



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:50 AM UTC

PDB ID : 5OCW / pdb_00005ocw
Title : Structure of Mycobacterium tuberculosis tryptophan synthase in space group F222
Authors : Fütterer, K.; Abrahams, K.; Cox, J.A.G.; Besra, G.S.
Deposited on : 2017-07-03
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

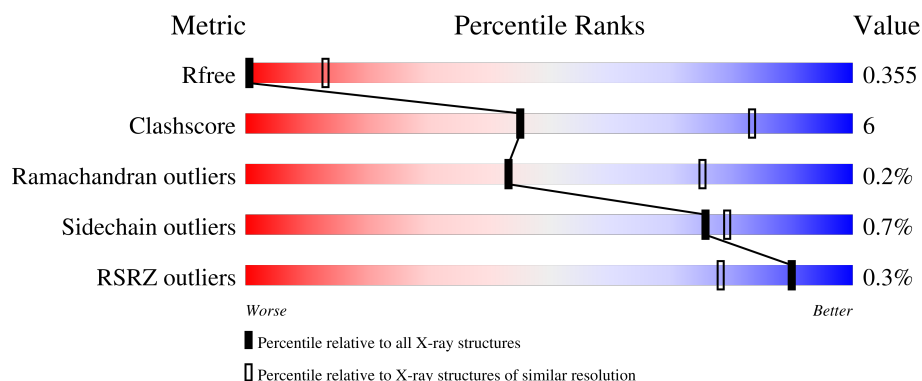
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



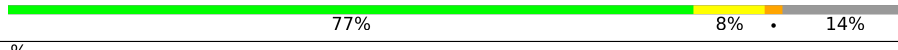
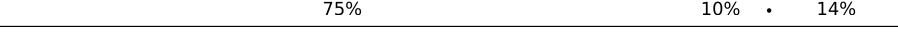
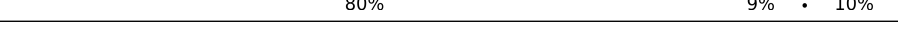
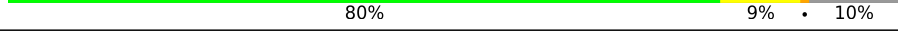
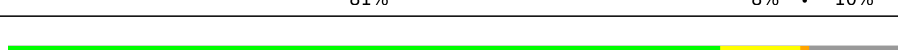
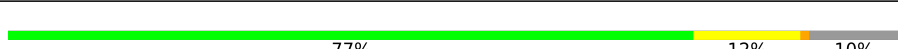
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	290	 79% 7% • 11%
1	C	290	 77% 7% • 14%
1	E	290	 78% 8% • 14%
1	G	290	 76% 9% • 14%
1	I	290	 77% 7% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	290	% 
1	M	290	
1	O	290	% 
1	Q	290	
1	S	290	
1	U	290	% 
1	W	290	
2	B	442	
2	D	442	
2	F	442	
2	H	442	
2	J	442	
2	L	442	% 
2	N	442	
2	P	442	
2	R	442	
2	T	442	
2	V	442	
2	X	442	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 57878 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1852	1159	335	353	5			
1	C	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	E	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	G	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	I	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	K	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	M	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	O	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	Q	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	S	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	U	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	W	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WFY1
A	-18	GLY	-	expression tag	UNP P9WFY1
A	-17	SER	-	expression tag	UNP P9WFY1
A	-16	SER	-	expression tag	UNP P9WFY1
A	-15	HIS	-	expression tag	UNP P9WFY1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P9WIFY1
A	-13	HIS	-	expression tag	UNP P9WIFY1
A	-12	HIS	-	expression tag	UNP P9WIFY1
A	-11	HIS	-	expression tag	UNP P9WIFY1
A	-10	HIS	-	expression tag	UNP P9WIFY1
A	-9	SER	-	expression tag	UNP P9WIFY1
A	-8	SER	-	expression tag	UNP P9WIFY1
A	-7	GLY	-	expression tag	UNP P9WIFY1
A	-6	LEU	-	expression tag	UNP P9WIFY1
A	-5	VAL	-	expression tag	UNP P9WIFY1
A	-4	PRO	-	expression tag	UNP P9WIFY1
A	-3	ARG	-	expression tag	UNP P9WIFY1
A	-2	GLY	-	expression tag	UNP P9WIFY1
A	-1	SER	-	expression tag	UNP P9WIFY1
A	0	HIS	-	expression tag	UNP P9WIFY1
C	-19	MET	-	initiating methionine	UNP P9WIFY1
C	-18	GLY	-	expression tag	UNP P9WIFY1
C	-17	SER	-	expression tag	UNP P9WIFY1
C	-16	SER	-	expression tag	UNP P9WIFY1
C	-15	HIS	-	expression tag	UNP P9WIFY1
C	-14	HIS	-	expression tag	UNP P9WIFY1
C	-13	HIS	-	expression tag	UNP P9WIFY1
C	-12	HIS	-	expression tag	UNP P9WIFY1
C	-11	HIS	-	expression tag	UNP P9WIFY1
C	-10	HIS	-	expression tag	UNP P9WIFY1
C	-9	SER	-	expression tag	UNP P9WIFY1
C	-8	SER	-	expression tag	UNP P9WIFY1
C	-7	GLY	-	expression tag	UNP P9WIFY1
C	-6	LEU	-	expression tag	UNP P9WIFY1
C	-5	VAL	-	expression tag	UNP P9WIFY1
C	-4	PRO	-	expression tag	UNP P9WIFY1
C	-3	ARG	-	expression tag	UNP P9WIFY1
C	-2	GLY	-	expression tag	UNP P9WIFY1
C	-1	SER	-	expression tag	UNP P9WIFY1
C	0	HIS	-	expression tag	UNP P9WIFY1
E	-19	MET	-	initiating methionine	UNP P9WIFY1
E	-18	GLY	-	expression tag	UNP P9WIFY1
E	-17	SER	-	expression tag	UNP P9WIFY1
E	-16	SER	-	expression tag	UNP P9WIFY1
E	-15	HIS	-	expression tag	UNP P9WIFY1
E	-14	HIS	-	expression tag	UNP P9WIFY1
E	-13	HIS	-	expression tag	UNP P9WIFY1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP P9WIFY1
E	-11	HIS	-	expression tag	UNP P9WIFY1
E	-10	HIS	-	expression tag	UNP P9WIFY1
E	-9	SER	-	expression tag	UNP P9WIFY1
E	-8	SER	-	expression tag	UNP P9WIFY1
E	-7	GLY	-	expression tag	UNP P9WIFY1
E	-6	LEU	-	expression tag	UNP P9WIFY1
E	-5	VAL	-	expression tag	UNP P9WIFY1
E	-4	PRO	-	expression tag	UNP P9WIFY1
E	-3	ARG	-	expression tag	UNP P9WIFY1
E	-2	GLY	-	expression tag	UNP P9WIFY1
E	-1	SER	-	expression tag	UNP P9WIFY1
E	0	HIS	-	expression tag	UNP P9WIFY1
G	-19	MET	-	initiating methionine	UNP P9WIFY1
G	-18	GLY	-	expression tag	UNP P9WIFY1
G	-17	SER	-	expression tag	UNP P9WIFY1
G	-16	SER	-	expression tag	UNP P9WIFY1
G	-15	HIS	-	expression tag	UNP P9WIFY1
G	-14	HIS	-	expression tag	UNP P9WIFY1
G	-13	HIS	-	expression tag	UNP P9WIFY1
G	-12	HIS	-	expression tag	UNP P9WIFY1
G	-11	HIS	-	expression tag	UNP P9WIFY1
G	-10	HIS	-	expression tag	UNP P9WIFY1
G	-9	SER	-	expression tag	UNP P9WIFY1
G	-8	SER	-	expression tag	UNP P9WIFY1
G	-7	GLY	-	expression tag	UNP P9WIFY1
G	-6	LEU	-	expression tag	UNP P9WIFY1
G	-5	VAL	-	expression tag	UNP P9WIFY1
G	-4	PRO	-	expression tag	UNP P9WIFY1
G	-3	ARG	-	expression tag	UNP P9WIFY1
G	-2	GLY	-	expression tag	UNP P9WIFY1
G	-1	SER	-	expression tag	UNP P9WIFY1
G	0	HIS	-	expression tag	UNP P9WIFY1
I	-19	MET	-	initiating methionine	UNP P9WIFY1
I	-18	GLY	-	expression tag	UNP P9WIFY1
I	-17	SER	-	expression tag	UNP P9WIFY1
I	-16	SER	-	expression tag	UNP P9WIFY1
I	-15	HIS	-	expression tag	UNP P9WIFY1
I	-14	HIS	-	expression tag	UNP P9WIFY1
I	-13	HIS	-	expression tag	UNP P9WIFY1
I	-12	HIS	-	expression tag	UNP P9WIFY1
I	-11	HIS	-	expression tag	UNP P9WIFY1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP P9WIFY1
I	-9	SER	-	expression tag	UNP P9WIFY1
I	-8	SER	-	expression tag	UNP P9WIFY1
I	-7	GLY	-	expression tag	UNP P9WIFY1
I	-6	LEU	-	expression tag	UNP P9WIFY1
I	-5	VAL	-	expression tag	UNP P9WIFY1
I	-4	PRO	-	expression tag	UNP P9WIFY1
I	-3	ARG	-	expression tag	UNP P9WIFY1
I	-2	GLY	-	expression tag	UNP P9WIFY1
I	-1	SER	-	expression tag	UNP P9WIFY1
I	0	HIS	-	expression tag	UNP P9WIFY1
K	-19	MET	-	initiating methionine	UNP P9WIFY1
K	-18	GLY	-	expression tag	UNP P9WIFY1
K	-17	SER	-	expression tag	UNP P9WIFY1
K	-16	SER	-	expression tag	UNP P9WIFY1
K	-15	HIS	-	expression tag	UNP P9WIFY1
K	-14	HIS	-	expression tag	UNP P9WIFY1
K	-13	HIS	-	expression tag	UNP P9WIFY1
K	-12	HIS	-	expression tag	UNP P9WIFY1
K	-11	HIS	-	expression tag	UNP P9WIFY1
K	-10	HIS	-	expression tag	UNP P9WIFY1
K	-9	SER	-	expression tag	UNP P9WIFY1
K	-8	SER	-	expression tag	UNP P9WIFY1
K	-7	GLY	-	expression tag	UNP P9WIFY1
K	-6	LEU	-	expression tag	UNP P9WIFY1
K	-5	VAL	-	expression tag	UNP P9WIFY1
K	-4	PRO	-	expression tag	UNP P9WIFY1
K	-3	ARG	-	expression tag	UNP P9WIFY1
K	-2	GLY	-	expression tag	UNP P9WIFY1
K	-1	SER	-	expression tag	UNP P9WIFY1
K	0	HIS	-	expression tag	UNP P9WIFY1
M	-19	MET	-	initiating methionine	UNP P9WIFY1
M	-18	GLY	-	expression tag	UNP P9WIFY1
M	-17	SER	-	expression tag	UNP P9WIFY1
M	-16	SER	-	expression tag	UNP P9WIFY1
M	-15	HIS	-	expression tag	UNP P9WIFY1
M	-14	HIS	-	expression tag	UNP P9WIFY1
M	-13	HIS	-	expression tag	UNP P9WIFY1
M	-12	HIS	-	expression tag	UNP P9WIFY1
M	-11	HIS	-	expression tag	UNP P9WIFY1
M	-10	HIS	-	expression tag	UNP P9WIFY1
M	-9	SER	-	expression tag	UNP P9WIFY1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	SER	-	expression tag	UNP P9WIFY1
M	-7	GLY	-	expression tag	UNP P9WIFY1
M	-6	LEU	-	expression tag	UNP P9WIFY1
M	-5	VAL	-	expression tag	UNP P9WIFY1
M	-4	PRO	-	expression tag	UNP P9WIFY1
M	-3	ARG	-	expression tag	UNP P9WIFY1
M	-2	GLY	-	expression tag	UNP P9WIFY1
M	-1	SER	-	expression tag	UNP P9WIFY1
M	0	HIS	-	expression tag	UNP P9WIFY1
O	-19	MET	-	initiating methionine	UNP P9WIFY1
O	-18	GLY	-	expression tag	UNP P9WIFY1
O	-17	SER	-	expression tag	UNP P9WIFY1
O	-16	SER	-	expression tag	UNP P9WIFY1
O	-15	HIS	-	expression tag	UNP P9WIFY1
O	-14	HIS	-	expression tag	UNP P9WIFY1
O	-13	HIS	-	expression tag	UNP P9WIFY1
O	-12	HIS	-	expression tag	UNP P9WIFY1
O	-11	HIS	-	expression tag	UNP P9WIFY1
O	-10	HIS	-	expression tag	UNP P9WIFY1
O	-9	SER	-	expression tag	UNP P9WIFY1
O	-8	SER	-	expression tag	UNP P9WIFY1
O	-7	GLY	-	expression tag	UNP P9WIFY1
O	-6	LEU	-	expression tag	UNP P9WIFY1
O	-5	VAL	-	expression tag	UNP P9WIFY1
O	-4	PRO	-	expression tag	UNP P9WIFY1
O	-3	ARG	-	expression tag	UNP P9WIFY1
O	-2	GLY	-	expression tag	UNP P9WIFY1
O	-1	SER	-	expression tag	UNP P9WIFY1
O	0	HIS	-	expression tag	UNP P9WIFY1
Q	-19	MET	-	initiating methionine	UNP P9WIFY1
Q	-18	GLY	-	expression tag	UNP P9WIFY1
Q	-17	SER	-	expression tag	UNP P9WIFY1
Q	-16	SER	-	expression tag	UNP P9WIFY1
Q	-15	HIS	-	expression tag	UNP P9WIFY1
Q	-14	HIS	-	expression tag	UNP P9WIFY1
Q	-13	HIS	-	expression tag	UNP P9WIFY1
Q	-12	HIS	-	expression tag	UNP P9WIFY1
Q	-11	HIS	-	expression tag	UNP P9WIFY1
Q	-10	HIS	-	expression tag	UNP P9WIFY1
Q	-9	SER	-	expression tag	UNP P9WIFY1
Q	-8	SER	-	expression tag	UNP P9WIFY1
Q	-7	GLY	-	expression tag	UNP P9WIFY1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Q	-6	LEU	-	expression tag	UNP P9WIFY1
Q	-5	VAL	-	expression tag	UNP P9WIFY1
Q	-4	PRO	-	expression tag	UNP P9WIFY1
Q	-3	ARG	-	expression tag	UNP P9WIFY1
Q	-2	GLY	-	expression tag	UNP P9WIFY1
Q	-1	SER	-	expression tag	UNP P9WIFY1
Q	0	HIS	-	expression tag	UNP P9WIFY1
S	-19	MET	-	initiating methionine	UNP P9WIFY1
S	-18	GLY	-	expression tag	UNP P9WIFY1
S	-17	SER	-	expression tag	UNP P9WIFY1
S	-16	SER	-	expression tag	UNP P9WIFY1
S	-15	HIS	-	expression tag	UNP P9WIFY1
S	-14	HIS	-	expression tag	UNP P9WIFY1
S	-13	HIS	-	expression tag	UNP P9WIFY1
S	-12	HIS	-	expression tag	UNP P9WIFY1
S	-11	HIS	-	expression tag	UNP P9WIFY1
S	-10	HIS	-	expression tag	UNP P9WIFY1
S	-9	SER	-	expression tag	UNP P9WIFY1
S	-8	SER	-	expression tag	UNP P9WIFY1
S	-7	GLY	-	expression tag	UNP P9WIFY1
S	-6	LEU	-	expression tag	UNP P9WIFY1
S	-5	VAL	-	expression tag	UNP P9WIFY1
S	-4	PRO	-	expression tag	UNP P9WIFY1
S	-3	ARG	-	expression tag	UNP P9WIFY1
S	-2	GLY	-	expression tag	UNP P9WIFY1
S	-1	SER	-	expression tag	UNP P9WIFY1
S	0	HIS	-	expression tag	UNP P9WIFY1
U	-19	MET	-	initiating methionine	UNP P9WIFY1
U	-18	GLY	-	expression tag	UNP P9WIFY1
U	-17	SER	-	expression tag	UNP P9WIFY1
U	-16	SER	-	expression tag	UNP P9WIFY1
U	-15	HIS	-	expression tag	UNP P9WIFY1
U	-14	HIS	-	expression tag	UNP P9WIFY1
U	-13	HIS	-	expression tag	UNP P9WIFY1
U	-12	HIS	-	expression tag	UNP P9WIFY1
U	-11	HIS	-	expression tag	UNP P9WIFY1
U	-10	HIS	-	expression tag	UNP P9WIFY1
U	-9	SER	-	expression tag	UNP P9WIFY1
U	-8	SER	-	expression tag	UNP P9WIFY1
U	-7	GLY	-	expression tag	UNP P9WIFY1
U	-6	LEU	-	expression tag	UNP P9WIFY1
U	-5	VAL	-	expression tag	UNP P9WIFY1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	-4	PRO	-	expression tag	UNP P9WIFY1
U	-3	ARG	-	expression tag	UNP P9WIFY1
U	-2	GLY	-	expression tag	UNP P9WIFY1
U	-1	SER	-	expression tag	UNP P9WIFY1
U	0	HIS	-	expression tag	UNP P9WIFY1
W	-19	MET	-	initiating methionine	UNP P9WIFY1
W	-18	GLY	-	expression tag	UNP P9WIFY1
W	-17	SER	-	expression tag	UNP P9WIFY1
W	-16	SER	-	expression tag	UNP P9WIFY1
W	-15	HIS	-	expression tag	UNP P9WIFY1
W	-14	HIS	-	expression tag	UNP P9WIFY1
W	-13	HIS	-	expression tag	UNP P9WIFY1
W	-12	HIS	-	expression tag	UNP P9WIFY1
W	-11	HIS	-	expression tag	UNP P9WIFY1
W	-10	HIS	-	expression tag	UNP P9WIFY1
W	-9	SER	-	expression tag	UNP P9WIFY1
W	-8	SER	-	expression tag	UNP P9WIFY1
W	-7	GLY	-	expression tag	UNP P9WIFY1
W	-6	LEU	-	expression tag	UNP P9WIFY1
W	-5	VAL	-	expression tag	UNP P9WIFY1
W	-4	PRO	-	expression tag	UNP P9WIFY1
W	-3	ARG	-	expression tag	UNP P9WIFY1
W	-2	GLY	-	expression tag	UNP P9WIFY1
W	-1	SER	-	expression tag	UNP P9WIFY1
W	0	HIS	-	expression tag	UNP P9WIFY1

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	D	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	F	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	H	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	J	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	L	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	N	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	R	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	T	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	V	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	X	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	MET	-	initiating methionine	UNP P9WFX9
B	-30	GLY	-	expression tag	UNP P9WFX9
B	-29	SER	-	expression tag	UNP P9WFX9
B	-28	SER	-	expression tag	UNP P9WFX9
B	-27	HIS	-	expression tag	UNP P9WFX9
B	-26	HIS	-	expression tag	UNP P9WFX9
B	-25	HIS	-	expression tag	UNP P9WFX9
B	-24	HIS	-	expression tag	UNP P9WFX9
B	-23	HIS	-	expression tag	UNP P9WFX9
B	-22	HIS	-	expression tag	UNP P9WFX9
B	-21	SER	-	expression tag	UNP P9WFX9
B	-20	SER	-	expression tag	UNP P9WFX9
B	-19	GLY	-	expression tag	UNP P9WFX9
B	-18	LEU	-	expression tag	UNP P9WFX9
B	-17	VAL	-	expression tag	UNP P9WFX9
B	-16	PRO	-	expression tag	UNP P9WFX9
B	-15	ARG	-	expression tag	UNP P9WFX9
B	-14	GLY	-	expression tag	UNP P9WFX9
B	-13	SER	-	expression tag	UNP P9WFX9
B	-12	HIS	-	expression tag	UNP P9WFX9
D	-31	MET	-	initiating methionine	UNP P9WFX9
D	-30	GLY	-	expression tag	UNP P9WFX9
D	-29	SER	-	expression tag	UNP P9WFX9
D	-28	SER	-	expression tag	UNP P9WFX9
D	-27	HIS	-	expression tag	UNP P9WFX9
D	-26	HIS	-	expression tag	UNP P9WFX9
D	-25	HIS	-	expression tag	UNP P9WFX9
D	-24	HIS	-	expression tag	UNP P9WFX9
D	-23	HIS	-	expression tag	UNP P9WFX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-22	HIS	-	expression tag	UNP P9WFX9
D	-21	SER	-	expression tag	UNP P9WFX9
D	-20	SER	-	expression tag	UNP P9WFX9
D	-19	GLY	-	expression tag	UNP P9WFX9
D	-18	LEU	-	expression tag	UNP P9WFX9
D	-17	VAL	-	expression tag	UNP P9WFX9
D	-16	PRO	-	expression tag	UNP P9WFX9
D	-15	ARG	-	expression tag	UNP P9WFX9
D	-14	GLY	-	expression tag	UNP P9WFX9
D	-13	SER	-	expression tag	UNP P9WFX9
D	-12	HIS	-	expression tag	UNP P9WFX9
F	-31	MET	-	initiating methionine	UNP P9WFX9
F	-30	GLY	-	expression tag	UNP P9WFX9
F	-29	SER	-	expression tag	UNP P9WFX9
F	-28	SER	-	expression tag	UNP P9WFX9
F	-27	HIS	-	expression tag	UNP P9WFX9
F	-26	HIS	-	expression tag	UNP P9WFX9
F	-25	HIS	-	expression tag	UNP P9WFX9
F	-24	HIS	-	expression tag	UNP P9WFX9
F	-23	HIS	-	expression tag	UNP P9WFX9
F	-22	HIS	-	expression tag	UNP P9WFX9
F	-21	SER	-	expression tag	UNP P9WFX9
F	-20	SER	-	expression tag	UNP P9WFX9
F	-19	GLY	-	expression tag	UNP P9WFX9
F	-18	LEU	-	expression tag	UNP P9WFX9
F	-17	VAL	-	expression tag	UNP P9WFX9
F	-16	PRO	-	expression tag	UNP P9WFX9
F	-15	ARG	-	expression tag	UNP P9WFX9
F	-14	GLY	-	expression tag	UNP P9WFX9
F	-13	SER	-	expression tag	UNP P9WFX9
F	-12	HIS	-	expression tag	UNP P9WFX9
H	-31	MET	-	initiating methionine	UNP P9WFX9
H	-30	GLY	-	expression tag	UNP P9WFX9
H	-29	SER	-	expression tag	UNP P9WFX9
H	-28	SER	-	expression tag	UNP P9WFX9
H	-27	HIS	-	expression tag	UNP P9WFX9
H	-26	HIS	-	expression tag	UNP P9WFX9
H	-25	HIS	-	expression tag	UNP P9WFX9
H	-24	HIS	-	expression tag	UNP P9WFX9
H	-23	HIS	-	expression tag	UNP P9WFX9
H	-22	HIS	-	expression tag	UNP P9WFX9
H	-21	SER	-	expression tag	UNP P9WFX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	SER	-	expression tag	UNP P9WFX9
H	-19	GLY	-	expression tag	UNP P9WFX9
H	-18	LEU	-	expression tag	UNP P9WFX9
H	-17	VAL	-	expression tag	UNP P9WFX9
H	-16	PRO	-	expression tag	UNP P9WFX9
H	-15	ARG	-	expression tag	UNP P9WFX9
H	-14	GLY	-	expression tag	UNP P9WFX9
H	-13	SER	-	expression tag	UNP P9WFX9
H	-12	HIS	-	expression tag	UNP P9WFX9
J	-31	MET	-	initiating methionine	UNP P9WFX9
J	-30	GLY	-	expression tag	UNP P9WFX9
J	-29	SER	-	expression tag	UNP P9WFX9
J	-28	SER	-	expression tag	UNP P9WFX9
J	-27	HIS	-	expression tag	UNP P9WFX9
J	-26	HIS	-	expression tag	UNP P9WFX9
J	-25	HIS	-	expression tag	UNP P9WFX9
J	-24	HIS	-	expression tag	UNP P9WFX9
J	-23	HIS	-	expression tag	UNP P9WFX9
J	-22	HIS	-	expression tag	UNP P9WFX9
J	-21	SER	-	expression tag	UNP P9WFX9
J	-20	SER	-	expression tag	UNP P9WFX9
J	-19	GLY	-	expression tag	UNP P9WFX9
J	-18	LEU	-	expression tag	UNP P9WFX9
J	-17	VAL	-	expression tag	UNP P9WFX9
J	-16	PRO	-	expression tag	UNP P9WFX9
J	-15	ARG	-	expression tag	UNP P9WFX9
J	-14	GLY	-	expression tag	UNP P9WFX9
J	-13	SER	-	expression tag	UNP P9WFX9
J	-12	HIS	-	expression tag	UNP P9WFX9
L	-31	MET	-	initiating methionine	UNP P9WFX9
L	-30	GLY	-	expression tag	UNP P9WFX9
L	-29	SER	-	expression tag	UNP P9WFX9
L	-28	SER	-	expression tag	UNP P9WFX9
L	-27	HIS	-	expression tag	UNP P9WFX9
L	-26	HIS	-	expression tag	UNP P9WFX9
L	-25	HIS	-	expression tag	UNP P9WFX9
L	-24	HIS	-	expression tag	UNP P9WFX9
L	-23	HIS	-	expression tag	UNP P9WFX9
L	-22	HIS	-	expression tag	UNP P9WFX9
L	-21	SER	-	expression tag	UNP P9WFX9
L	-20	SER	-	expression tag	UNP P9WFX9
L	-19	GLY	-	expression tag	UNP P9WFX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-18	LEU	-	expression tag	UNP P9WFX9
L	-17	VAL	-	expression tag	UNP P9WFX9
L	-16	PRO	-	expression tag	UNP P9WFX9
L	-15	ARG	-	expression tag	UNP P9WFX9
L	-14	GLY	-	expression tag	UNP P9WFX9
L	-13	SER	-	expression tag	UNP P9WFX9
L	-12	HIS	-	expression tag	UNP P9WFX9
N	-31	MET	-	initiating methionine	UNP P9WFX9
N	-30	GLY	-	expression tag	UNP P9WFX9
N	-29	SER	-	expression tag	UNP P9WFX9
N	-28	SER	-	expression tag	UNP P9WFX9
N	-27	HIS	-	expression tag	UNP P9WFX9
N	-26	HIS	-	expression tag	UNP P9WFX9
N	-25	HIS	-	expression tag	UNP P9WFX9
N	-24	HIS	-	expression tag	UNP P9WFX9
N	-23	HIS	-	expression tag	UNP P9WFX9
N	-22	HIS	-	expression tag	UNP P9WFX9
N	-21	SER	-	expression tag	UNP P9WFX9
N	-20	SER	-	expression tag	UNP P9WFX9
N	-19	GLY	-	expression tag	UNP P9WFX9
N	-18	LEU	-	expression tag	UNP P9WFX9
N	-17	VAL	-	expression tag	UNP P9WFX9
N	-16	PRO	-	expression tag	UNP P9WFX9
N	-15	ARG	-	expression tag	UNP P9WFX9
N	-14	GLY	-	expression tag	UNP P9WFX9
N	-13	SER	-	expression tag	UNP P9WFX9
N	-12	HIS	-	expression tag	UNP P9WFX9
P	-31	MET	-	initiating methionine	UNP P9WFX9
P	-30	GLY	-	expression tag	UNP P9WFX9
P	-29	SER	-	expression tag	UNP P9WFX9
P	-28	SER	-	expression tag	UNP P9WFX9
P	-27	HIS	-	expression tag	UNP P9WFX9
P	-26	HIS	-	expression tag	UNP P9WFX9
P	-25	HIS	-	expression tag	UNP P9WFX9
P	-24	HIS	-	expression tag	UNP P9WFX9
P	-23	HIS	-	expression tag	UNP P9WFX9
P	-22	HIS	-	expression tag	UNP P9WFX9
P	-21	SER	-	expression tag	UNP P9WFX9
P	-20	SER	-	expression tag	UNP P9WFX9
P	-19	GLY	-	expression tag	UNP P9WFX9
P	-18	LEU	-	expression tag	UNP P9WFX9
P	-17	VAL	-	expression tag	UNP P9WFX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	-16	PRO	-	expression tag	UNP P9WFX9
P	-15	ARG	-	expression tag	UNP P9WFX9
P	-14	GLY	-	expression tag	UNP P9WFX9
P	-13	SER	-	expression tag	UNP P9WFX9
P	-12	HIS	-	expression tag	UNP P9WFX9
R	-31	MET	-	initiating methionine	UNP P9WFX9
R	-30	GLY	-	expression tag	UNP P9WFX9
R	-29	SER	-	expression tag	UNP P9WFX9
R	-28	SER	-	expression tag	UNP P9WFX9
R	-27	HIS	-	expression tag	UNP P9WFX9
R	-26	HIS	-	expression tag	UNP P9WFX9
R	-25	HIS	-	expression tag	UNP P9WFX9
R	-24	HIS	-	expression tag	UNP P9WFX9
R	-23	HIS	-	expression tag	UNP P9WFX9
R	-22	HIS	-	expression tag	UNP P9WFX9
R	-21	SER	-	expression tag	UNP P9WFX9
R	-20	SER	-	expression tag	UNP P9WFX9
R	-19	GLY	-	expression tag	UNP P9WFX9
R	-18	LEU	-	expression tag	UNP P9WFX9
R	-17	VAL	-	expression tag	UNP P9WFX9
R	-16	PRO	-	expression tag	UNP P9WFX9
R	-15	ARG	-	expression tag	UNP P9WFX9
R	-14	GLY	-	expression tag	UNP P9WFX9
R	-13	SER	-	expression tag	UNP P9WFX9
R	-12	HIS	-	expression tag	UNP P9WFX9
T	-31	MET	-	initiating methionine	UNP P9WFX9
T	-30	GLY	-	expression tag	UNP P9WFX9
T	-29	SER	-	expression tag	UNP P9WFX9
T	-28	SER	-	expression tag	UNP P9WFX9
T	-27	HIS	-	expression tag	UNP P9WFX9
T	-26	HIS	-	expression tag	UNP P9WFX9
T	-25	HIS	-	expression tag	UNP P9WFX9
T	-24	HIS	-	expression tag	UNP P9WFX9
T	-23	HIS	-	expression tag	UNP P9WFX9
T	-22	HIS	-	expression tag	UNP P9WFX9
T	-21	SER	-	expression tag	UNP P9WFX9
T	-20	SER	-	expression tag	UNP P9WFX9
T	-19	GLY	-	expression tag	UNP P9WFX9
T	-18	LEU	-	expression tag	UNP P9WFX9
T	-17	VAL	-	expression tag	UNP P9WFX9
T	-16	PRO	-	expression tag	UNP P9WFX9
T	-15	ARG	-	expression tag	UNP P9WFX9

Continued on next page...

Continued from previous page...

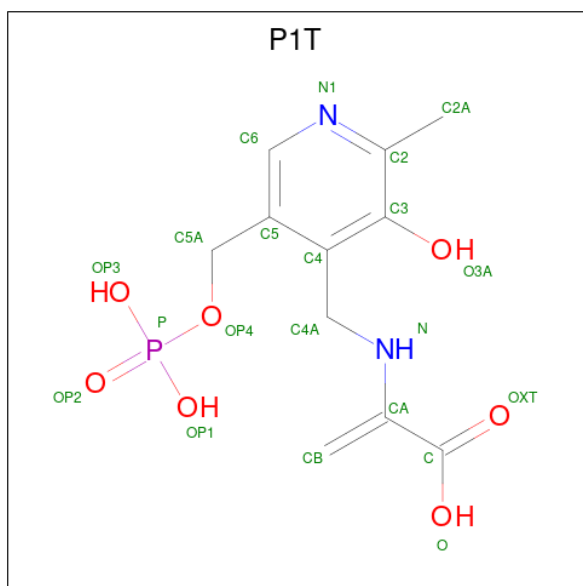
Chain	Residue	Modelled	Actual	Comment	Reference
T	-14	GLY	-	expression tag	UNP P9WFX9
T	-13	SER	-	expression tag	UNP P9WFX9
T	-12	HIS	-	expression tag	UNP P9WFX9
V	-31	MET	-	initiating methionine	UNP P9WFX9
V	-30	GLY	-	expression tag	UNP P9WFX9
V	-29	SER	-	expression tag	UNP P9WFX9
V	-28	SER	-	expression tag	UNP P9WFX9
V	-27	HIS	-	expression tag	UNP P9WFX9
V	-26	HIS	-	expression tag	UNP P9WFX9
V	-25	HIS	-	expression tag	UNP P9WFX9
V	-24	HIS	-	expression tag	UNP P9WFX9
V	-23	HIS	-	expression tag	UNP P9WFX9
V	-22	HIS	-	expression tag	UNP P9WFX9
V	-21	SER	-	expression tag	UNP P9WFX9
V	-20	SER	-	expression tag	UNP P9WFX9
V	-19	GLY	-	expression tag	UNP P9WFX9
V	-18	LEU	-	expression tag	UNP P9WFX9
V	-17	VAL	-	expression tag	UNP P9WFX9
V	-16	PRO	-	expression tag	UNP P9WFX9
V	-15	ARG	-	expression tag	UNP P9WFX9
V	-14	GLY	-	expression tag	UNP P9WFX9
V	-13	SER	-	expression tag	UNP P9WFX9
V	-12	HIS	-	expression tag	UNP P9WFX9
X	-31	MET	-	initiating methionine	UNP P9WFX9
X	-30	GLY	-	expression tag	UNP P9WFX9
X	-29	SER	-	expression tag	UNP P9WFX9
X	-28	SER	-	expression tag	UNP P9WFX9
X	-27	HIS	-	expression tag	UNP P9WFX9
X	-26	HIS	-	expression tag	UNP P9WFX9
X	-25	HIS	-	expression tag	UNP P9WFX9
X	-24	HIS	-	expression tag	UNP P9WFX9
X	-23	HIS	-	expression tag	UNP P9WFX9
X	-22	HIS	-	expression tag	UNP P9WFX9
X	-21	SER	-	expression tag	UNP P9WFX9
X	-20	SER	-	expression tag	UNP P9WFX9
X	-19	GLY	-	expression tag	UNP P9WFX9
X	-18	LEU	-	expression tag	UNP P9WFX9
X	-17	VAL	-	expression tag	UNP P9WFX9
X	-16	PRO	-	expression tag	UNP P9WFX9
X	-15	ARG	-	expression tag	UNP P9WFX9
X	-14	GLY	-	expression tag	UNP P9WFX9
X	-13	SER	-	expression tag	UNP P9WFX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	-12	HIS	-	expression tag	UNP P9WFX9

- Molecule 3 is 2-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL)METHYL)AMINO]ACRYLIC ACID (CCD ID: P1T) (formula: C₁₁H₁₅N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	F	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	H	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	J	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	L	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	N	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	P	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	R	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	T	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

Continued on next page...

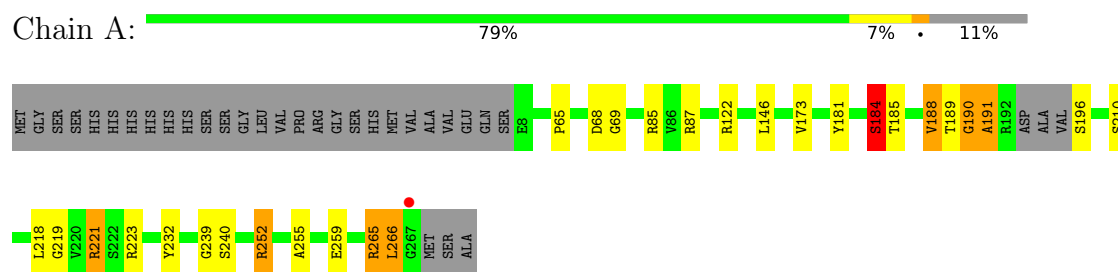
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	V	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	X	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

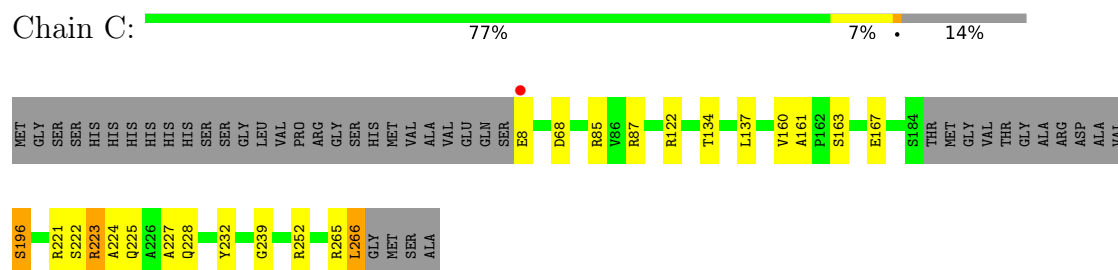
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

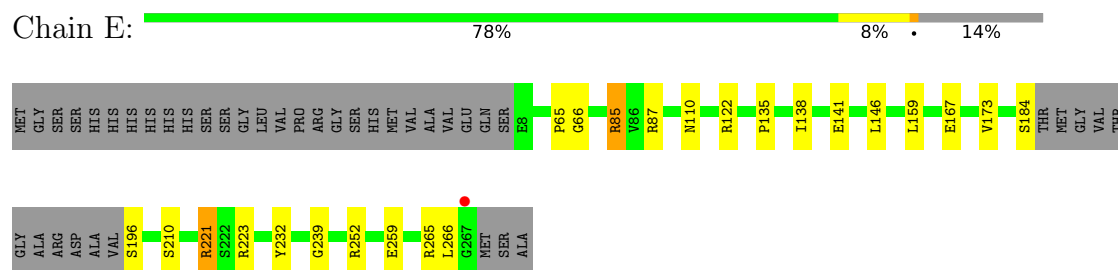
• Molecule 1: Tryptophan synthase alpha chain



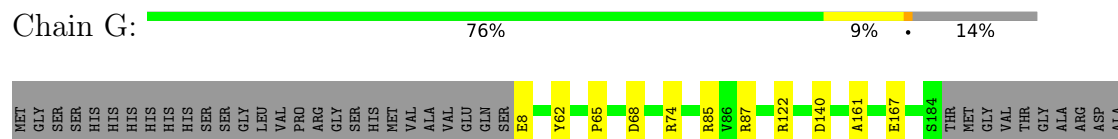
• Molecule 1: Tryptophan synthase alpha chain



• Molecule 1: Tryptophan synthase alpha chain



• Molecule 1: Tryptophan synthase alpha chain

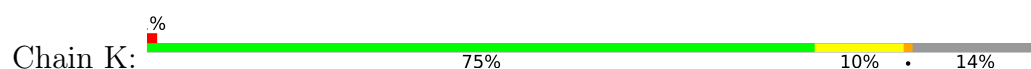




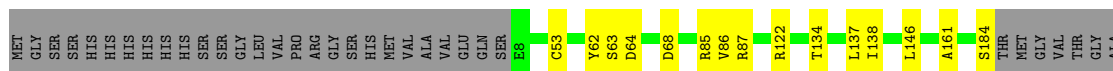
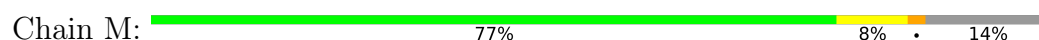
- Molecule 1: Tryptophan synthase alpha chain



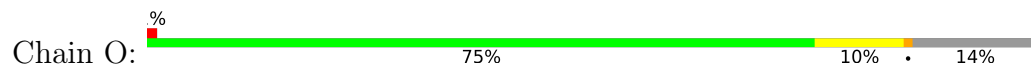
- Molecule 1: Tryptophan synthase alpha chain



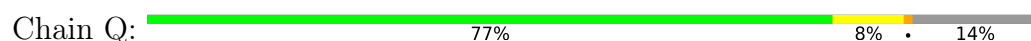
- Molecule 1: Tryptophan synthase alpha chain

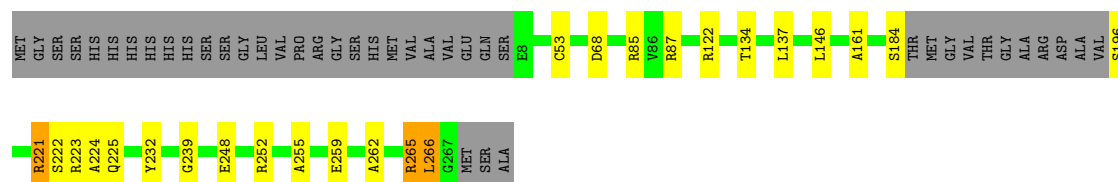


- Molecule 1: Tryptophan synthase alpha chain

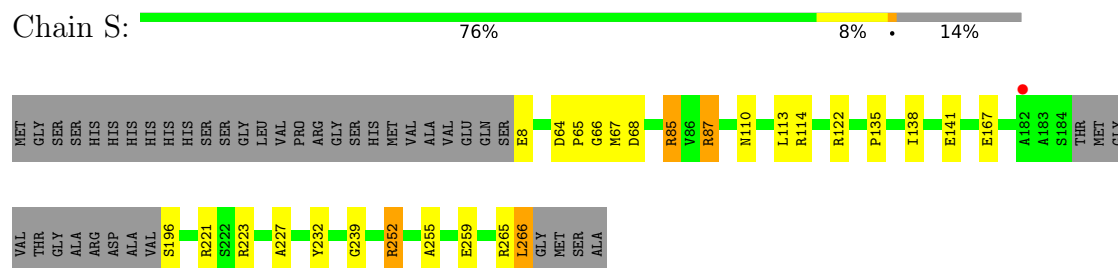


- Molecule 1: Tryptophan synthase alpha chain

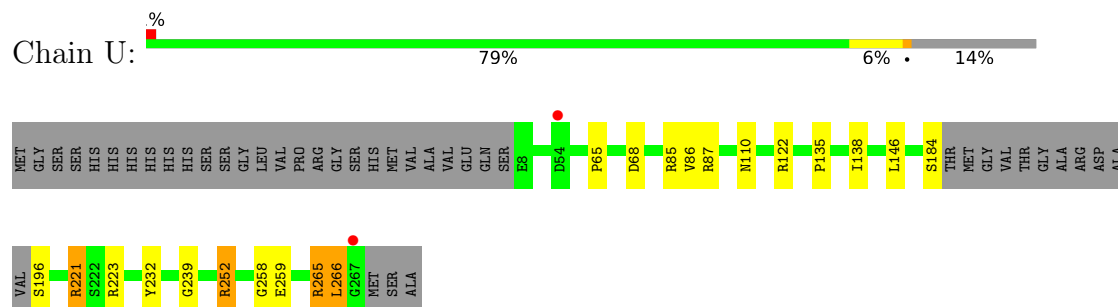




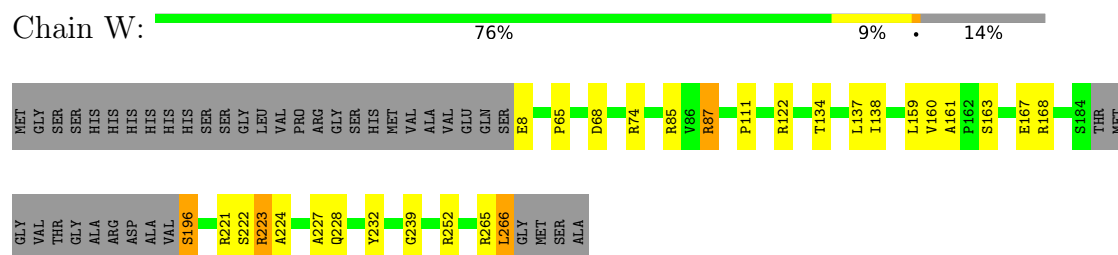
- Molecule 1: Tryptophan synthase alpha chain



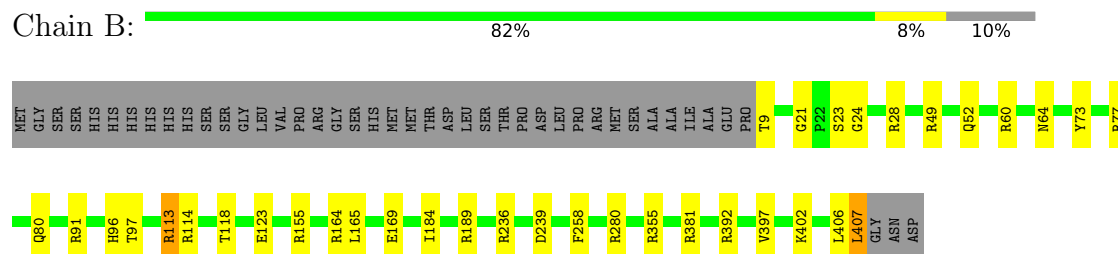
- Molecule 1: Tryptophan synthase alpha chain



- Molecule 1: Tryptophan synthase alpha chain

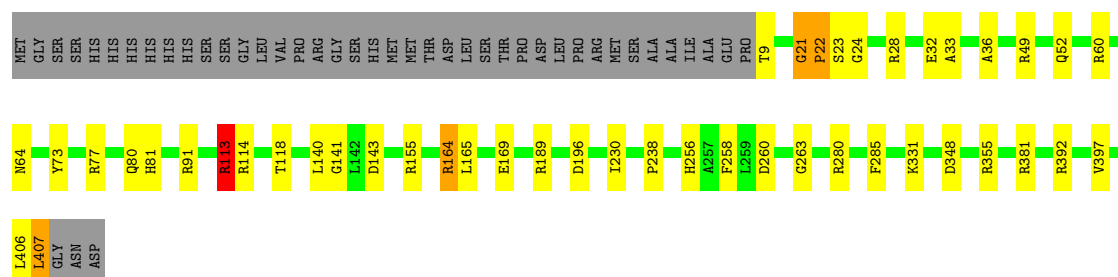


- Molecule 2: Tryptophan synthase beta chain



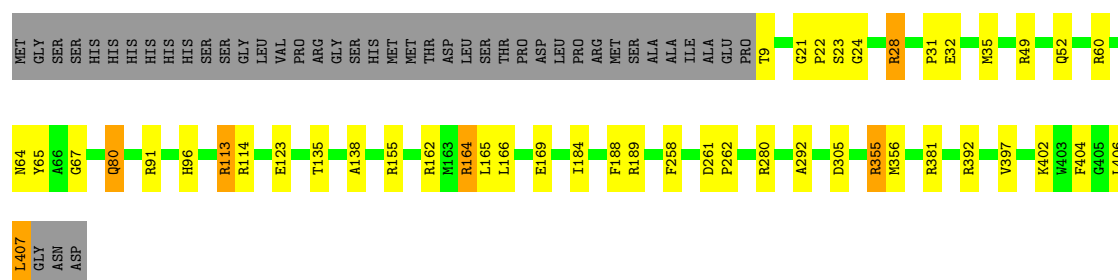
- Molecule 2: Tryptophan synthase beta chain

Chain D:  80% 9% 10%



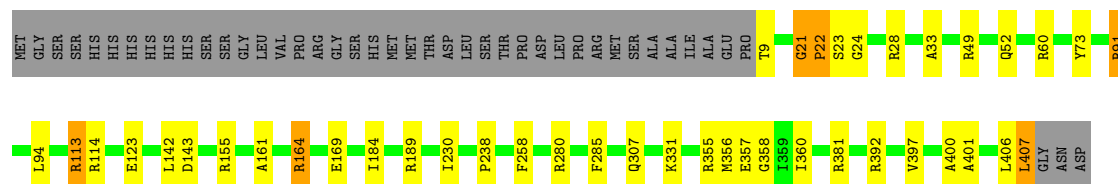
- Molecule 2: Tryptophan synthase beta chain

Chain F:  80% 9% 10%



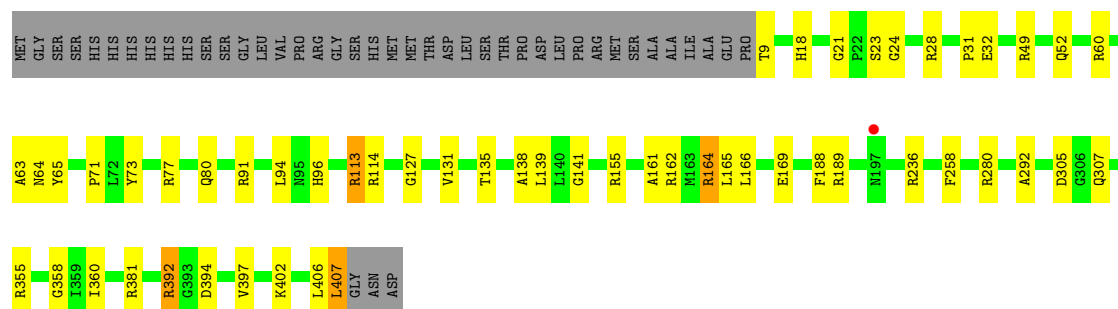
- Molecule 2: Tryptophan synthase beta chain

Chain H:  81% 8% 10%

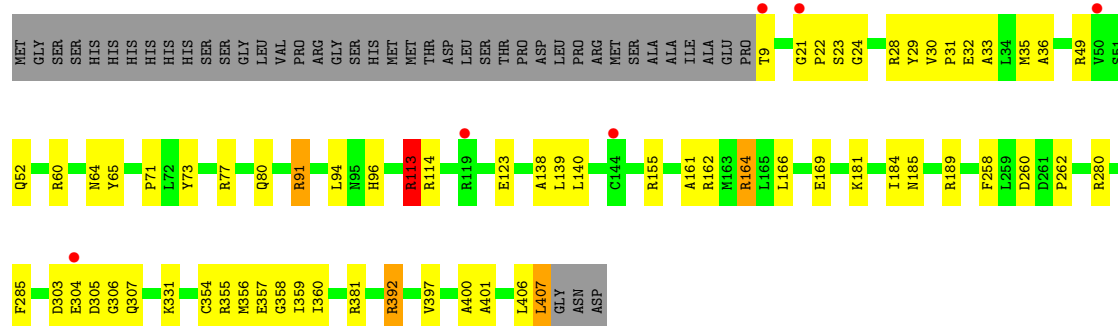
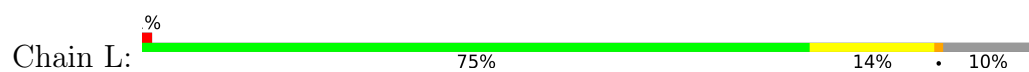


- Molecule 2: Tryptophan synthase beta chain

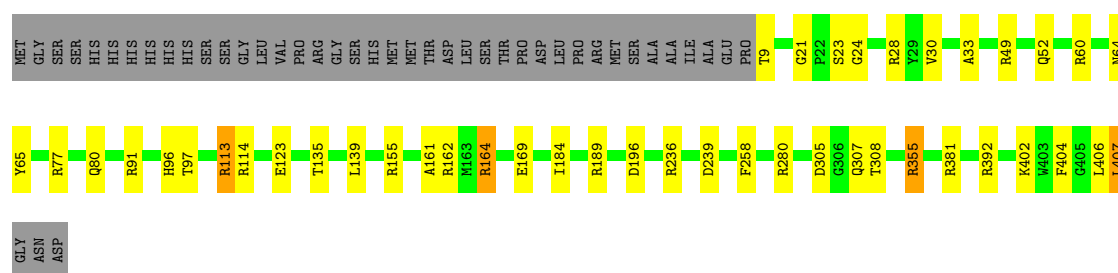
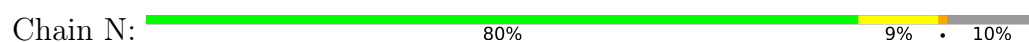
Chain J:  78% 11% 10%



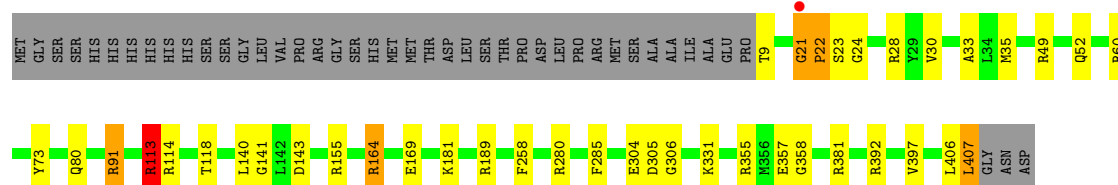
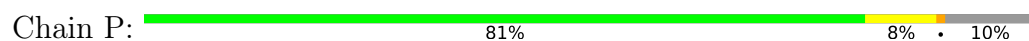
- Molecule 2: Tryptophan synthase beta chain



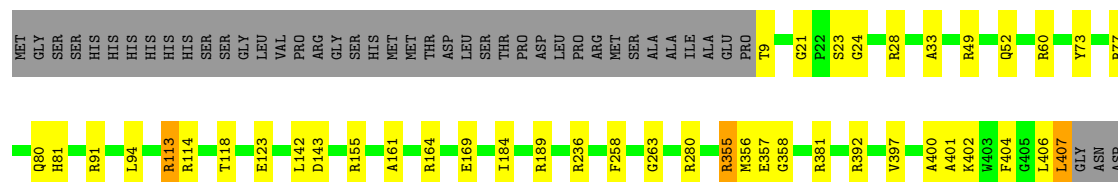
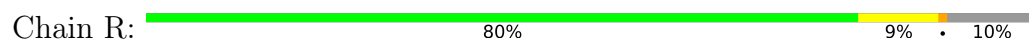
• Molecule 2: Tryptophan synthase beta chain



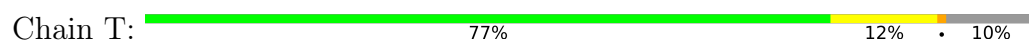
• Molecule 2: Tryptophan synthase beta chain

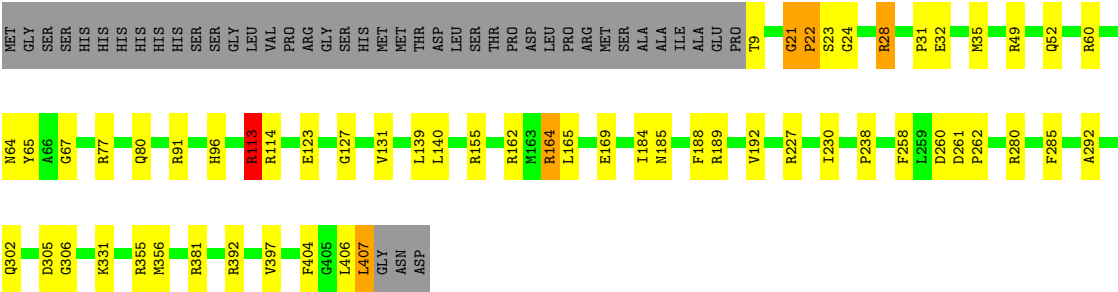


• Molecule 2: Tryptophan synthase beta chain

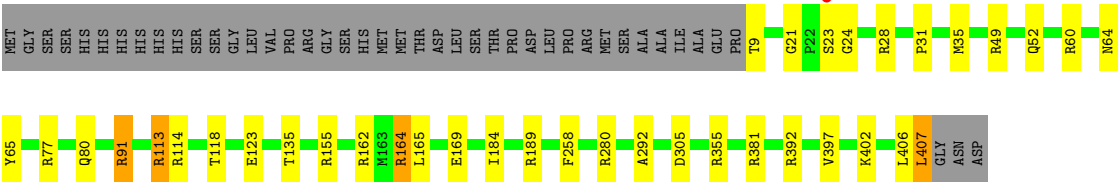
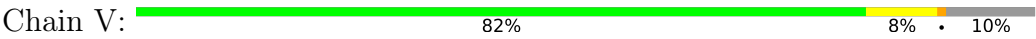


• Molecule 2: Tryptophan synthase beta chain

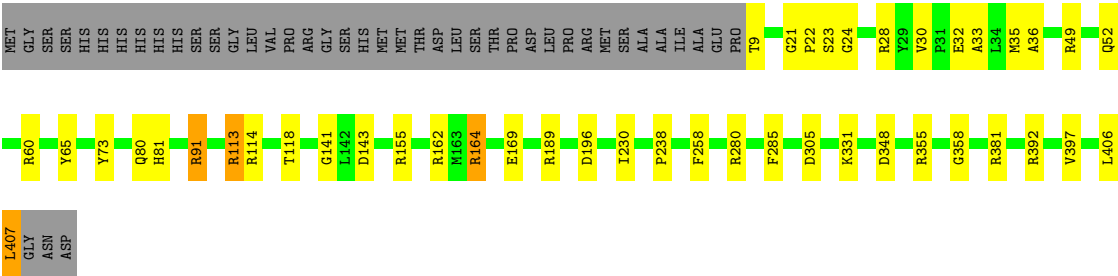
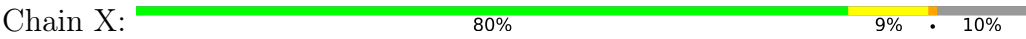




• Molecule 2: Tryptophan synthase beta chain



• Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	426.05Å 432.11Å 434.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 4.00 49.80 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.80-4.00) 95.1 (49.80-4.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.358 , 0.368 0.346 , 0.355	Depositor DCC
R_{free} test set	8243 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	171.2	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 363.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.108 for -h,l,k 0.036 for l,-k,h 0.060 for -k,-h,-l 0.029 for -k,-l,h 0.029 for l,-h,-k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	57878	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P1T

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	1.36	28/1881 (1.5%)	1.28	23/2566 (0.9%)
1	C	1.29	21/1828 (1.1%)	1.20	16/2495 (0.6%)
1	E	1.33	22/1843 (1.2%)	1.24	20/2514 (0.8%)
1	G	1.28	23/1828 (1.3%)	1.22	17/2495 (0.7%)
1	I	1.34	26/1843 (1.4%)	1.26	22/2514 (0.9%)
1	K	1.30	22/1828 (1.2%)	1.22	17/2495 (0.7%)
1	M	1.34	25/1843 (1.4%)	1.25	21/2514 (0.8%)
1	O	1.30	23/1828 (1.3%)	1.22	16/2495 (0.6%)
1	Q	1.34	26/1843 (1.4%)	1.25	20/2514 (0.8%)
1	S	1.32	22/1827 (1.2%)	1.25	19/2492 (0.8%)
1	U	1.33	25/1843 (1.4%)	1.26	22/2514 (0.9%)
1	W	1.29	22/1828 (1.2%)	1.21	16/2495 (0.6%)
2	B	1.33	38/3062 (1.2%)	1.13	29/4148 (0.7%)
2	D	1.31	39/3043 (1.3%)	1.10	25/4123 (0.6%)
2	F	1.35	40/3062 (1.3%)	1.11	28/4148 (0.7%)
2	H	1.27	38/3043 (1.2%)	1.14	26/4123 (0.6%)
2	J	1.33	38/3062 (1.2%)	1.12	29/4148 (0.7%)
2	L	1.32	40/3043 (1.3%)	1.12	26/4123 (0.6%)
2	N	1.33	38/3062 (1.2%)	1.13	30/4148 (0.7%)
2	P	1.33	39/3043 (1.3%)	1.12	27/4123 (0.7%)
2	R	1.34	38/3062 (1.2%)	1.12	27/4148 (0.7%)
2	T	1.33	40/3043 (1.3%)	1.12	29/4123 (0.7%)
2	V	1.33	37/3062 (1.2%)	1.13	28/4148 (0.7%)
2	X	1.31	39/3043 (1.3%)	1.11	27/4123 (0.7%)
All	All	1.32	749/58693 (1.3%)	1.17	560/79729 (0.7%)

The worst 5 of 749 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	23	SER	CA-CB	-18.89	1.26	1.53
2	V	24	GLY	N-CA	-17.96	1.19	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	221	ARG	CZ-NH2	-17.80	1.10	1.33
1	Q	221	ARG	CZ-NH2	-17.78	1.10	1.33
1	U	221	ARG	CZ-NH2	-17.66	1.10	1.33

The worst 5 of 560 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	164	ARG	NE-CZ-NH2	15.03	132.72	119.20
1	E	221	ARG	NE-CZ-NH2	-13.26	107.27	119.20
1	M	221	ARG	NE-CZ-NH2	-13.08	107.43	119.20
1	U	221	ARG	NE-CZ-NH2	-13.02	107.48	119.20
1	E	221	ARG	NE-CZ-NH1	12.99	134.49	121.50

There are no chirality outliers.

There are no planarity outliers.

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	1852	0	1855	52	0
1	C	1799	0	1819	10	22
1	E	1814	0	1834	16	2
1	G	1799	0	1816	60	0
1	I	1814	0	1834	33	0
1	K	1799	0	1819	65	3
1	M	1814	0	1834	40	0
1	O	1799	0	1819	23	14
1	Q	1814	0	1829	30	0
1	S	1799	0	1818	38	3
1	U	1814	0	1834	23	0
1	W	1799	0	1819	20	22
2	B	3002	0	2929	29	9
2	D	2983	0	2908	48	13
2	F	3002	0	2926	76	4
2	H	2983	0	2908	55	2
2	J	3002	0	2929	103	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2983	0	2908	155	0
2	N	3002	0	2929	28	13
2	P	2983	0	2908	46	5
2	R	3002	0	2929	76	3
2	T	2983	0	2906	117	0
2	V	3002	0	2929	28	10
2	X	2983	0	2908	45	12
3	B	21	0	11	0	0
3	D	21	0	11	0	0
3	F	21	0	11	0	0
3	H	21	0	11	0	0
3	J	21	0	11	0	0
3	L	21	0	11	0	0
3	N	21	0	11	0	0
3	P	21	0	11	0	0
3	R	21	0	11	0	0
3	T	21	0	11	0	0
3	V	21	0	11	0	0
3	X	21	0	11	0	0
All	All	57878	0	57079	682	70

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 6.

The worst 5 of 682 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:A:69:GLY:HA3	1:A:188:VAL:CB	1.25	1.67
2:L:80:GLN:HE22	1:U:259:GLU:CG	1.03	1.59
1:G:228:GLN:NE2	2:R:118:THR:CB	1.69	1.53
2:L:80:GLN:NE2	1:U:259:GLU:HG2	1.26	1.47
1:G:262:ALA:HB2	2:T:80:GLN:NE2	1.30	1.47

The worst 5 of 70 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:NE2	2:D:118:THR:CG2[2_555]	0.66	1.54
1:W:228:GLN:NE2	2:X:118:THR:CG2[3_555]	0.68	1.52
1:O:228:GLN:NE2	2:P:118:THR:CG2[2_555]	0.69	1.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ARG:CZ	1:C:223:ARG:NH2[2_555]	0.73	1.47
1:C:228:GLN:CD	2:D:118:THR:CG2[2_555]	0.76	1.44

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/290 (88%)	246 (97%)	4 (2%)	4 (2%)	7	37
1	C	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	30	65
1	E	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	30	65
1	G	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	30	65
1	I	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	30	65
1	K	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	30	65
1	M	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	30	65
1	O	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	30	65
1	Q	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	30	65
1	S	242/290 (83%)	239 (99%)	2 (1%)	1 (0%)	30	65
1	U	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	30	65
1	W	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	30	65
2	B	400/442 (90%)	392 (98%)	8 (2%)	0	100	100
2	D	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	F	400/442 (90%)	392 (98%)	8 (2%)	0	100	100
2	H	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	J	400/442 (90%)	393 (98%)	7 (2%)	0	100	100
2	L	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	N	400/442 (90%)	392 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	R	400/442 (90%)	393 (98%)	7 (2%)	0	100	100
2	T	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	V	400/442 (90%)	392 (98%)	8 (2%)	0	100	100
2	X	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
All	All	7734/8784 (88%)	7576 (98%)	143 (2%)	15 (0%)	43	75

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	THR
1	A	188	VAL
1	A	191	ALA
1	C	239	GLY
1	G	239	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/211 (85%)	177 (98%)	3 (2%)	53	68
1	C	179/211 (85%)	179 (100%)	0	100	100
1	E	180/211 (85%)	177 (98%)	3 (2%)	53	68
1	G	179/211 (85%)	178 (99%)	1 (1%)	78	81
1	I	180/211 (85%)	177 (98%)	3 (2%)	53	68
1	K	179/211 (85%)	179 (100%)	0	100	100
1	M	180/211 (85%)	176 (98%)	4 (2%)	45	65
1	O	179/211 (85%)	178 (99%)	1 (1%)	78	81
1	Q	180/211 (85%)	176 (98%)	4 (2%)	45	65
1	S	179/211 (85%)	179 (100%)	0	100	100
1	U	180/211 (85%)	177 (98%)	3 (2%)	53	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	179/211 (85%)	179 (100%)	0	100	100
2	B	298/331 (90%)	296 (99%)	2 (1%)	76	79
2	D	296/331 (89%)	294 (99%)	2 (1%)	76	79
2	F	298/331 (90%)	296 (99%)	2 (1%)	76	79
2	H	296/331 (89%)	295 (100%)	1 (0%)	86	85
2	J	298/331 (90%)	296 (99%)	2 (1%)	76	79
2	L	296/331 (89%)	295 (100%)	1 (0%)	86	85
2	N	298/331 (90%)	296 (99%)	2 (1%)	76	79
2	P	296/331 (89%)	295 (100%)	1 (0%)	86	85
2	R	298/331 (90%)	296 (99%)	2 (1%)	76	79
2	T	296/331 (89%)	295 (100%)	1 (0%)	86	85
2	V	298/331 (90%)	296 (99%)	2 (1%)	76	79
2	X	296/331 (89%)	295 (100%)	1 (0%)	86	85
All	All	5718/6504 (88%)	5677 (99%)	41 (1%)	76	79

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	53	CYS
1	U	146	LEU
1	Q	146	LEU
2	R	80	GLN
1	U	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	T	81	HIS
2	V	52	GLN
2	X	81	HIS
2	L	18	HIS
1	I	228	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	P1T	X	501	-	20,21,21	2.53	5 (25%)	29,30,30	1.35	4 (13%)
3	P1T	F	501	-	20,21,21	2.52	4 (20%)	29,30,30	1.34	4 (13%)
3	P1T	B	501	-	20,21,21	2.52	4 (20%)	29,30,30	1.31	4 (13%)
3	P1T	H	501	-	20,21,21	2.51	4 (20%)	29,30,30	1.29	3 (10%)
3	P1T	N	501	-	20,21,21	2.57	4 (20%)	29,30,30	1.33	4 (13%)
3	P1T	D	501	-	20,21,21	2.53	5 (25%)	29,30,30	1.35	3 (10%)
3	P1T	R	501	-	20,21,21	2.56	4 (20%)	29,30,30	1.29	4 (13%)
3	P1T	L	501	-	20,21,21	2.66	4 (20%)	29,30,30	1.37	4 (13%)
3	P1T	V	501	-	20,21,21	2.59	4 (20%)	29,30,30	1.31	3 (10%)
3	P1T	P	501	-	20,21,21	2.54	4 (20%)	29,30,30	1.33	3 (10%)
3	P1T	T	501	-	20,21,21	2.48	4 (20%)	29,30,30	1.40	4 (13%)
3	P1T	J	501	-	20,21,21	2.60	4 (20%)	29,30,30	1.28	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P1T	X	501	-	-	3/14/15/15	0/1/1/1
3	P1T	F	501	-	-	3/14/15/15	0/1/1/1
3	P1T	B	501	-	-	3/14/15/15	0/1/1/1
3	P1T	H	501	-	-	3/14/15/15	0/1/1/1
3	P1T	N	501	-	-	3/14/15/15	0/1/1/1
3	P1T	D	501	-	-	3/14/15/15	0/1/1/1
3	P1T	R	501	-	-	3/14/15/15	0/1/1/1
3	P1T	L	501	-	-	3/14/15/15	0/1/1/1
3	P1T	V	501	-	-	3/14/15/15	0/1/1/1
3	P1T	P	501	-	-	3/14/15/15	0/1/1/1
3	P1T	T	501	-	-	3/14/15/15	0/1/1/1
3	P1T	J	501	-	-	3/14/15/15	0/1/1/1

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	501	P1T	C3-C2	7.71	1.49	1.41
3	R	501	P1T	C3-C2	7.46	1.48	1.41
3	V	501	P1T	C3-C2	7.35	1.48	1.41
3	F	501	P1T	C3-C2	7.18	1.48	1.41
3	P	501	P1T	C3-C2	7.17	1.48	1.41

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	P1T	C4A-C4-C3	3.04	124.03	119.98
3	N	501	P1T	C4A-C4-C3	2.79	123.69	119.98
3	T	501	P1T	C6-N1-C2	2.78	124.24	119.20
3	B	501	P1T	C6-N1-C2	2.76	124.20	119.20
3	X	501	P1T	C4A-C4-C3	2.75	123.64	119.98

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

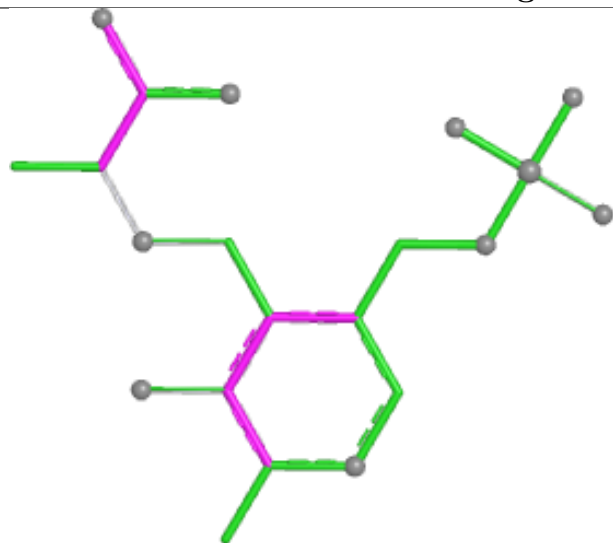
Mol	Chain	Res	Type	Atoms
3	B	501	P1T	C5-C4-C4A-N
3	D	501	P1T	C5-C4-C4A-N
3	F	501	P1T	C5-C4-C4A-N
3	H	501	P1T	C5-C4-C4A-N
3	J	501	P1T	C5-C4-C4A-N

There are no ring outliers.

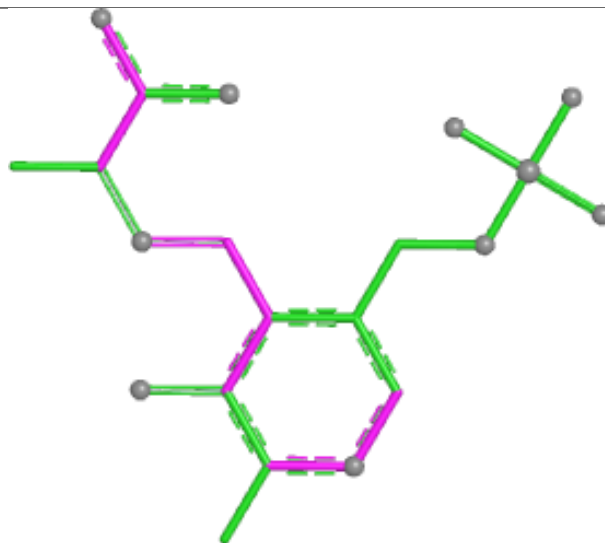
No monomer is involved in short contacts.

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.

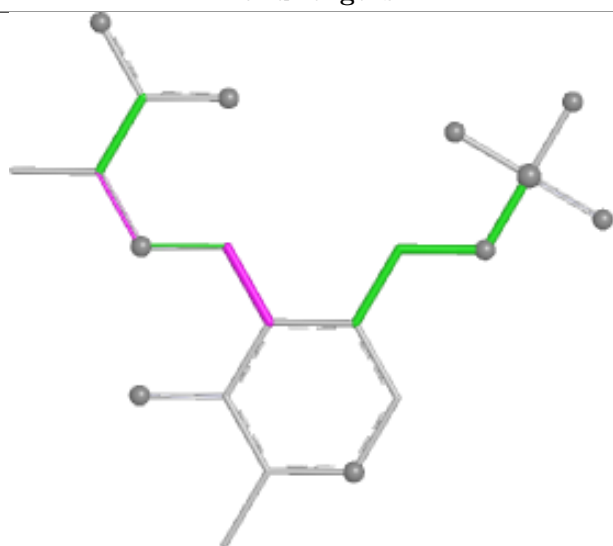
Ligand P1T X 501



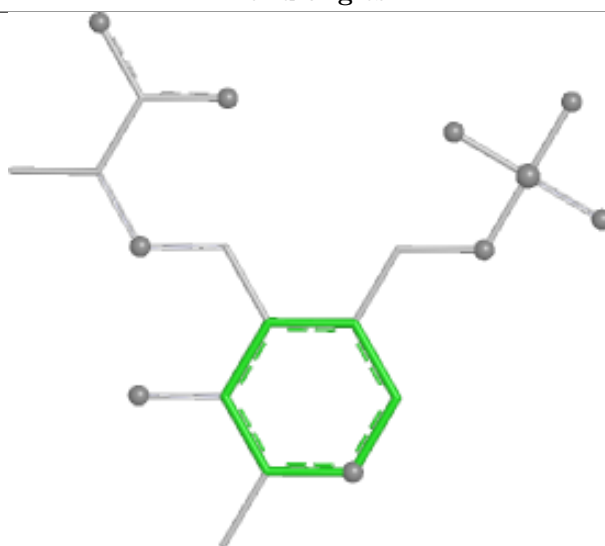
Bond lengths



Bond angles

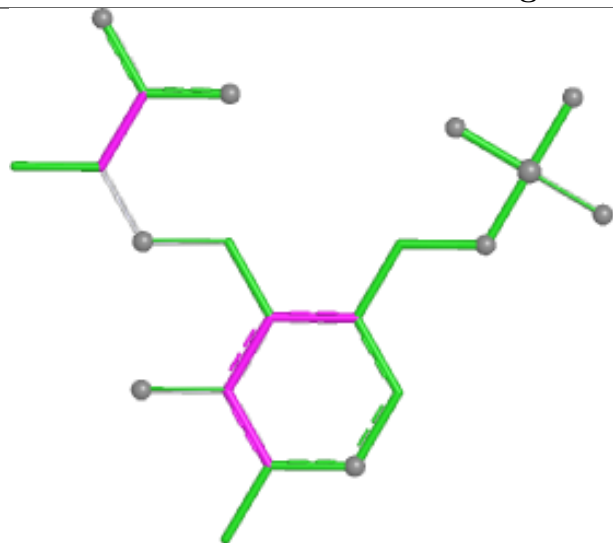


Torsions

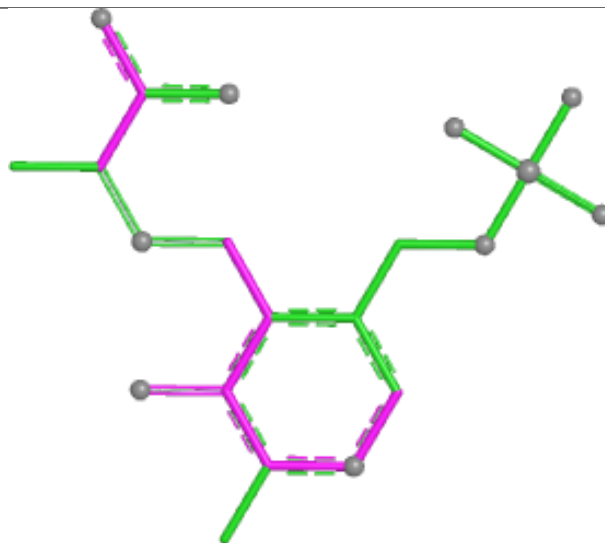


Rings

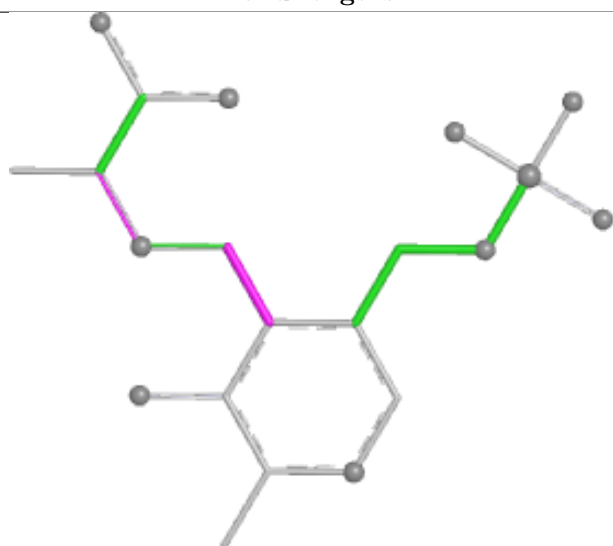
Ligand P1T F 501



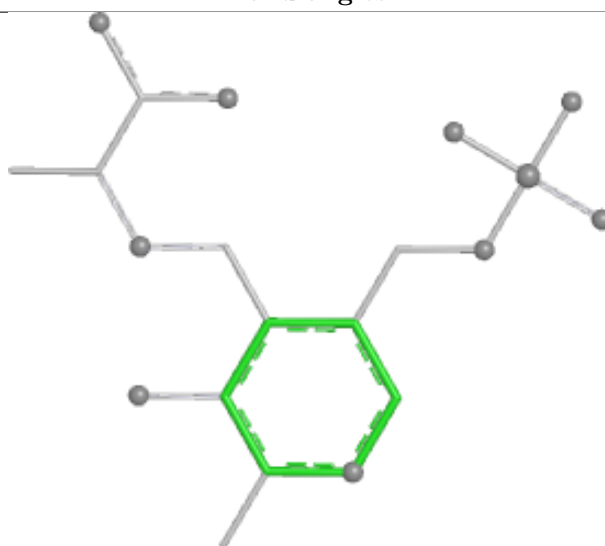
Bond lengths



Bond angles

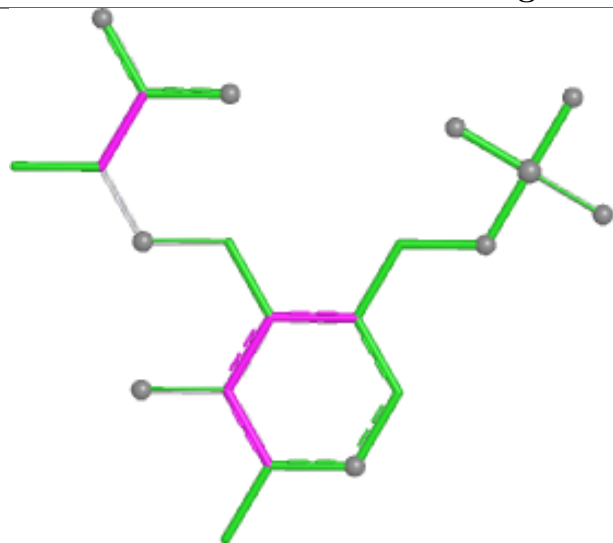


Torsions

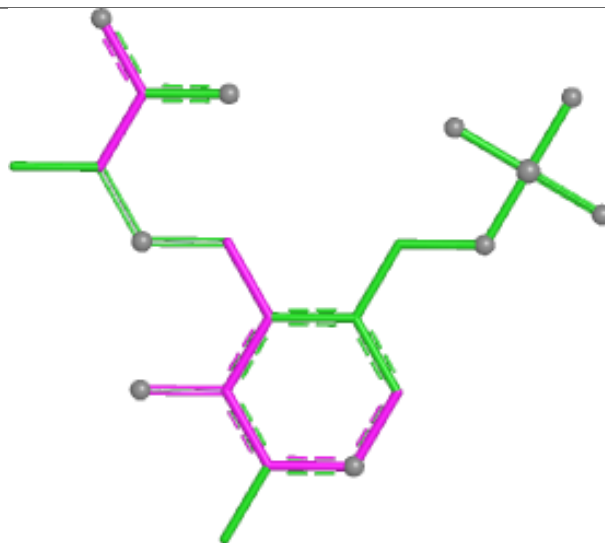


Rings

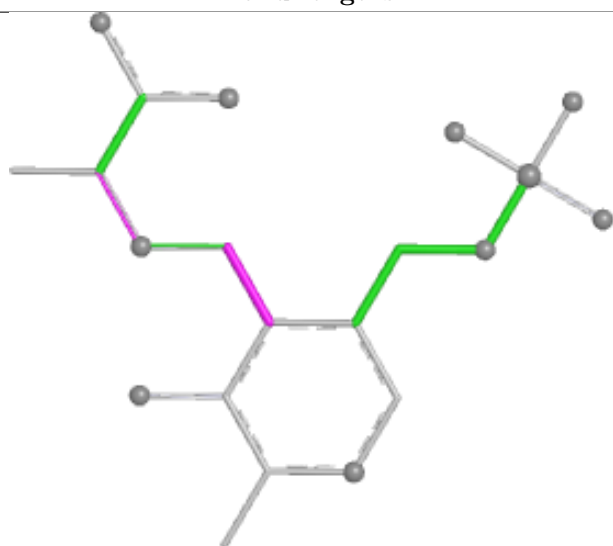
Ligand P1T B 501



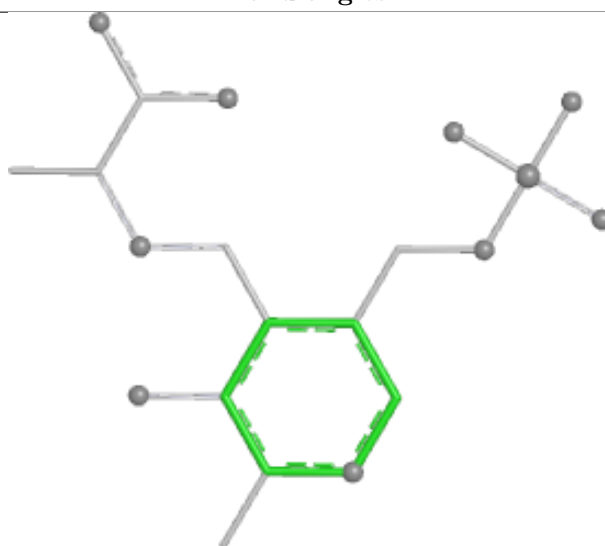
Bond lengths



Bond angles

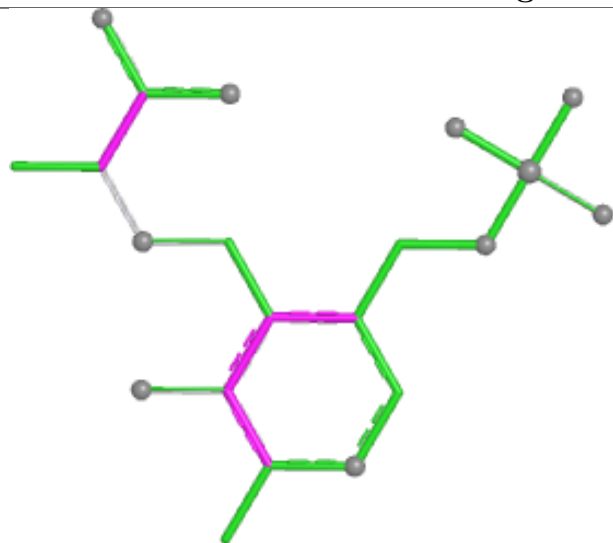


Torsions

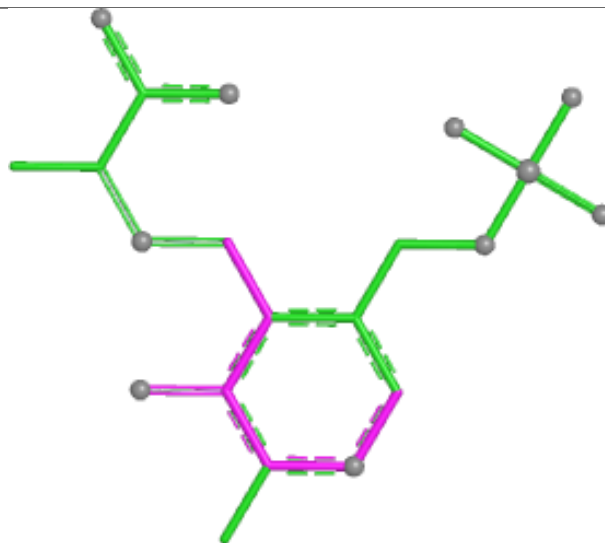


Rings

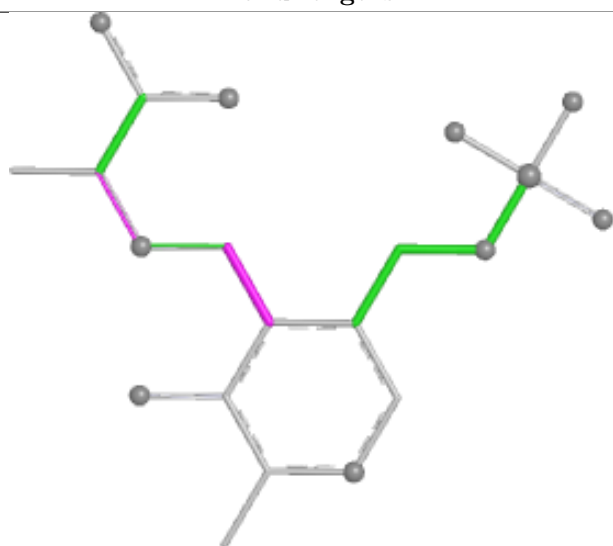
Ligand P1T H 501



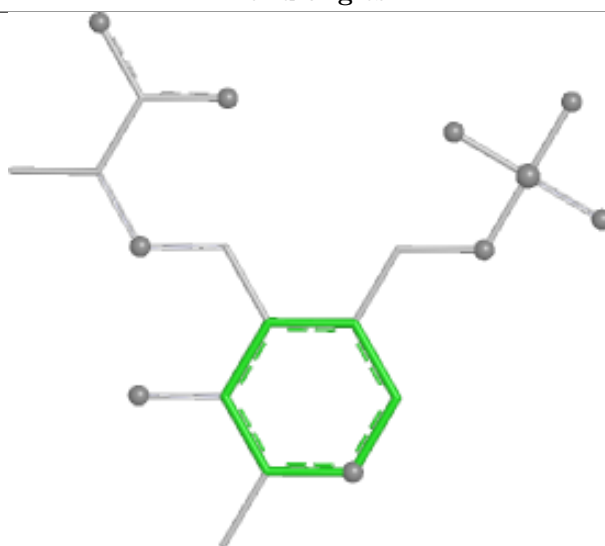
Bond lengths



Bond angles

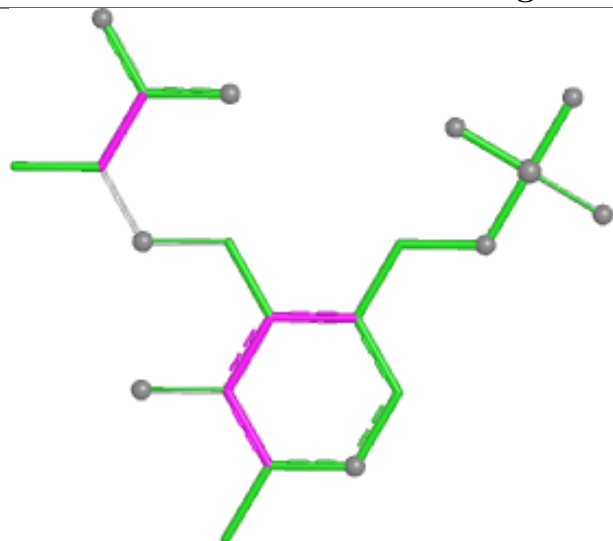


Torsions

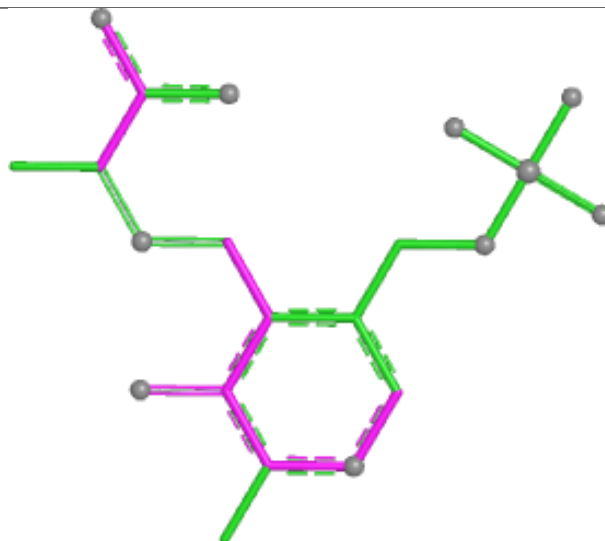


Rings

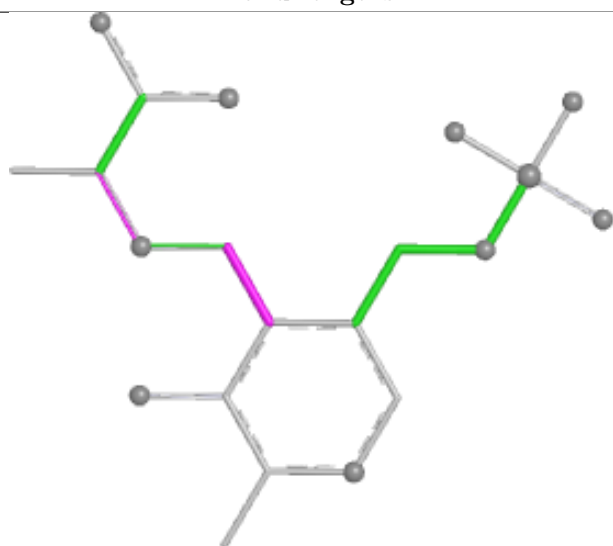
Ligand P1T N 501



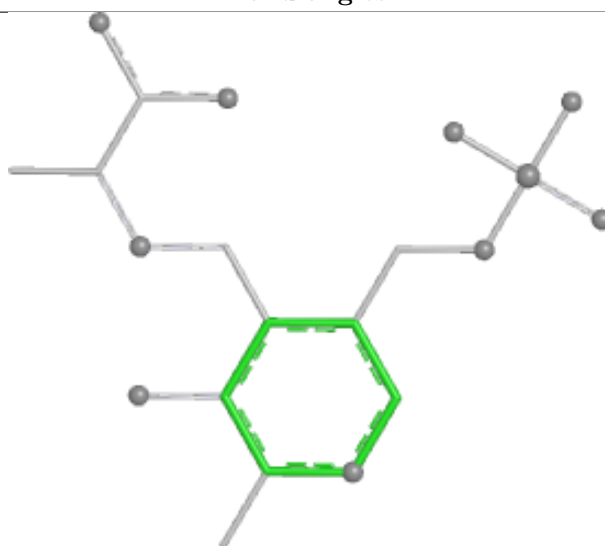
Bond lengths



Bond angles

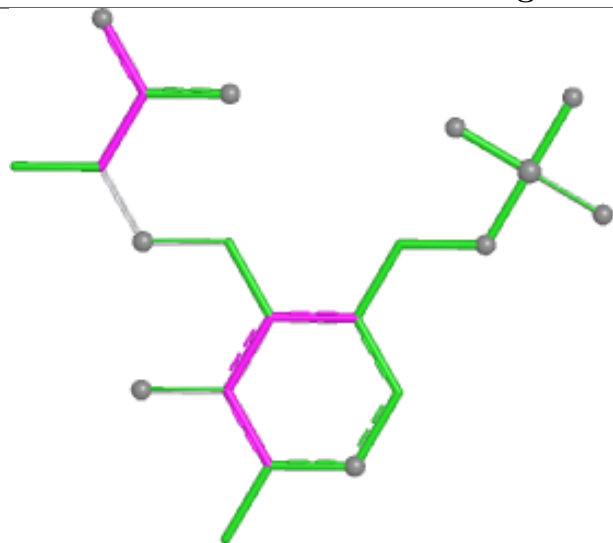


Torsions

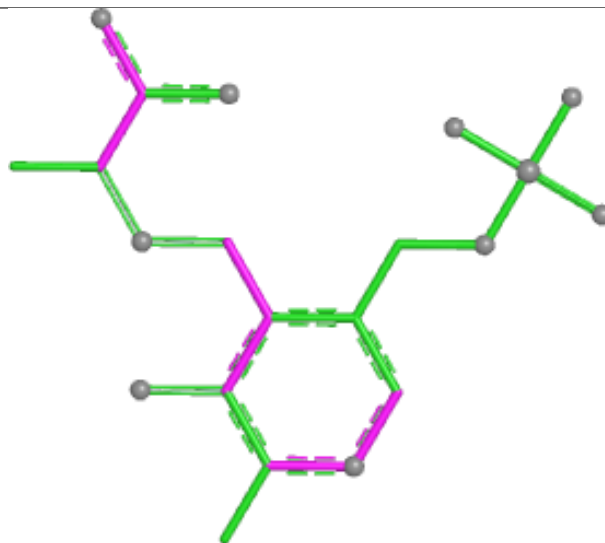


Rings

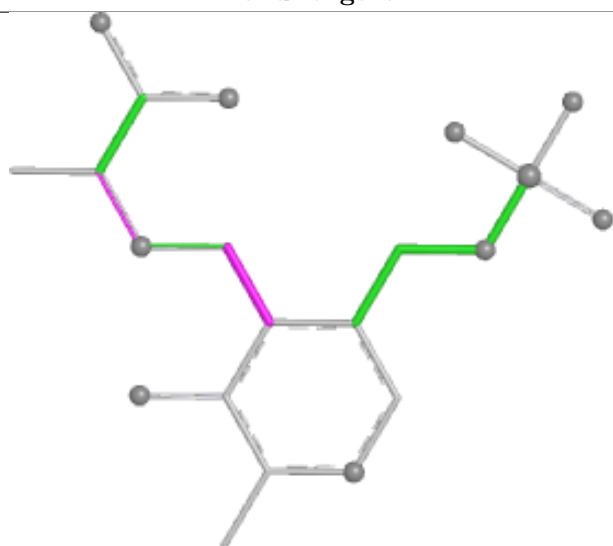
Ligand P1T D 501



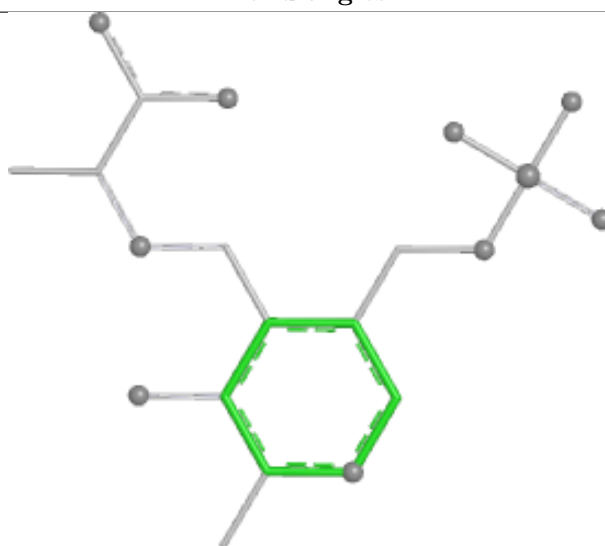
Bond lengths



Bond angles

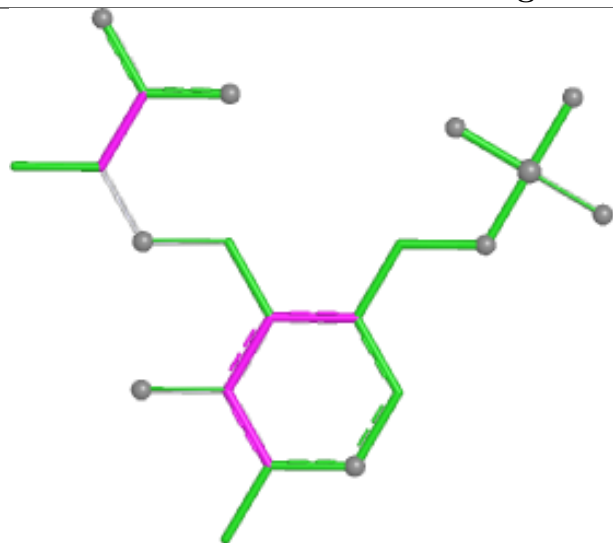


Torsions

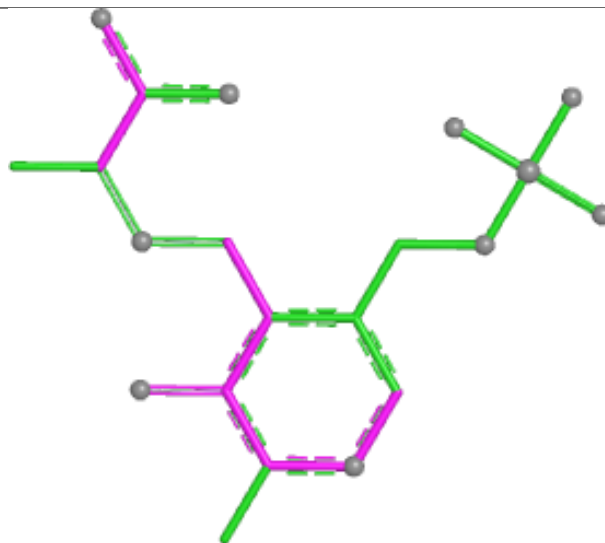


Rings

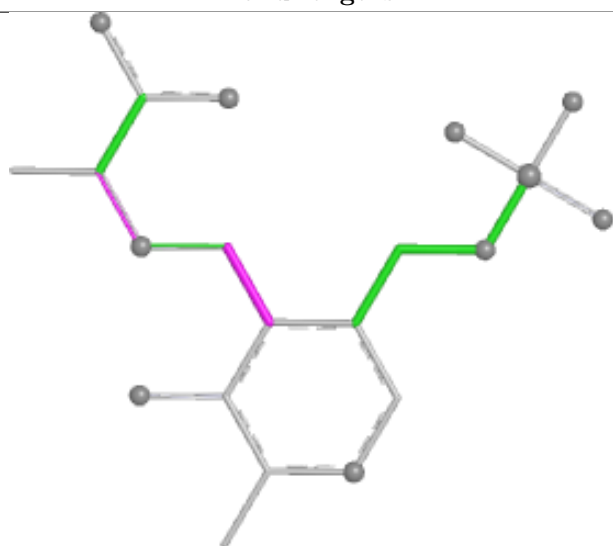
Ligand P1T R 501



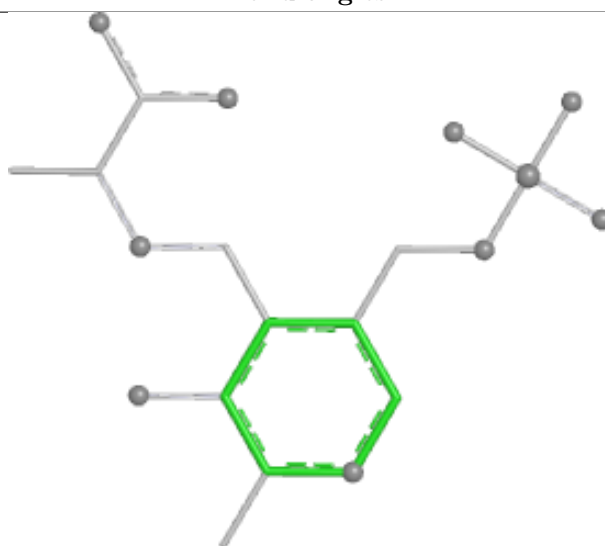
Bond lengths



Bond angles

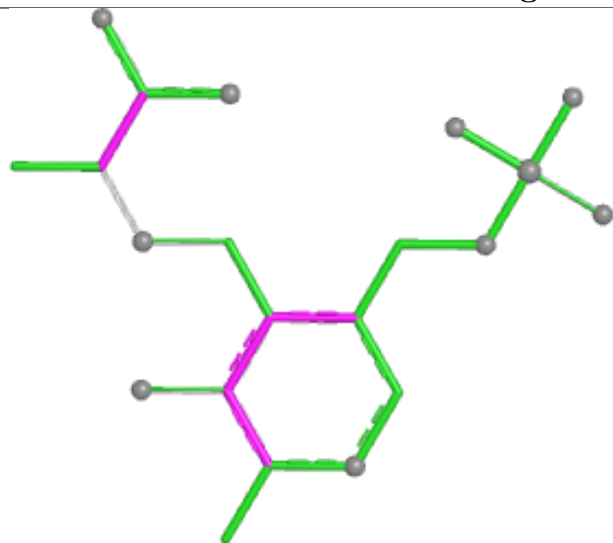


Torsions

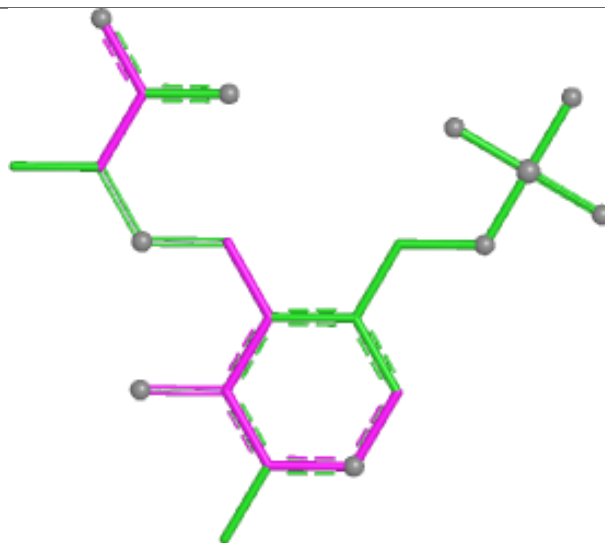


Rings

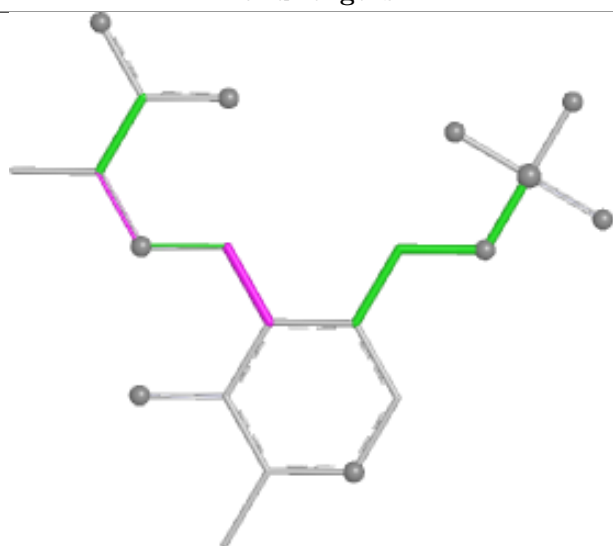
Ligand P1T L 501



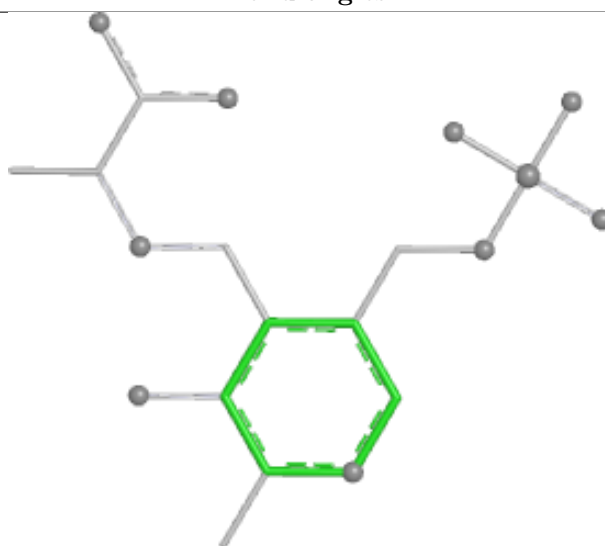
Bond lengths



Bond angles

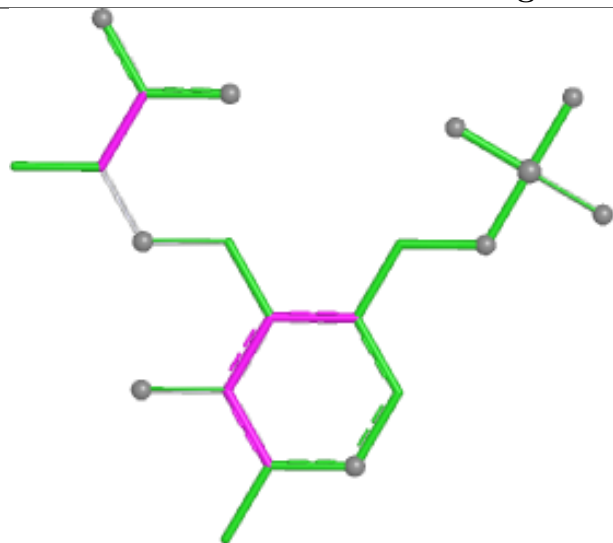


Torsions

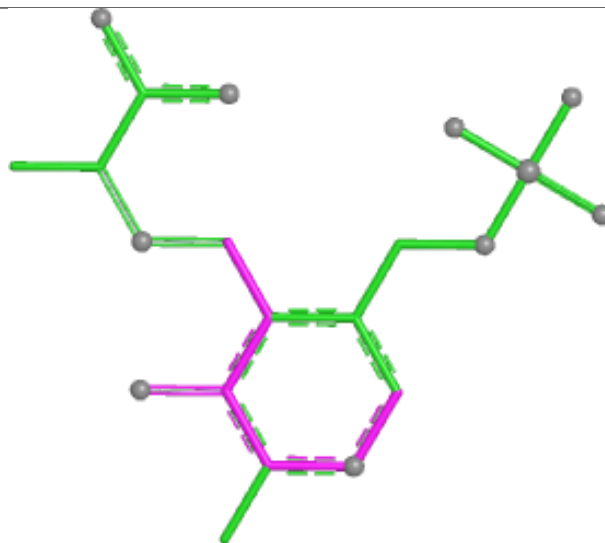


Rings

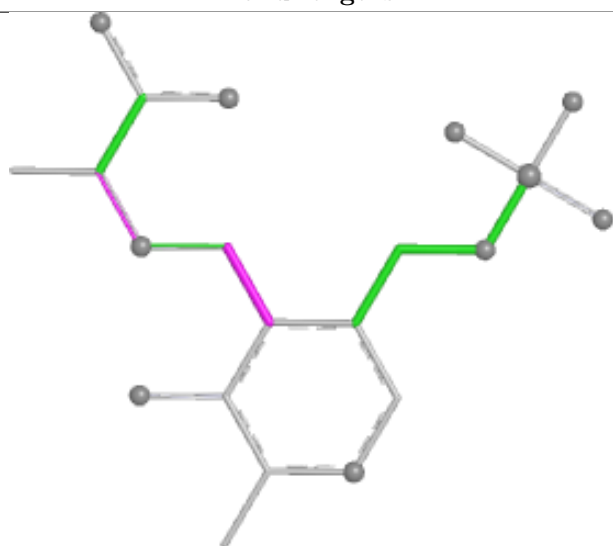
Ligand P1T V 501



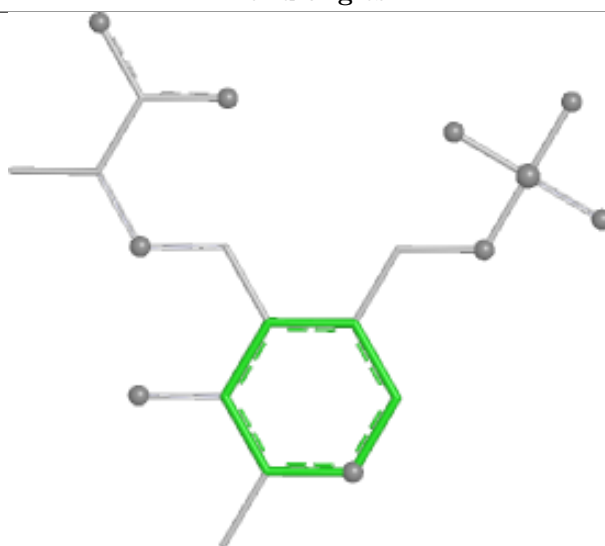
Bond lengths



Bond angles

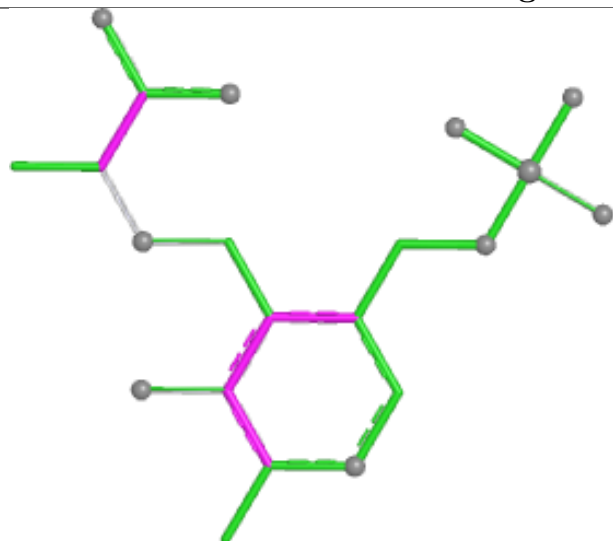


Torsions

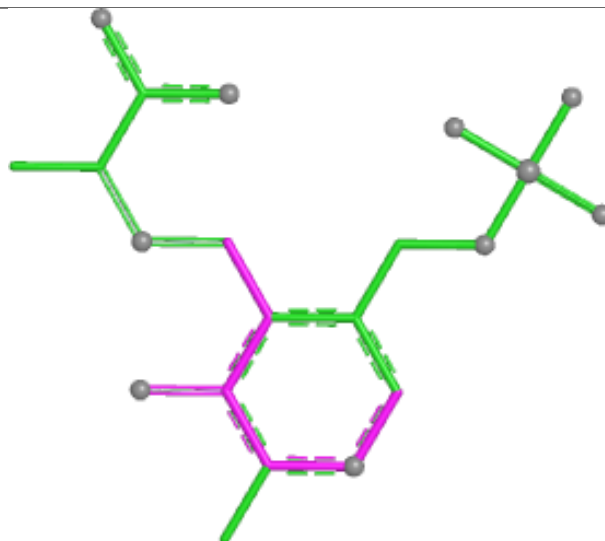


Rings

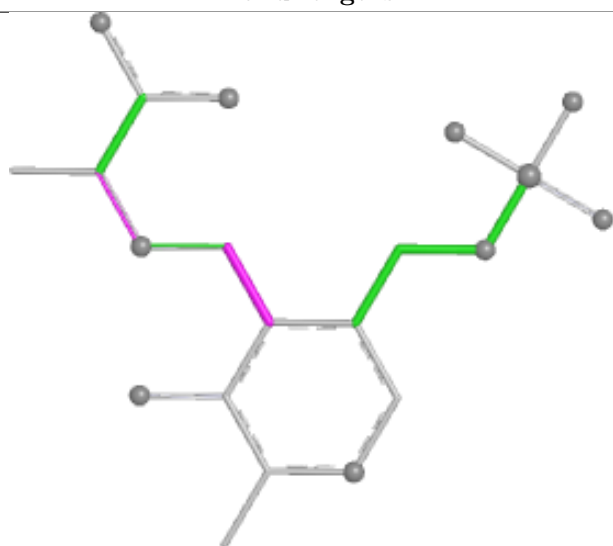
Ligand P1T P 501



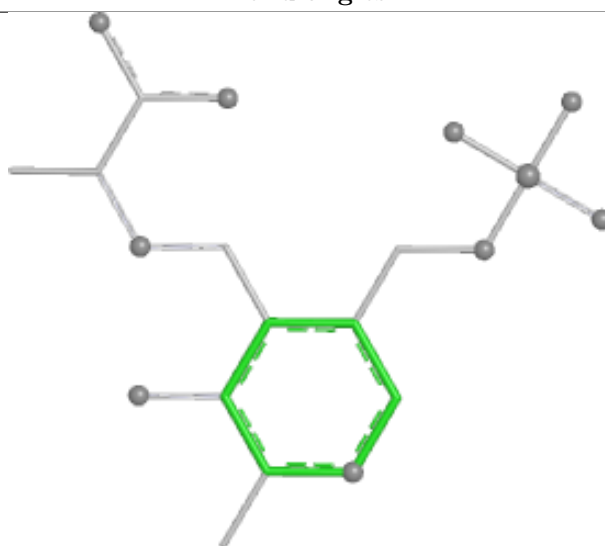
Bond lengths



Bond angles

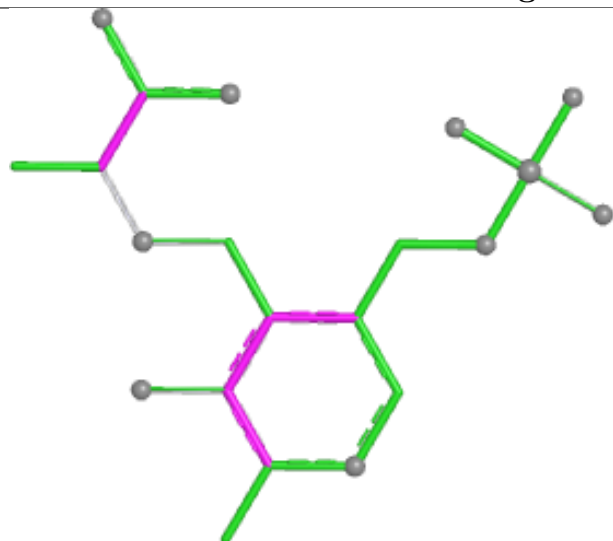


Torsions

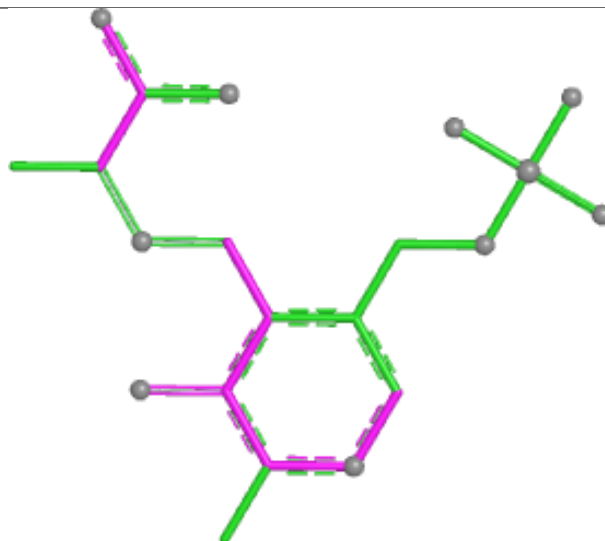


Rings

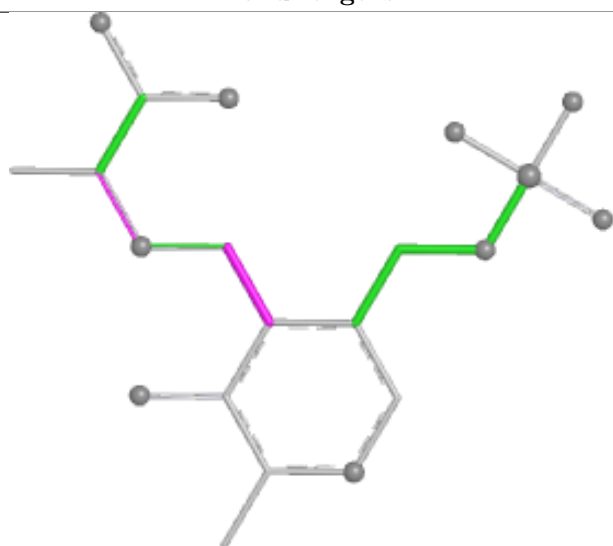
Ligand P1T T 501



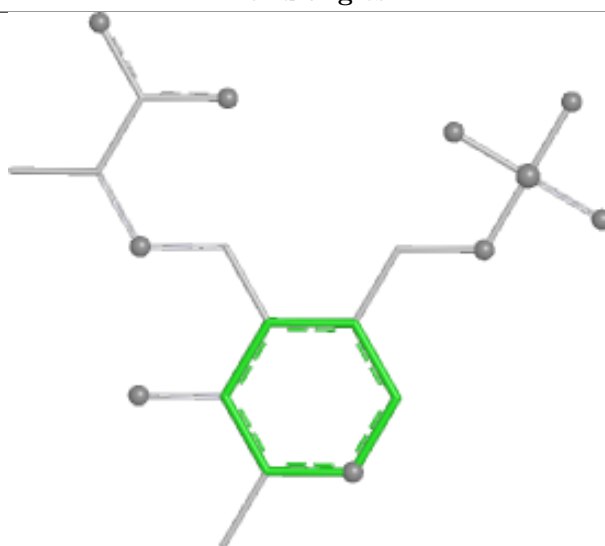
Bond lengths



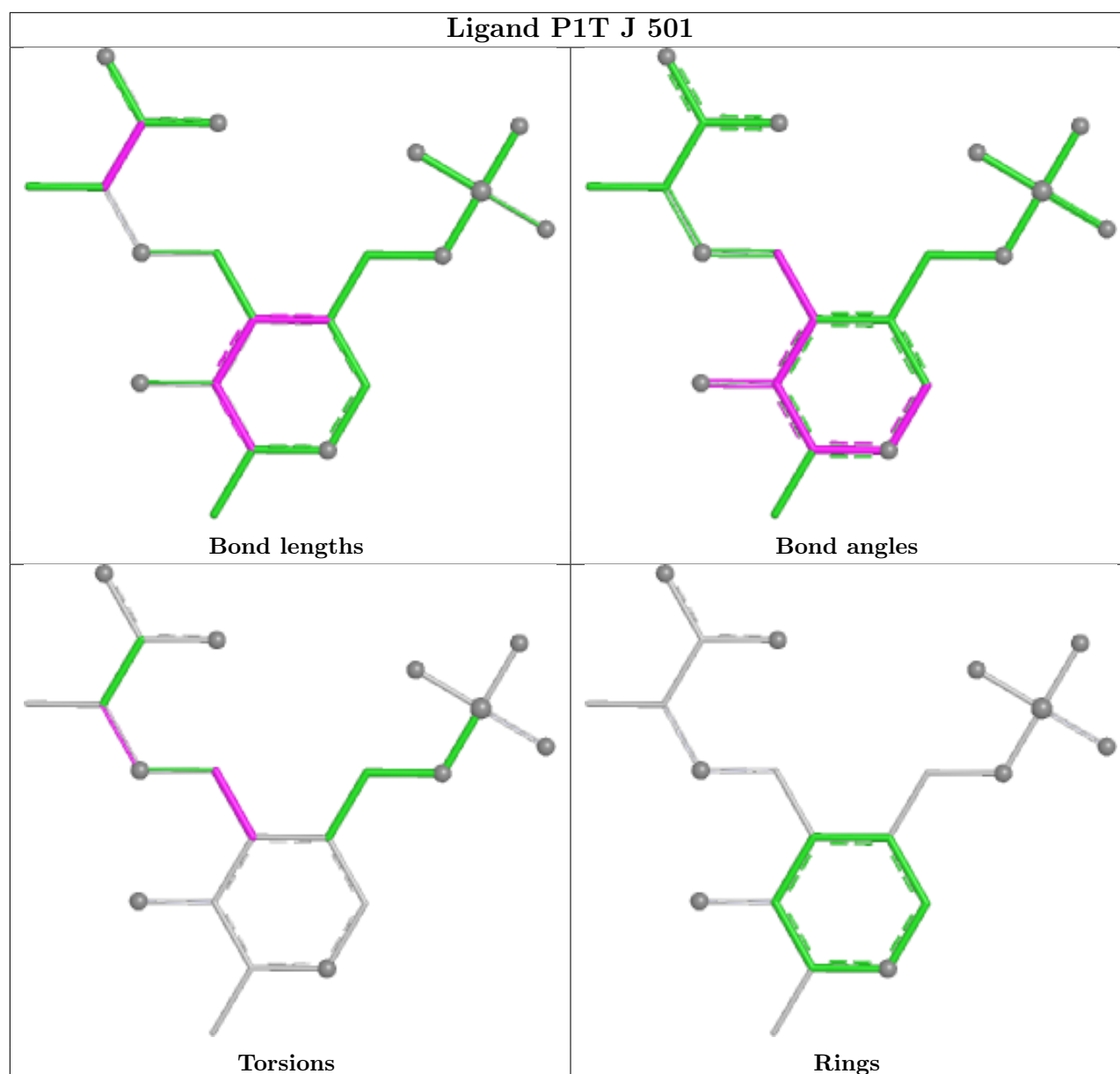
Bond angles



Torsions



Rings



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	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	9:ALA	C	10:SER	N	3.34

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	257/290 (88%)	-0.49	1 (0%) 88 75	93, 141, 184, 206	1 (0%)
1	C	248/290 (85%)	-0.80	1 (0%) 88 75	58, 86, 106, 117	0
1	E	249/290 (85%)	-0.27	1 (0%) 88 75	102, 176, 211, 238	1 (0%)
1	G	248/290 (85%)	-0.61	0 100 100	111, 138, 159, 173	0
1	I	249/290 (85%)	-0.43	0 100 100	79, 169, 200, 211	1 (0%)
1	K	248/290 (85%)	0.04	4 (1%) 70 52	149, 199, 236, 255	0
1	M	249/290 (85%)	-0.49	1 (0%) 88 75	70, 127, 142, 156	1 (0%)
1	O	248/290 (85%)	-0.44	2 (0%) 82 65	122, 144, 161, 171	0
1	Q	249/290 (85%)	-0.53	0 100 100	77, 135, 156, 170	1 (0%)
1	S	248/290 (85%)	-0.38	1 (0%) 88 75	118, 148, 178, 188	0
1	U	249/290 (85%)	-0.12	2 (0%) 82 65	123, 213, 264, 302	1 (0%)
1	W	248/290 (85%)	-0.67	0 100 100	88, 117, 145, 162	0
2	B	399/442 (90%)	-0.74	0 100 100	39, 78, 101, 123	3 (0%)
2	D	399/442 (90%)	-0.82	0 100 100	29, 61, 81, 91	1 (0%)
2	F	399/442 (90%)	-0.58	0 100 100	55, 113, 137, 149	3 (0%)
2	H	399/442 (90%)	-0.66	0 100 100	55, 108, 119, 126	1 (0%)
2	J	399/442 (90%)	-0.25	1 (0%) 90 78	79, 155, 188, 200	3 (0%)
2	L	399/442 (90%)	-0.10	6 (1%) 72 54	81, 165, 198, 208	1 (0%)
2	N	399/442 (90%)	-0.42	0 100 100	63, 118, 137, 149	3 (0%)
2	P	399/442 (90%)	-0.42	1 (0%) 90 78	62, 125, 140, 147	1 (0%)
2	R	399/442 (90%)	-0.71	0 100 100	47, 100, 111, 123	3 (0%)
2	T	399/442 (90%)	-0.69	0 100 100	58, 103, 118, 135	1 (0%)
2	V	399/442 (90%)	-0.68	1 (0%) 90 78	62, 122, 162, 180	3 (0%)
2	X	399/442 (90%)	-0.79	0 100 100	45, 97, 121, 136	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7778/8784 (88%)	-0.52	22 (0%) 90 78	29, 122, 197, 302	30 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	21	GLY	3.4
2	L	9	THR	3.3
2	P	21	GLY	3.1
1	K	8	GLU	2.8
1	C	8	GLU	2.7

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

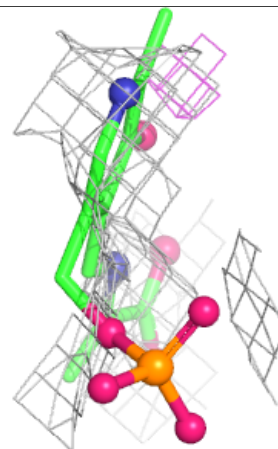
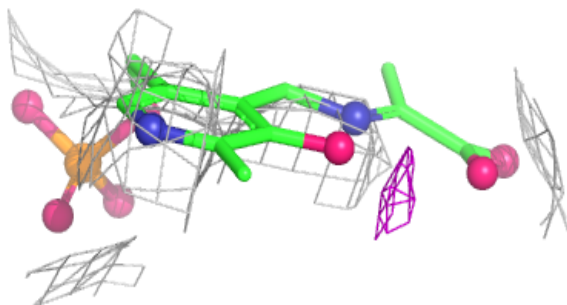
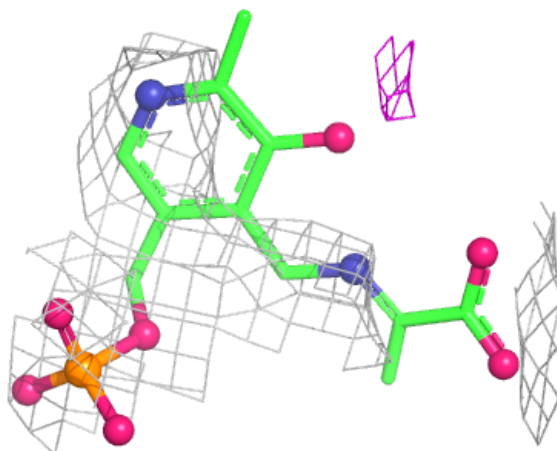
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	P1T	L	501	21/21	0.98	0.09	175,175,175,175	0
3	P1T	D	501	21/21	0.99	0.09	175,175,175,175	0
3	P1T	F	501	21/21	0.99	0.06	175,175,175,175	0
3	P1T	H	501	21/21	0.99	0.06	175,175,175,175	0
3	P1T	J	501	21/21	0.99	0.08	175,175,175,175	0
3	P1T	B	501	21/21	0.99	0.07	175,175,175,175	0
3	P1T	N	501	21/21	0.99	0.07	175,175,175,175	0
3	P1T	P	501	21/21	0.99	0.07	175,175,175,175	0
3	P1T	R	501	21/21	0.99	0.08	175,175,175,175	0
3	P1T	T	501	21/21	0.99	0.06	175,175,175,175	0
3	P1T	V	501	21/21	0.99	0.06	175,175,175,175	0
3	P1T	X	501	21/21	1.00	0.04	175,175,175,175	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

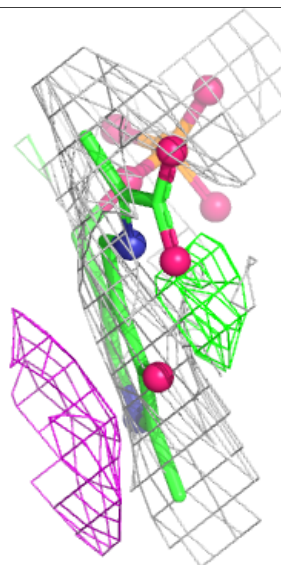
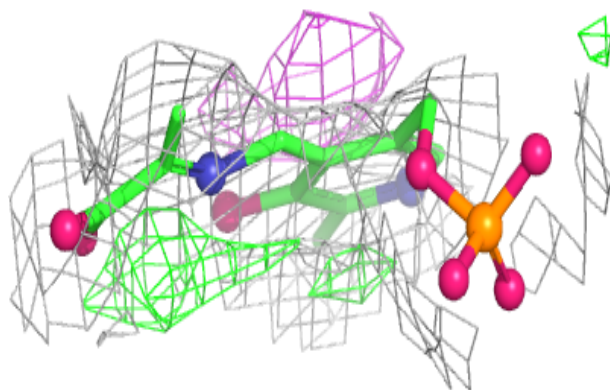
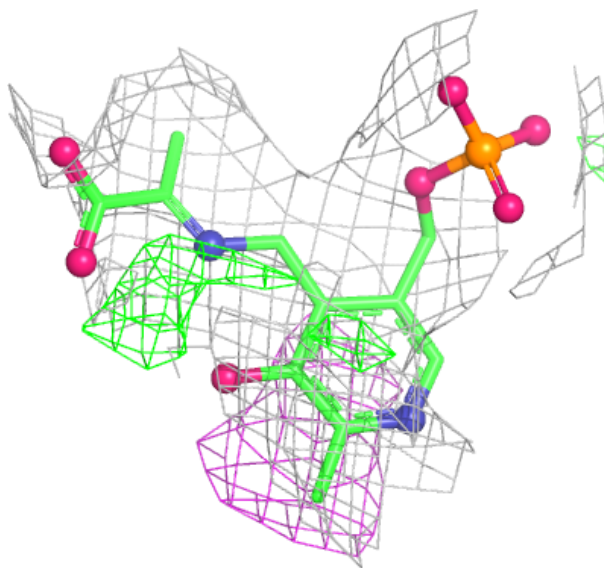
Electron density around P1T L 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



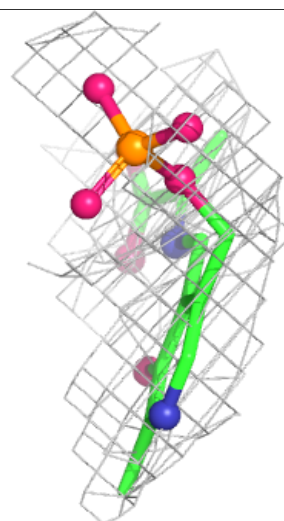
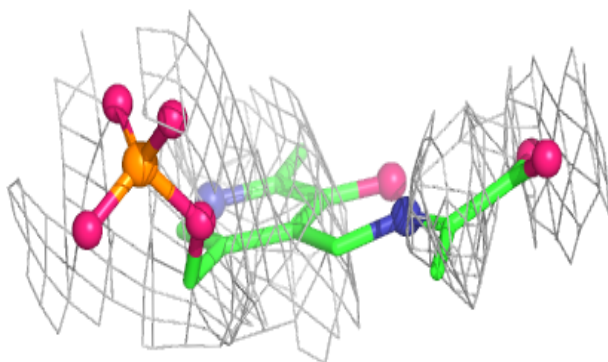
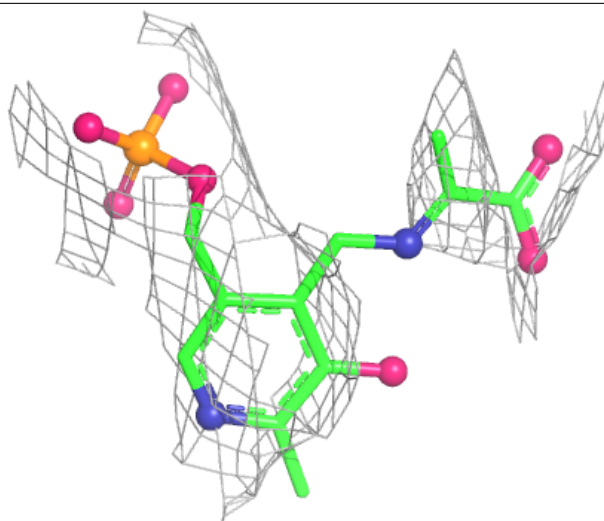
Electron density around P1T D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



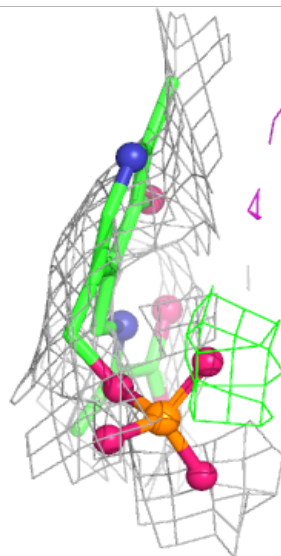
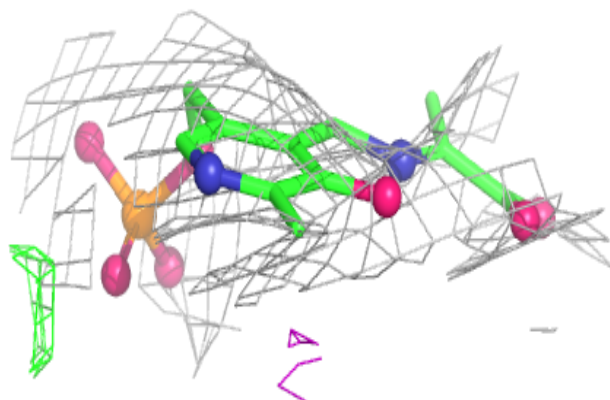
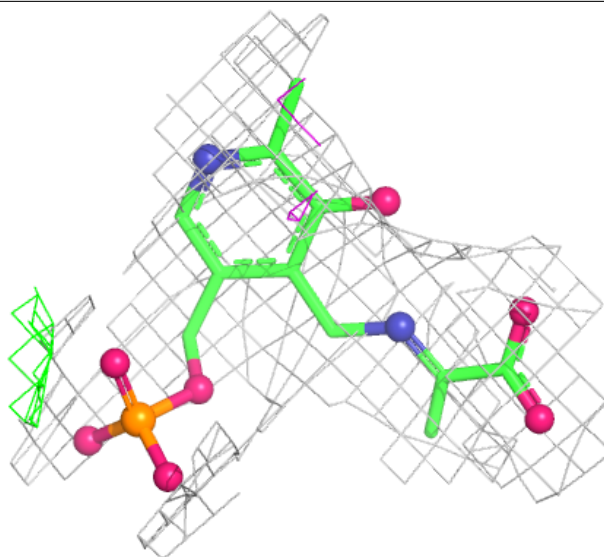
Electron density around P1T F 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



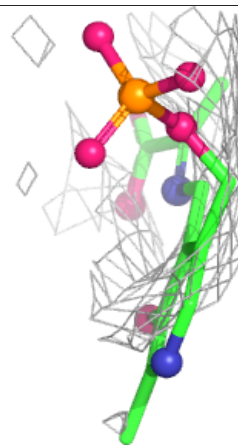
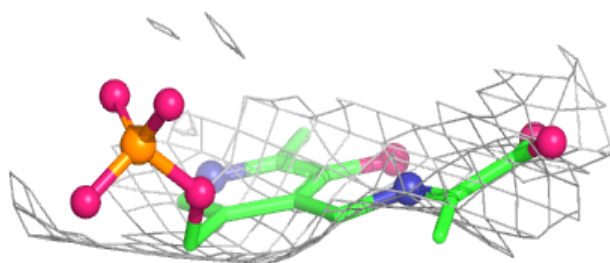
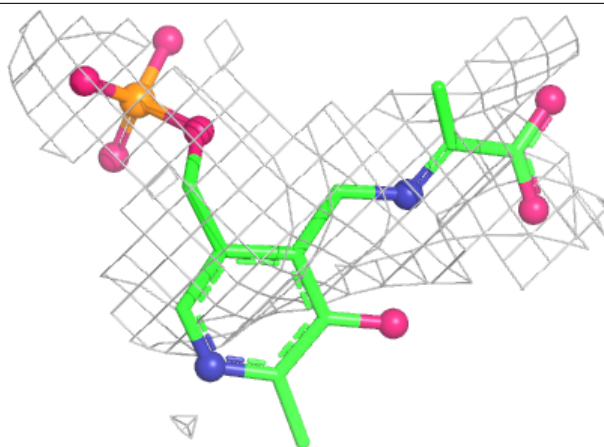
Electron density around P1T H 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



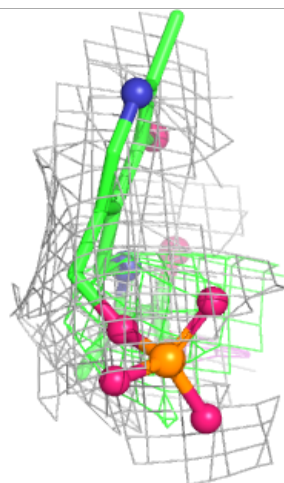
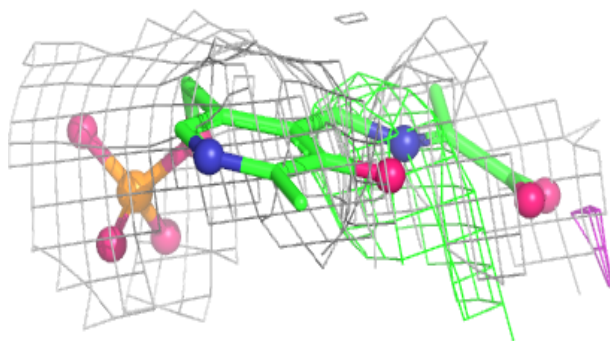
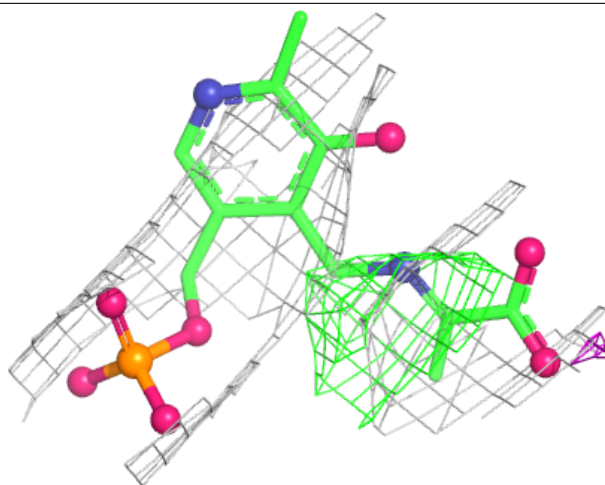
Electron density around P1T J 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



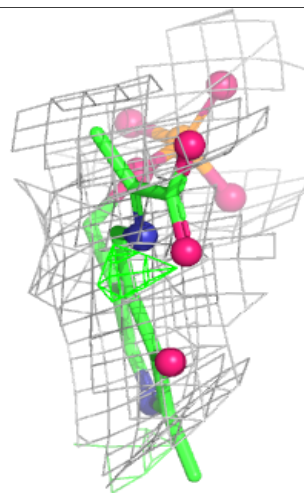
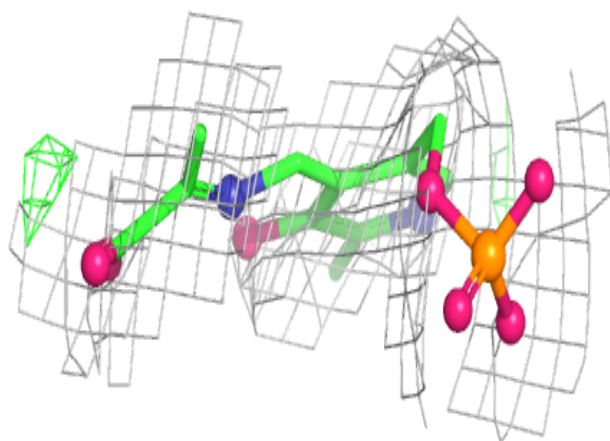
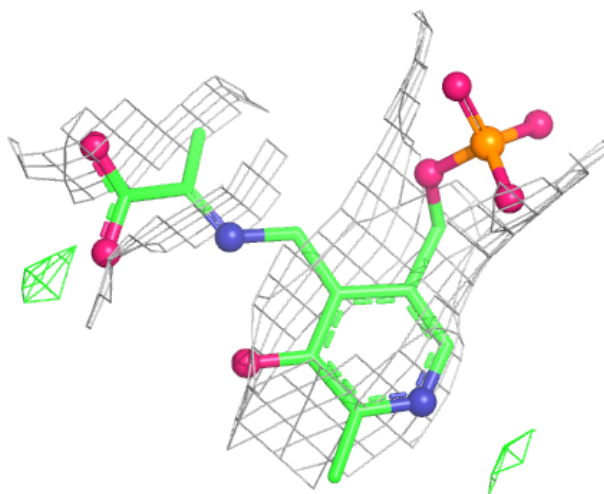
Electron density around P1T B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



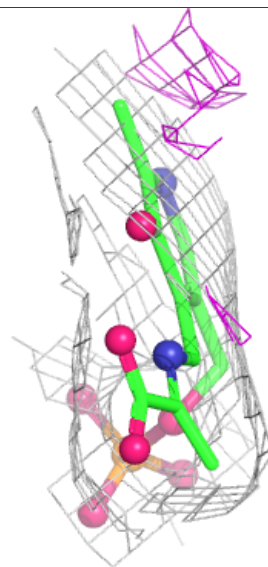
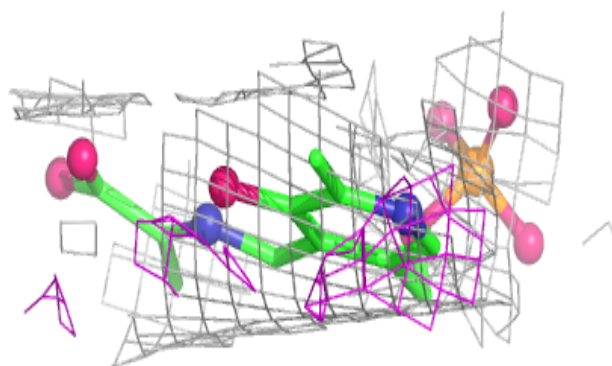
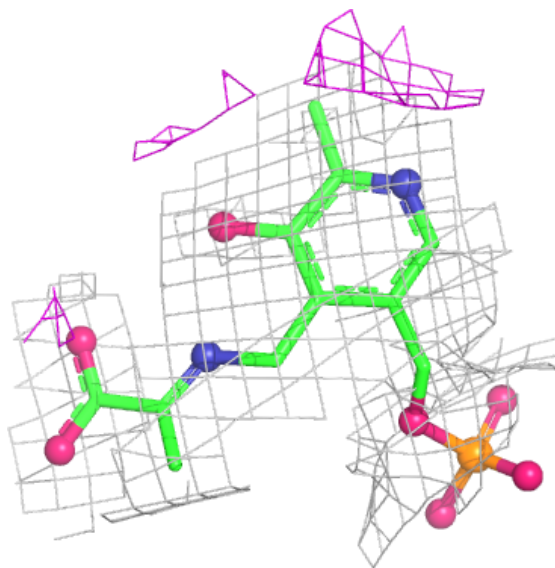
Electron density around P1T N 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



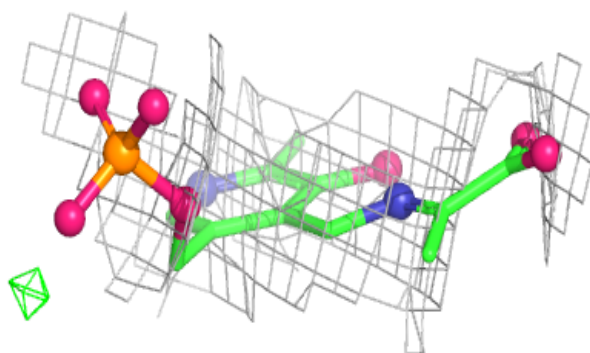
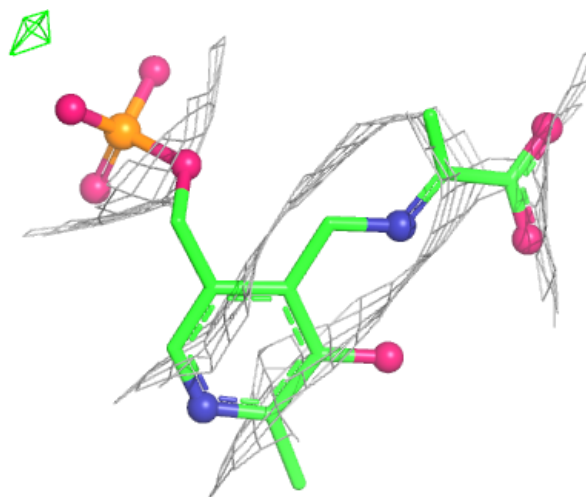
Electron density around P1T P 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



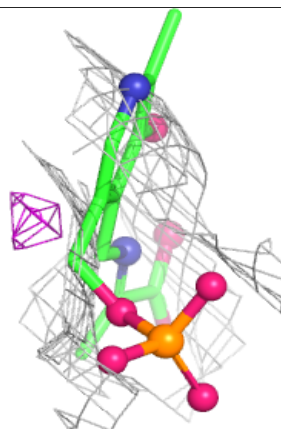
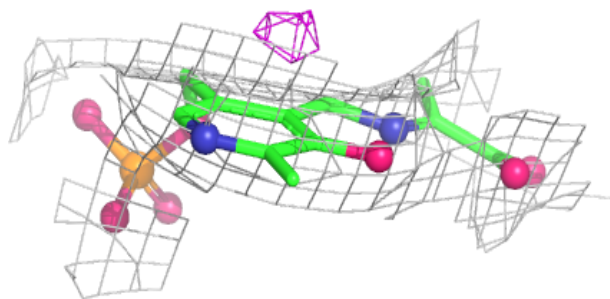
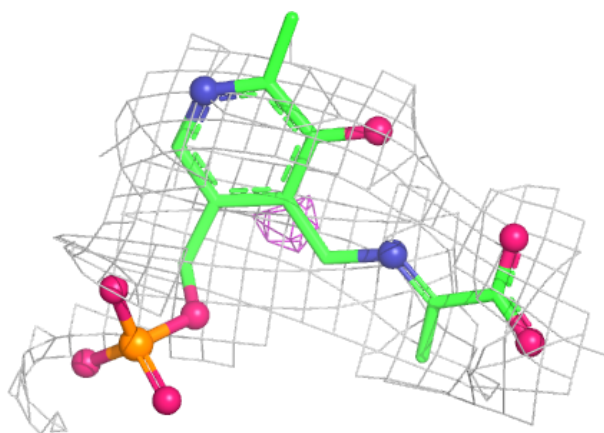
Electron density around P1T R 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



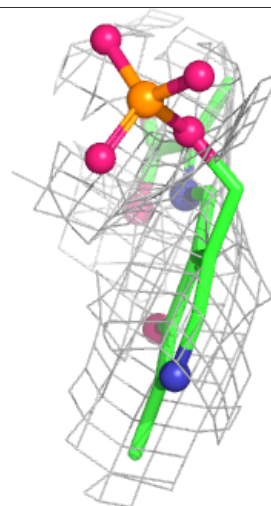
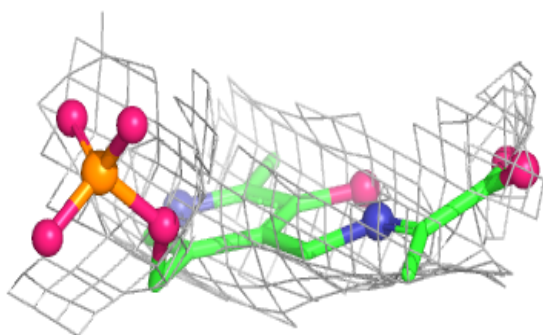
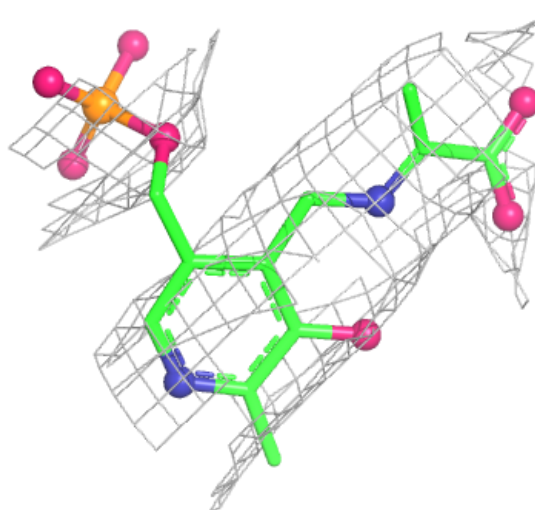
Electron density around P1T T 501:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



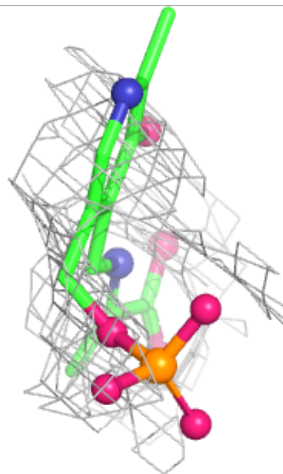
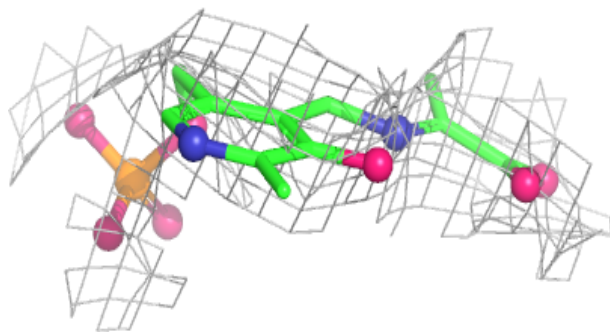
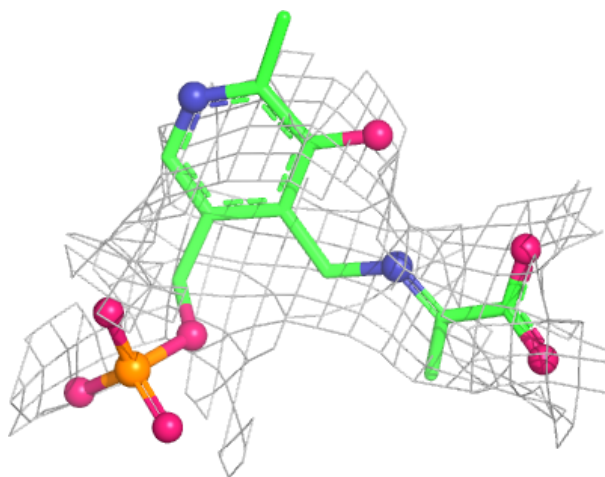
Electron density around P1T V 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P1T X 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.