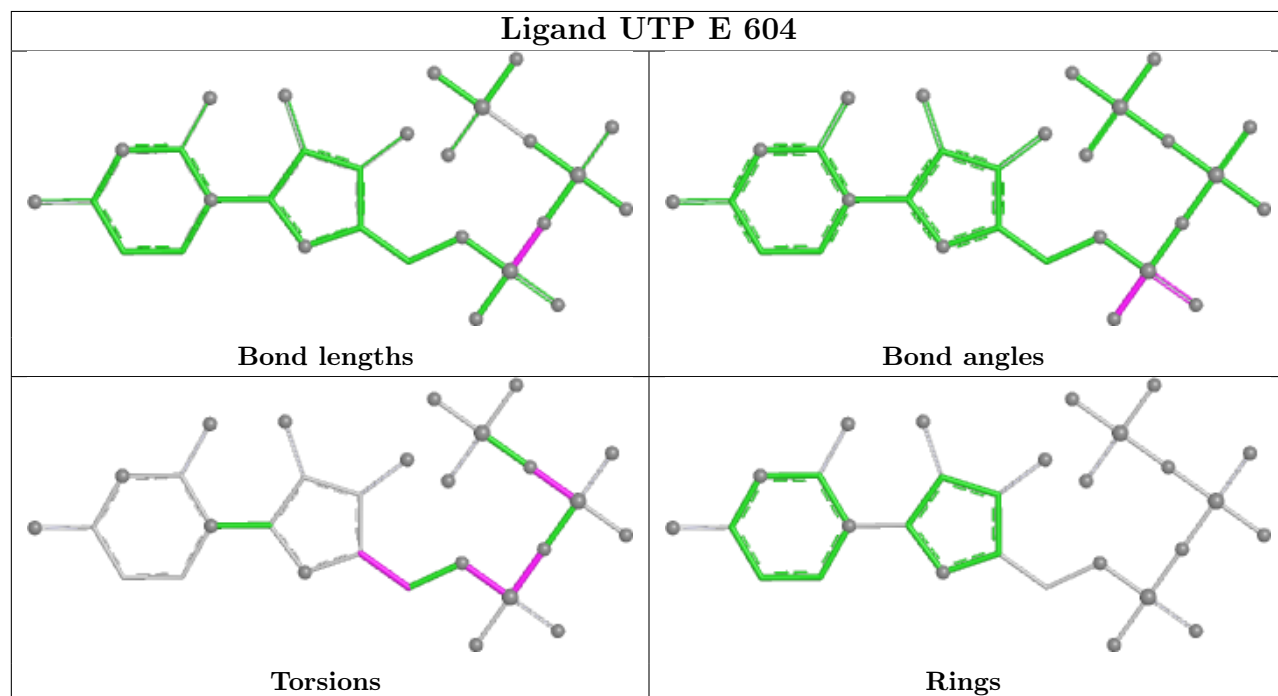


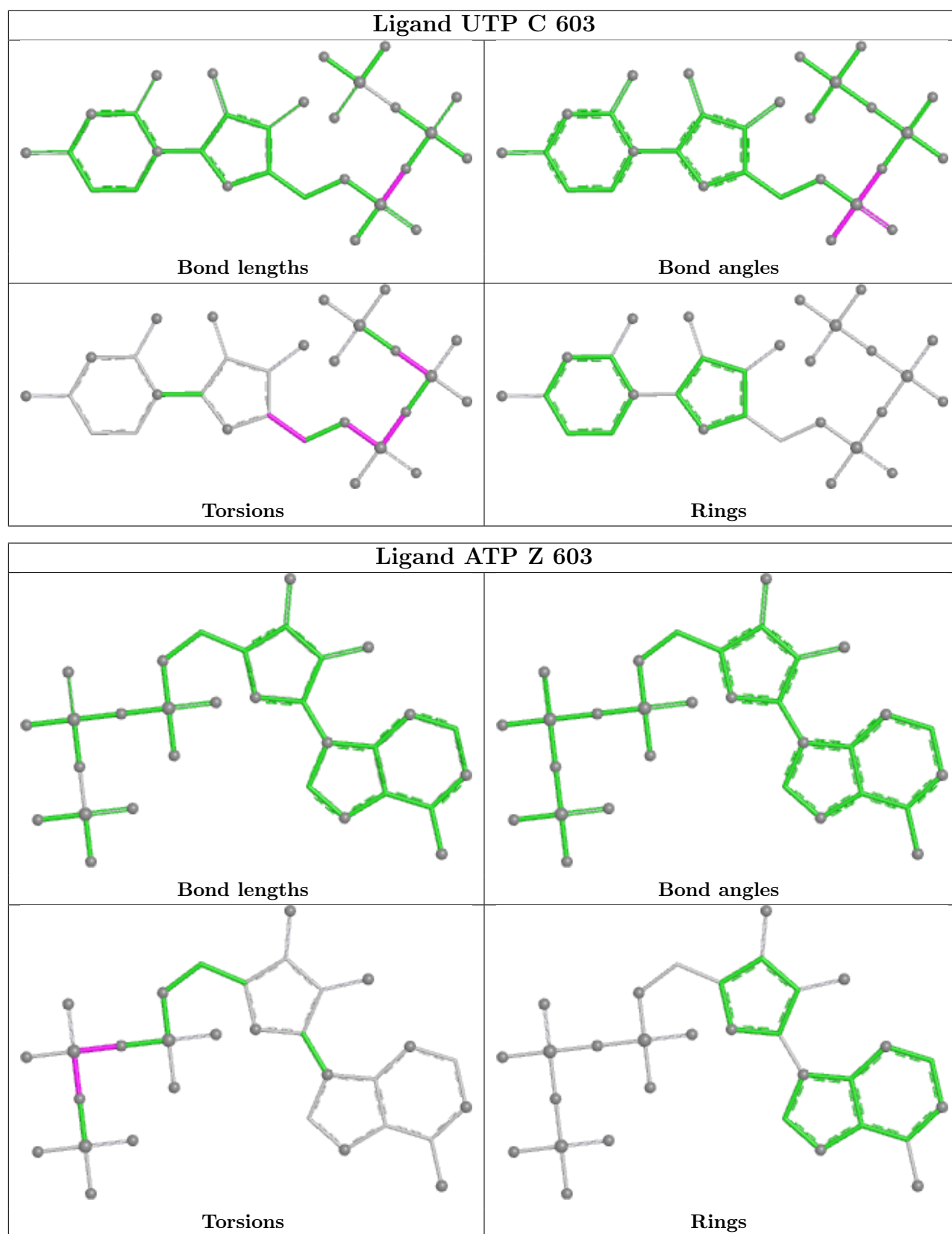


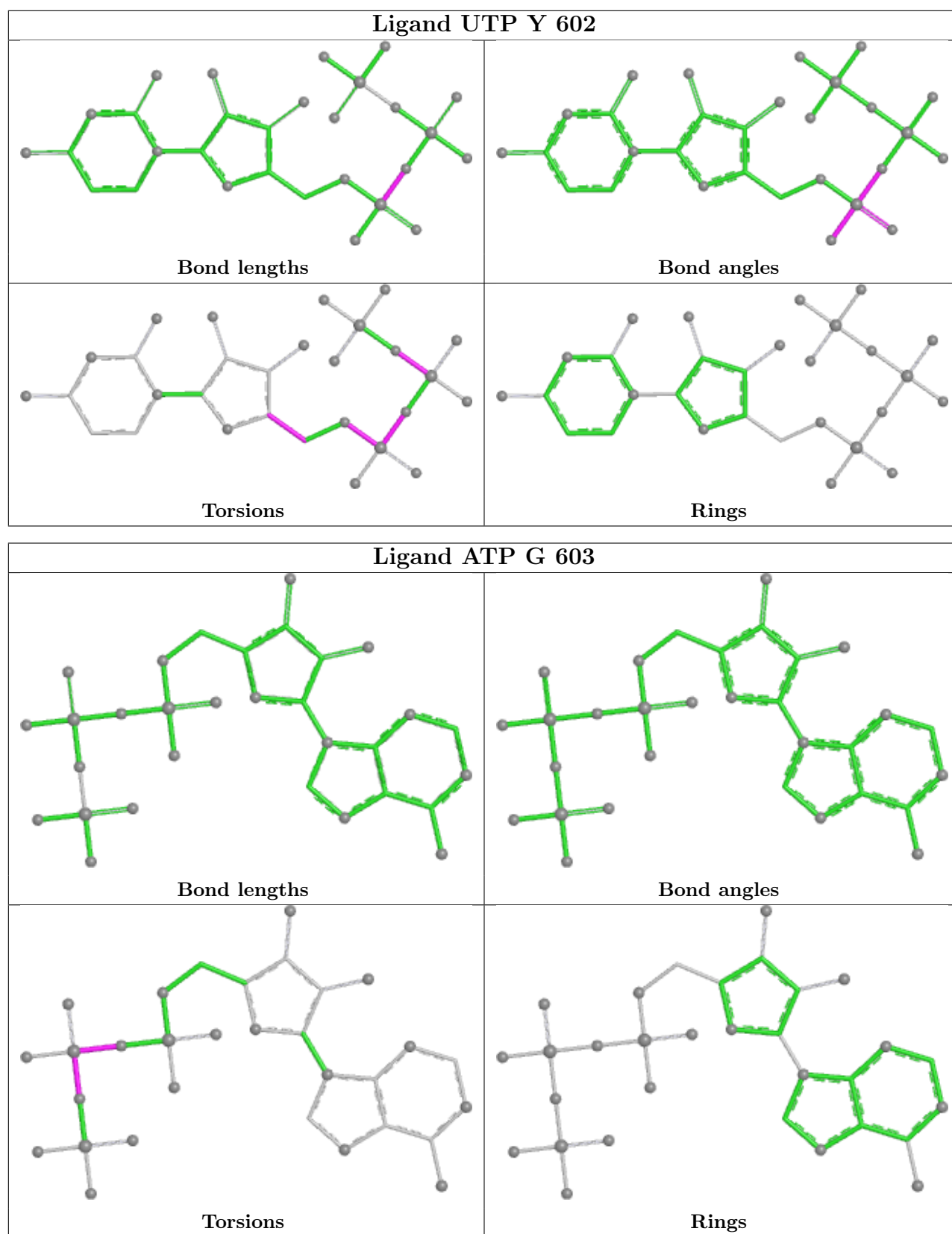
Ligand ATP E 602

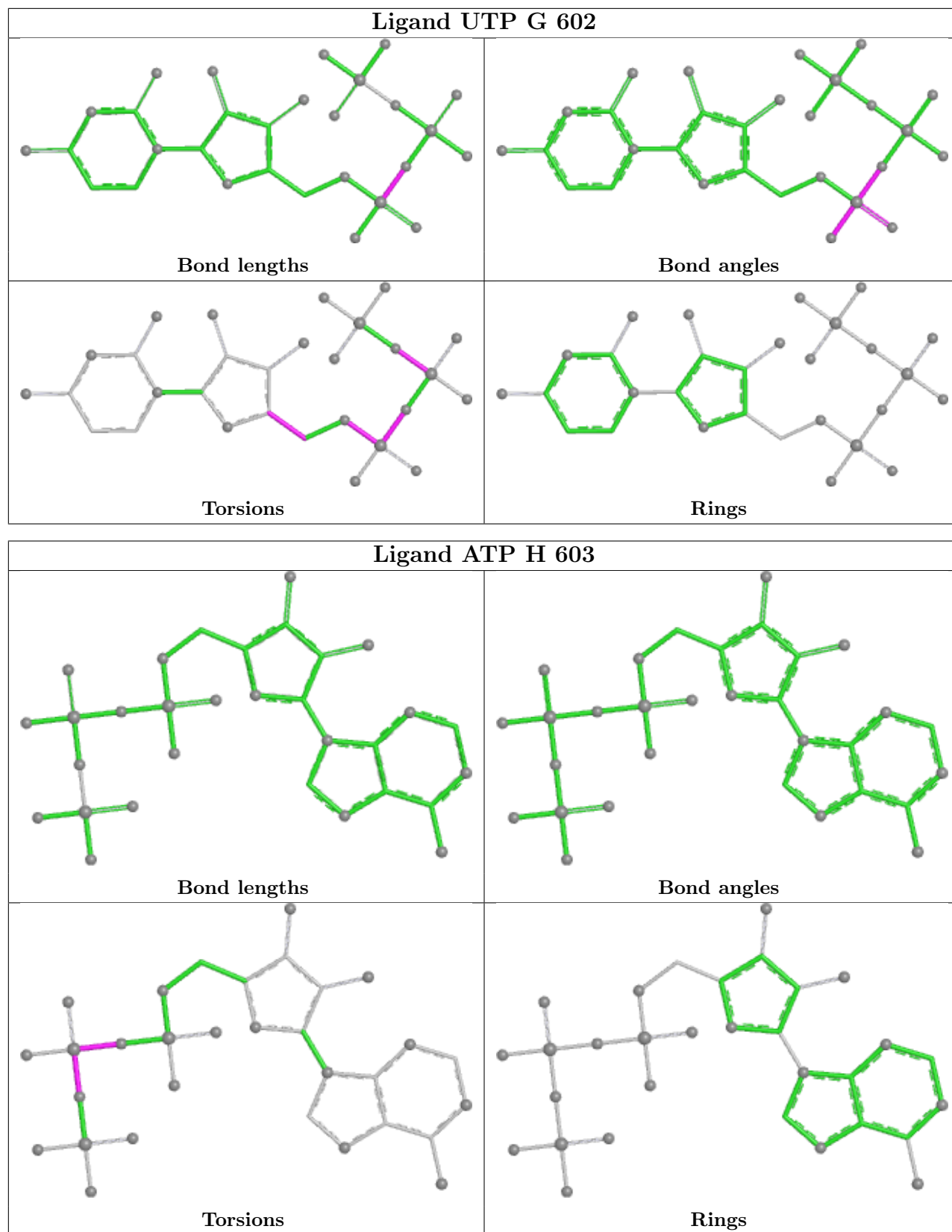


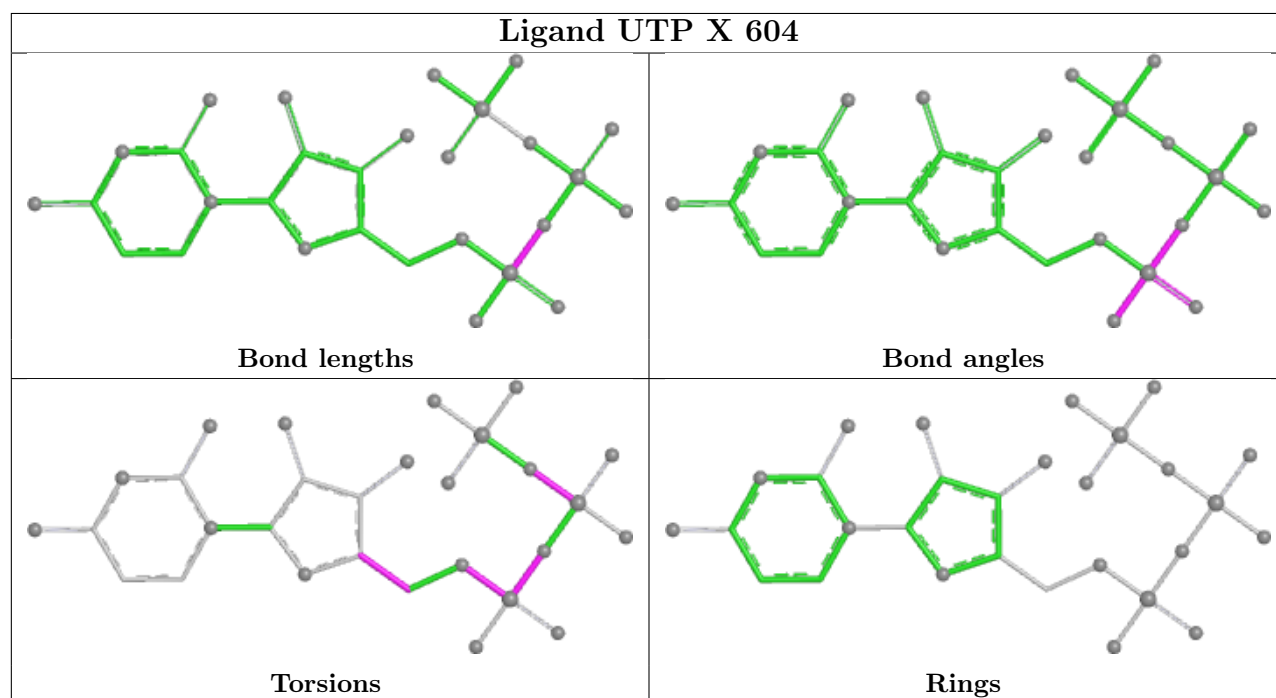
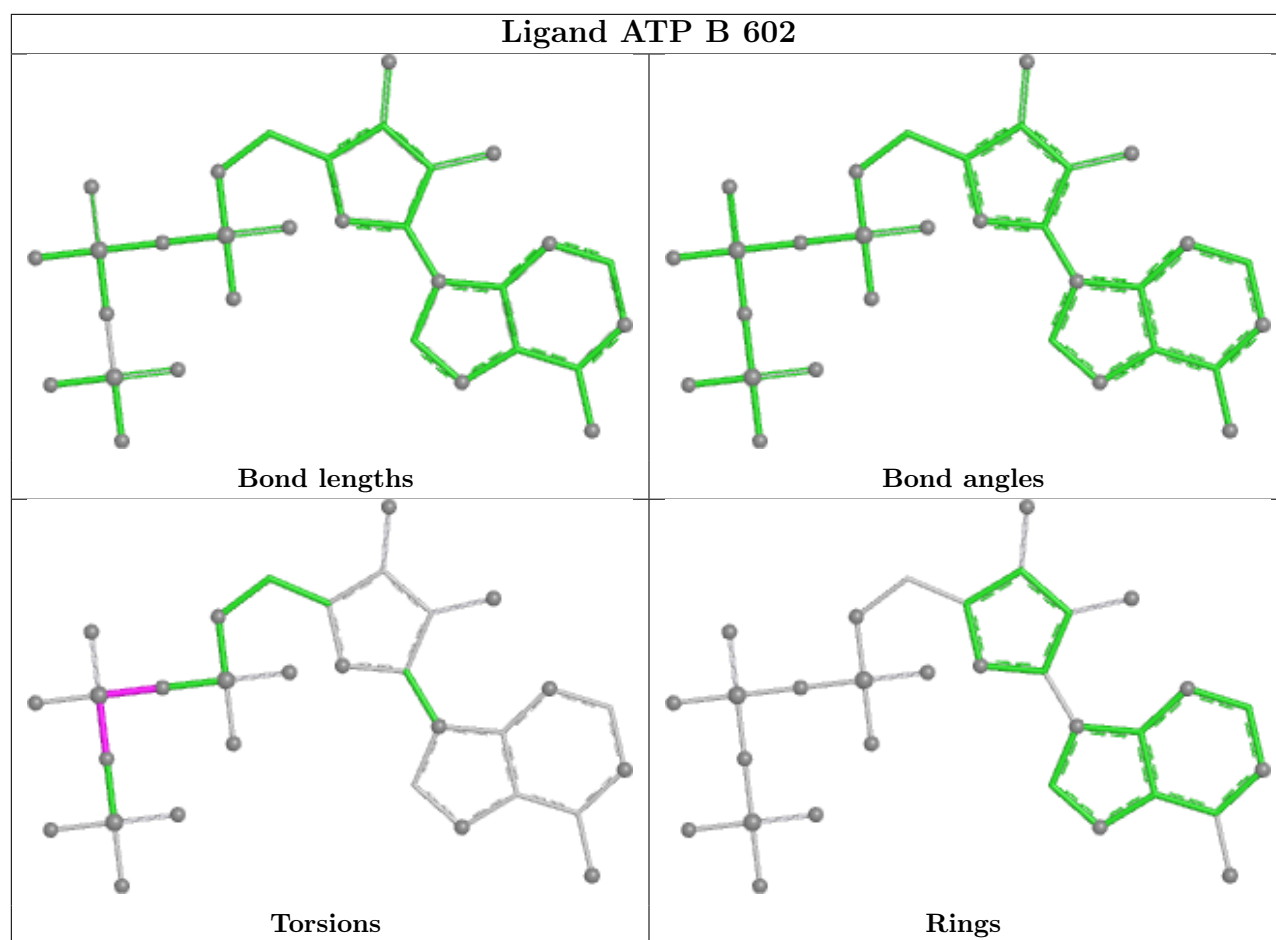
Ligand UTP E 604

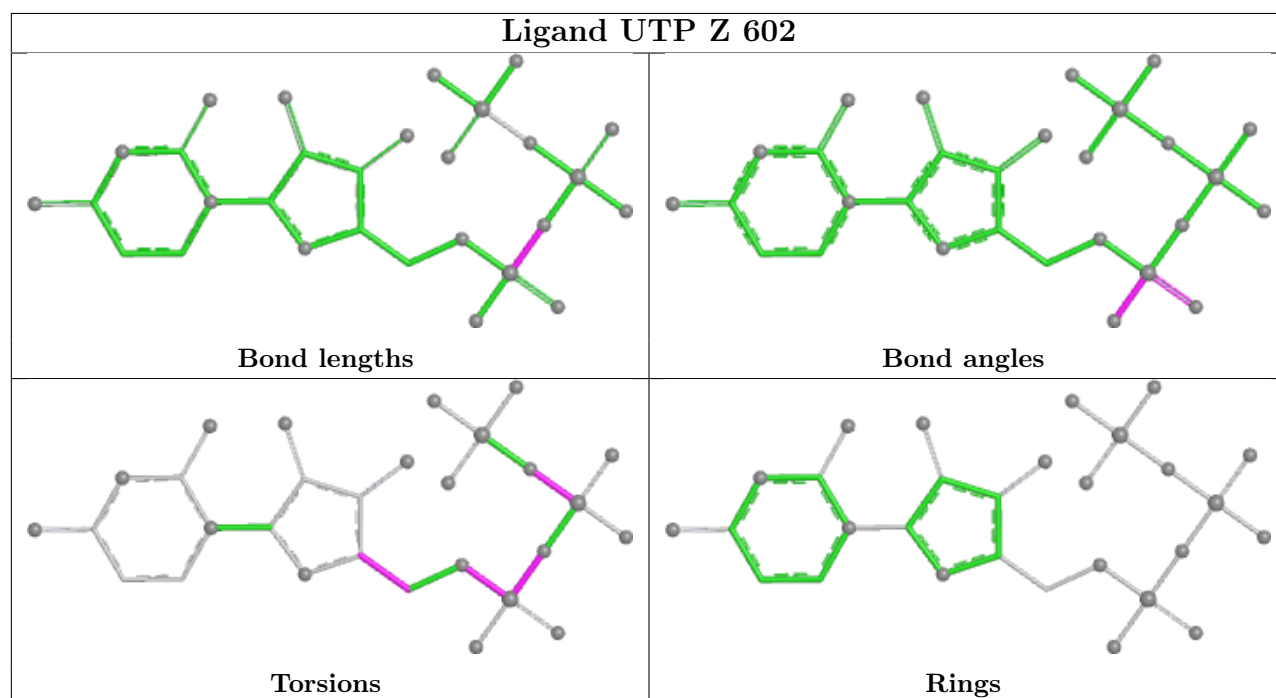
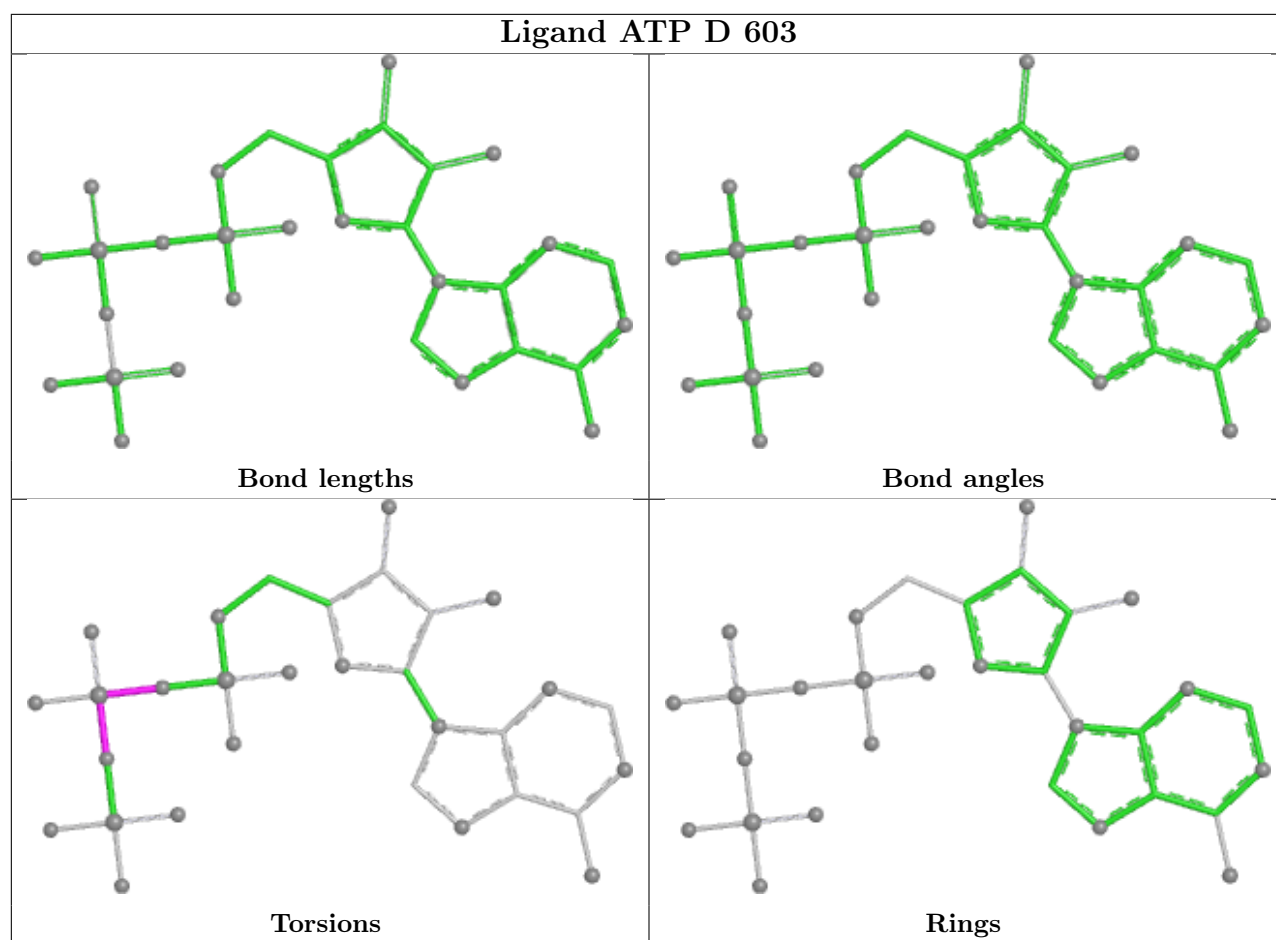


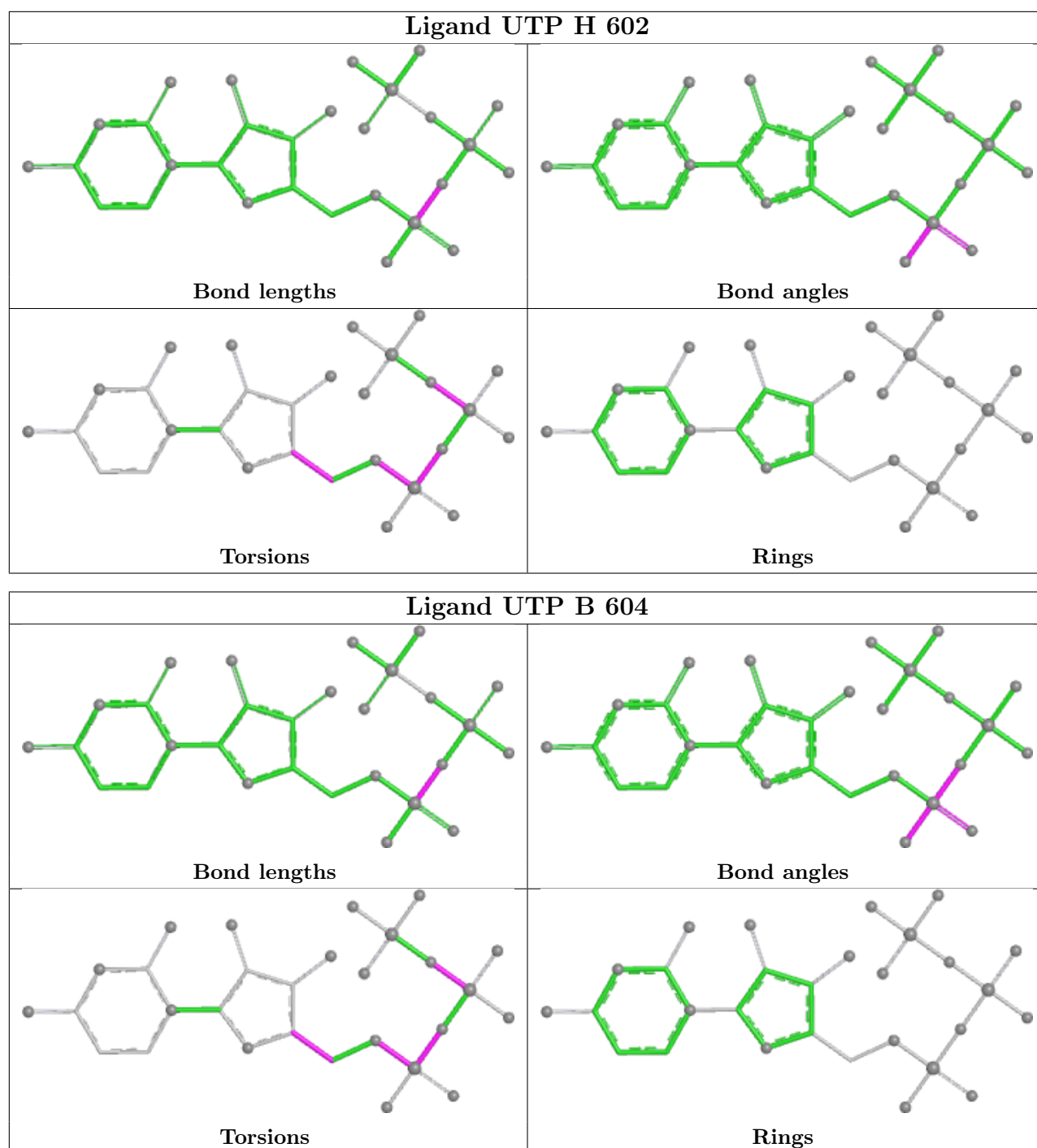


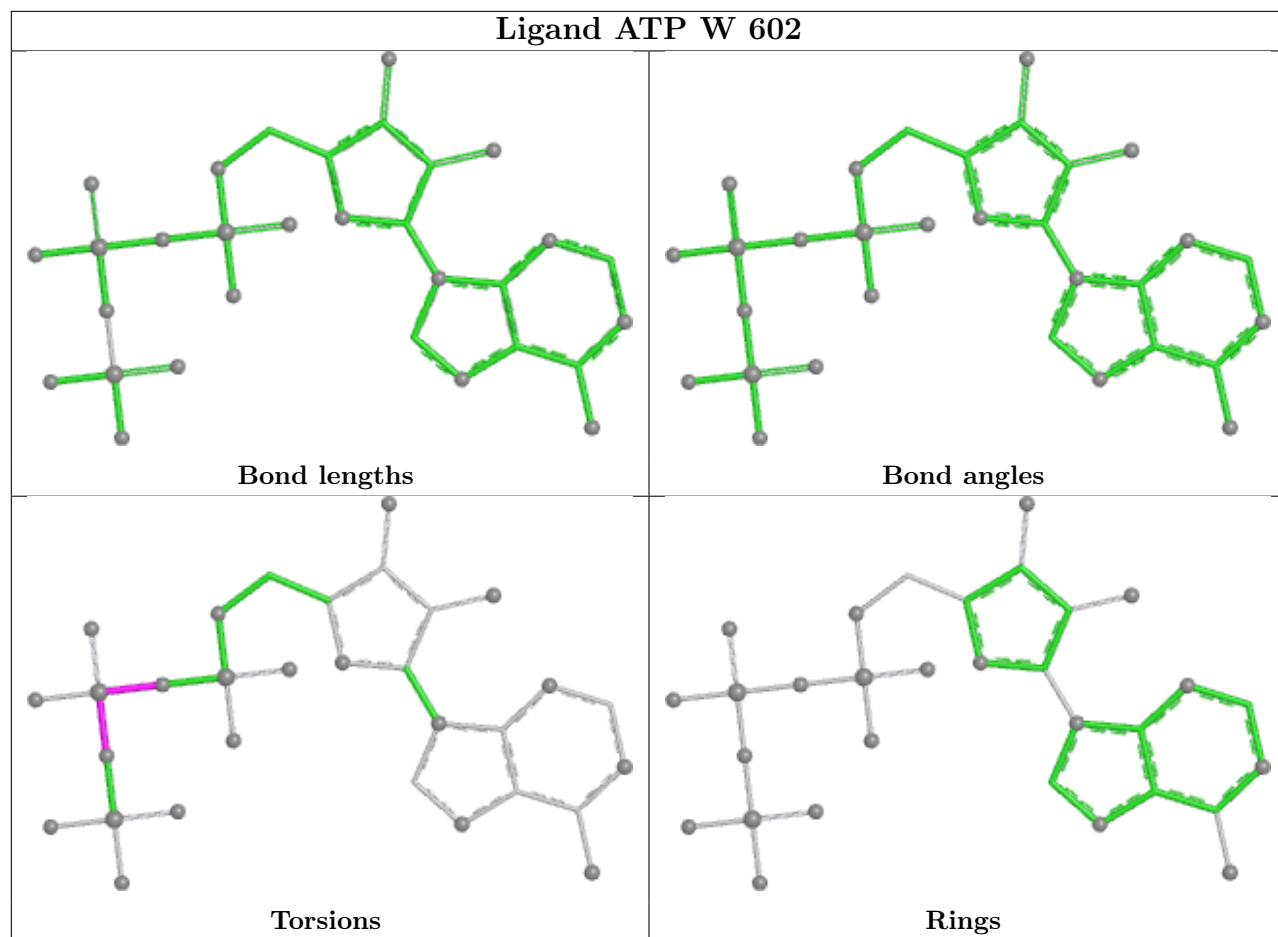


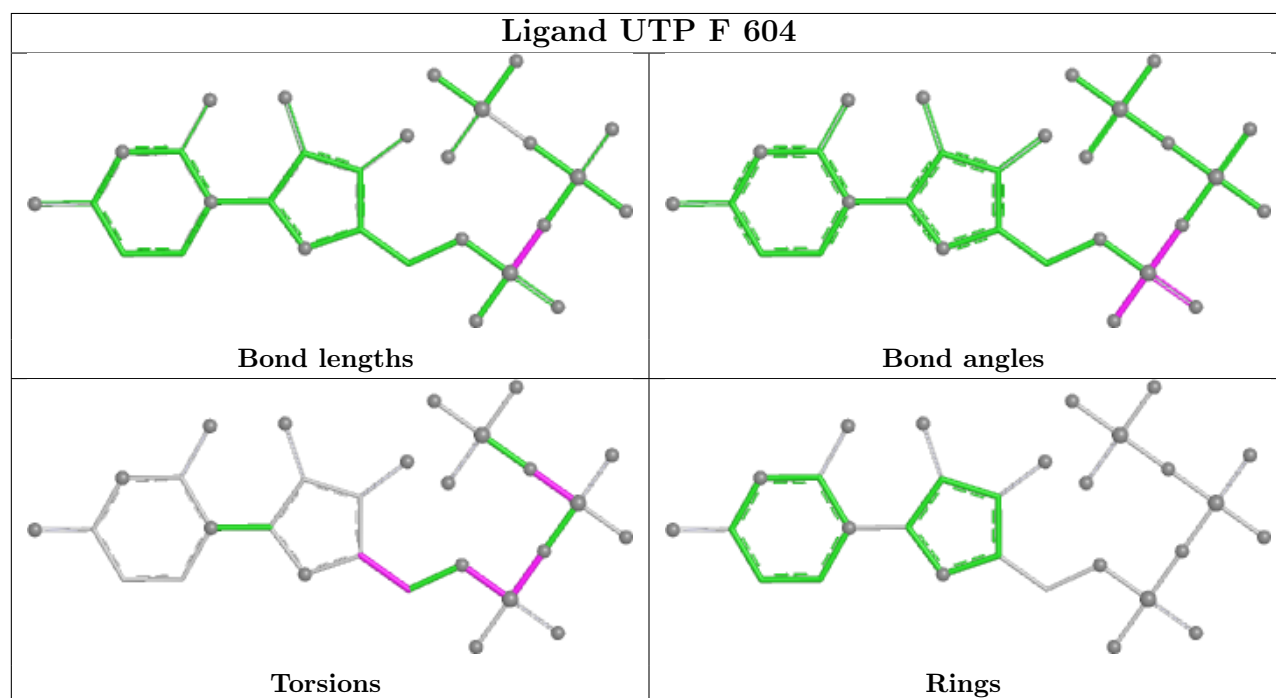
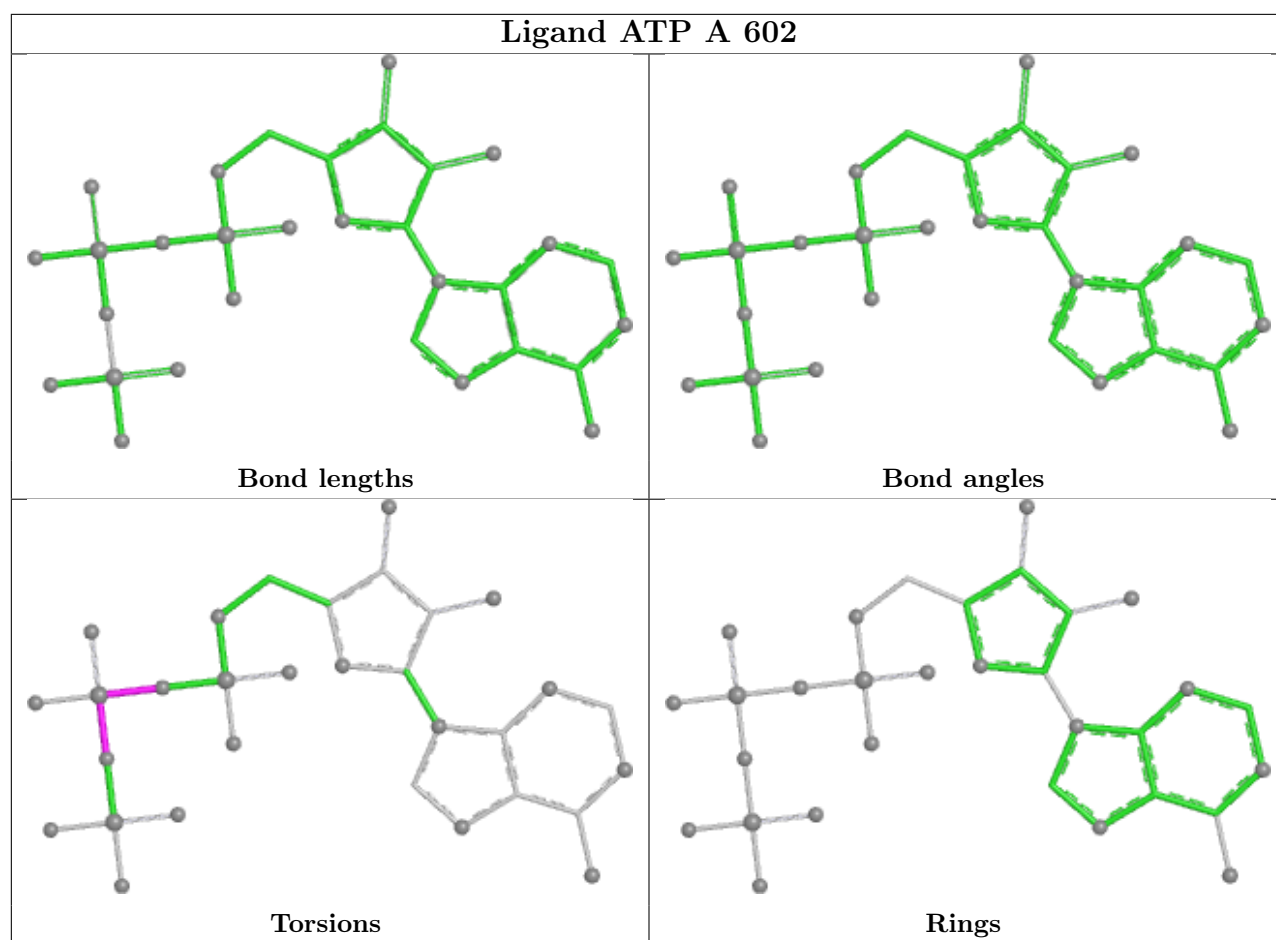


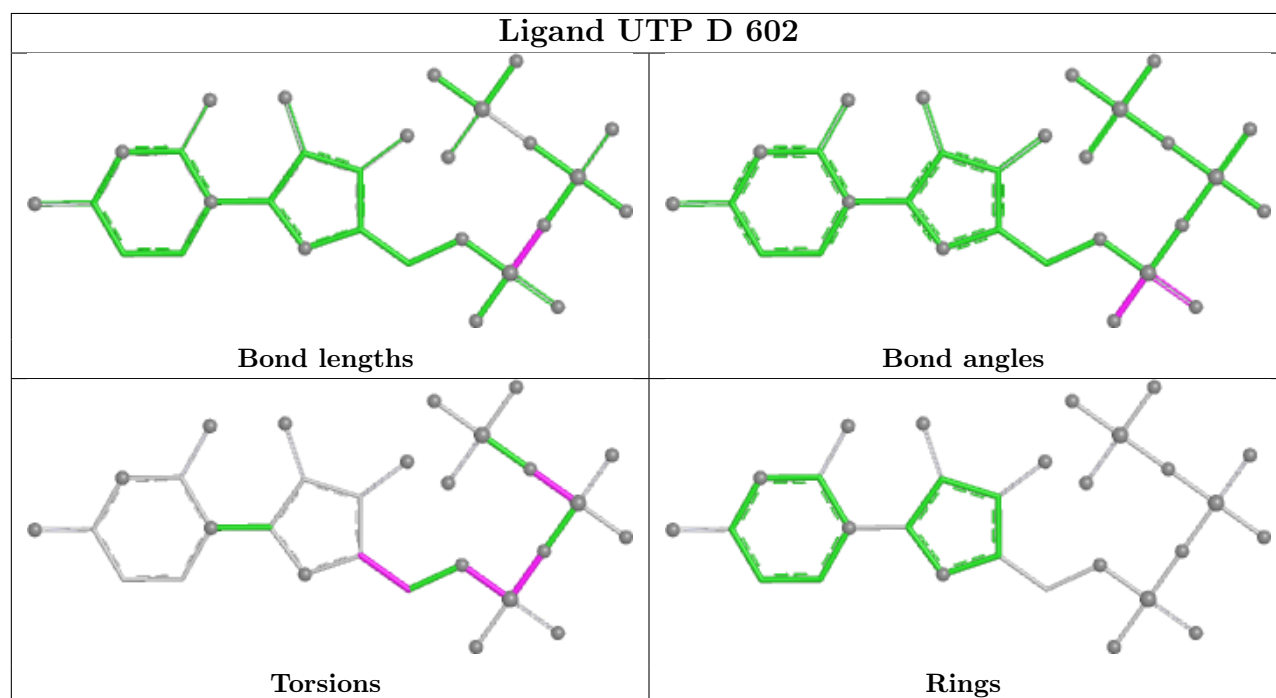
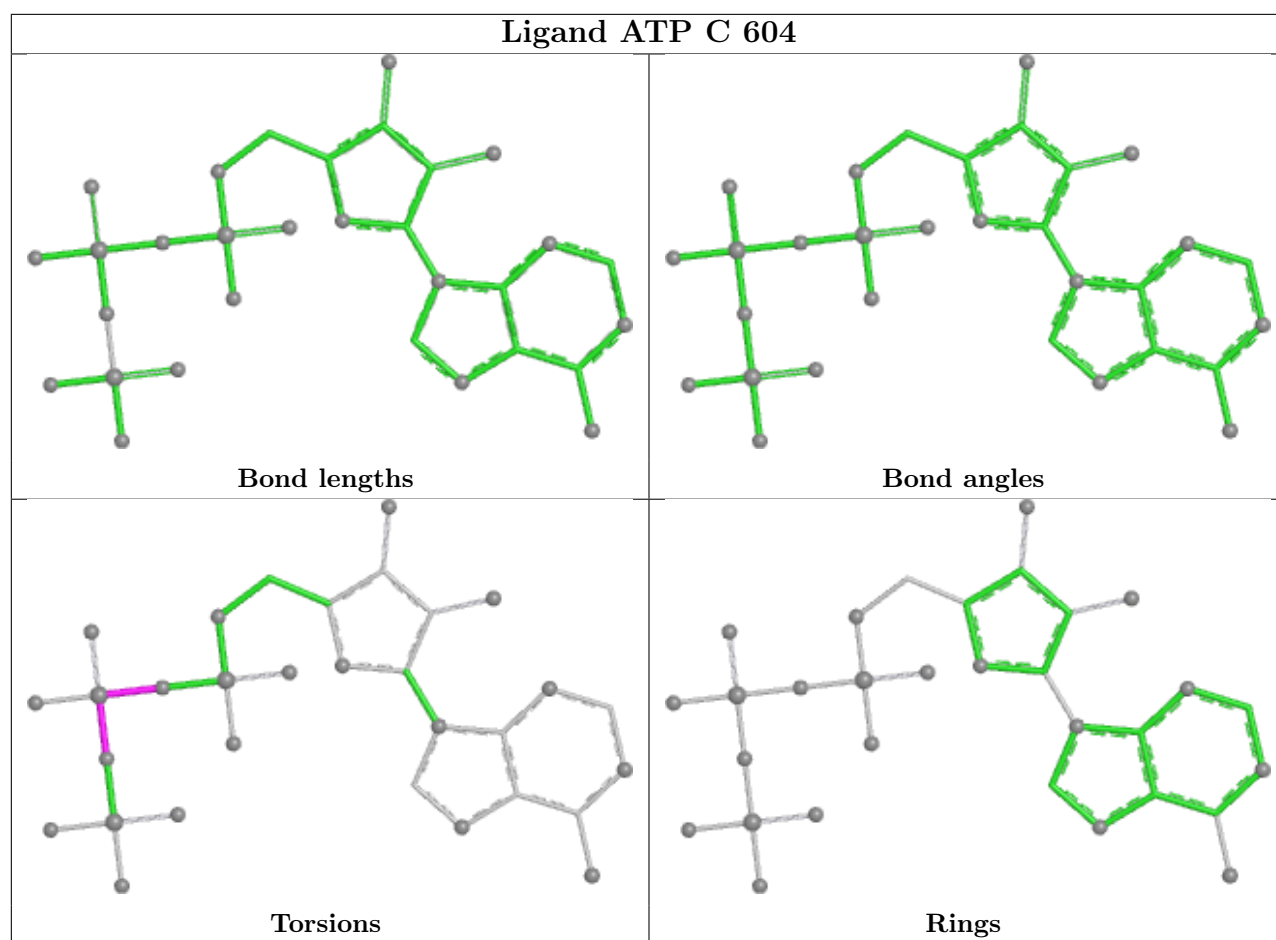












5.7 Other polymers [i](#)

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

All 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
1	F	443:ILE	C	456:THR	N	8.92
1	G	443:ILE	C	456:THR	N	8.92
1	H	443:ILE	C	456:THR	N	8.92
1	W	443:ILE	C	456:THR	N	8.92
1	X	443:ILE	C	456:THR	N	8.92
1	Y	443:ILE	C	456:THR	N	8.92
1	Z	443:ILE	C	456:THR	N	8.92

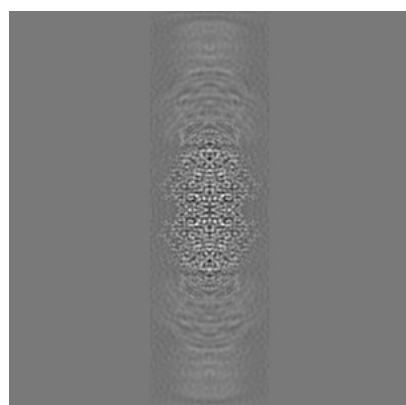
6 Map visualisation [i](#)

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.

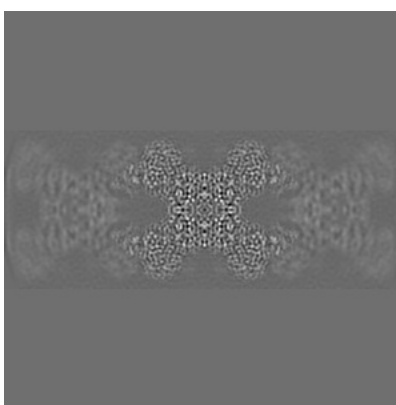
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

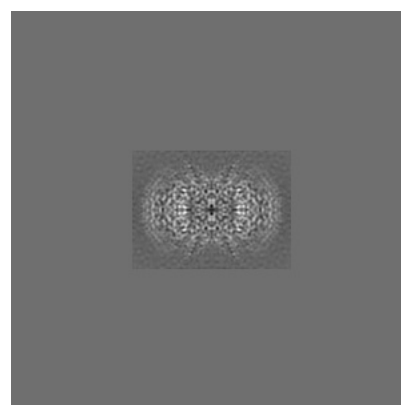
6.1.1 Primary map



X



Y

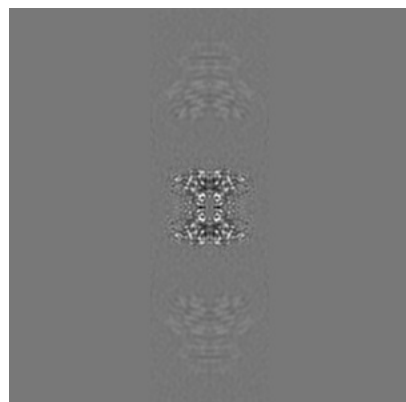


Z

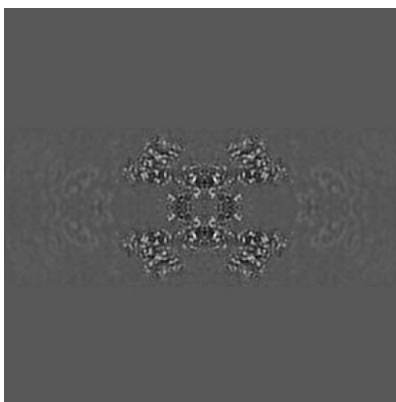
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

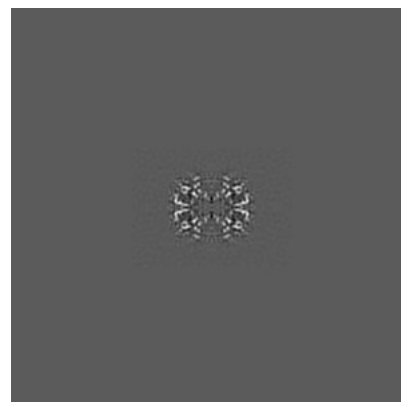
6.2.1 Primary map



X Index: 160



Y Index: 160

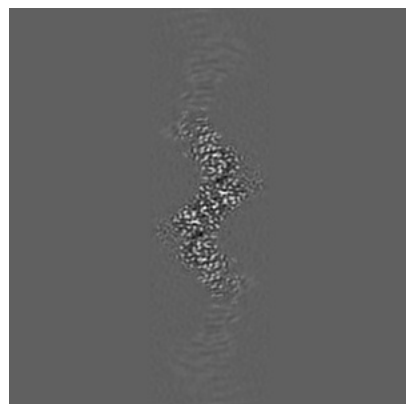


Z Index: 160

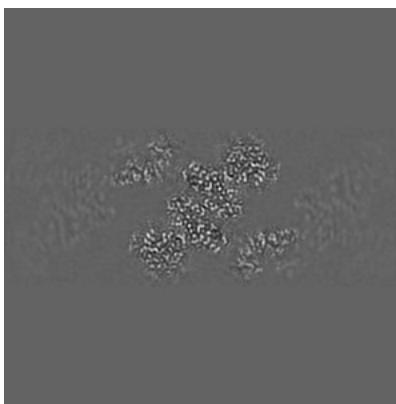
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

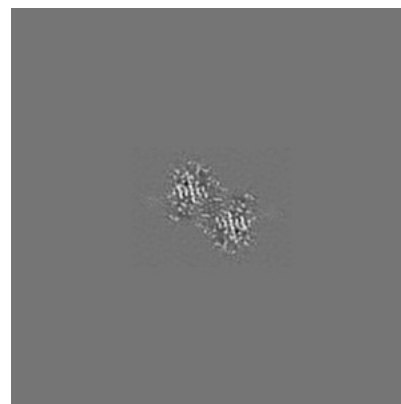
6.3.1 Primary map



X Index: 135



Y Index: 153

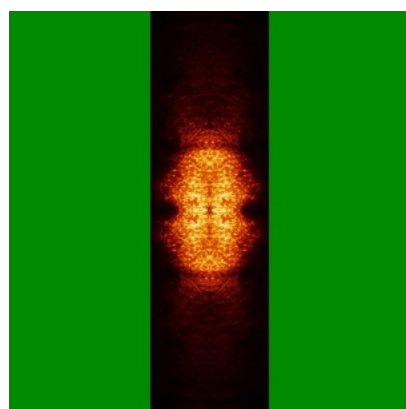


Z Index: 172

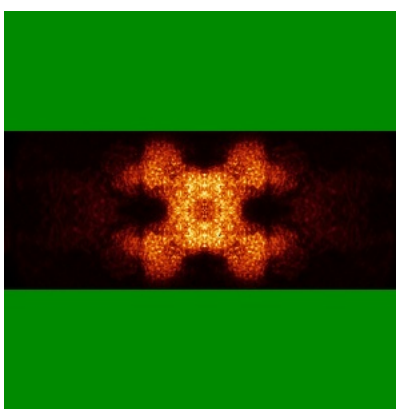
The images above show the largest variance slices of the map in three orthogonal directions.

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

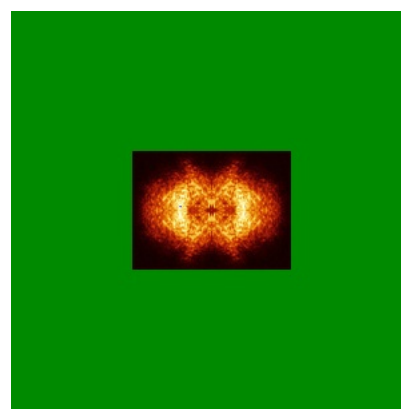
6.4.1 Primary map



X



Y

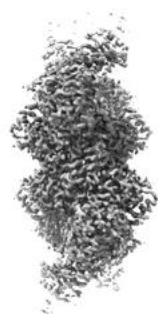


Z

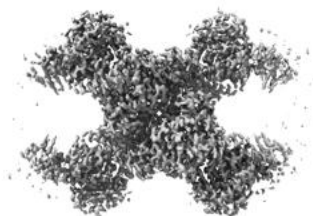
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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.

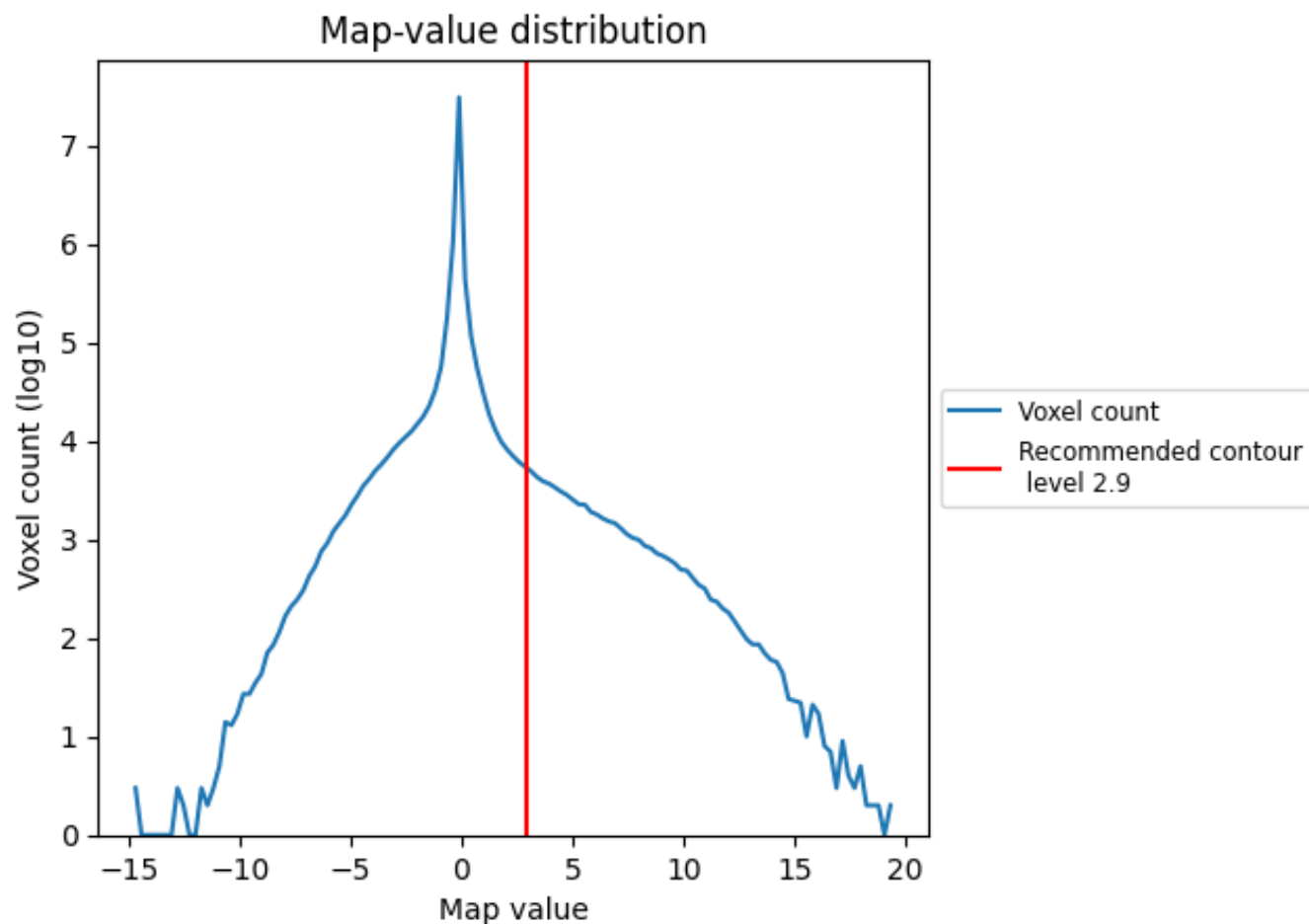
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

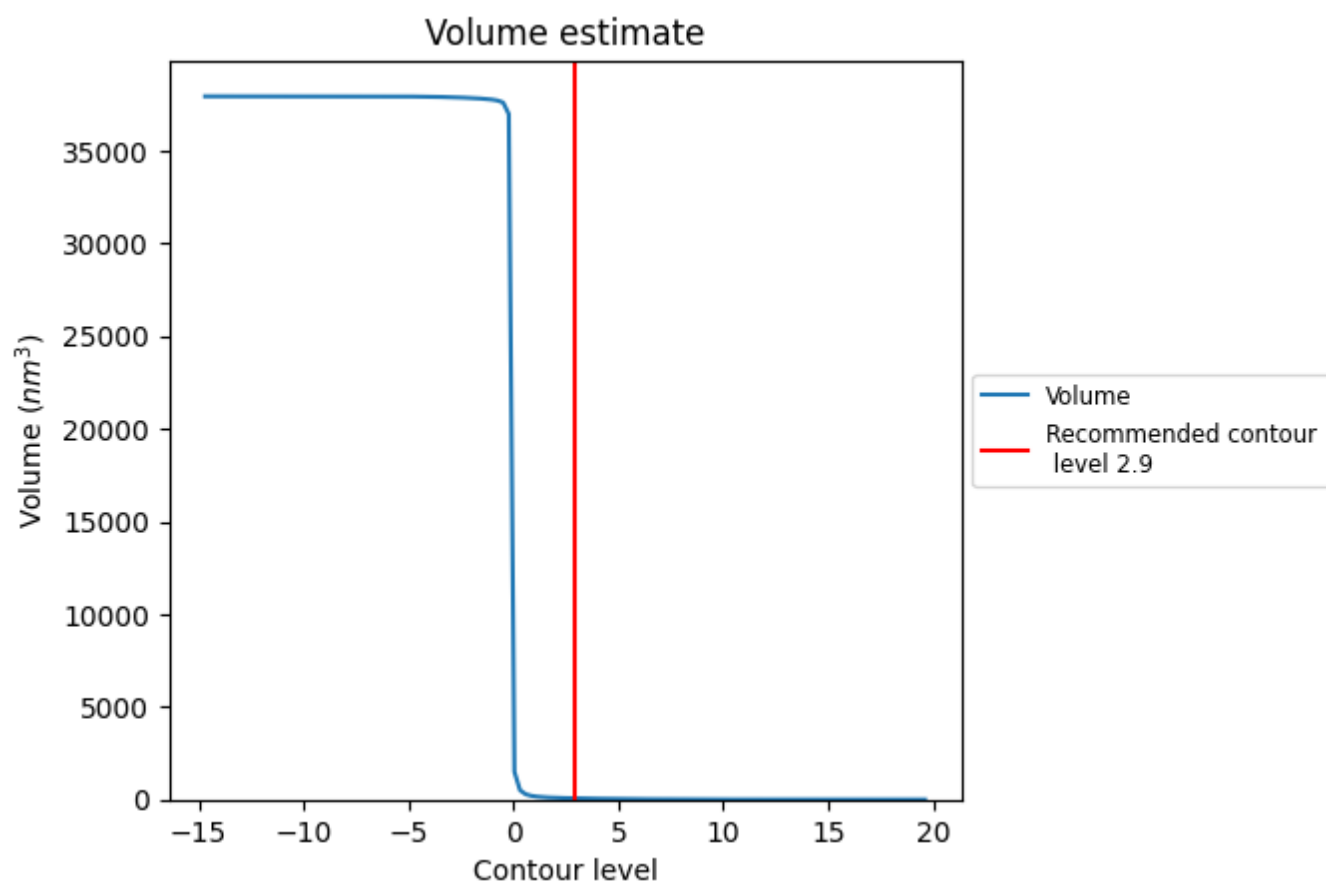
This section contains the results of statistical analysis of the map.

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.

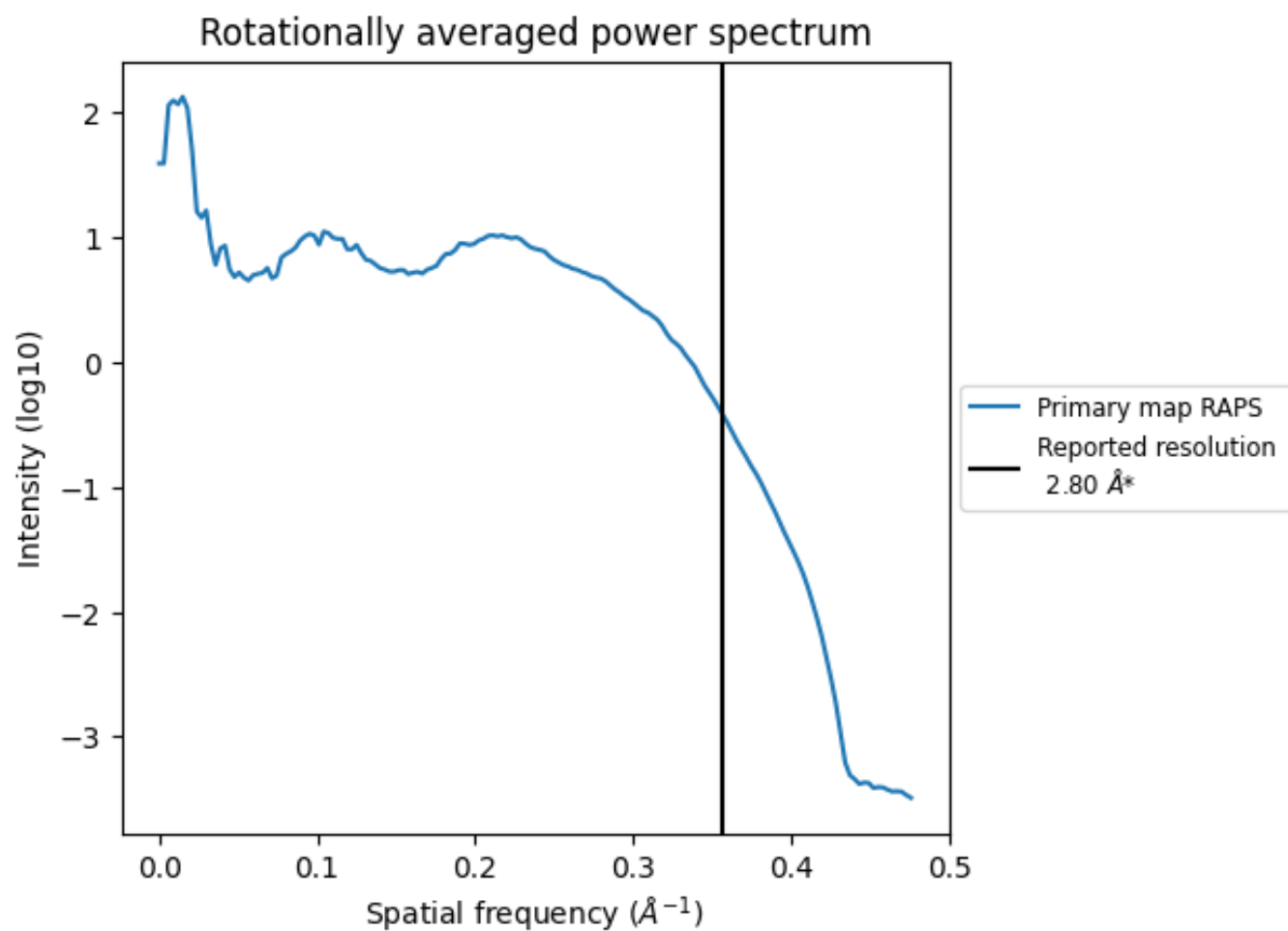
7.2 Volume estimate [i](#)



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 ⓘ



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

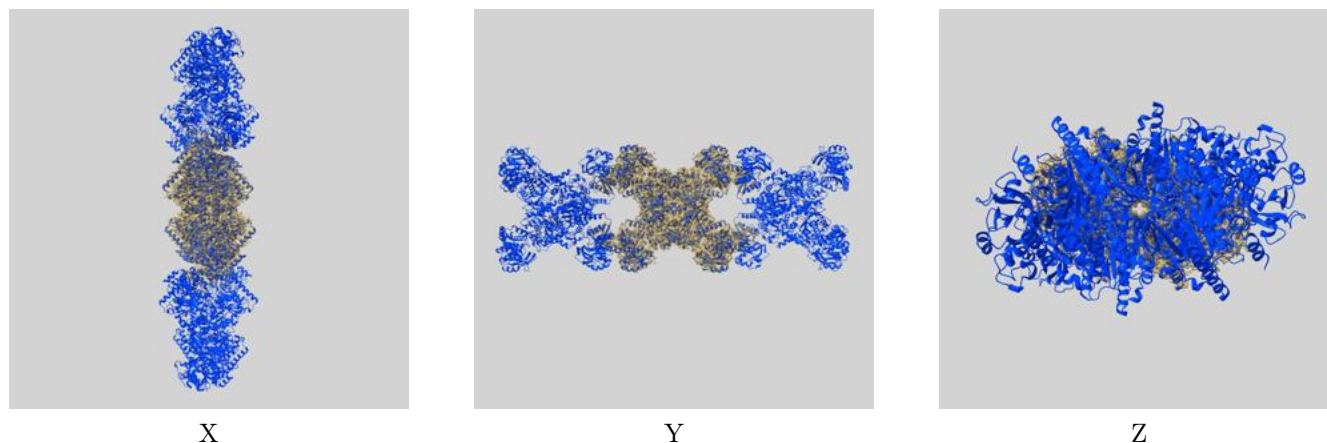
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

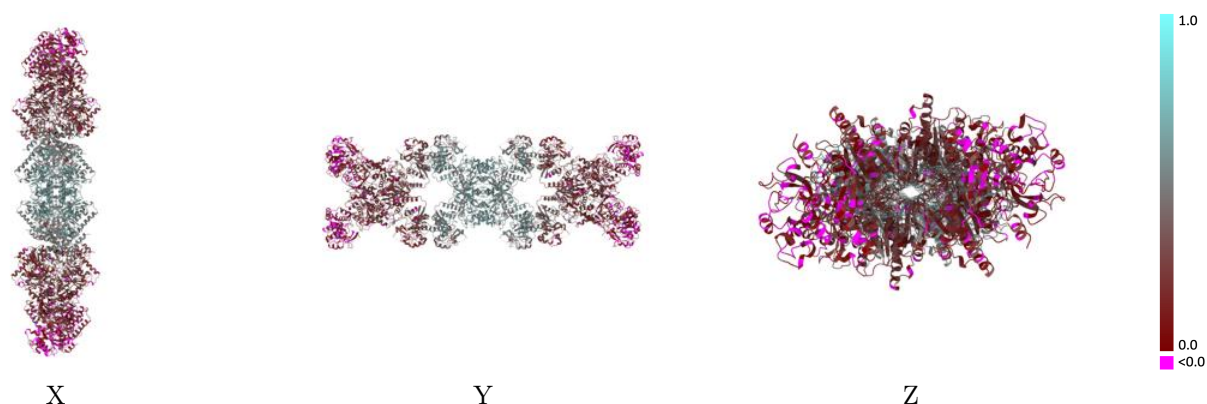
This section contains information regarding the fit between EMDB map EMD-24512 and PDB model 7RL0. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



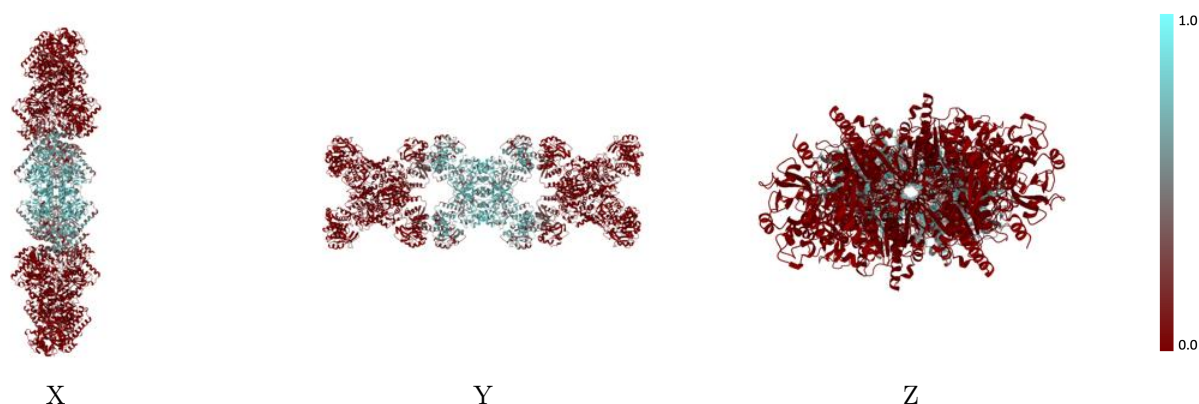
The images above show the 3D surface view of the map at the recommended contour level 2.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



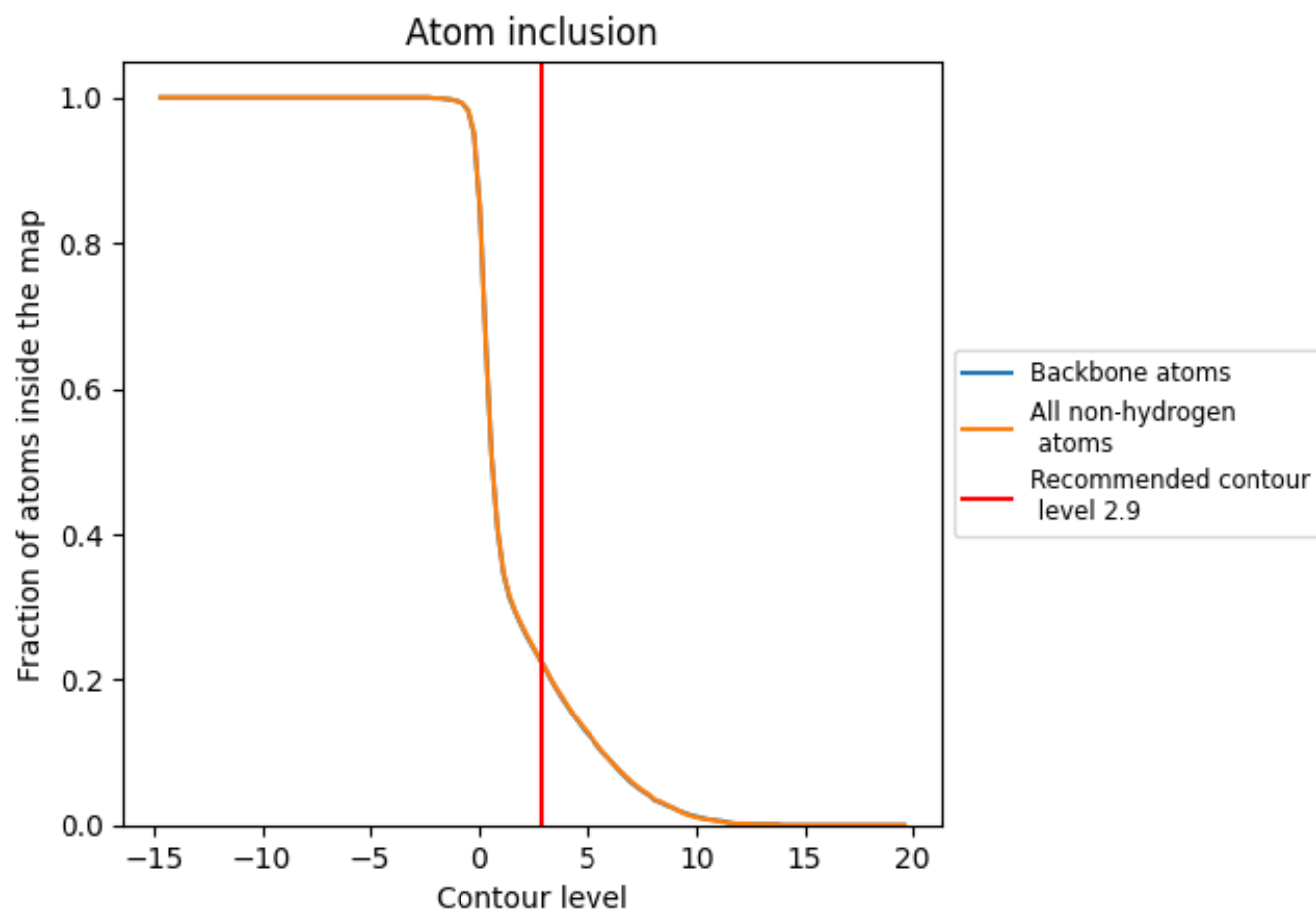
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

