



wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 02:15 am BST

PDB ID : 5OCW
Title : Structure of Mycobacterium tuberculosis tryptophan synthase in space group F222
Authors : Futterer, 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 (i) symbol.

The following versions of software and data (see [references \(1\)](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

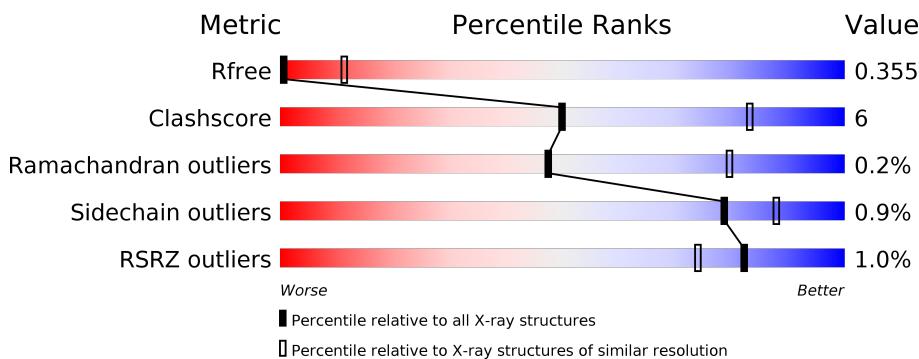
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



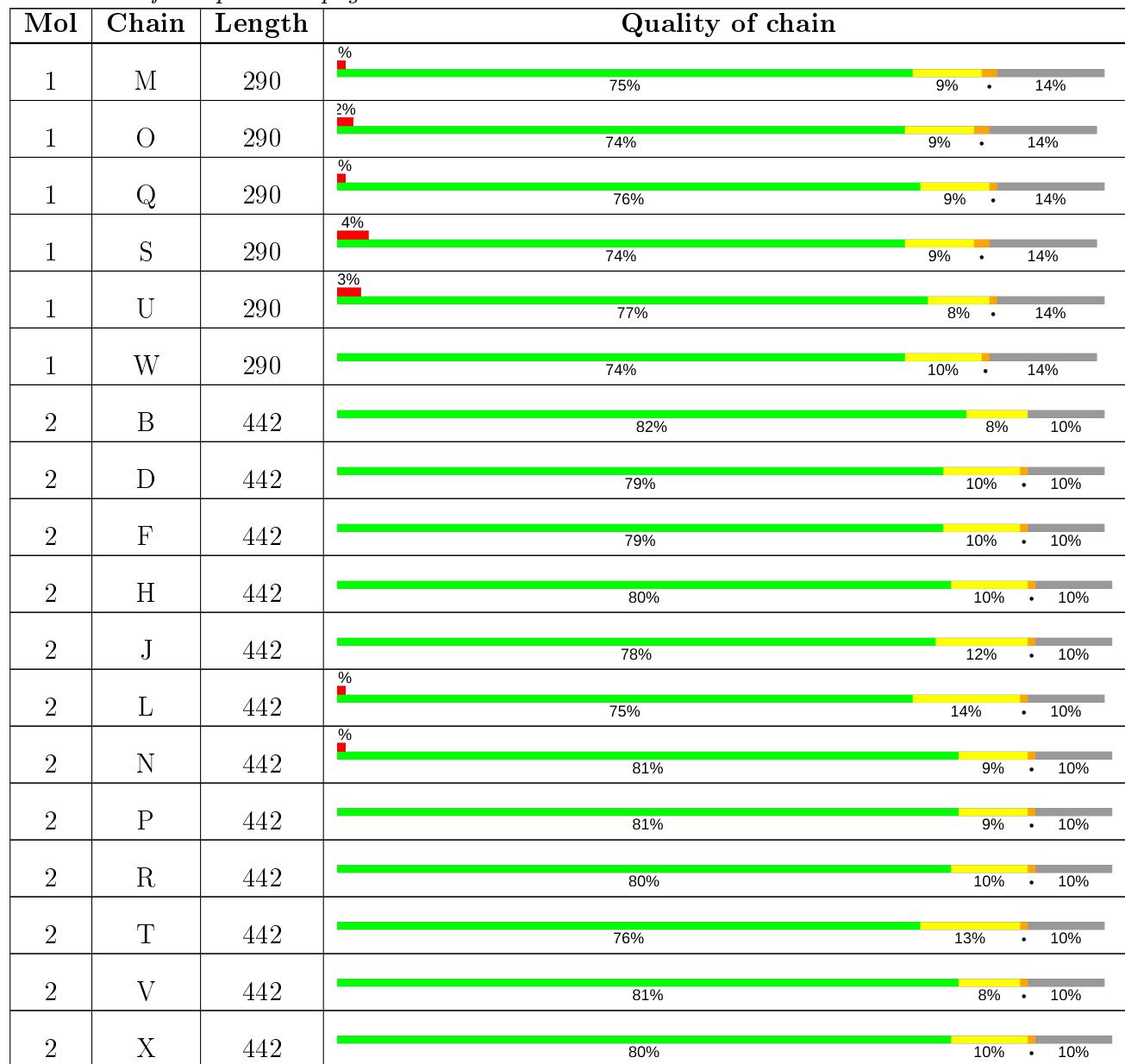
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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.



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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	P1T	D	501	-	-	-	X
3	P1T	P	501	-	-	-	X

2 Entry composition i

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 1852	N 1159	O 335	S 353	5	0	1	0
1	C	248	Total	C 1799	N 1129	O 322	S 343	5	0	0	0
1	E	249	Total	C 1814	N 1137	O 327	S 345	5	0	1	0
1	G	248	Total	C 1799	N 1129	O 322	S 343	5	0	0	0
1	I	249	Total	C 1814	N 1137	O 327	S 345	5	0	1	0
1	K	248	Total	C 1799	N 1129	O 322	S 343	5	0	0	0
1	M	249	Total	C 1814	N 1137	O 327	S 345	5	0	1	0
1	O	248	Total	C 1799	N 1129	O 322	S 343	5	0	0	0
1	Q	249	Total	C 1814	N 1137	O 327	S 345	5	0	1	0
1	S	248	Total	C 1799	N 1129	O 322	S 343	5	0	0	0
1	U	249	Total	C 1814	N 1137	O 327	S 345	5	0	1	0
1	W	248	Total	C 1799	N 1129	O 322	S 343	5	0	0	0

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P9WFY1
A	-13	HIS	-	expression tag	UNP P9WFY1
A	-12	HIS	-	expression tag	UNP P9WFY1
A	-11	HIS	-	expression tag	UNP P9WFY1
A	-10	HIS	-	expression tag	UNP P9WFY1
A	-9	SER	-	expression tag	UNP P9WFY1
A	-8	SER	-	expression tag	UNP P9WFY1
A	-7	GLY	-	expression tag	UNP P9WFY1
A	-6	LEU	-	expression tag	UNP P9WFY1
A	-5	VAL	-	expression tag	UNP P9WFY1
A	-4	PRO	-	expression tag	UNP P9WFY1
A	-3	ARG	-	expression tag	UNP P9WFY1
A	-2	GLY	-	expression tag	UNP P9WFY1
A	-1	SER	-	expression tag	UNP P9WFY1
A	0	HIS	-	expression tag	UNP P9WFY1
C	-19	MET	-	initiating methionine	UNP P9WFY1
C	-18	GLY	-	expression tag	UNP P9WFY1
C	-17	SER	-	expression tag	UNP P9WFY1
C	-16	SER	-	expression tag	UNP P9WFY1
C	-15	HIS	-	expression tag	UNP P9WFY1
C	-14	HIS	-	expression tag	UNP P9WFY1
C	-13	HIS	-	expression tag	UNP P9WFY1
C	-12	HIS	-	expression tag	UNP P9WFY1
C	-11	HIS	-	expression tag	UNP P9WFY1
C	-10	HIS	-	expression tag	UNP P9WFY1
C	-9	SER	-	expression tag	UNP P9WFY1
C	-8	SER	-	expression tag	UNP P9WFY1
C	-7	GLY	-	expression tag	UNP P9WFY1
C	-6	LEU	-	expression tag	UNP P9WFY1
C	-5	VAL	-	expression tag	UNP P9WFY1
C	-4	PRO	-	expression tag	UNP P9WFY1
C	-3	ARG	-	expression tag	UNP P9WFY1
C	-2	GLY	-	expression tag	UNP P9WFY1
C	-1	SER	-	expression tag	UNP P9WFY1
C	0	HIS	-	expression tag	UNP P9WFY1
E	-19	MET	-	initiating methionine	UNP P9WFY1
E	-18	GLY	-	expression tag	UNP P9WFY1
E	-17	SER	-	expression tag	UNP P9WFY1
E	-16	SER	-	expression tag	UNP P9WFY1
E	-15	HIS	-	expression tag	UNP P9WFY1
E	-14	HIS	-	expression tag	UNP P9WFY1
E	-13	HIS	-	expression tag	UNP P9WFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP P9WFY1
E	-11	HIS	-	expression tag	UNP P9WFY1
E	-10	HIS	-	expression tag	UNP P9WFY1
E	-9	SER	-	expression tag	UNP P9WFY1
E	-8	SER	-	expression tag	UNP P9WFY1
E	-7	GLY	-	expression tag	UNP P9WFY1
E	-6	LEU	-	expression tag	UNP P9WFY1
E	-5	VAL	-	expression tag	UNP P9WFY1
E	-4	PRO	-	expression tag	UNP P9WFY1
E	-3	ARG	-	expression tag	UNP P9WFY1
E	-2	GLY	-	expression tag	UNP P9WFY1
E	-1	SER	-	expression tag	UNP P9WFY1
E	0	HIS	-	expression tag	UNP P9WFY1
G	-19	MET	-	initiating methionine	UNP P9WFY1
G	-18	GLY	-	expression tag	UNP P9WFY1
G	-17	SER	-	expression tag	UNP P9WFY1
G	-16	SER	-	expression tag	UNP P9WFY1
G	-15	HIS	-	expression tag	UNP P9WFY1
G	-14	HIS	-	expression tag	UNP P9WFY1
G	-13	HIS	-	expression tag	UNP P9WFY1
G	-12	HIS	-	expression tag	UNP P9WFY1
G	-11	HIS	-	expression tag	UNP P9WFY1
G	-10	HIS	-	expression tag	UNP P9WFY1
G	-9	SER	-	expression tag	UNP P9WFY1
G	-8	SER	-	expression tag	UNP P9WFY1
G	-7	GLY	-	expression tag	UNP P9WFY1
G	-6	LEU	-	expression tag	UNP P9WFY1
G	-5	VAL	-	expression tag	UNP P9WFY1
G	-4	PRO	-	expression tag	UNP P9WFY1
G	-3	ARG	-	expression tag	UNP P9WFY1
G	-2	GLY	-	expression tag	UNP P9WFY1
G	-1	SER	-	expression tag	UNP P9WFY1
G	0	HIS	-	expression tag	UNP P9WFY1
I	-19	MET	-	initiating methionine	UNP P9WFY1
I	-18	GLY	-	expression tag	UNP P9WFY1
I	-17	SER	-	expression tag	UNP P9WFY1
I	-16	SER	-	expression tag	UNP P9WFY1
I	-15	HIS	-	expression tag	UNP P9WFY1
I	-14	HIS	-	expression tag	UNP P9WFY1
I	-13	HIS	-	expression tag	UNP P9WFY1
I	-12	HIS	-	expression tag	UNP P9WFY1
I	-11	HIS	-	expression tag	UNP P9WFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP P9WFY1
I	-9	SER	-	expression tag	UNP P9WFY1
I	-8	SER	-	expression tag	UNP P9WFY1
I	-7	GLY	-	expression tag	UNP P9WFY1
I	-6	LEU	-	expression tag	UNP P9WFY1
I	-5	VAL	-	expression tag	UNP P9WFY1
I	-4	PRO	-	expression tag	UNP P9WFY1
I	-3	ARG	-	expression tag	UNP P9WFY1
I	-2	GLY	-	expression tag	UNP P9WFY1
I	-1	SER	-	expression tag	UNP P9WFY1
I	0	HIS	-	expression tag	UNP P9WFY1
K	-19	MET	-	initiating methionine	UNP P9WFY1
K	-18	GLY	-	expression tag	UNP P9WFY1
K	-17	SER	-	expression tag	UNP P9WFY1
K	-16	SER	-	expression tag	UNP P9WFY1
K	-15	HIS	-	expression tag	UNP P9WFY1
K	-14	HIS	-	expression tag	UNP P9WFY1
K	-13	HIS	-	expression tag	UNP P9WFY1
K	-12	HIS	-	expression tag	UNP P9WFY1
K	-11	HIS	-	expression tag	UNP P9WFY1
K	-10	HIS	-	expression tag	UNP P9WFY1
K	-9	SER	-	expression tag	UNP P9WFY1
K	-8	SER	-	expression tag	UNP P9WFY1
K	-7	GLY	-	expression tag	UNP P9WFY1
K	-6	LEU	-	expression tag	UNP P9WFY1
K	-5	VAL	-	expression tag	UNP P9WFY1
K	-4	PRO	-	expression tag	UNP P9WFY1
K	-3	ARG	-	expression tag	UNP P9WFY1
K	-2	GLY	-	expression tag	UNP P9WFY1
K	-1	SER	-	expression tag	UNP P9WFY1
K	0	HIS	-	expression tag	UNP P9WFY1
M	-19	MET	-	initiating methionine	UNP P9WFY1
M	-18	GLY	-	expression tag	UNP P9WFY1
M	-17	SER	-	expression tag	UNP P9WFY1
M	-16	SER	-	expression tag	UNP P9WFY1
M	-15	HIS	-	expression tag	UNP P9WFY1
M	-14	HIS	-	expression tag	UNP P9WFY1
M	-13	HIS	-	expression tag	UNP P9WFY1
M	-12	HIS	-	expression tag	UNP P9WFY1
M	-11	HIS	-	expression tag	UNP P9WFY1
M	-10	HIS	-	expression tag	UNP P9WFY1
M	-9	SER	-	expression tag	UNP P9WFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	SER	-	expression tag	UNP P9WFY1
M	-7	GLY	-	expression tag	UNP P9WFY1
M	-6	LEU	-	expression tag	UNP P9WFY1
M	-5	VAL	-	expression tag	UNP P9WFY1
M	-4	PRO	-	expression tag	UNP P9WFY1
M	-3	ARG	-	expression tag	UNP P9WFY1
M	-2	GLY	-	expression tag	UNP P9WFY1
M	-1	SER	-	expression tag	UNP P9WFY1
M	0	HIS	-	expression tag	UNP P9WFY1
O	-19	MET	-	initiating methionine	UNP P9WFY1
O	-18	GLY	-	expression tag	UNP P9WFY1
O	-17	SER	-	expression tag	UNP P9WFY1
O	-16	SER	-	expression tag	UNP P9WFY1
O	-15	HIS	-	expression tag	UNP P9WFY1
O	-14	HIS	-	expression tag	UNP P9WFY1
O	-13	HIS	-	expression tag	UNP P9WFY1
O	-12	HIS	-	expression tag	UNP P9WFY1
O	-11	HIS	-	expression tag	UNP P9WFY1
O	-10	HIS	-	expression tag	UNP P9WFY1
O	-9	SER	-	expression tag	UNP P9WFY1
O	-8	SER	-	expression tag	UNP P9WFY1
O	-7	GLY	-	expression tag	UNP P9WFY1
O	-6	LEU	-	expression tag	UNP P9WFY1
O	-5	VAL	-	expression tag	UNP P9WFY1
O	-4	PRO	-	expression tag	UNP P9WFY1
O	-3	ARG	-	expression tag	UNP P9WFY1
O	-2	GLY	-	expression tag	UNP P9WFY1
O	-1	SER	-	expression tag	UNP P9WFY1
O	0	HIS	-	expression tag	UNP P9WFY1
Q	-19	MET	-	initiating methionine	UNP P9WFY1
Q	-18	GLY	-	expression tag	UNP P9WFY1
Q	-17	SER	-	expression tag	UNP P9WFY1
Q	-16	SER	-	expression tag	UNP P9WFY1
Q	-15	HIS	-	expression tag	UNP P9WFY1
Q	-14	HIS	-	expression tag	UNP P9WFY1
Q	-13	HIS	-	expression tag	UNP P9WFY1
Q	-12	HIS	-	expression tag	UNP P9WFY1
Q	-11	HIS	-	expression tag	UNP P9WFY1
Q	-10	HIS	-	expression tag	UNP P9WFY1
Q	-9	SER	-	expression tag	UNP P9WFY1
Q	-8	SER	-	expression tag	UNP P9WFY1
Q	-7	GLY	-	expression tag	UNP P9WFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-6	LEU	-	expression tag	UNP P9WFY1
Q	-5	VAL	-	expression tag	UNP P9WFY1
Q	-4	PRO	-	expression tag	UNP P9WFY1
Q	-3	ARG	-	expression tag	UNP P9WFY1
Q	-2	GLY	-	expression tag	UNP P9WFY1
Q	-1	SER	-	expression tag	UNP P9WFY1
Q	0	HIS	-	expression tag	UNP P9WFY1
S	-19	MET	-	initiating methionine	UNP P9WFY1
S	-18	GLY	-	expression tag	UNP P9WFY1
S	-17	SER	-	expression tag	UNP P9WFY1
S	-16	SER	-	expression tag	UNP P9WFY1
S	-15	HIS	-	expression tag	UNP P9WFY1
S	-14	HIS	-	expression tag	UNP P9WFY1
S	-13	HIS	-	expression tag	UNP P9WFY1
S	-12	HIS	-	expression tag	UNP P9WFY1
S	-11	HIS	-	expression tag	UNP P9WFY1
S	-10	HIS	-	expression tag	UNP P9WFY1
S	-9	SER	-	expression tag	UNP P9WFY1
S	-8	SER	-	expression tag	UNP P9WFY1
S	-7	GLY	-	expression tag	UNP P9WFY1
S	-6	LEU	-	expression tag	UNP P9WFY1
S	-5	VAL	-	expression tag	UNP P9WFY1
S	-4	PRO	-	expression tag	UNP P9WFY1
S	-3	ARG	-	expression tag	UNP P9WFY1
S	-2	GLY	-	expression tag	UNP P9WFY1
S	-1	SER	-	expression tag	UNP P9WFY1
S	0	HIS	-	expression tag	UNP P9WFY1
U	-19	MET	-	initiating methionine	UNP P9WFY1
U	-18	GLY	-	expression tag	UNP P9WFY1
U	-17	SER	-	expression tag	UNP P9WFY1
U	-16	SER	-	expression tag	UNP P9WFY1
U	-15	HIS	-	expression tag	UNP P9WFY1
U	-14	HIS	-	expression tag	UNP P9WFY1
U	-13	HIS	-	expression tag	UNP P9WFY1
U	-12	HIS	-	expression tag	UNP P9WFY1
U	-11	HIS	-	expression tag	UNP P9WFY1
U	-10	HIS	-	expression tag	UNP P9WFY1
U	-9	SER	-	expression tag	UNP P9WFY1
U	-8	SER	-	expression tag	UNP P9WFY1
U	-7	GLY	-	expression tag	UNP P9WFY1
U	-6	LEU	-	expression tag	UNP P9WFY1
U	-5	VAL	-	expression tag	UNP P9WFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-4	PRO	-	expression tag	UNP P9WFY1
U	-3	ARG	-	expression tag	UNP P9WFY1
U	-2	GLY	-	expression tag	UNP P9WFY1
U	-1	SER	-	expression tag	UNP P9WFY1
U	0	HIS	-	expression tag	UNP P9WFY1
W	-19	MET	-	initiating methionine	UNP P9WFY1
W	-18	GLY	-	expression tag	UNP P9WFY1
W	-17	SER	-	expression tag	UNP P9WFY1
W	-16	SER	-	expression tag	UNP P9WFY1
W	-15	HIS	-	expression tag	UNP P9WFY1
W	-14	HIS	-	expression tag	UNP P9WFY1
W	-13	HIS	-	expression tag	UNP P9WFY1
W	-12	HIS	-	expression tag	UNP P9WFY1
W	-11	HIS	-	expression tag	UNP P9WFY1
W	-10	HIS	-	expression tag	UNP P9WFY1
W	-9	SER	-	expression tag	UNP P9WFY1
W	-8	SER	-	expression tag	UNP P9WFY1
W	-7	GLY	-	expression tag	UNP P9WFY1
W	-6	LEU	-	expression tag	UNP P9WFY1
W	-5	VAL	-	expression tag	UNP P9WFY1
W	-4	PRO	-	expression tag	UNP P9WFY1
W	-3	ARG	-	expression tag	UNP P9WFY1
W	-2	GLY	-	expression tag	UNP P9WFY1
W	-1	SER	-	expression tag	UNP P9WFY1
W	0	HIS	-	expression tag	UNP P9WFY1

- 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			

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

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

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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

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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

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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

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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

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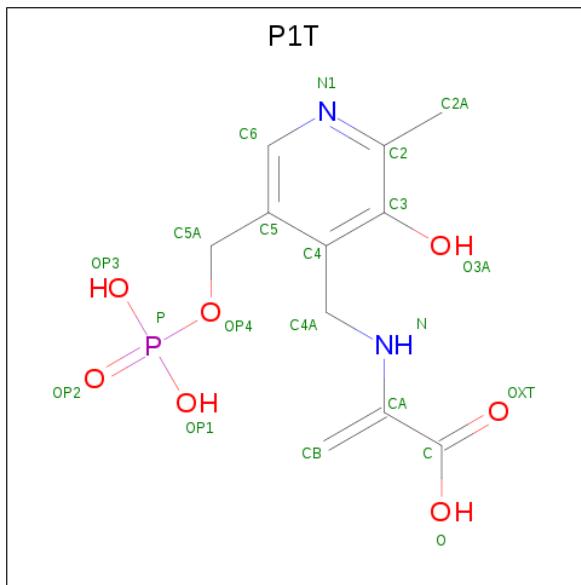
Chain	Residue	Modelled	Actual	Comment	Reference
T	-14	GLY	-	expression tag	UNP P9WFX9
T	-13	SER	-	expression tag	UNP P9WFX9
T	-12	HIS	-	expression tag	UNP P9WFX9
V	-31	MET	-	initiating methionine	UNP P9WFX9
V	-30	GLY	-	expression tag	UNP P9WFX9
V	-29	SER	-	expression tag	UNP P9WFX9
V	-28	SER	-	expression 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

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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]AMINOACRYLIC ACID (three-letter code: P1T) (formula: C₁₁H₁₅N₂O₇P).



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

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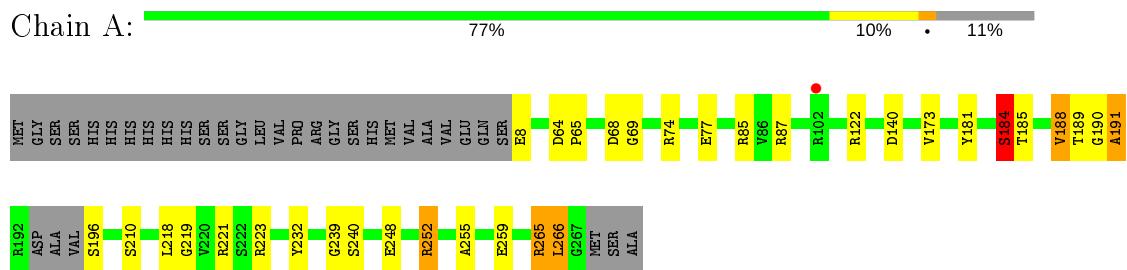
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	V	1	21	11	2	7	1	0	0
3	X	1	21	11	2	7	1	0	0

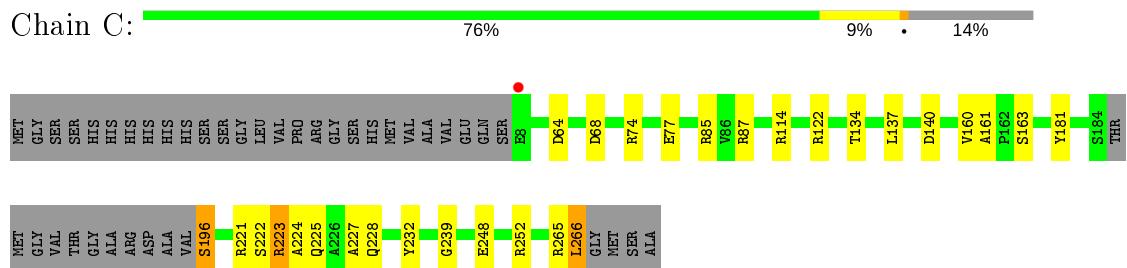
3 Residue-property plots

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

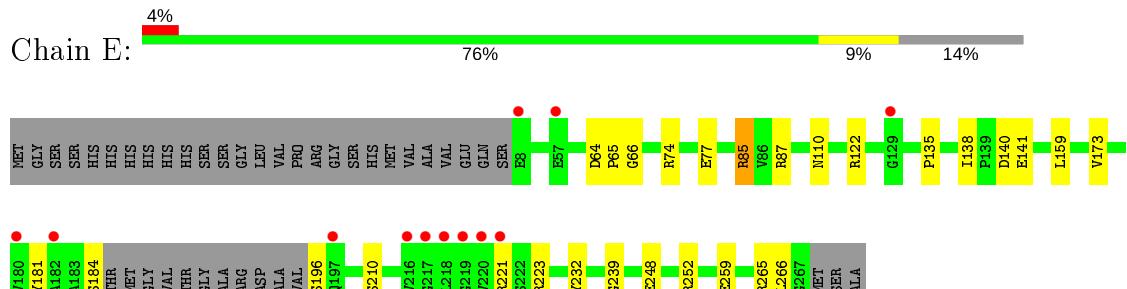
- Molecule 1: Tryptophan synthase alpha chain



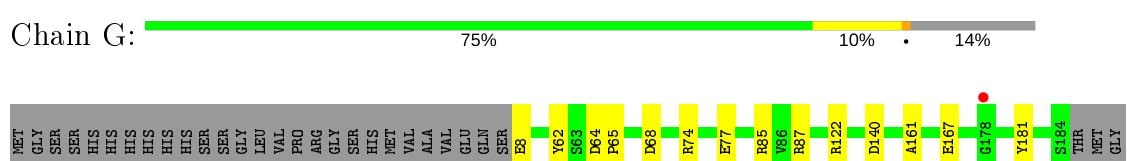
- Molecule 1: Tryptophan synthase alpha chain



- Molecule 1: Tryptophan synthase alpha chain

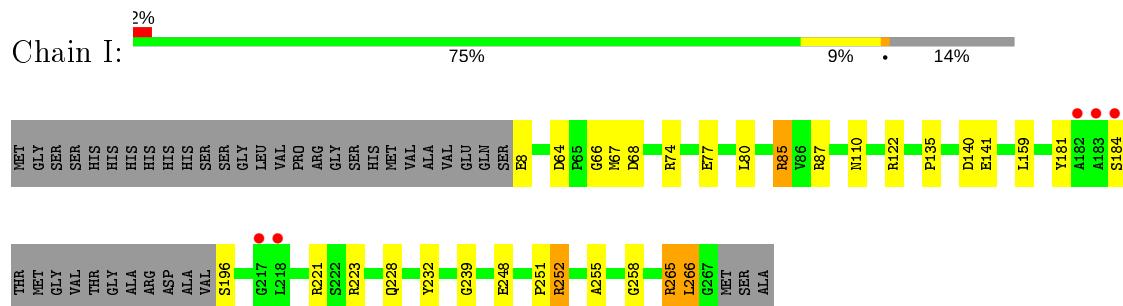


- Molecule 1: Tryptophan synthase alpha chain

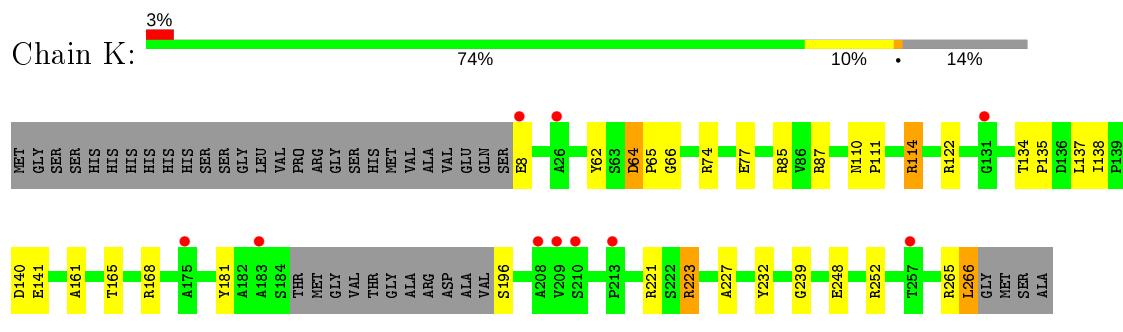




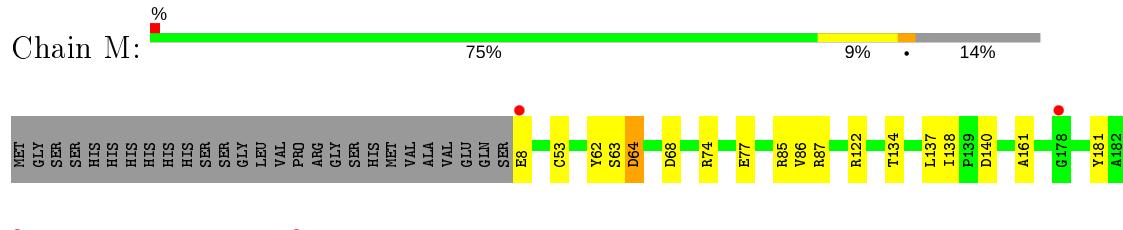
- Molecule 1: Tryptophan synthase alpha chain



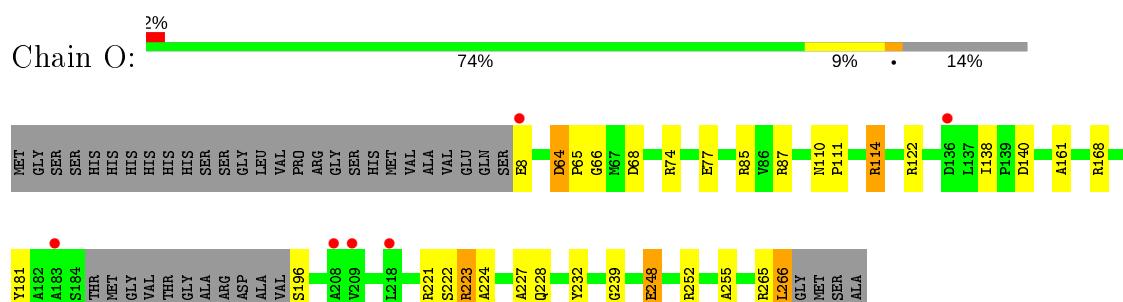
- Molecule 1: Tryptophan synthase alpha chain



- Molecule 1: Tryptophan synthase alpha chain

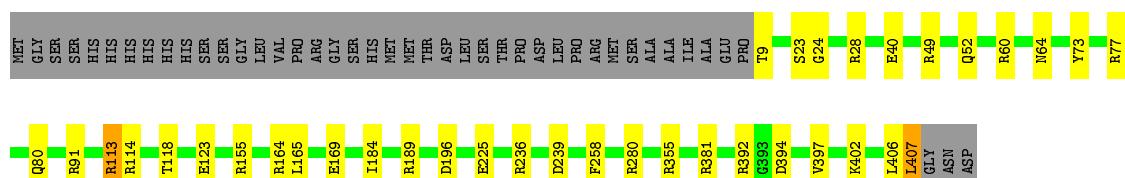
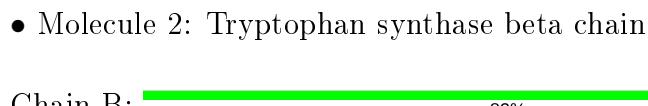
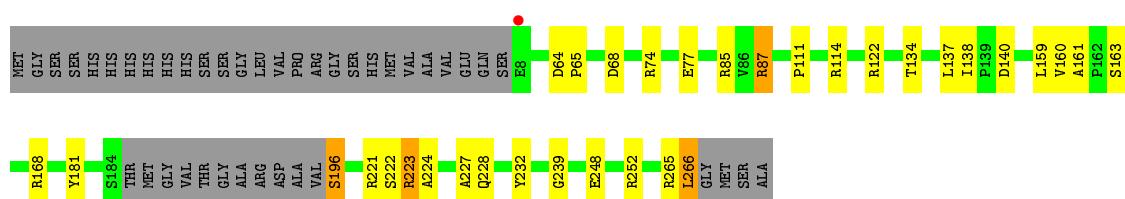
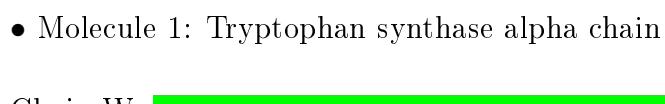
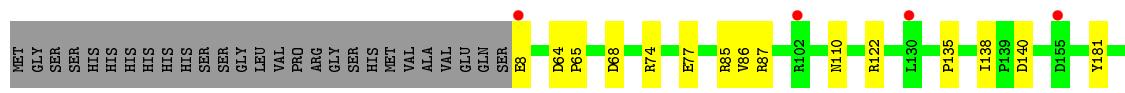
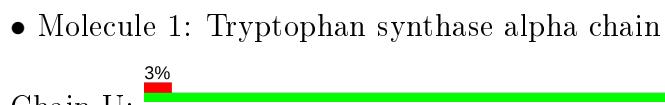
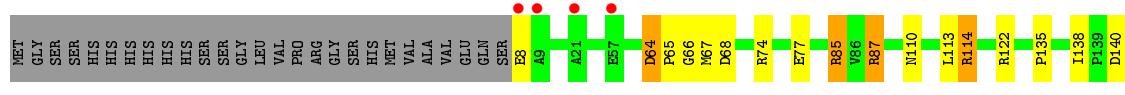
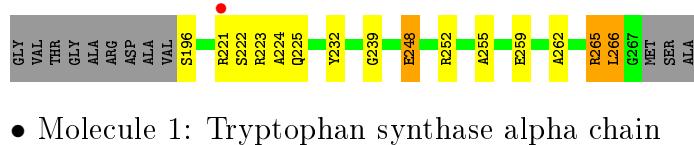


- Molecule 1: Tryptophan synthase alpha chain



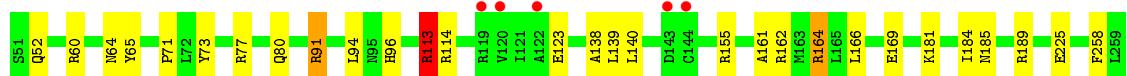
- Molecule 1: Tryptophan synthase alpha chain



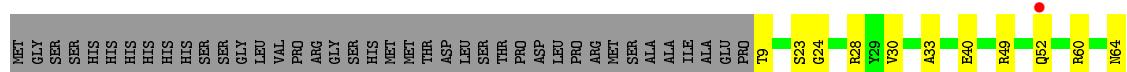
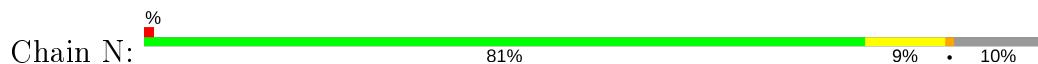




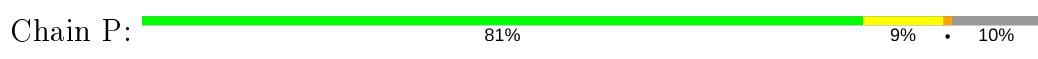
- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain





- Molecule 2: Tryptophan synthase beta chain

Chain T:



- Molecule 2: Tryptophan synthase beta chain

Chain V:



- Molecule 2: Tryptophan synthase beta chain

Chain X:



4 Data and refinement statistics i

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	426.05 Å 432.11 Å 434.03 Å 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 4.00 Å)	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)	0.20 , -9.9	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	0.85	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 i

5.1 Standard geometry i

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	1.37	29/1881 (1.5%)	1.54	34/2566 (1.3%)
1	C	1.32	25/1828 (1.4%)	1.42	29/2495 (1.2%)
1	E	1.33	24/1843 (1.3%)	1.52	30/2514 (1.2%)
1	G	1.33	30/1828 (1.6%)	1.43	29/2495 (1.2%)
1	I	1.36	26/1843 (1.4%)	1.55	34/2514 (1.4%)
1	K	1.34	27/1828 (1.5%)	1.43	31/2495 (1.2%)
1	M	1.37	27/1843 (1.5%)	1.55	34/2514 (1.4%)
1	O	1.33	25/1828 (1.4%)	1.43	30/2495 (1.2%)
1	Q	1.37	28/1843 (1.5%)	1.54	34/2514 (1.4%)
1	S	1.37	27/1827 (1.5%)	1.46	33/2492 (1.3%)
1	U	1.36	28/1843 (1.5%)	1.55	34/2514 (1.4%)
1	W	1.32	24/1828 (1.3%)	1.43	30/2495 (1.2%)
2	B	1.27	42/3062 (1.4%)	1.24	40/4148 (1.0%)
2	D	1.24	40/3043 (1.3%)	1.26	37/4123 (0.9%)
2	F	1.29	40/3062 (1.3%)	1.22	39/4148 (0.9%)
2	H	1.22	40/3043 (1.3%)	1.30	35/4123 (0.8%)
2	J	1.28	42/3062 (1.4%)	1.23	39/4148 (0.9%)
2	L	1.25	42/3043 (1.4%)	1.27	37/4123 (0.9%)
2	N	1.28	41/3062 (1.3%)	1.24	39/4148 (0.9%)
2	P	1.25	43/3043 (1.4%)	1.27	35/4123 (0.8%)
2	R	1.28	42/3062 (1.4%)	1.23	36/4148 (0.9%)
2	T	1.25	42/3043 (1.4%)	1.27	37/4123 (0.9%)
2	V	1.27	42/3062 (1.4%)	1.24	40/4148 (1.0%)
2	X	1.24	42/3043 (1.4%)	1.27	38/4123 (0.9%)
All	All	1.29	818/58693 (1.4%)	1.35	834/79729 (1.0%)

The worst 5 of 818 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	24	GLY	N-CA	-17.82	1.19	1.46
2	B	24	GLY	N-CA	-17.53	1.19	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	221	ARG	CZ-NH2	-17.50	1.10	1.33
2	J	24	GLY	N-CA	-17.49	1.19	1.46
1	Q	221	ARG	CZ-NH2	-17.47	1.10	1.33

The worst 5 of 834 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	ARG	NE-CZ-NH1	28.37	134.49	120.30
1	M	221	ARG	NE-CZ-NH1	28.25	134.43	120.30
1	Q	221	ARG	NE-CZ-NH1	28.08	134.34	120.30
1	I	221	ARG	NE-CZ-NH1	28.03	134.32	120.30
1	A	221	ARG	NE-CZ-NH1	28.02	134.31	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1852	0	1855	50	0
1	C	1799	0	1819	10	22
1	E	1814	0	1834	16	2
1	G	1799	0	1816	57	0
1	I	1814	0	1834	32	0
1	K	1799	0	1819	63	3
1	M	1814	0	1834	40	0
1	O	1799	0	1819	20	14
1	Q	1814	0	1829	32	0
1	S	1799	0	1818	37	3
1	U	1814	0	1834	23	0
1	W	1799	0	1819	18	22
2	B	3002	0	2929	28	9
2	D	2983	0	2908	47	13
2	F	3002	0	2926	78	4
2	H	2983	0	2908	54	2
2	J	3002	0	2929	102	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2983	0	2908	152	0
2	N	3002	0	2929	26	13
2	P	2983	0	2908	41	5
2	R	3002	0	2929	72	3
2	T	2983	0	2906	113	0
2	V	3002	0	2929	27	10
2	X	2983	0	2908	43	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	663	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 663 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:H2	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

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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%)	9 44
1	C	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34 71
1	E	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34 71
1	G	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34 71
1	I	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34 71
1	K	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34 71
1	M	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34 71
1	O	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34 71
1	Q	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34 71
1	S	242/290 (83%)	239 (99%)	2 (1%)	1 (0%)	34 71
1	U	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34 71
1	W	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34 71
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

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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%)	47	79

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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/211 (85%)	177 (98%)	3 (2%)	60	78
1	C	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	E	180/211 (85%)	177 (98%)	3 (2%)	60	78
1	G	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	I	180/211 (85%)	177 (98%)	3 (2%)	60	78
1	K	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	M	180/211 (85%)	176 (98%)	4 (2%)	52	71
1	O	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	Q	180/211 (85%)	176 (98%)	4 (2%)	52	71
1	S	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	U	180/211 (85%)	177 (98%)	3 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	179/211 (85%)	177 (99%)	2 (1%)	73	85
2	B	298/331 (90%)	295 (99%)	3 (1%)	76	86
2	D	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	F	298/331 (90%)	296 (99%)	2 (1%)	84	90
2	H	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	J	298/331 (90%)	295 (99%)	3 (1%)	76	86
2	L	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	N	298/331 (90%)	295 (99%)	3 (1%)	76	86
2	P	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	R	298/331 (90%)	296 (99%)	2 (1%)	84	90
2	T	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	V	298/331 (90%)	295 (99%)	3 (1%)	76	86
2	X	296/331 (89%)	295 (100%)	1 (0%)	92	95
All	All	5718/6504 (88%)	5664 (99%)	54 (1%)	78	88

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	181	TYR
2	N	80	GLN
2	V	355	ARG
2	L	113	ARG
1	M	140	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	80	GLN
2	X	81	HIS
2	T	80	GLN
2	L	81	HIS
2	P	81	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [\(i\)](#)

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	H	501	-	18,21,21	2.73	4 (22%)	23,30,30	1.37	3 (13%)
3	P1T	B	501	-	18,21,21	2.73	4 (22%)	23,30,30	1.38	3 (13%)
3	P1T	L	501	-	18,21,21	2.87	4 (22%)	23,30,30	1.44	3 (13%)
3	P1T	V	501	-	18,21,21	2.80	4 (22%)	23,30,30	1.40	3 (13%)
3	P1T	P	501	-	18,21,21	2.76	4 (22%)	23,30,30	1.42	3 (13%)
3	P1T	J	501	-	18,21,21	2.80	4 (22%)	23,30,30	1.38	3 (13%)
3	P1T	T	501	-	18,21,21	2.68	4 (22%)	23,30,30	1.46	3 (13%)
3	P1T	X	501	-	18,21,21	2.72	4 (22%)	23,30,30	1.41	3 (13%)
3	P1T	R	501	-	18,21,21	2.77	4 (22%)	23,30,30	1.35	3 (13%)
3	P1T	F	501	-	18,21,21	2.73	4 (22%)	23,30,30	1.38	3 (13%)
3	P1T	D	501	-	18,21,21	2.73	4 (22%)	23,30,30	1.43	2 (8%)
3	P1T	N	501	-	18,21,21	2.76	4 (22%)	23,30,30	1.41	2 (8%)

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	H	501	-	-	3/10/15/15	0/1/1/1
3	P1T	B	501	-	-	3/10/15/15	0/1/1/1
3	P1T	L	501	-	-	3/10/15/15	0/1/1/1
3	P1T	V	501	-	-	3/10/15/15	0/1/1/1
3	P1T	P	501	-	-	3/10/15/15	0/1/1/1
3	P1T	J	501	-	-	3/10/15/15	0/1/1/1
3	P1T	T	501	-	-	3/10/15/15	0/1/1/1
3	P1T	X	501	-	-	3/10/15/15	0/1/1/1
3	P1T	R	501	-	-	3/10/15/15	0/1/1/1
3	P1T	F	501	-	-	3/10/15/15	0/1/1/1
3	P1T	D	501	-	-	3/10/15/15	0/1/1/1
3	P1T	N	501	-	-	3/10/15/15	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	501	P1T	C3-C2	8.06	1.49	1.40
3	R	501	P1T	C3-C2	7.80	1.48	1.40
3	V	501	P1T	C3-C2	7.69	1.48	1.40
3	F	501	P1T	C3-C2	7.52	1.48	1.40
3	P	501	P1T	C3-C2	7.50	1.48	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	P1T	C4A-C4-C3	3.72	124.03	120.04
3	N	501	P1T	C4A-C4-C3	3.41	123.69	120.04
3	X	501	P1T	C4A-C4-C3	3.36	123.64	120.04
3	V	501	P1T	C4A-C4-C3	3.33	123.61	120.04
3	P	501	P1T	C4A-C4-C3	3.32	123.59	120.04

There are no chirality outliers.

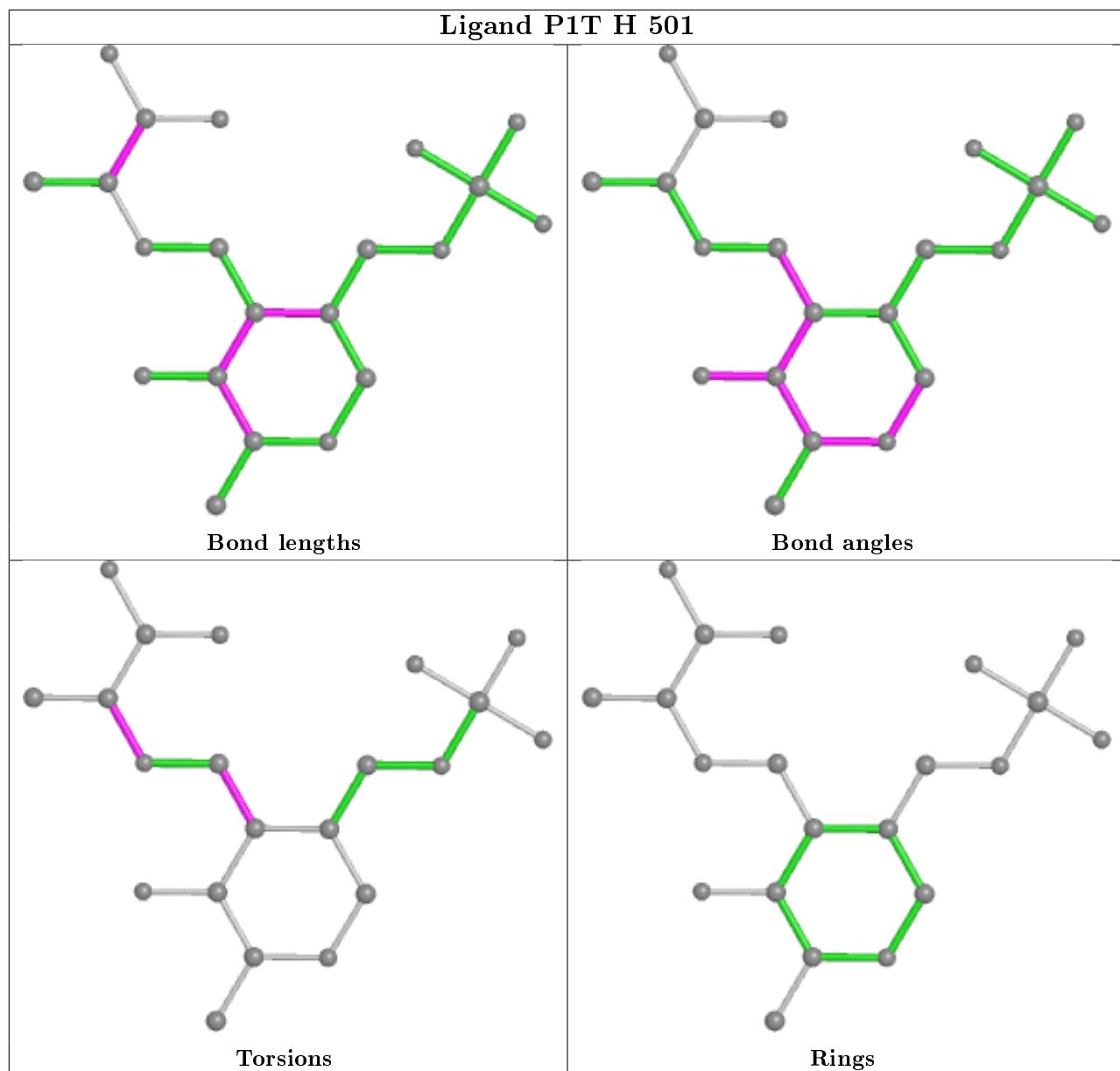
5 of 36 torsion outliers are listed below:

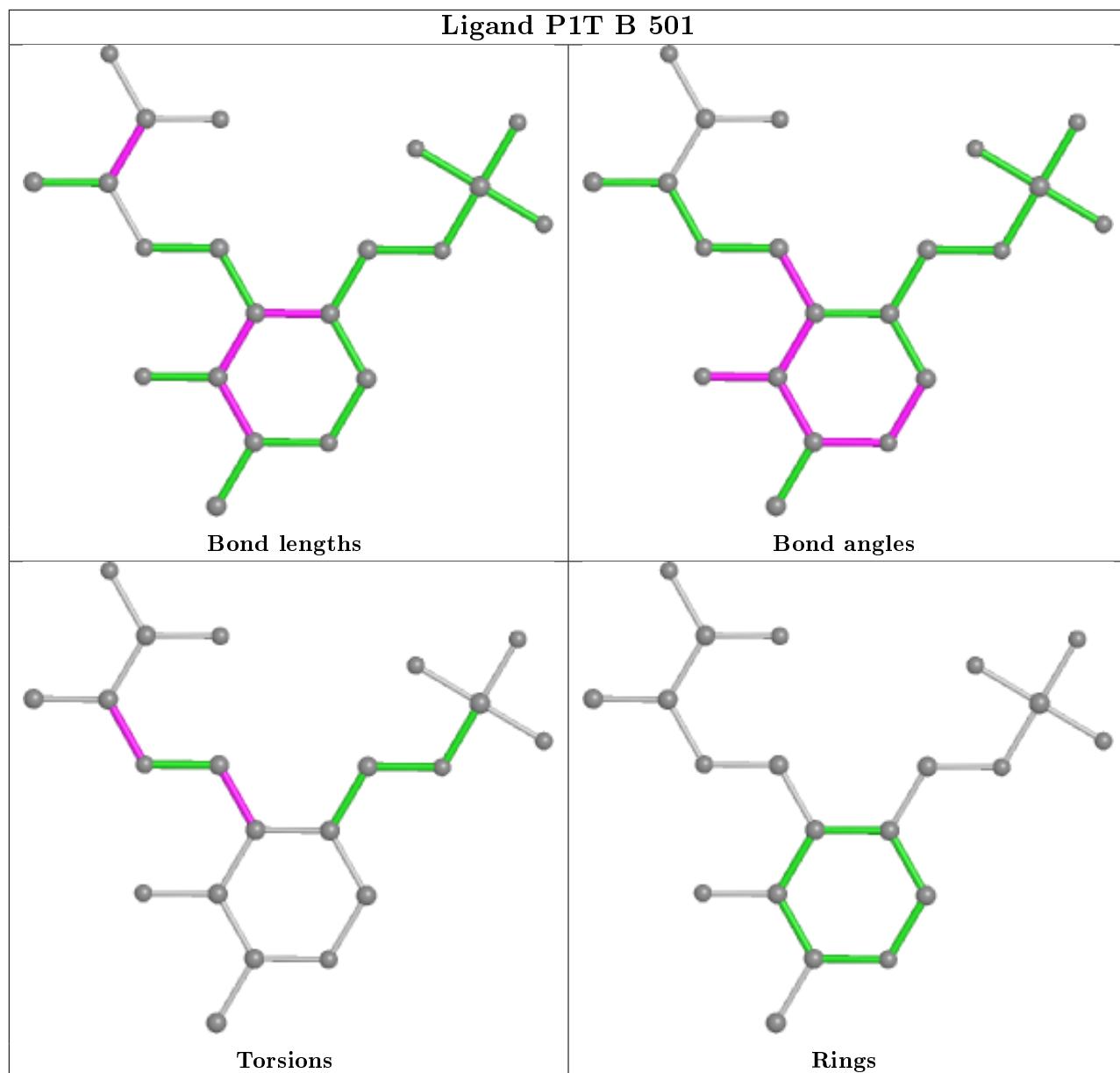
Mol	Chain	Res	Type	Atoms
3	H	501	P1T	C5-C4-C4A-N
3	B	501	P1T	C5-C4-C4A-N
3	L	501	P1T	C5-C4-C4A-N
3	V	501	P1T	C5-C4-C4A-N
3	P	501	P1T	C5-C4-C4A-N

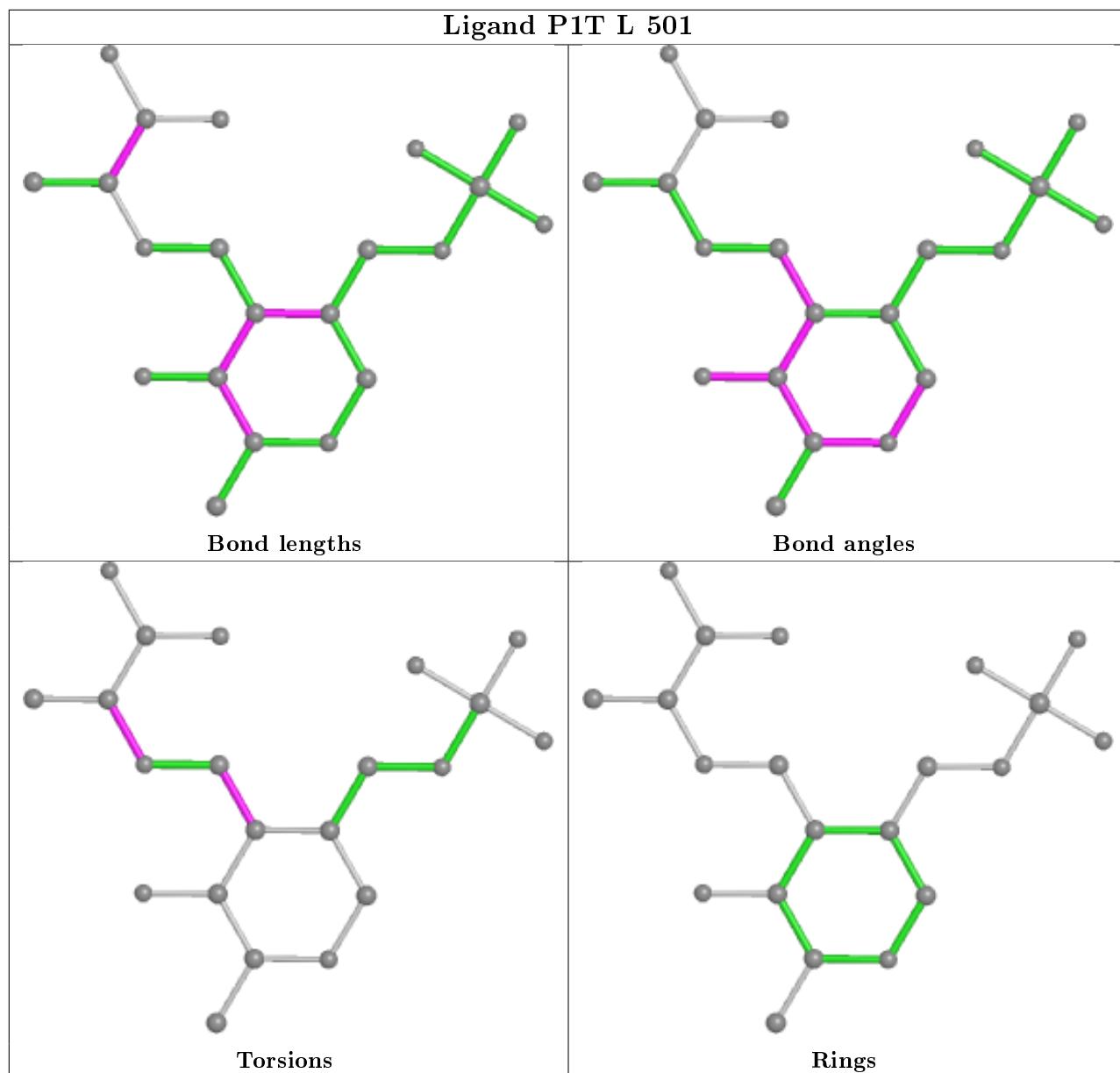
There are no ring outliers.

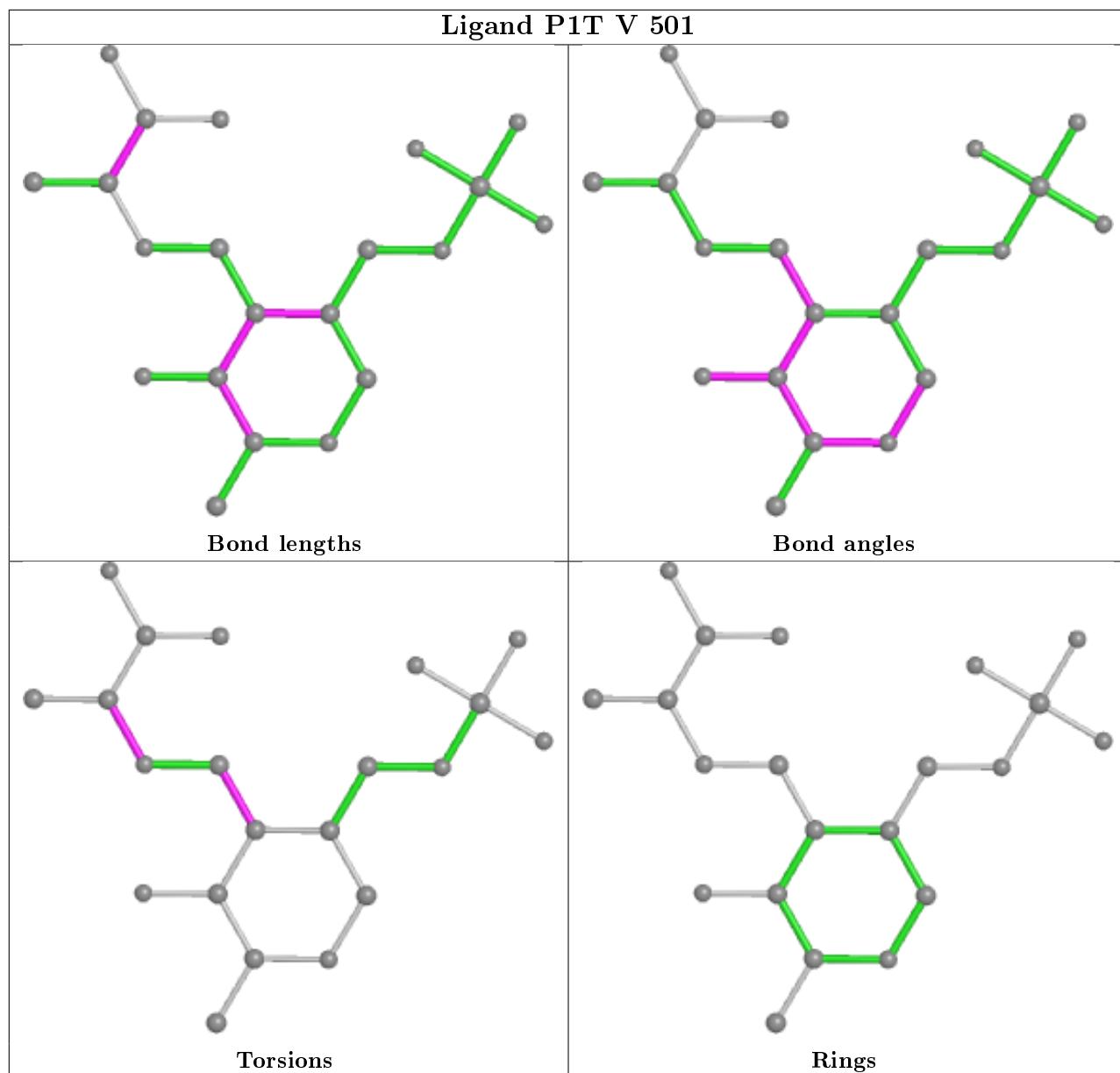
No monomer is involved in short contacts.

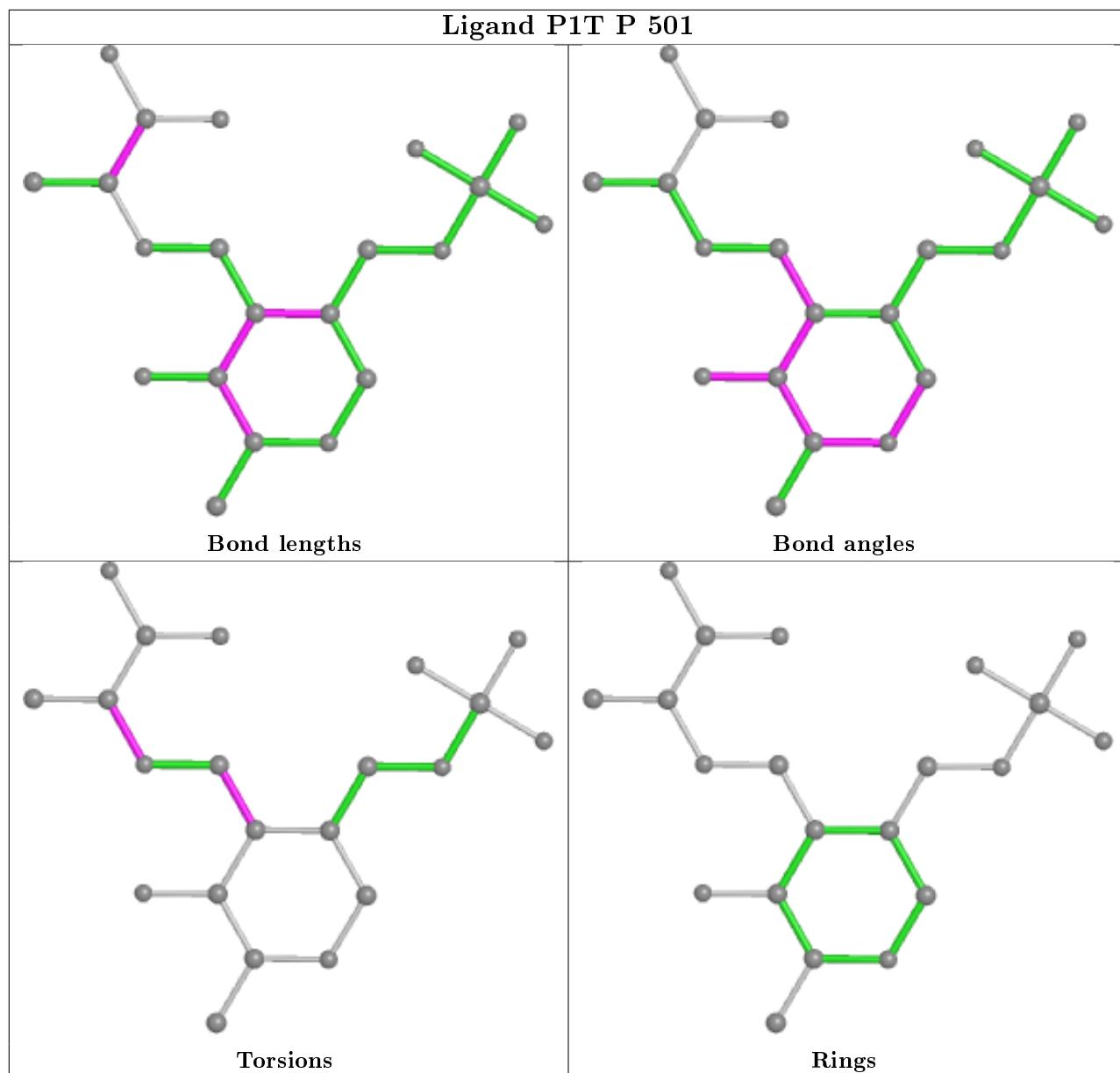
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

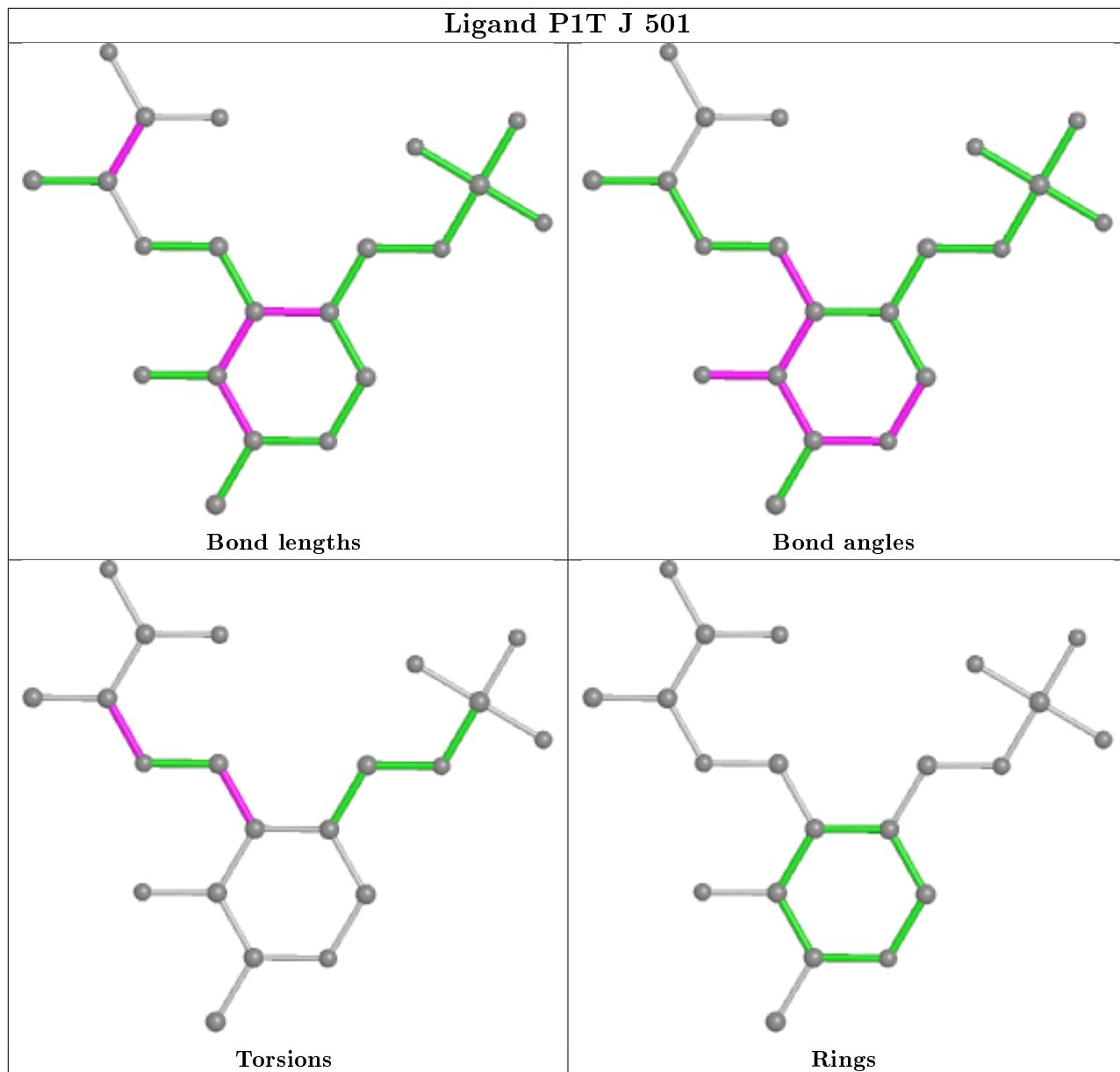


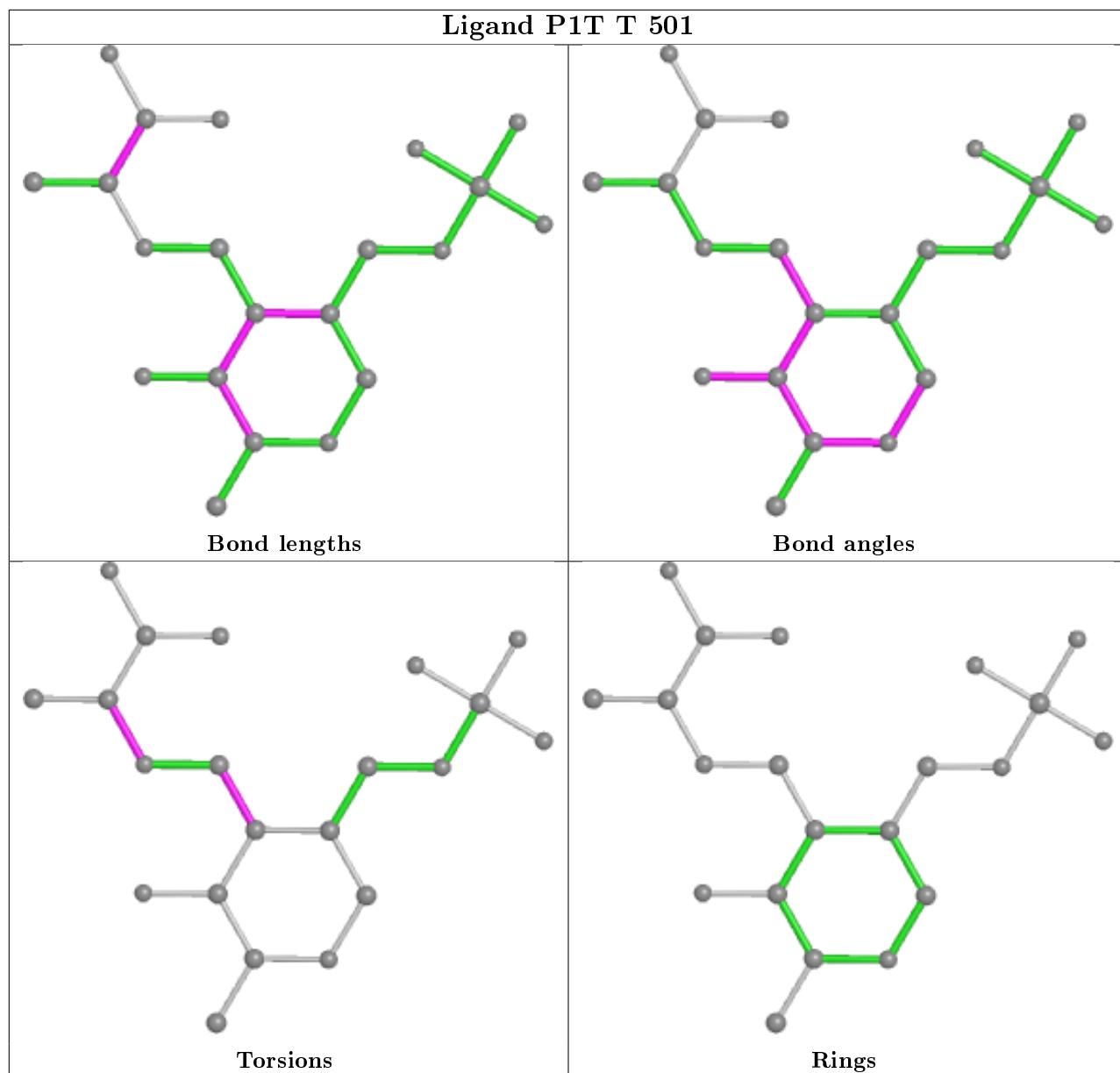


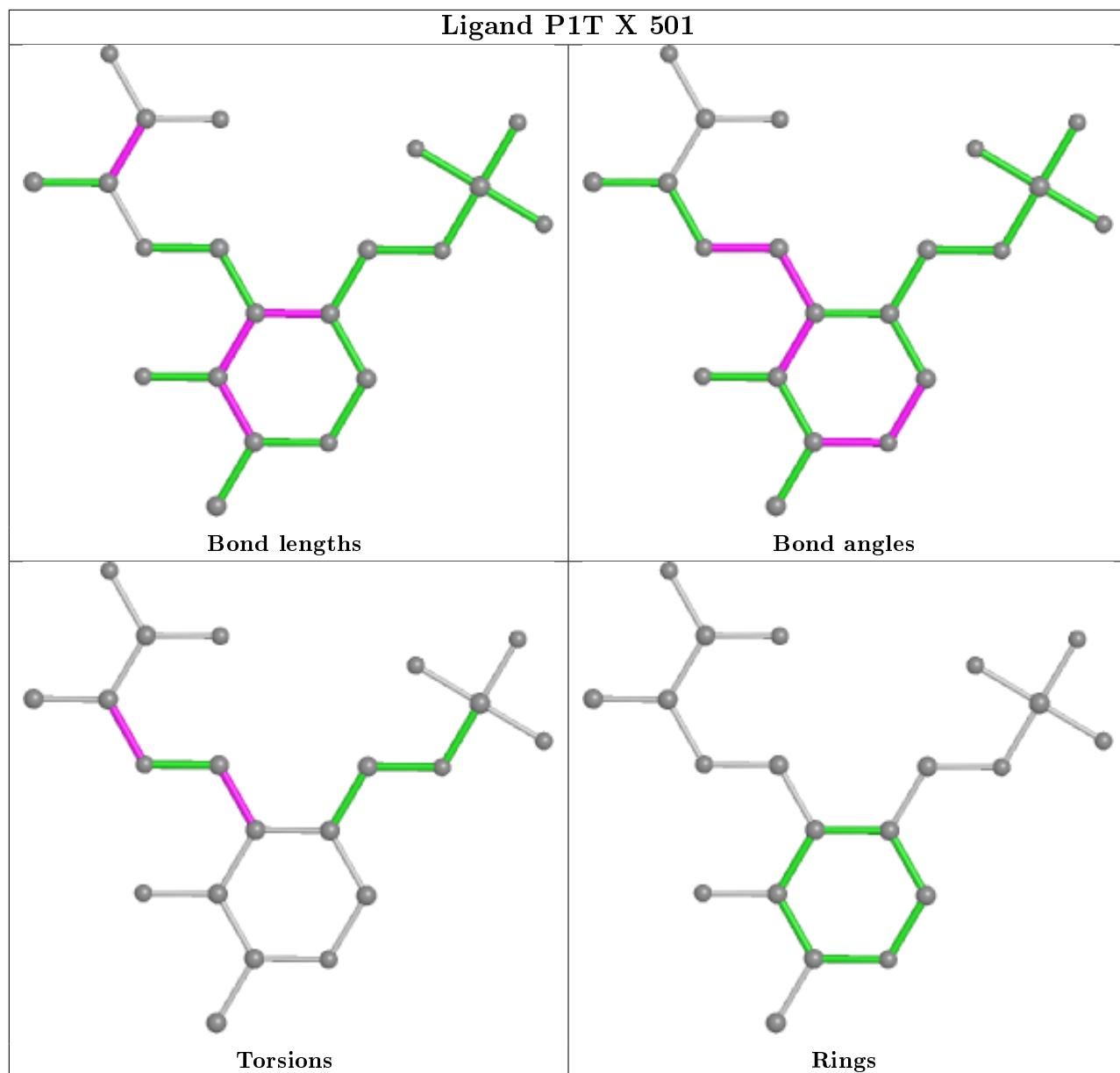


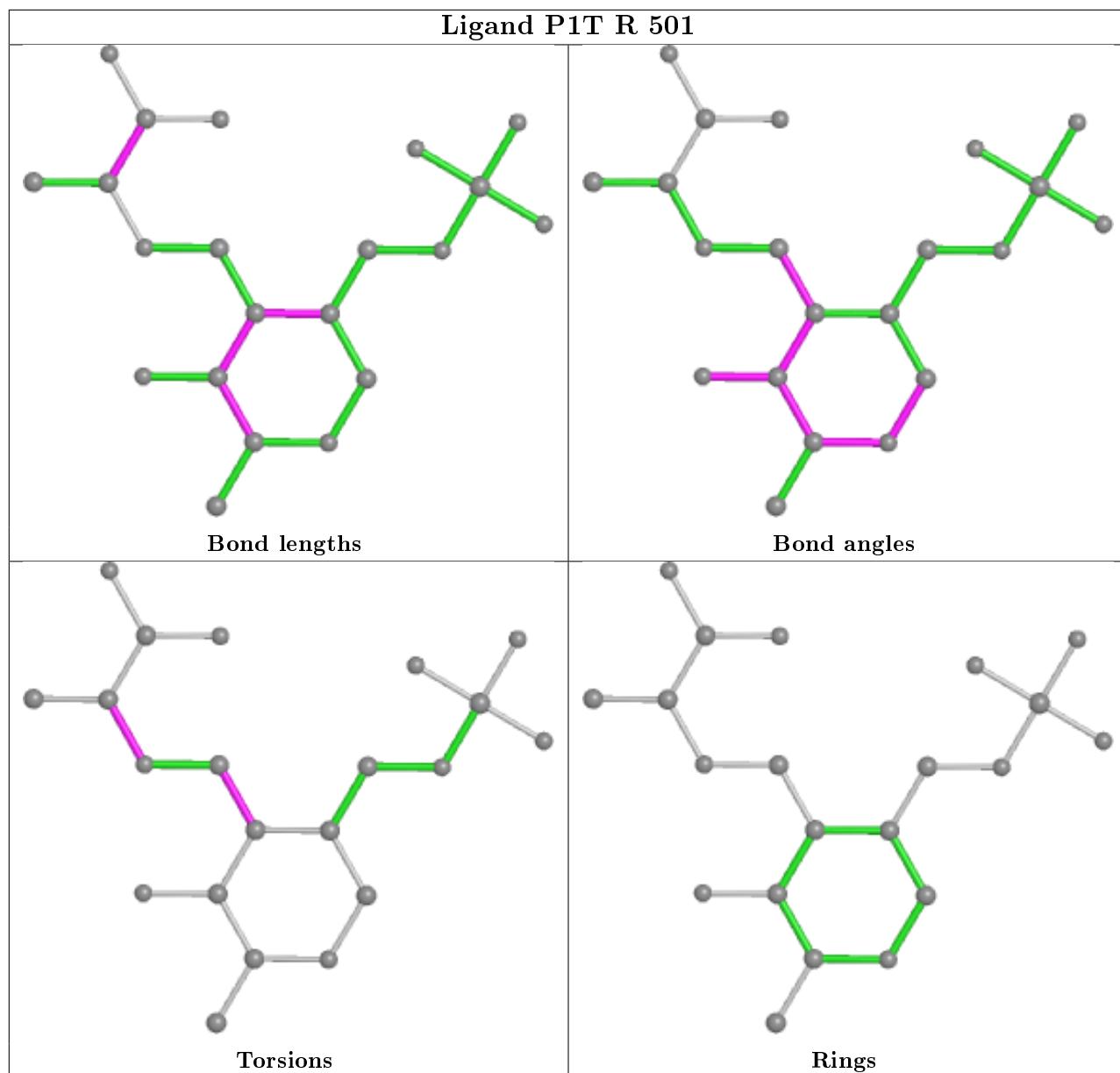


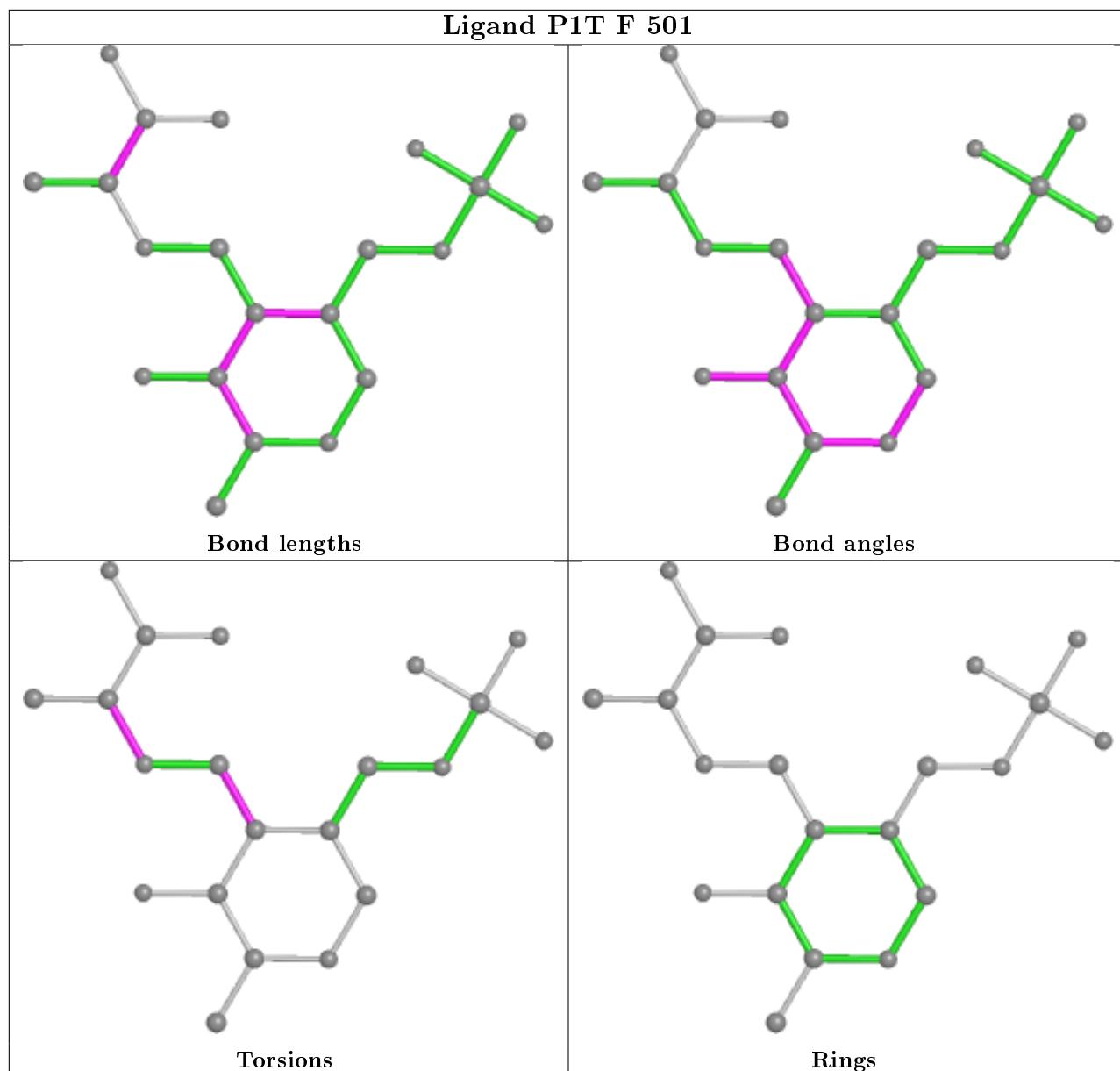


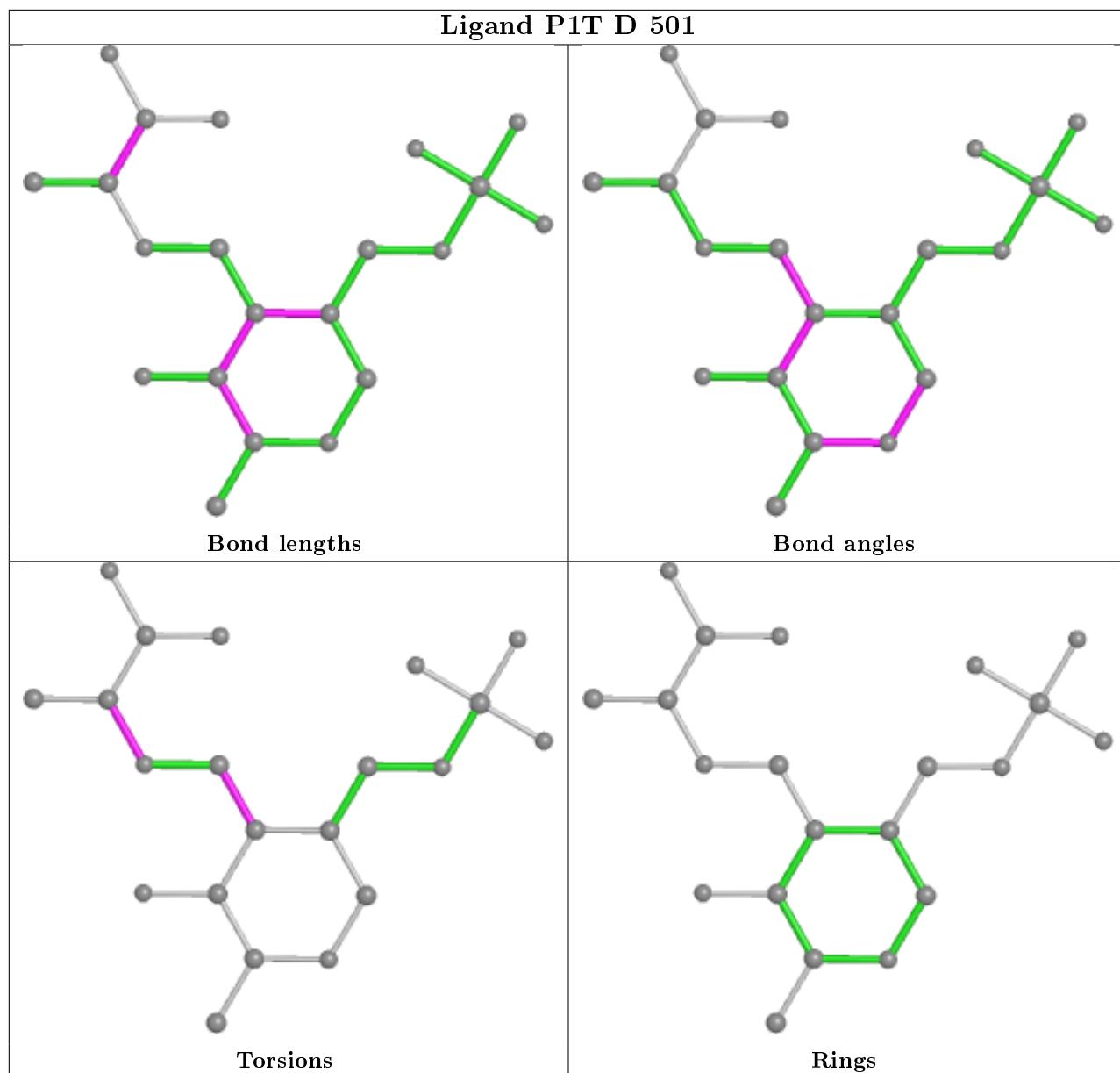


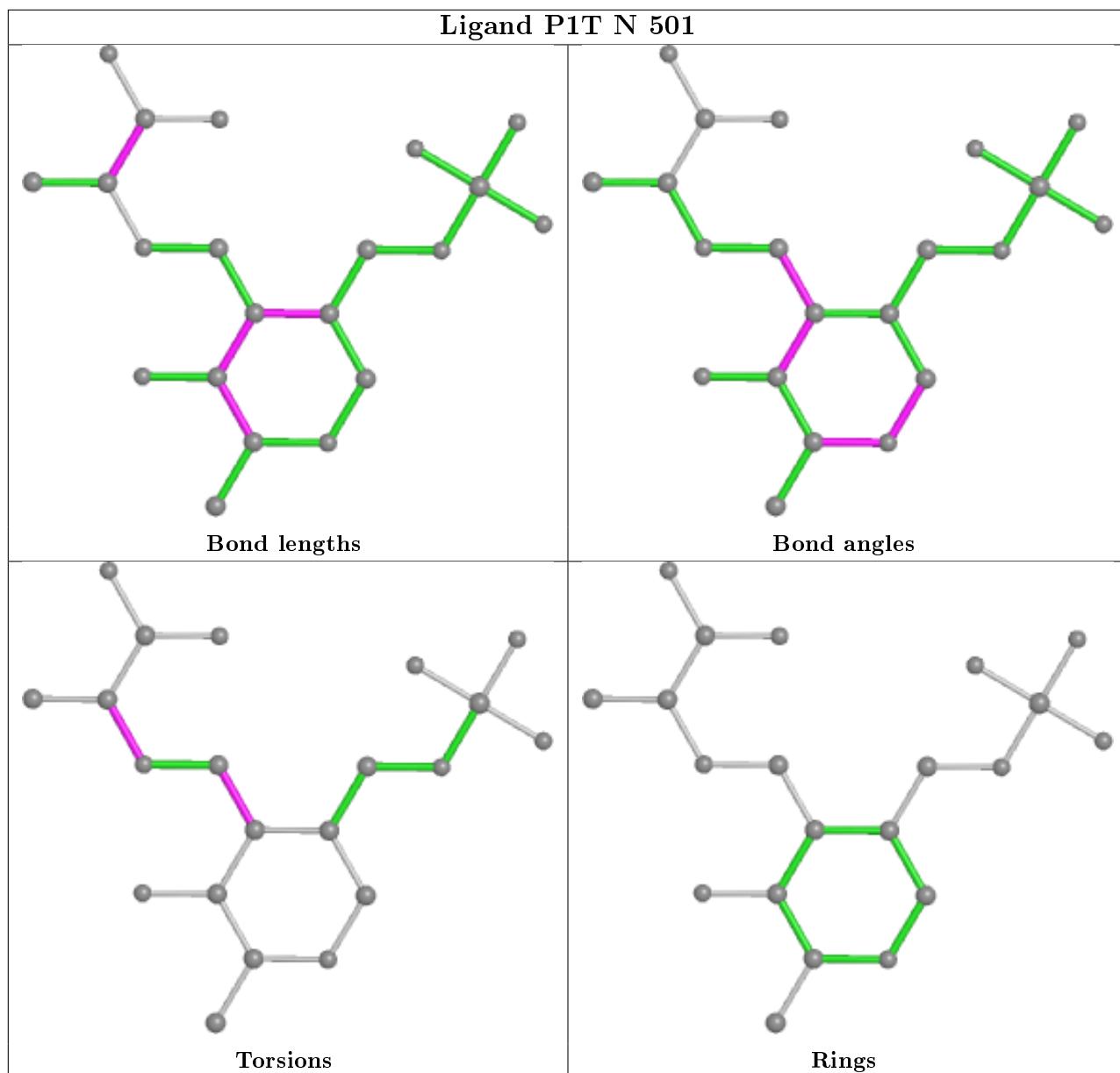












5.7 Other polymers [\(i\)](#)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.37	1 (0%)	92	87	94, 142, 184, 206
1	C	248/290 (85%)	-0.49	1 (0%)	92	87	58, 86, 106, 117
1	E	249/290 (85%)	0.08	12 (4%)	30	25	132, 176, 211, 238
1	G	248/290 (85%)	-0.22	1 (0%)	92	87	111, 138, 159, 173
1	I	249/290 (85%)	-0.25	5 (2%)	65	56	130, 169, 200, 211
1	K	248/290 (85%)	0.02	10 (4%)	38	30	149, 199, 236, 255
1	M	249/290 (85%)	-0.24	4 (1%)	72	62	112, 127, 142, 156
1	O	248/290 (85%)	-0.22	6 (2%)	59	49	122, 144, 161, 171
1	Q	249/290 (85%)	-0.17	2 (0%)	86	79	109, 135, 156, 170
1	S	248/290 (85%)	0.16	11 (4%)	34	28	118, 148, 178, 188
1	U	249/290 (85%)	0.04	8 (3%)	47	37	146, 214, 264, 302
1	W	248/290 (85%)	-0.41	1 (0%)	92	87	88, 117, 145, 162
2	B	399/442 (90%)	-0.58	0	100	100	53, 79, 101, 123
2	D	399/442 (90%)	-0.57	0	100	100	49, 61, 81, 91
2	F	399/442 (90%)	-0.41	1 (0%)	94	90	98, 113, 137, 149
2	H	399/442 (90%)	-0.42	1 (0%)	94	90	97, 108, 119, 126
2	J	399/442 (90%)	-0.32	2 (0%)	91	85	125, 156, 188, 200
2	L	399/442 (90%)	-0.09	6 (1%)	73	64	126, 165, 198, 208
2	N	399/442 (90%)	-0.35	3 (0%)	86	79	109, 118, 137, 149
2	P	399/442 (90%)	-0.34	1 (0%)	94	90	110, 125, 140, 147
2	R	399/442 (90%)	-0.40	0	100	100	89, 101, 111, 123
2	T	399/442 (90%)	-0.34	0	100	100	89, 103, 118, 135
2	V	399/442 (90%)	-0.46	0	100	100	91, 123, 162, 181
2	X	399/442 (90%)	-0.48	0	100	100	83, 97, 121, 136

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7778/8784 (88%)	-0.31	76 (0%) 82 74	49, 122, 198, 302	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	218	LEU	7.6
1	S	217	GLY	5.5
1	E	218	LEU	5.3
1	E	217	GLY	4.7
1	E	57	GLU	4.7

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

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

6.3 Carbohydrates [\(i\)](#)

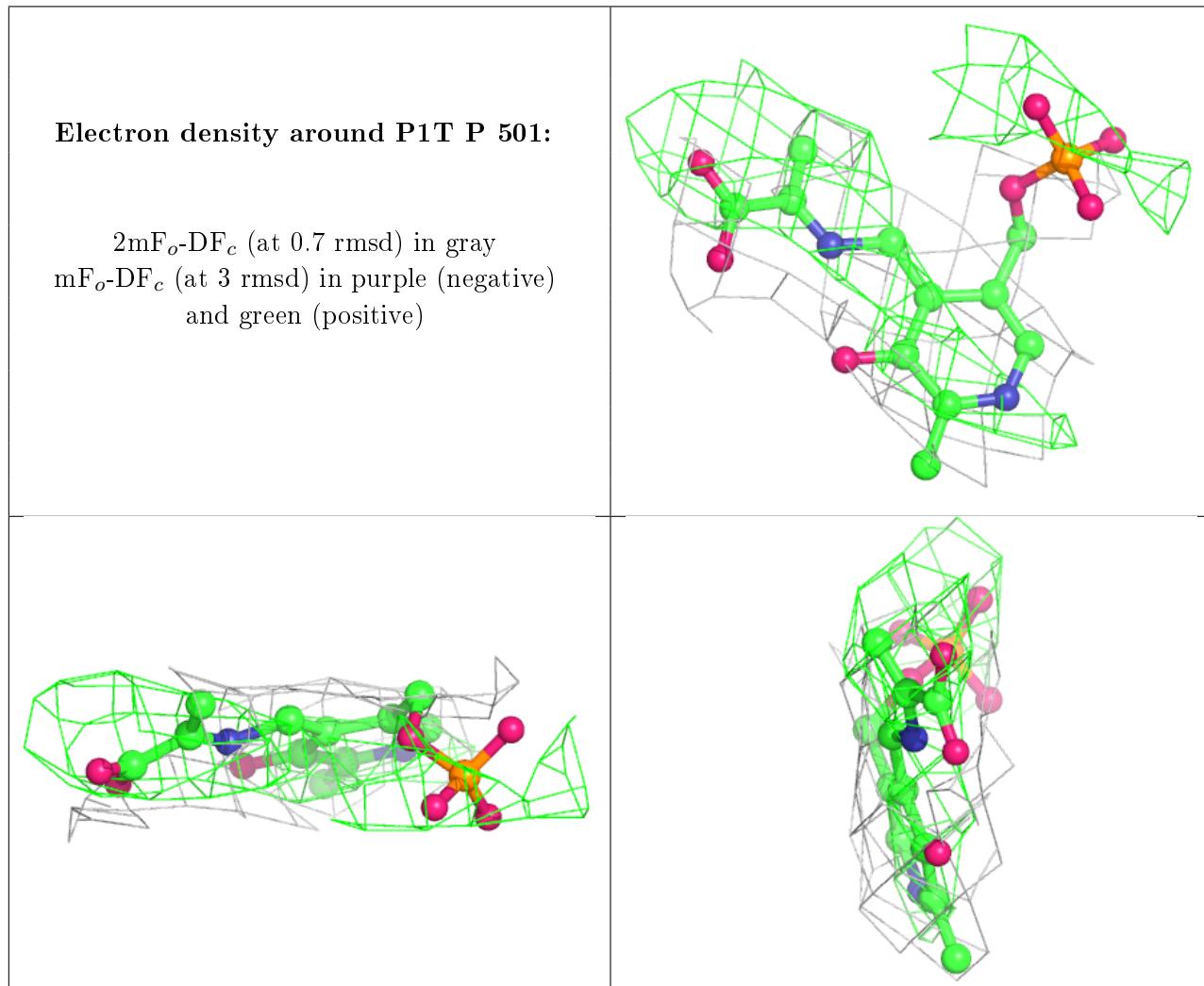
There are no carbohydrates in this entry.

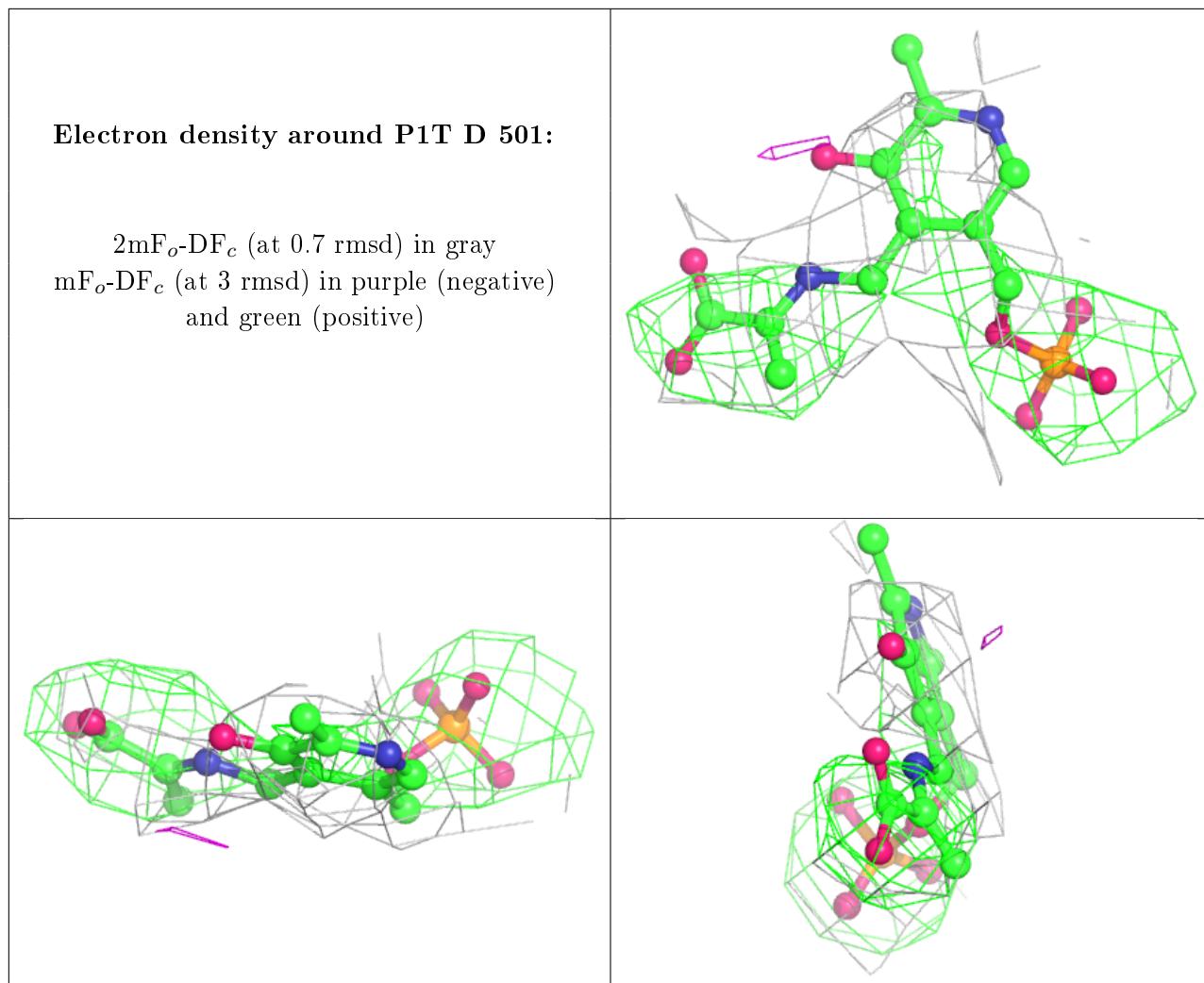
6.4 Ligands [\(i\)](#)

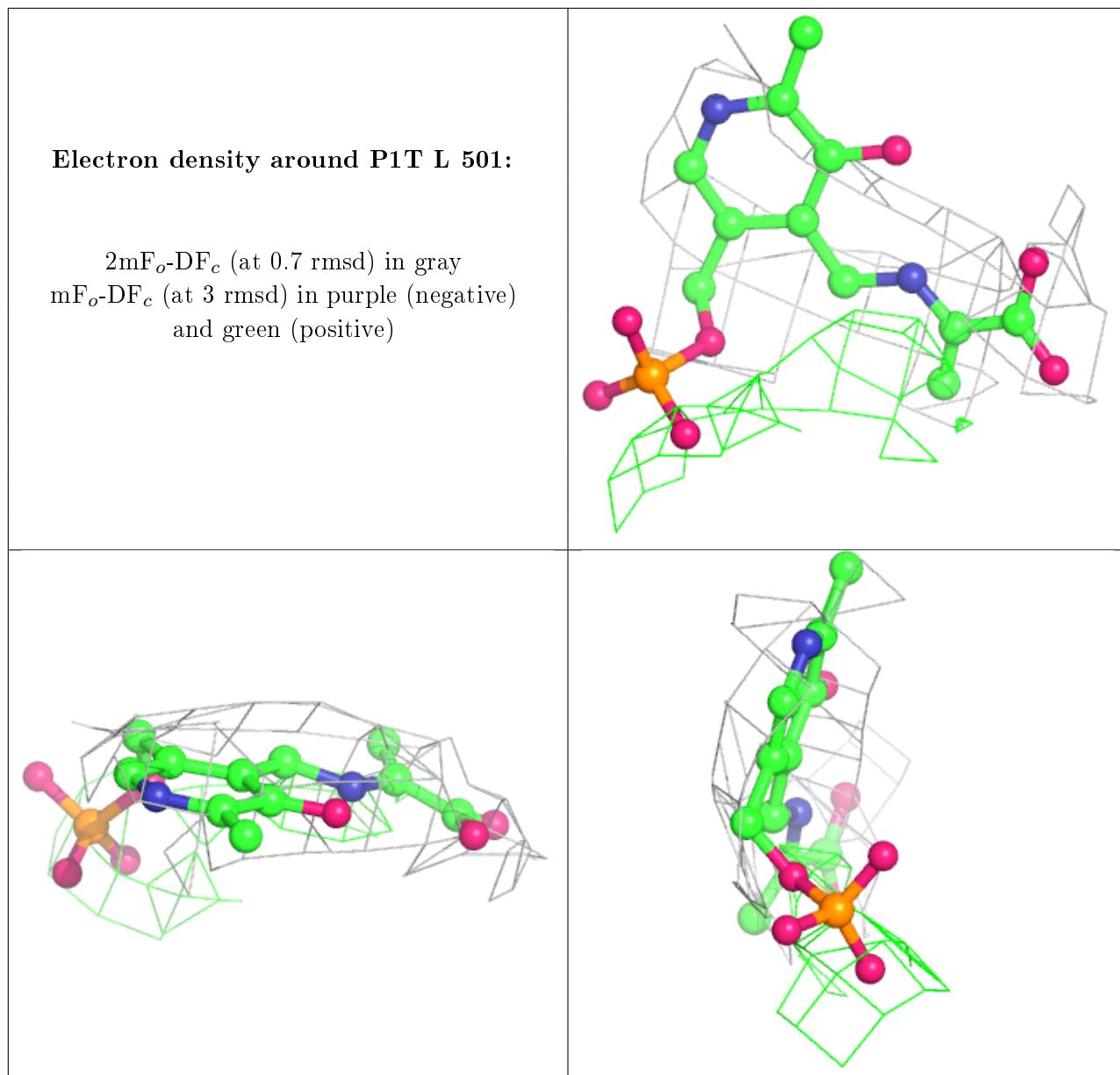
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

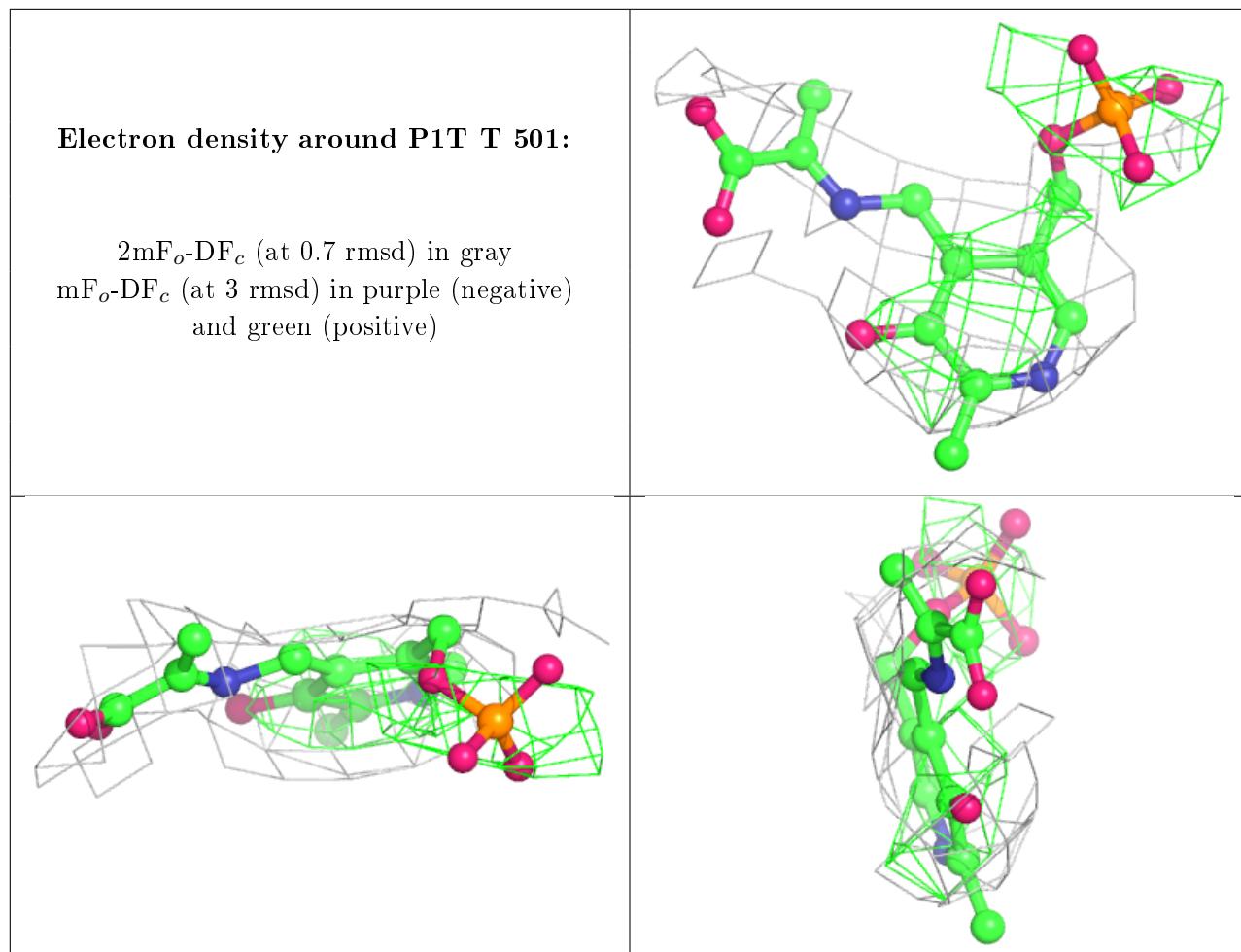
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	P1T	P	501	21/21	0.76	0.45	175,175,175,175	0
3	P1T	D	501	21/21	0.79	0.45	175,175,175,175	0
3	P1T	L	501	21/21	0.81	0.32	175,175,175,175	0
3	P1T	T	501	21/21	0.86	0.36	175,175,175,175	0
3	P1T	B	501	21/21	0.86	0.41	175,175,175,175	0
3	P1T	N	501	21/21	0.87	0.30	175,175,175,175	0
3	P1T	F	501	21/21	0.88	0.34	175,175,175,175	0
3	P1T	J	501	21/21	0.88	0.30	175,175,175,175	0
3	P1T	X	501	21/21	0.88	0.36	175,175,175,175	0
3	P1T	V	501	21/21	0.90	0.30	175,175,175,175	0
3	P1T	R	501	21/21	0.91	0.32	175,175,175,175	0
3	P1T	H	501	21/21	0.91	0.30	175,175,175,175	0

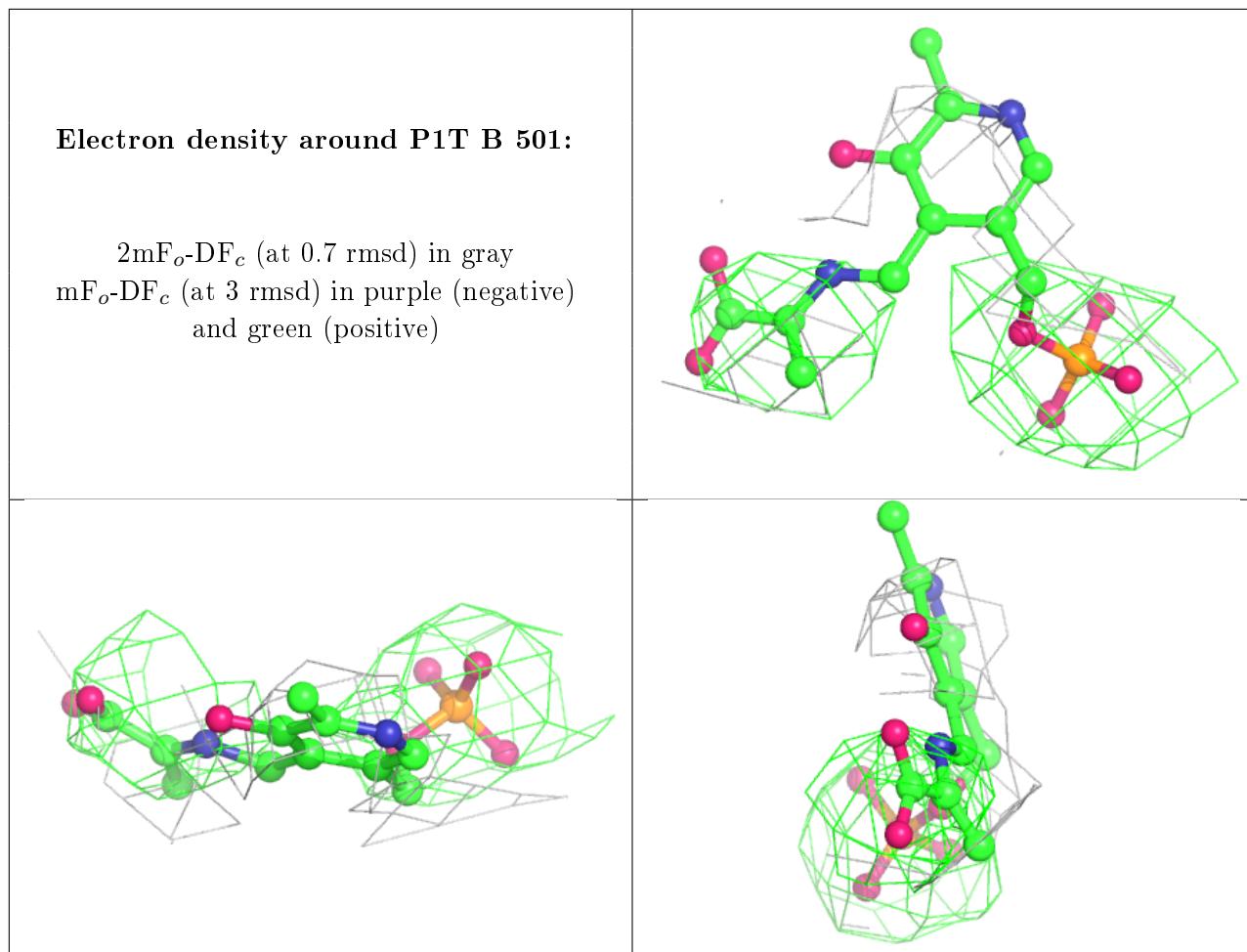
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

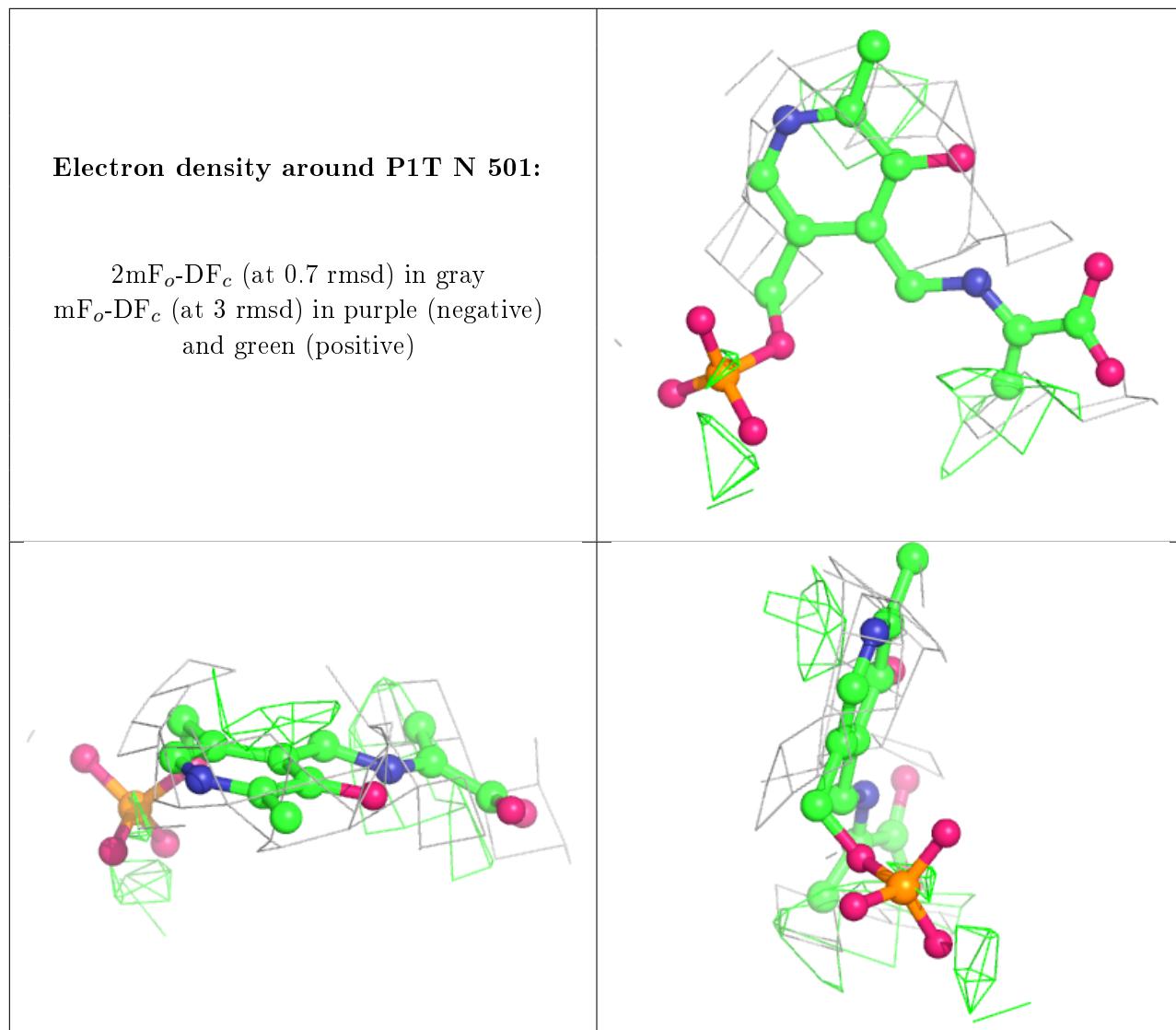


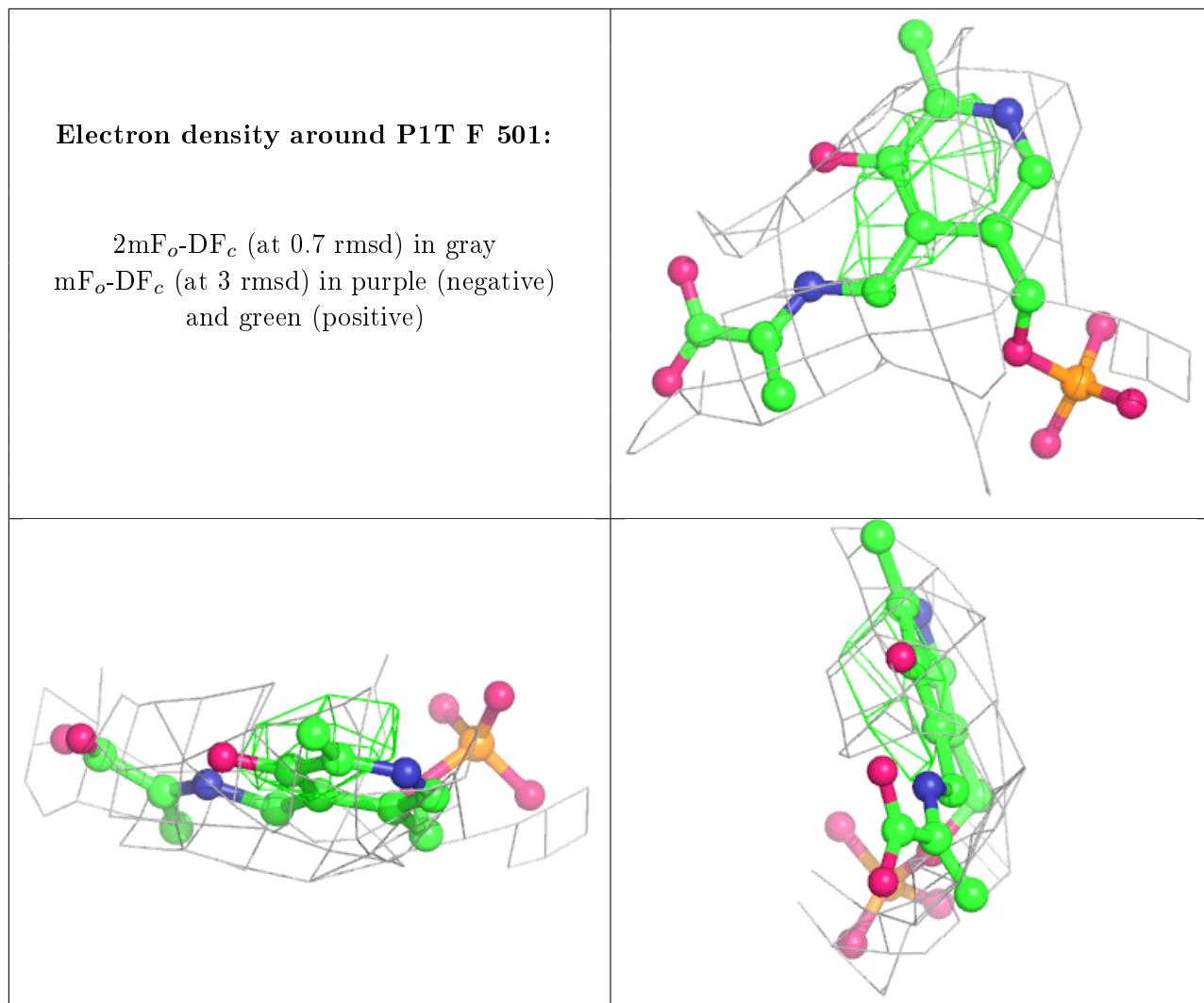


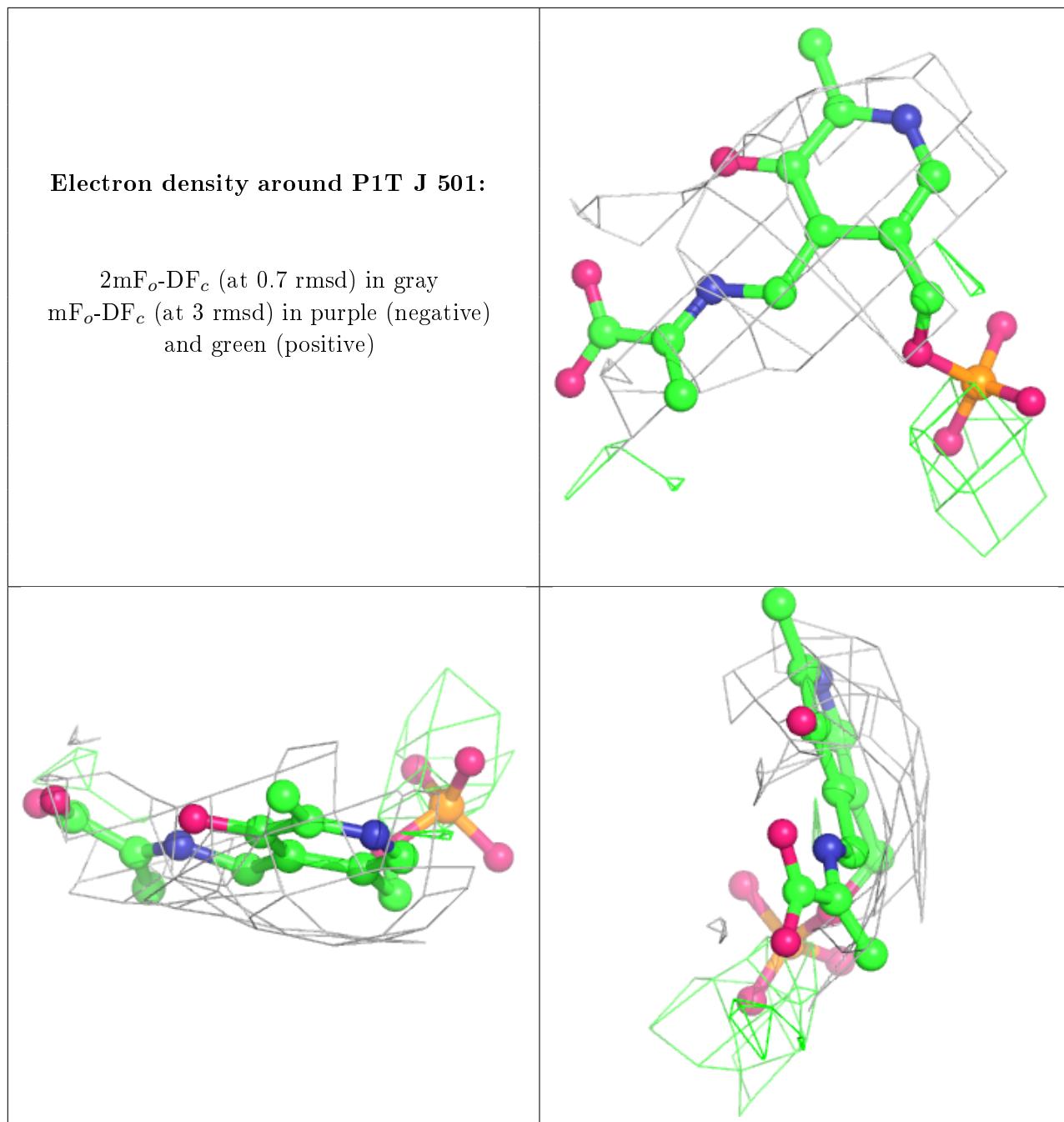


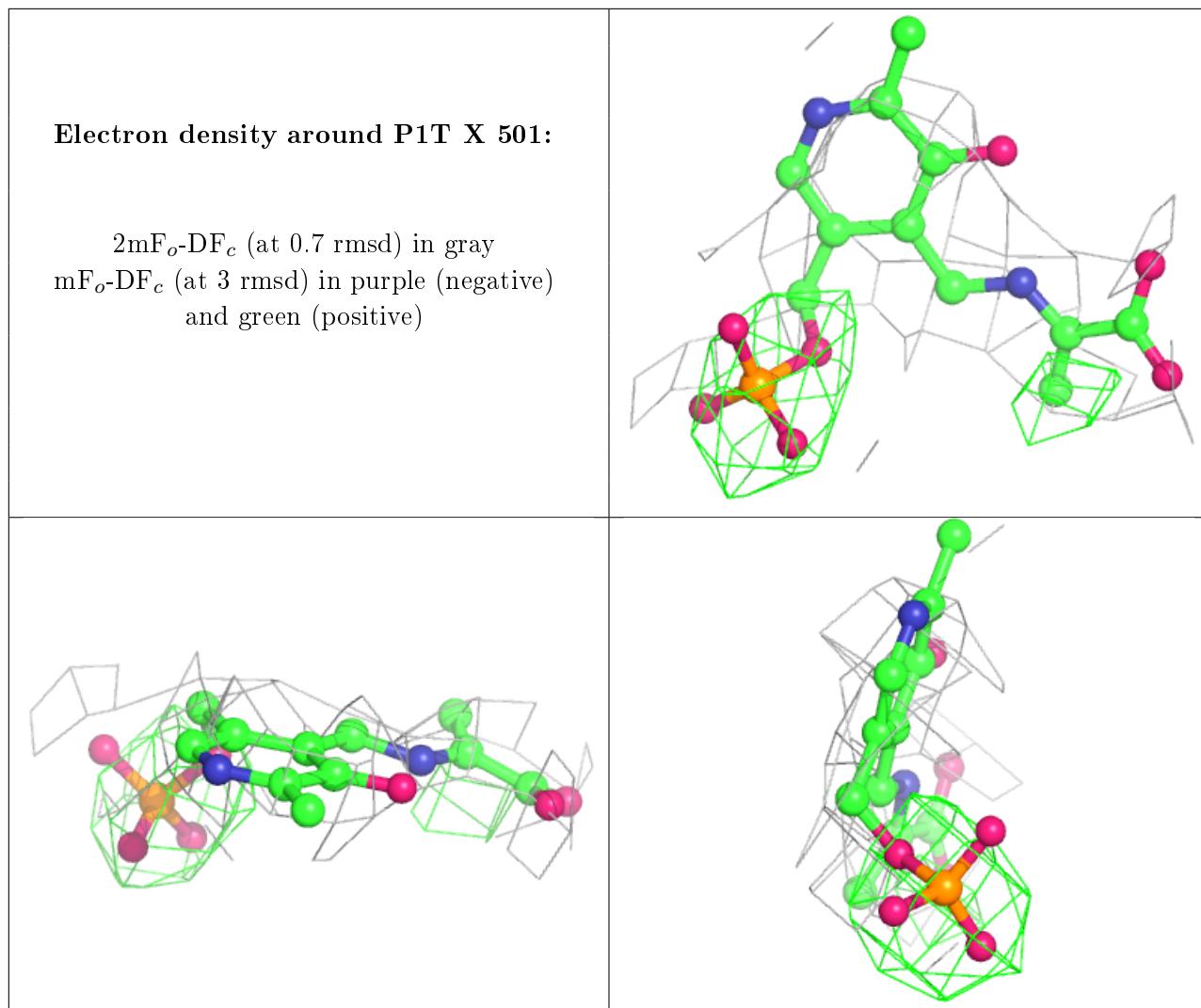


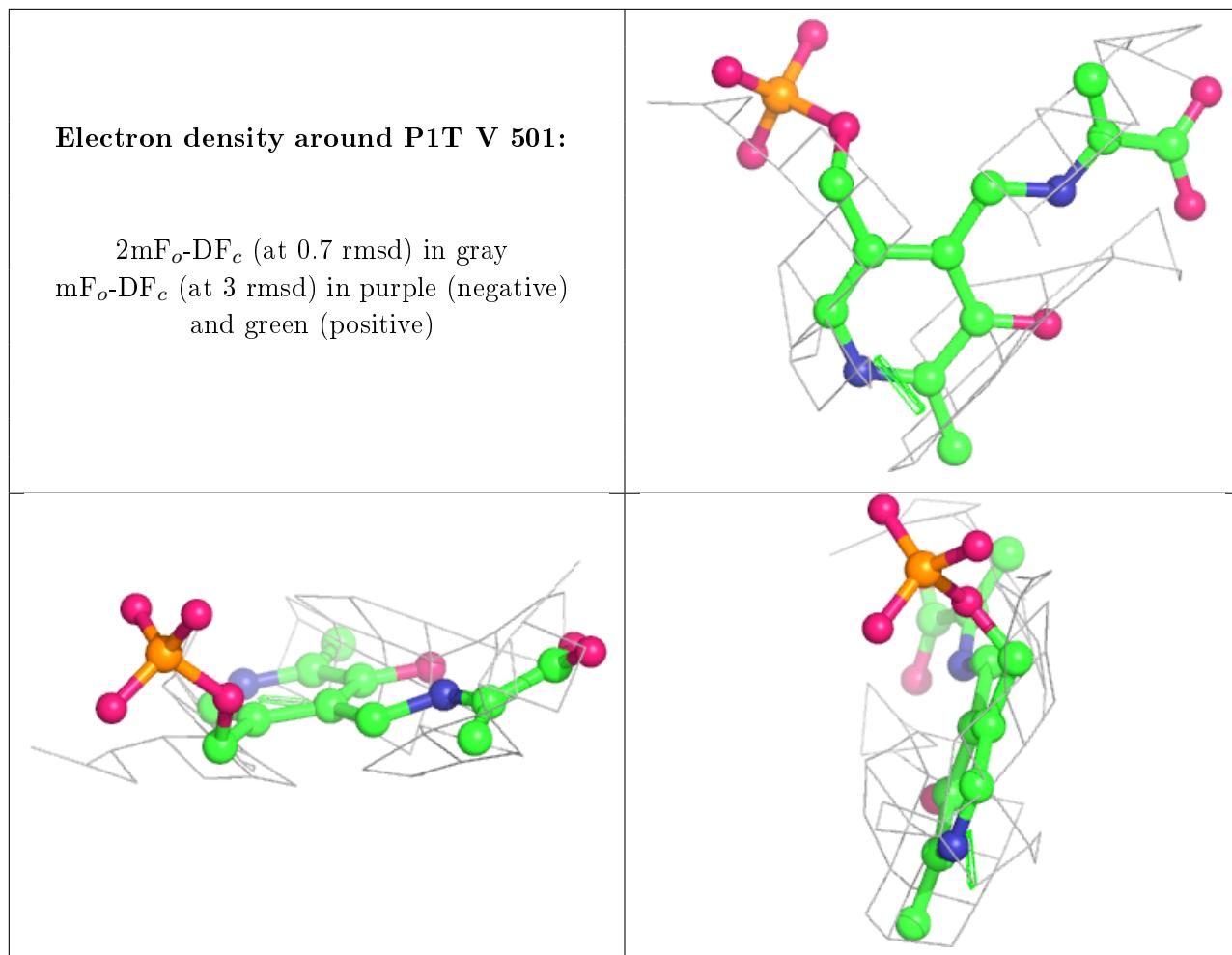


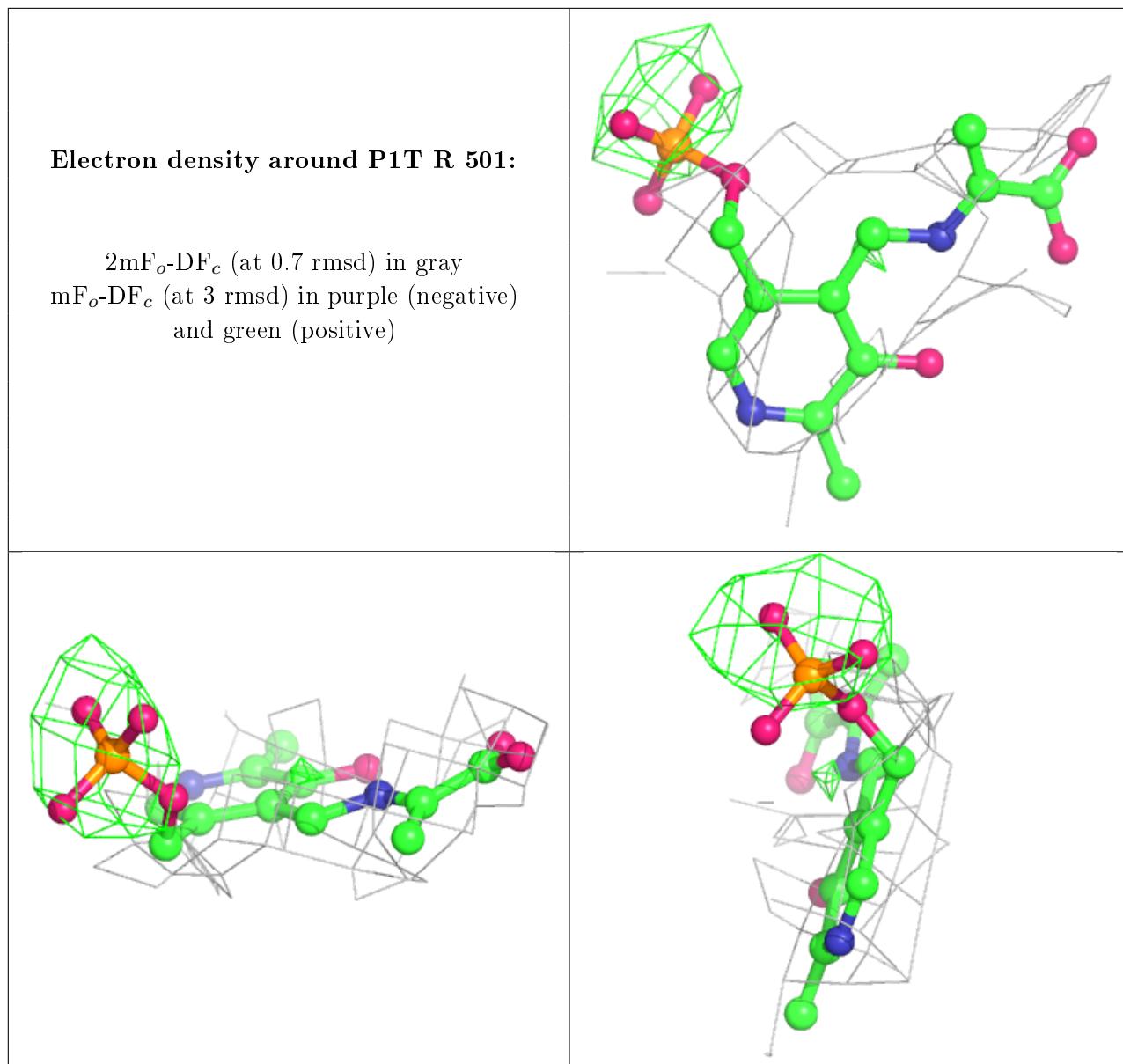


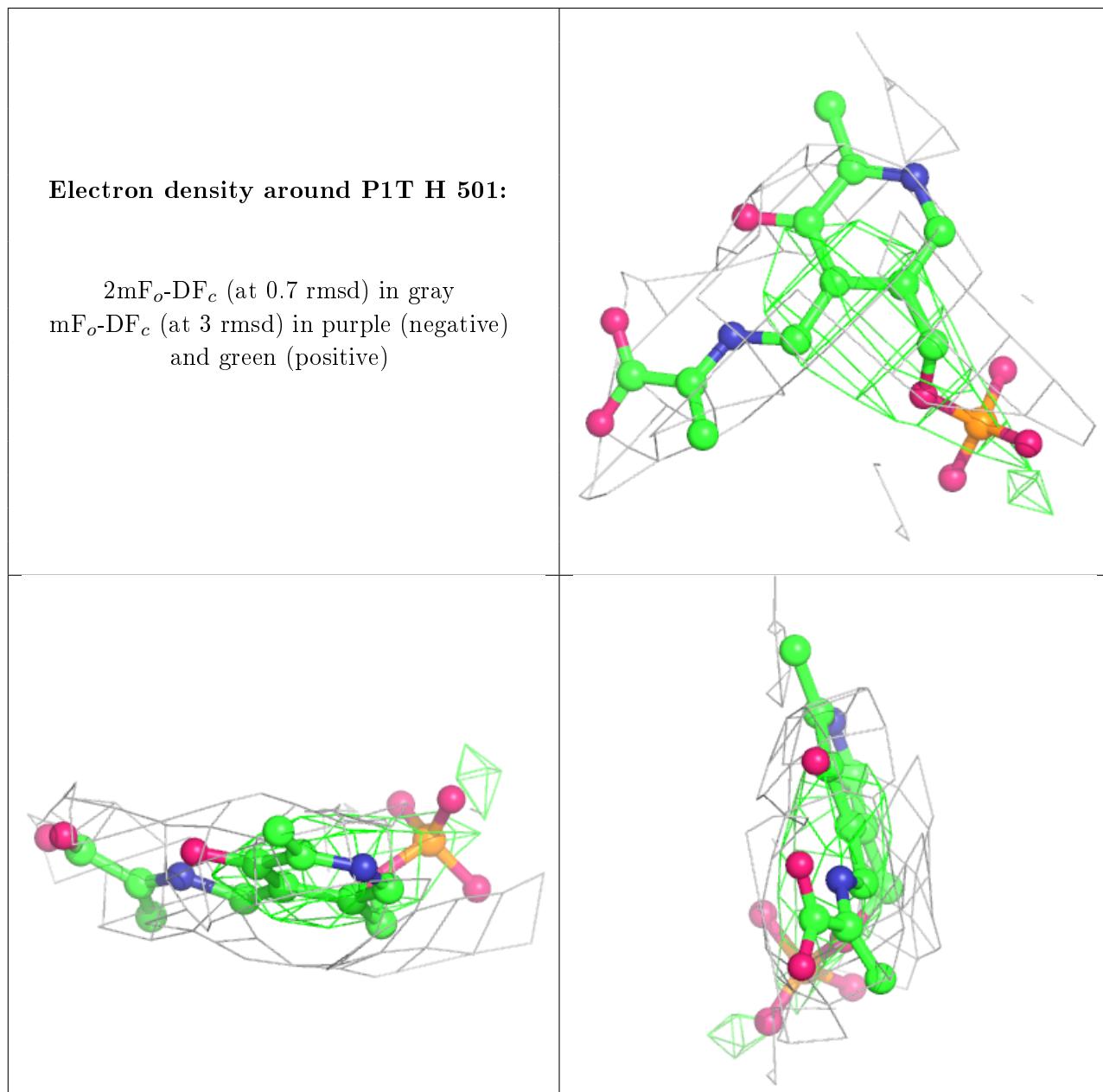












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.