



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2022 – 10:48 AM EDT

PDB ID : 6USA  
Title : Crystal structure of tryptophan synthase from *M. tuberculosis* - aminoacylate- and GSK1-bound form  
Authors : Chang, C.; Michalska, K.; Maltseva, N.I.; Jedrzejczak, R.; McCarren, P.; Nag, P.P.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2019-10-25  
Resolution : 2.41 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](mailto: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>.

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

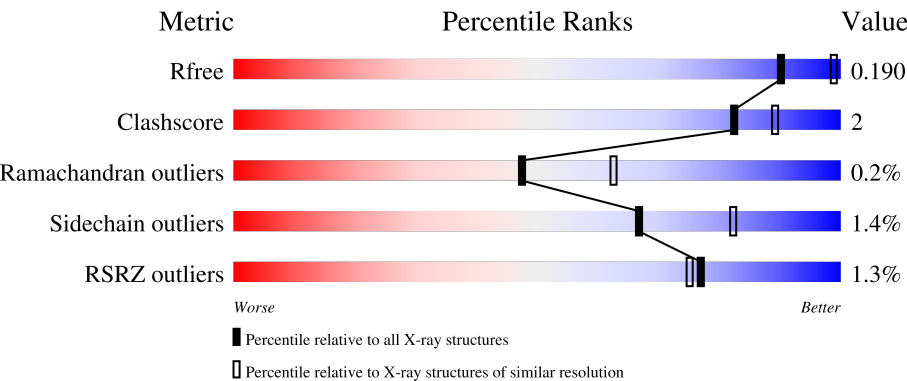
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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.



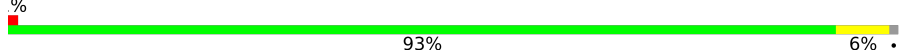
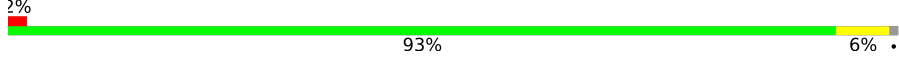
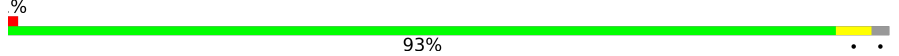
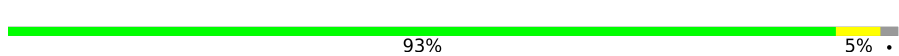
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	276	<div><div>3%</div><div>84%</div><div>5%</div><div>10%</div></div>
1	C	276	<div><div>2%</div><div>84%</div><div>6%</div><div>10%</div></div>
1	E	276	<div><div>2%</div><div>82%</div><div>7%</div><div>11%</div></div>
1	G	276	<div><div>%</div><div>85%</div><div>.</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
2	B	410	 93% 6% •
2	D	410	 93% 6% •
2	F	410	 93% • •
2	H	410	 93% 5% •

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	FMT	E	301	-	-	-	X
7	K	D	512	-	-	-	X
9	PEG	C	301	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21114 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	249	Total	C	N	O	S	0	1	0
			1812	1136	324	347	5			
1	C	249	Total	C	N	O	S	0	3	0
			1833	1148	332	347	6			
1	E	245	Total	C	N	O	S	0	2	0
			1795	1126	324	339	6			
1	G	248	Total	C	N	O	S	0	3	0
			1824	1143	331	344	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP P9WIFY1
A	272	HIS	-	expression tag	UNP P9WIFY1
A	273	HIS	-	expression tag	UNP P9WIFY1
A	274	HIS	-	expression tag	UNP P9WIFY1
A	275	HIS	-	expression tag	UNP P9WIFY1
A	276	HIS	-	expression tag	UNP P9WIFY1
C	271	HIS	-	expression tag	UNP P9WIFY1
C	272	HIS	-	expression tag	UNP P9WIFY1
C	273	HIS	-	expression tag	UNP P9WIFY1
C	274	HIS	-	expression tag	UNP P9WIFY1
C	275	HIS	-	expression tag	UNP P9WIFY1
C	276	HIS	-	expression tag	UNP P9WIFY1
E	271	HIS	-	expression tag	UNP P9WIFY1
E	272	HIS	-	expression tag	UNP P9WIFY1
E	273	HIS	-	expression tag	UNP P9WIFY1
E	274	HIS	-	expression tag	UNP P9WIFY1
E	275	HIS	-	expression tag	UNP P9WIFY1
E	276	HIS	-	expression tag	UNP P9WIFY1
G	271	HIS	-	expression tag	UNP P9WIFY1
G	272	HIS	-	expression tag	UNP P9WIFY1
G	273	HIS	-	expression tag	UNP P9WIFY1

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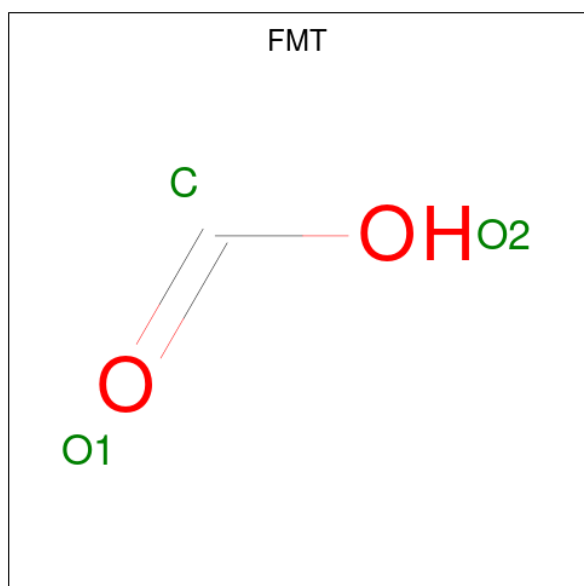
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Chain	Residue	Modelled	Actual	Comment	Reference
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	5	0
			3047	1900	553	580	14			
2	D	404	Total	C	N	O	S	0	4	0
			3048	1902	557	576	13			
2	F	400	Total	C	N	O	S	0	5	0
			3028	1889	555	571	13			
2	H	403	Total	C	N	O	S	0	15	0
			3127	1951	572	590	14			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

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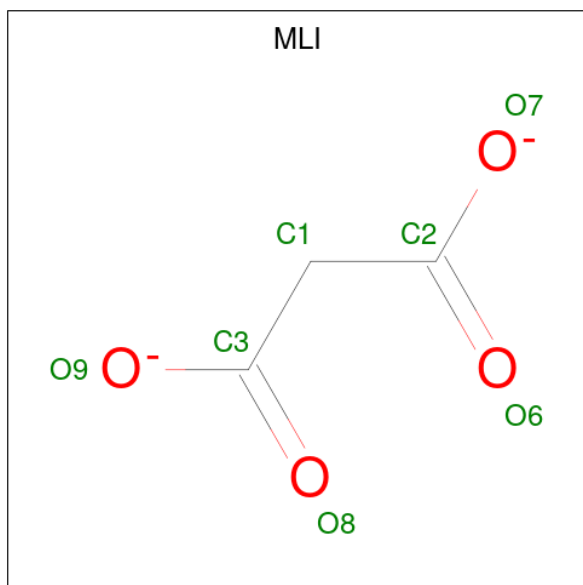
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	F	1	Total	C	O	0	0
			3	1	2		
3	G	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		

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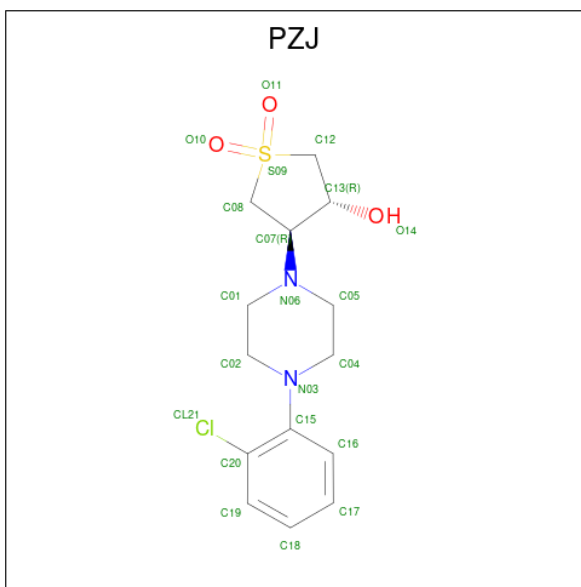
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



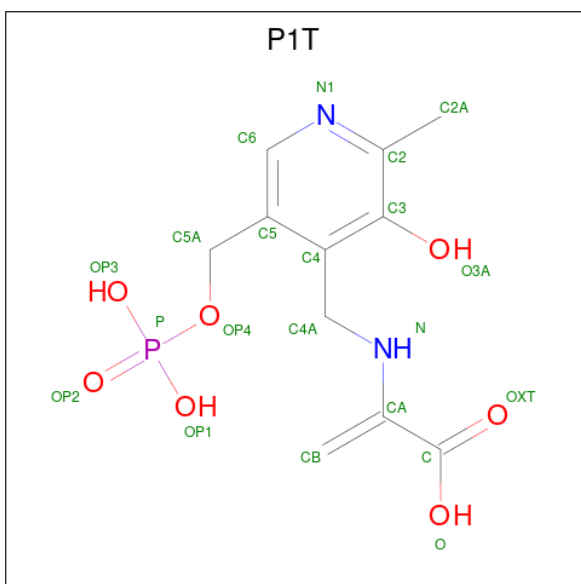
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	C	1	Total	C	O	0	0
			7	3	4		
4	D	1	Total	C	O	0	0
			7	3	4		
4	E	1	Total	C	O	0	0
			7	3	4		
4	F	1	Total	C	O	0	0
			7	3	4		
4	G	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is (3R,4R)-4-[4-(2-Chlorophenyl)piperazin-1-yl]-1,1-dioxothiolan-3-ol (three-letter code: PZJ) (formula:  $C_{14}H_{19}ClN_2O_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total 21	C 14	Cl 1	N 2	O 3	S 1	0	0
5	D	1	Total 21	C 14	Cl 1	N 2	O 3	S 1	0	0
5	F	1	Total 21	C 14	Cl 1	N 2	O 3	S 1	0	0
5	H	1	Total 21	C 14	Cl 1	N 2	O 3	S 1	0	0

- Molecule 6 is 2-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)AMINO]ACRYLIC ACID (three-letter code: P1T) (formula:  $C_{11}H_{15}N_2O_7P$ ).



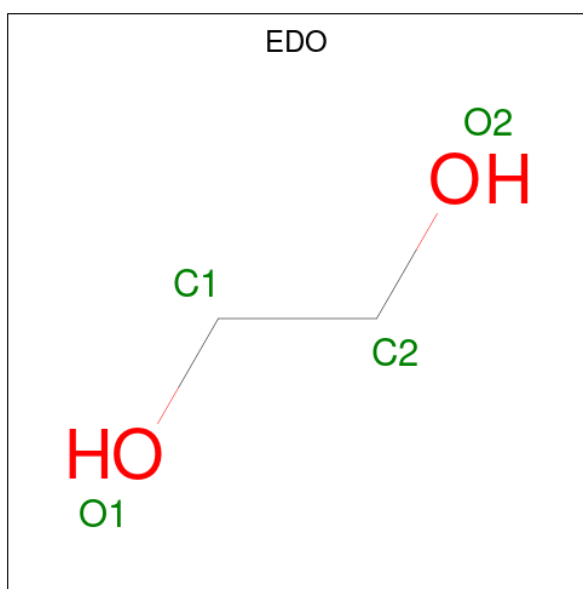


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
6	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
6	F	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
6	H	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	K	0	0
			1	1		
7	D	3	Total	K	0	0
			3	3		
7	F	4	Total	K	0	0
			4	4		
7	G	1	Total	K	0	0
			1	1		
7	H	1	Total	K	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



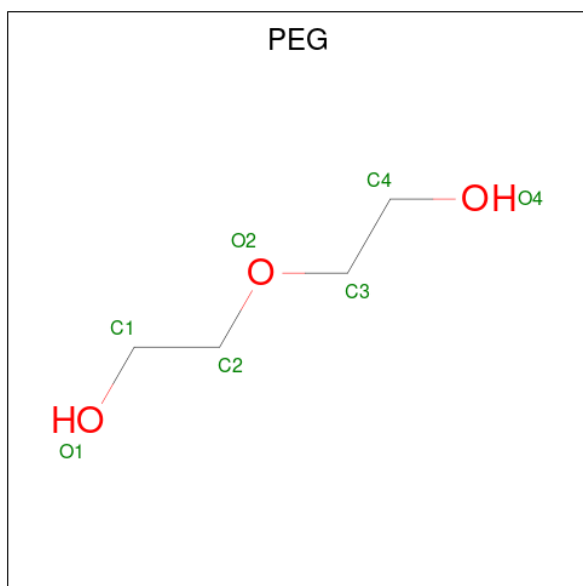
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

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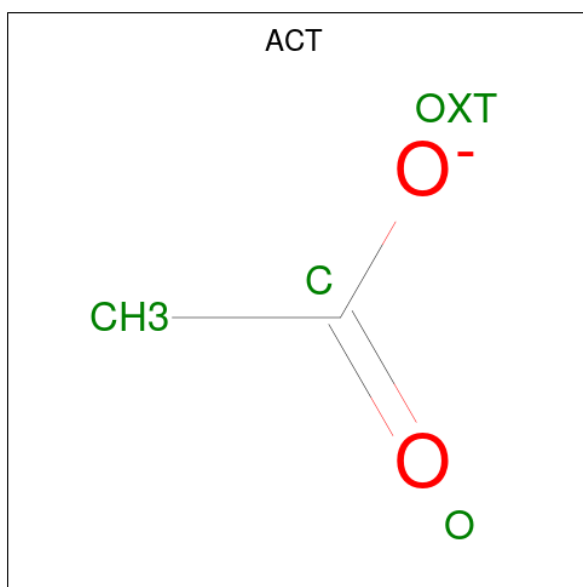
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		
8	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



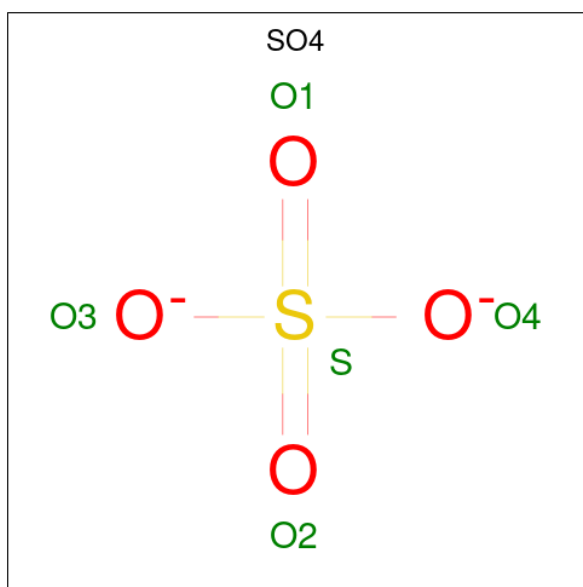
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	2	Total 2	Na 2	0	0

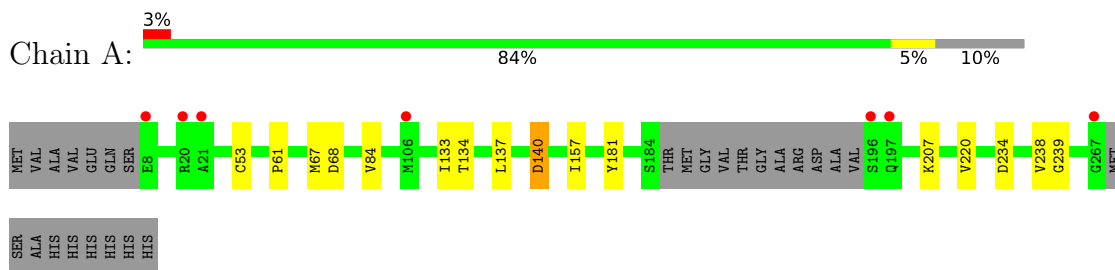
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	72	Total 72	O 72	0	0
13	B	234	Total 234	O 234	0	0
13	C	90	Total 90	O 90	0	0
13	D	223	Total 223	O 223	0	0
13	E	60	Total 60	O 60	0	0
13	F	200	Total 200	O 200	0	0
13	G	110	Total 110	O 110	0	0
13	H	245	Total 245	O 245	0	0

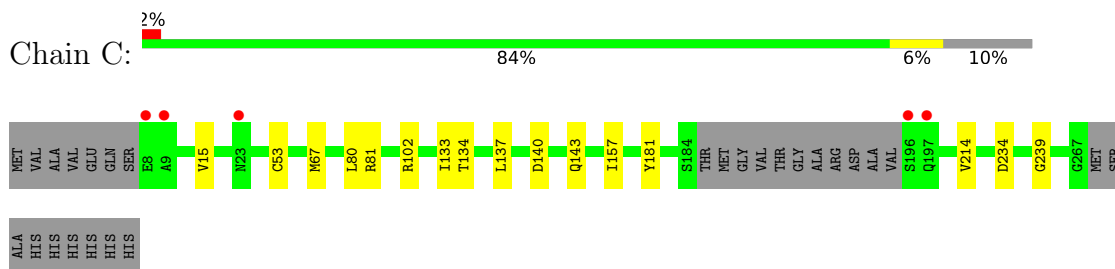
### 3 Residue-property plots [i](#)

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.

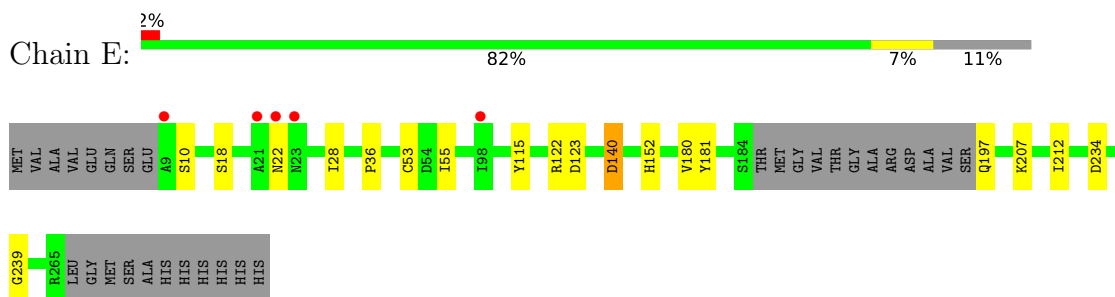
- Molecule 1: Tryptophan synthase alpha chain



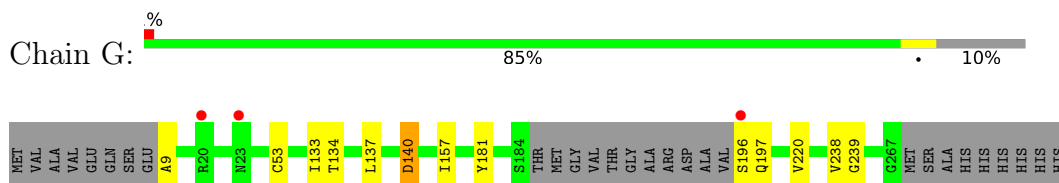
- Molecule 1: Tryptophan synthase alpha chain



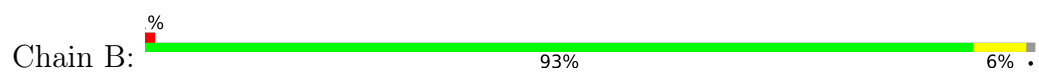
- Molecule 1: Tryptophan synthase alpha chain



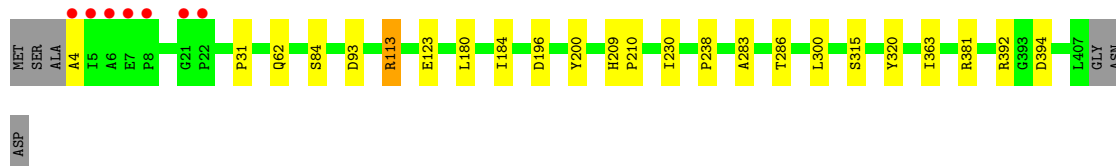
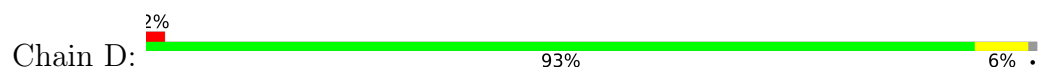
- Molecule 1: Tryptophan synthase alpha chain



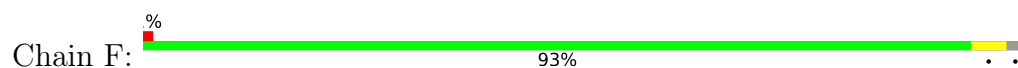
- Molecule 2: Tryptophan synthase beta chain



• 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	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.92Å 160.04Å 165.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.41 29.89 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.89-2.41) 99.4 (29.89-2.41)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.158 , 0.192 0.158 , 0.190	Depositor DCC
$R_{free}$ test set	2678 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, PEG, FMT, K, PZJ, MLI, EDO, P1T, SO4, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/1841	0.43	0/2512
1	C	0.25	0/1862	0.43	0/2538
1	E	0.25	0/1824	0.43	0/2488
1	G	0.25	0/1853	0.44	0/2526
2	B	0.27	0/3108	0.45	0/4211
2	D	0.27	0/3109	0.45	0/4212
2	F	0.27	0/3090	0.45	0/4185
2	H	0.27	0/3192	0.45	0/4324
All	All	0.26	0/19879	0.45	0/26996

There are no bond length outliers.

There are no bond angle outliers.

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	1812	0	1827	8	0
1	C	1833	0	1854	7	0
1	E	1795	0	1817	9	0
1	G	1824	0	1848	7	0
2	B	3047	0	2956	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3048	0	2973	13	0
2	F	3028	0	2948	13	0
2	H	3127	0	3031	14	0
3	A	6	0	2	0	0
3	B	15	0	5	0	0
3	C	3	0	1	0	0
3	D	15	0	5	0	0
3	E	6	0	2	1	0
3	F	18	0	6	0	0
3	G	3	0	1	0	0
3	H	18	0	6	0	0
4	A	7	0	2	0	0
4	C	7	0	2	0	0
4	D	7	0	2	0	0
4	E	7	0	2	0	0
4	F	7	0	2	0	0
4	G	7	0	2	0	0
5	B	21	0	0	4	0
5	D	21	0	0	3	0
5	F	21	0	0	3	0
5	H	21	0	0	4	0
6	B	21	0	11	0	0
6	D	21	0	11	1	0
6	F	21	0	11	0	0
6	H	21	0	11	2	0
7	B	1	0	0	0	0
7	D	3	0	0	0	0
7	F	4	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	B	8	0	12	0	0
8	D	8	0	12	0	0
8	F	16	0	24	4	0
8	G	4	0	6	0	0
9	C	7	0	10	1	0
10	D	8	0	6	0	0
10	F	4	0	3	0	0
11	H	5	0	0	0	0
12	H	2	0	0	0	0
13	A	72	0	0	0	0
13	B	234	0	0	5	0
13	C	90	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	223	0	0	2	0
13	E	60	0	0	1	0
13	F	200	0	0	3	0
13	G	110	0	0	2	0
13	H	245	0	0	4	0
All	All	21114	0	19411	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 97 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)
5:B:501:PZJ:C13	5:B:501:PZJ:C07	1.78	1.50
5:H:501:PZJ:C13	5:H:501:PZJ:C07	1.78	1.48
5:D:501:PZJ:C13	5:D:501:PZJ:C07	1.78	1.44
5:F:501:PZJ:C13	5:F:501:PZJ:C07	1.78	1.41
5:H:501:PZJ:C13	5:H:501:PZJ:N06	2.24	1.01

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	246/276 (89%)	241 (98%)	4 (2%)	1 (0%)	34	48
1	C	248/276 (90%)	244 (98%)	3 (1%)	1 (0%)	34	48
1	E	243/276 (88%)	238 (98%)	4 (2%)	1 (0%)	34	48
1	G	247/276 (90%)	243 (98%)	3 (1%)	1 (0%)	34	48
2	B	407/410 (99%)	400 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	406/410 (99%)	395 (97%)	11 (3%)	0	100	100
2	F	403/410 (98%)	393 (98%)	10 (2%)	0	100	100
2	H	416/410 (102%)	407 (98%)	9 (2%)	0	100	100
All	All	2616/2744 (95%)	2561 (98%)	51 (2%)	4 (0%)	47	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	239	GLY
1	A	239	GLY
1	E	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	180/200 (90%)	177 (98%)	3 (2%)	60	78
1	C	182/200 (91%)	178 (98%)	4 (2%)	52	71
1	E	178/200 (89%)	174 (98%)	4 (2%)	52	71
1	G	181/200 (90%)	178 (98%)	3 (2%)	60	78
2	B	302/302 (100%)	298 (99%)	4 (1%)	69	84
2	D	302/302 (100%)	298 (99%)	4 (1%)	69	84
2	F	301/302 (100%)	298 (99%)	3 (1%)	76	88
2	H	309/302 (102%)	305 (99%)	4 (1%)	69	84
All	All	1935/2008 (96%)	1906 (98%)	29 (2%)	67	80

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	300	LEU
2	H	200	TYR

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Mol	Chain	Res	Type
1	E	140	ASP
1	G	181	TYR
1	E	53	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 12 are monoatomic - leaving 56 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	FMT	D	503	-	2,2,2	0.74	0	1,1,1	0.27	0
3	FMT	H	503	-	2,2,2	0.70	0	1,1,1	0.21	0
11	SO4	H	510	-	4,4,4	0.13	0	6,6,6	0.06	0
9	PEG	C	301	-	6,6,6	0.12	0	5,5,5	0.09	0
3	FMT	B	503	-	2,2,2	0.73	0	1,1,1	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	ACT	F	506	-	3,3,3	1.36	0	3,3,3	1.55	0
8	EDO	F	515	-	3,3,3	0.46	0	2,2,2	0.28	0
3	FMT	D	506	-	2,2,2	0.71	0	1,1,1	0.21	0
8	EDO	D	515	-	3,3,3	0.48	0	2,2,2	0.31	0
3	FMT	F	504	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	H	504	-	2,2,2	0.70	0	1,1,1	0.20	0
4	MLI	F	514	-	6,6,6	1.09	0	7,7,7	0.98	0
3	FMT	D	508	-	2,2,2	0.70	0	1,1,1	0.21	0
6	P1T	B	502	-	20,21,21	2.68	4 (20%)	28,30,30	1.51	5 (17%)
3	FMT	D	507	-	2,2,2	0.71	0	1,1,1	0.21	0
3	FMT	F	509	-	2,2,2	0.72	0	1,1,1	0.22	0
8	EDO	D	514	-	3,3,3	0.48	0	2,2,2	0.28	0
4	MLI	E	303	-	6,6,6	1.09	0	7,7,7	0.94	0
5	PZJ	D	501	-	22,23,23	6.76	8 (36%)	28,34,34	2.75	10 (35%)
8	EDO	F	518	-	3,3,3	0.46	0	2,2,2	0.27	0
5	PZJ	B	501	-	22,23,23	6.67	8 (36%)	28,34,34	2.63	9 (32%)
3	FMT	H	508	-	2,2,2	0.69	0	1,1,1	0.19	0
3	FMT	B	506	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	H	505	-	2,2,2	0.71	0	1,1,1	0.22	0
6	P1T	D	502	-	20,21,21	2.77	4 (20%)	28,30,30	2.11	8 (28%)
3	FMT	F	505	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	E	302	-	2,2,2	0.70	0	1,1,1	0.22	0
3	FMT	E	301	-	2,2,2	0.71	0	1,1,1	0.20	0
3	FMT	B	507	-	2,2,2	0.73	0	1,1,1	0.28	0
3	FMT	D	504	-	2,2,2	0.71	0	1,1,1	0.23	0
6	P1T	H	502	-	20,21,21	2.65	4 (20%)	28,30,30	2.00	7 (25%)
8	EDO	F	516	-	3,3,3	0.46	0	2,2,2	0.34	0
3	FMT	C	302	-	2,2,2	0.70	0	1,1,1	0.20	0
6	P1T	F	502	-	20,21,21	2.60	4 (20%)	28,30,30	1.48	5 (17%)
3	FMT	A	302	-	2,2,2	0.71	0	1,1,1	0.18	0
4	MLI	G	303	-	6,6,6	1.08	0	7,7,7	0.98	0
3	FMT	A	301	-	2,2,2	0.72	0	1,1,1	0.26	0
8	EDO	B	510	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EDO	G	304	-	3,3,3	0.46	0	2,2,2	0.33	0
3	FMT	B	505	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	H	506	-	2,2,2	0.71	0	1,1,1	0.21	0
3	FMT	F	508	-	2,2,2	0.71	0	1,1,1	0.18	0
4	MLI	C	303	-	6,6,6	1.08	0	7,7,7	1.07	0
10	ACT	D	509	-	3,3,3	1.36	0	3,3,3	1.48	0
3	FMT	H	507	-	2,2,2	0.71	0	1,1,1	0.24	0
4	MLI	A	303	-	6,6,6	1.10	0	7,7,7	1.01	0
3	FMT	G	301	-	2,2,2	0.71	0	1,1,1	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	B	509	-	3,3,3	0.47	0	2,2,2	0.35	0
3	FMT	F	507	-	2,2,2	0.70	0	1,1,1	0.23	0
5	PZJ	F	501	-	22,23,23	6.73	8 (36%)	28,34,34	2.71	11 (39%)
3	FMT	F	503	-	2,2,2	0.73	0	1,1,1	0.25	0
5	PZJ	H	501	-	22,23,23	6.66	8 (36%)	28,34,34	2.68	9 (32%)
3	FMT	B	504	-	2,2,2	0.70	0	1,1,1	0.22	0
8	EDO	F	517	-	3,3,3	0.46	0	2,2,2	0.34	0
4	MLI	D	513	-	6,6,6	1.10	0	7,7,7	1.03	0
10	ACT	D	505	-	3,3,3	1.39	0	3,3,3	1.45	0

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
9	PEG	C	301	-	-	0/4/4/4	-
8	EDO	F	515	-	-	1/1/1/1	-
8	EDO	D	515	-	-	0/1/1/1	-
4	MLI	F	514	-	-	4/4/4/4	-
6	P1T	B	502	-	-	3/14/15/15	0/1/1/1
8	EDO	D	514	-	-	0/1/1/1	-
4	MLI	E	303	-	-	2/4/4/4	-
5	PZJ	D	501	-	-	2/8/32/32	0/3/3/3
8	EDO	F	518	-	-	0/1/1/1	-
5	PZJ	B	501	-	-	4/8/32/32	0/3/3/3
6	P1T	D	502	-	-	3/14/15/15	0/1/1/1
6	P1T	H	502	-	-	3/14/15/15	0/1/1/1
8	EDO	F	516	-	-	0/1/1/1	-
6	P1T	F	502	-	-	4/14/15/15	0/1/1/1
4	MLI	G	303	-	-	0/4/4/4	-
8	EDO	B	510	-	-	0/1/1/1	-
8	EDO	G	304	-	-	0/1/1/1	-
4	MLI	C	303	-	-	4/4/4/4	-
4	MLI	A	303	-	-	0/4/4/4	-
8	EDO	B	509	-	-	0/1/1/1	-
5	PZJ	H	501	-	-	5/8/32/32	0/3/3/3
5	PZJ	F	501	-	-	0/8/32/32	0/3/3/3
8	EDO	F	517	-	-	0/1/1/1	-
4	MLI	D	513	-	-	0/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	PZJ	C08-S09	-20.98	1.52	1.78
5	F	501	PZJ	C13-C07	20.62	1.78	1.53
5	B	501	PZJ	C13-C07	20.55	1.78	1.53
5	F	501	PZJ	C08-S09	-20.53	1.53	1.78
5	H	501	PZJ	C13-C07	20.44	1.78	1.53

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	PZJ	C12-S09-C08	9.14	106.66	96.11
5	H	501	PZJ	C12-S09-C08	9.02	106.52	96.11
5	F	501	PZJ	C12-S09-C08	8.70	106.15	96.11
5	B	501	PZJ	C12-S09-C08	8.69	106.14	96.11
5	H	501	PZJ	C08-C07-N06	7.24	133.94	116.84

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

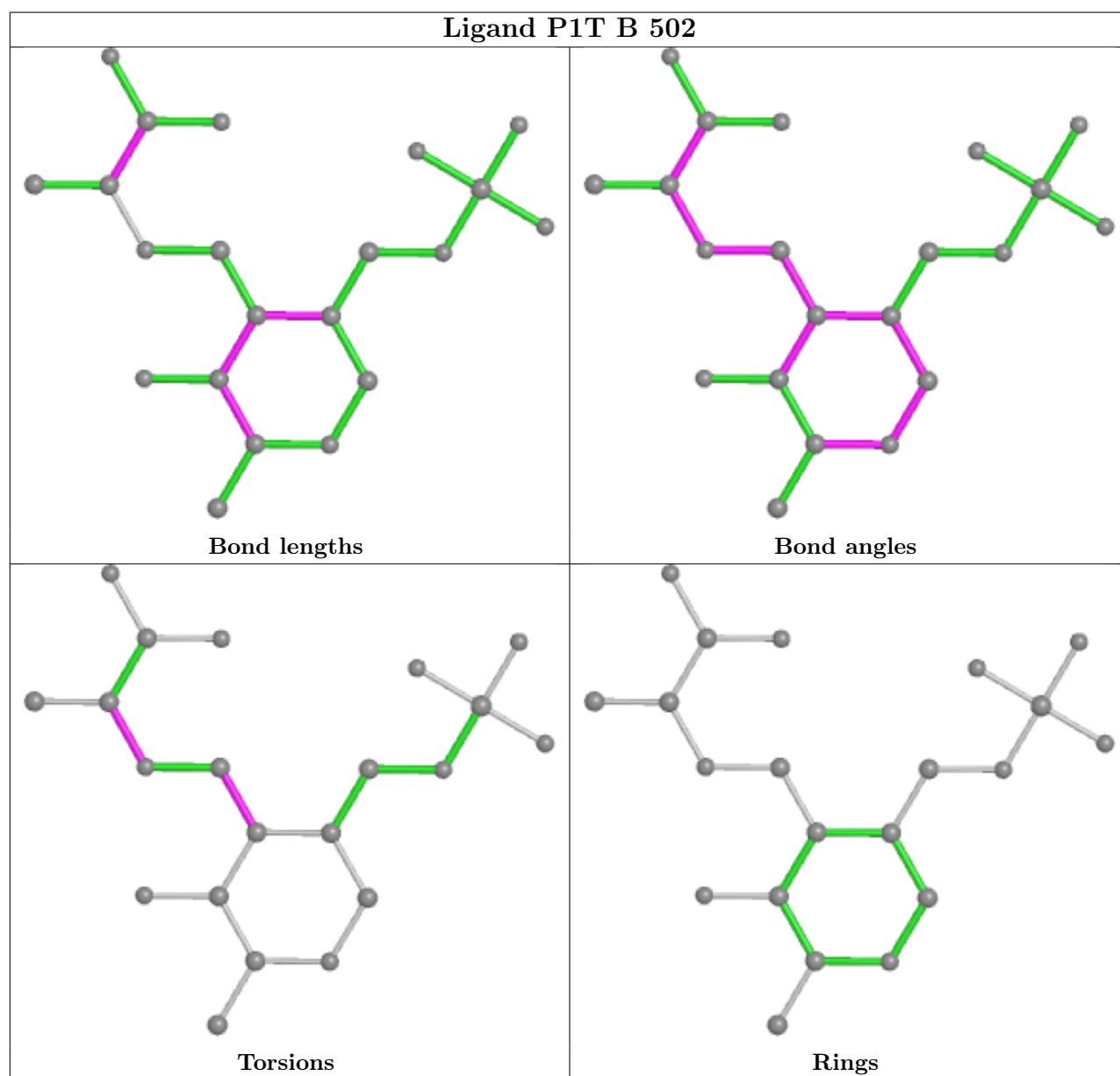
Mol	Chain	Res	Type	Atoms
5	B	501	PZJ	C20-C15-N03-C02
5	H	501	PZJ	C20-C15-N03-C02
6	B	502	P1T	C5-C4-C4A-N
6	B	502	P1T	C3-C4-C4A-N
6	D	502	P1T	C5-C4-C4A-N

There are no ring outliers.

11 monomers are involved in 23 short contacts:

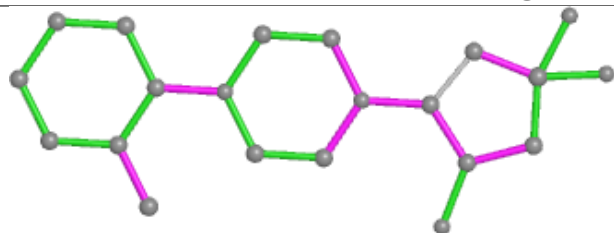
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	301	PEG	1	0
8	F	515	EDO	1	0
5	D	501	PZJ	3	0
8	F	518	EDO	2	0
5	B	501	PZJ	4	0
6	D	502	P1T	1	0
3	E	301	FMT	1	0
6	H	502	P1T	2	0
5	F	501	PZJ	3	0
5	H	501	PZJ	4	0
8	F	517	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

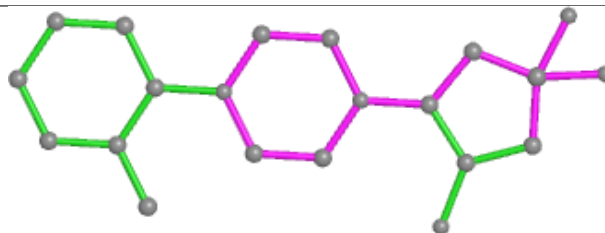




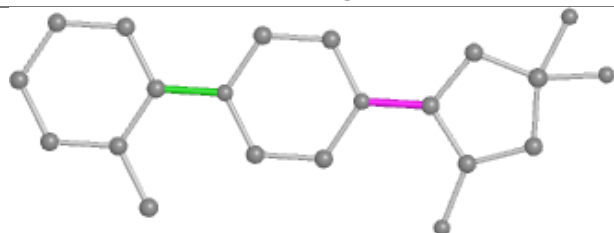
## Ligand PZJ D 501



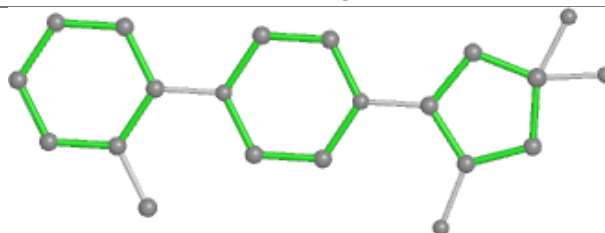
Bond lengths



Bond angles

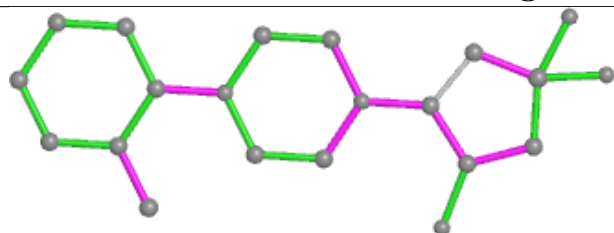


Torsions

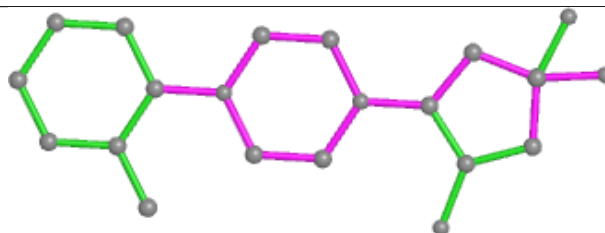


Rings

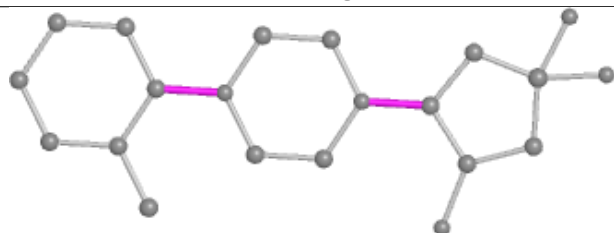
## Ligand PZJ B 501



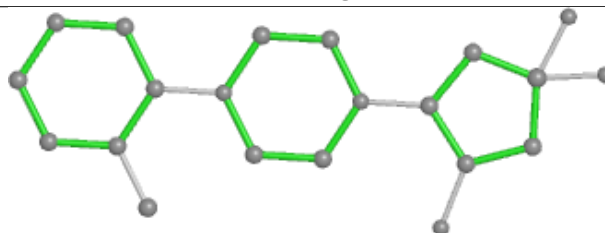
Bond lengths



Bond angles

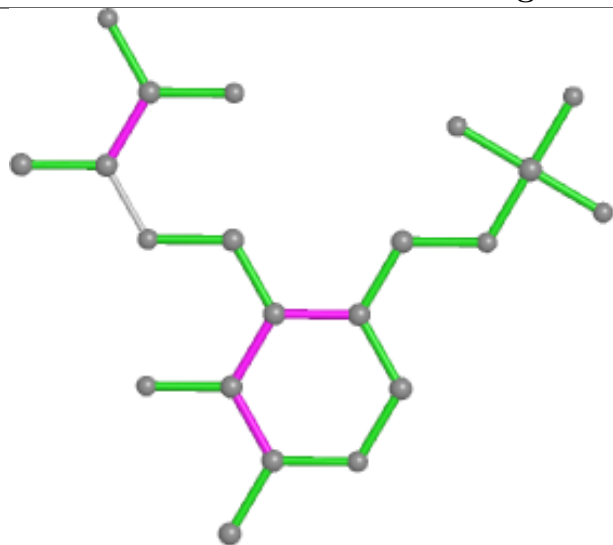


Torsions

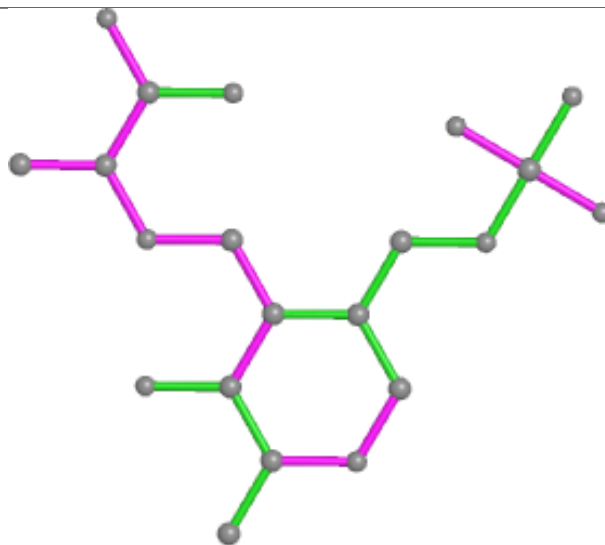


Rings

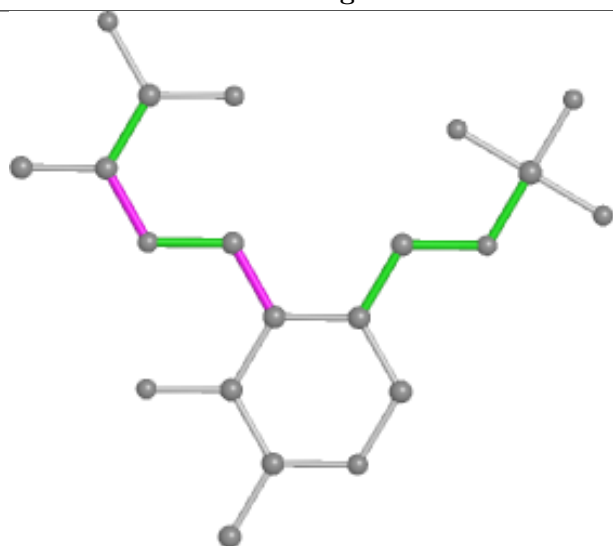
## Ligand P1T D 502



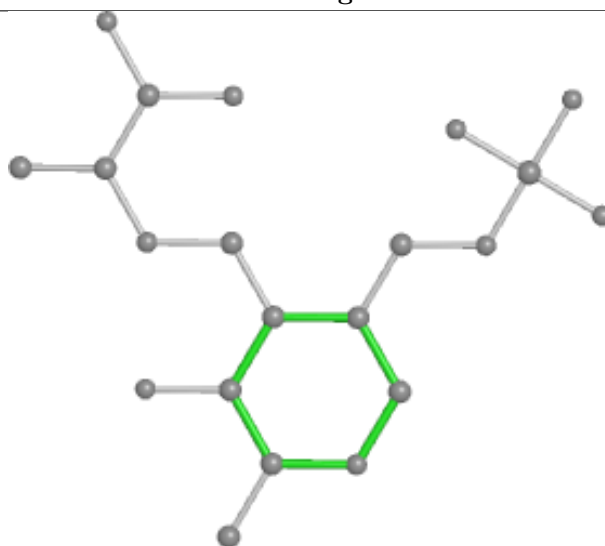
Bond lengths



Bond angles

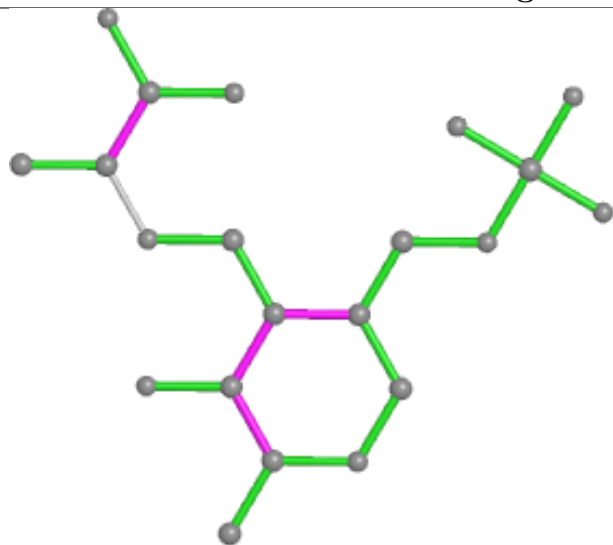


Torsions

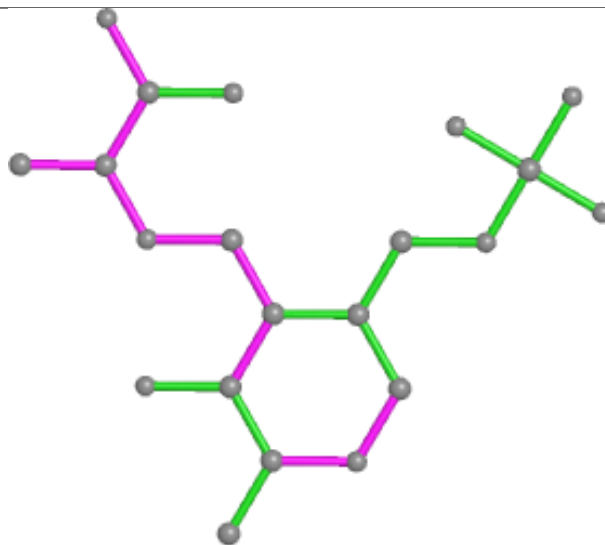


Rings

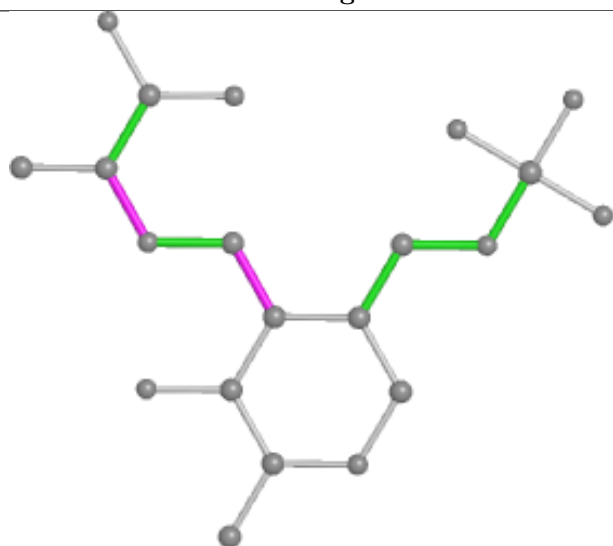
## Ligand P1T H 502



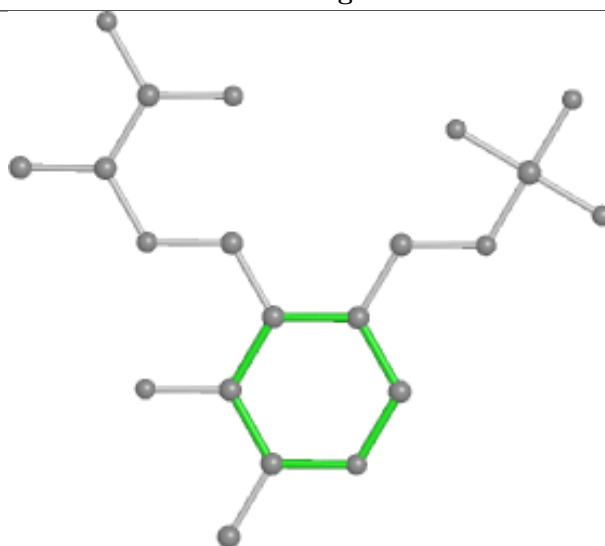
Bond lengths



Bond angles

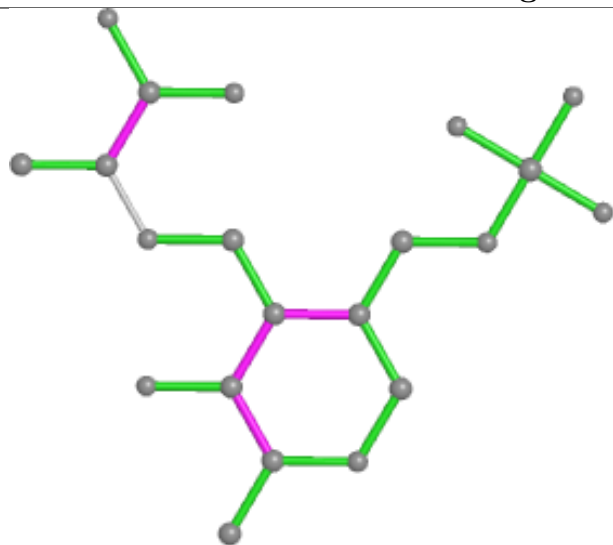


Torsions

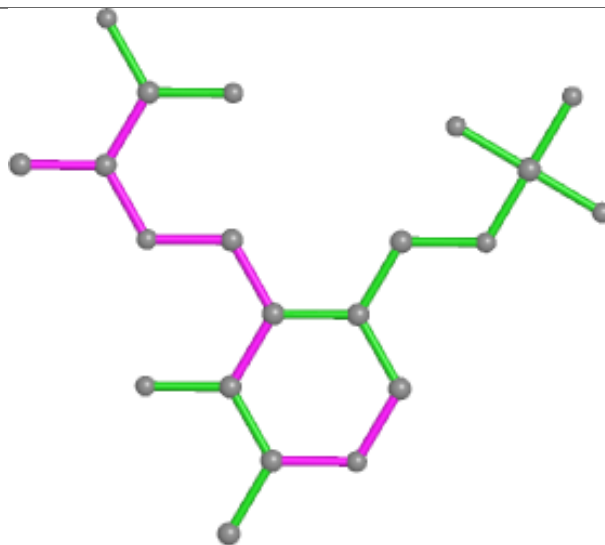


Rings

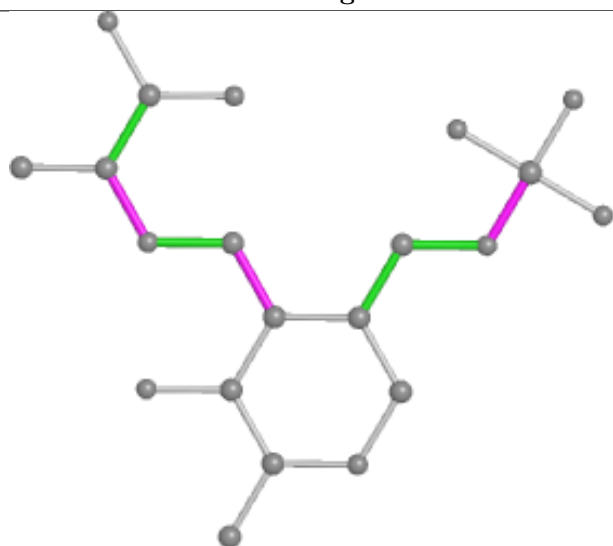
## Ligand P1T F 502



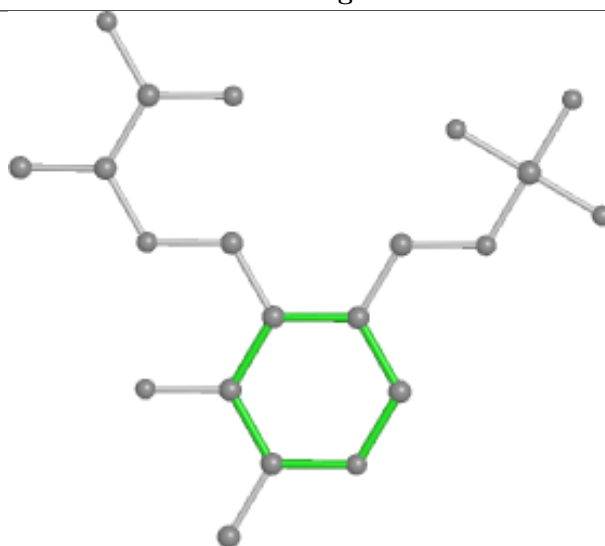
Bond lengths



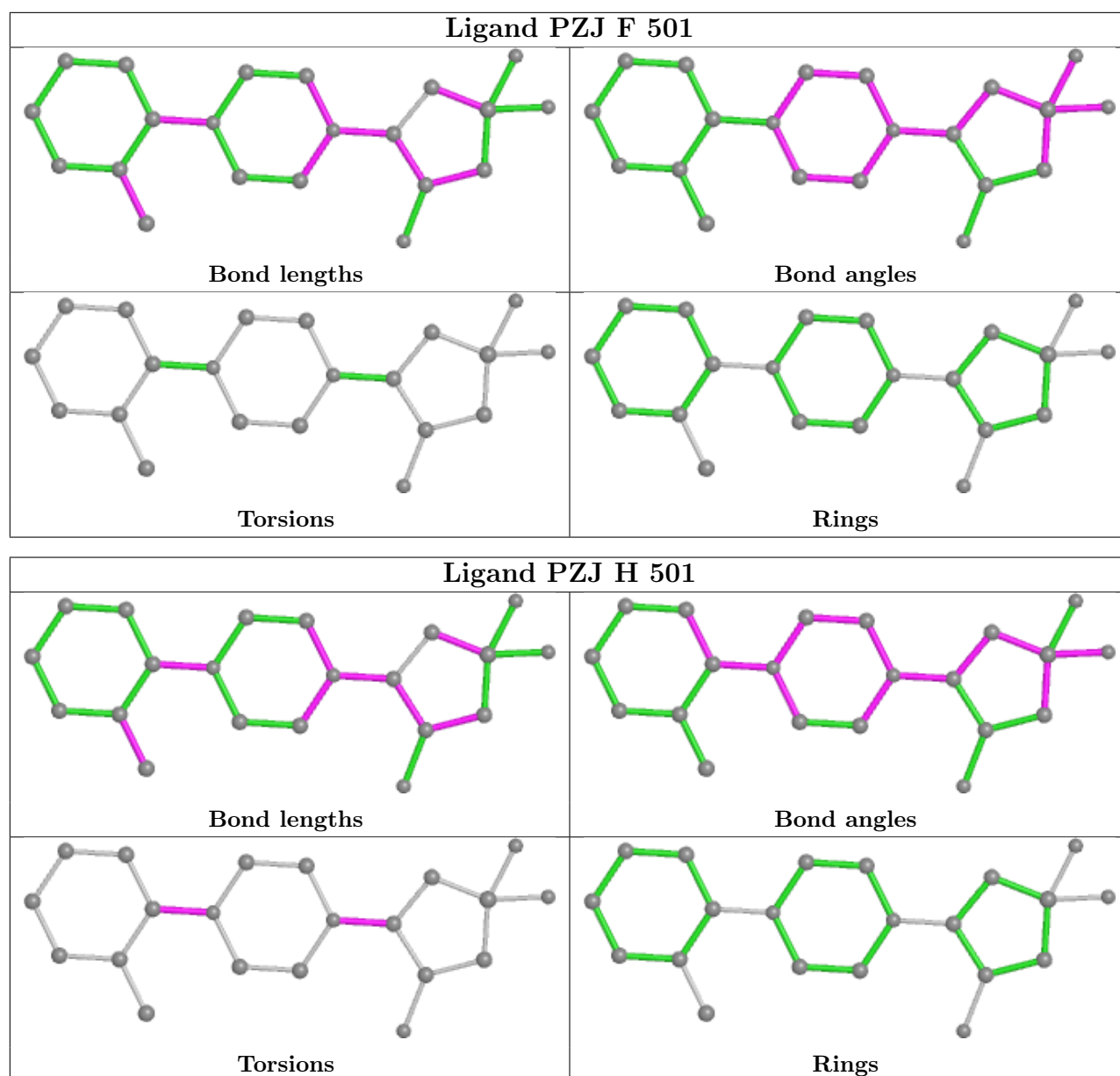
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	249/276 (90%)	-0.39	7 (2%) 53 51	31, 45, 69, 127	0
1	C	249/276 (90%)	-0.45	5 (2%) 65 63	25, 42, 75, 122	0
1	E	245/276 (88%)	-0.29	5 (2%) 65 63	32, 53, 80, 102	0
1	G	248/276 (89%)	-0.60	3 (1%) 79 77	24, 40, 62, 94	0
2	B	404/410 (98%)	-0.78	3 (0%) 87 86	18, 28, 49, 100	0
2	D	404/410 (98%)	-0.69	7 (1%) 70 68	18, 27, 46, 152	0
2	F	400/410 (97%)	-0.80	4 (1%) 82 80	19, 28, 49, 110	0
2	H	403/410 (98%)	-0.78	1 (0%) 95 94	15, 26, 44, 115	0
All	All	2602/2744 (94%)	-0.64	35 (1%) 77 75	15, 32, 67, 152	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	8	PRO	5.1
2	D	7	GLU	4.8
1	C	8	GLU	4.4
1	A	8	GLU	4.3
2	D	4	ALA	4.1

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	K	D	512	1/1	0.63	0.46	120,120,120,120	0
3	FMT	G	301	3/3	0.69	0.26	71,71,72,73	0
9	PEG	C	301	7/7	0.73	0.59	75,77,81,82	0
3	FMT	H	505	3/3	0.74	0.23	73,73,74,74	0
3	FMT	B	505	3/3	0.75	0.17	64,64,65,66	0
8	EDO	F	516	4/4	0.76	0.16	62,63,66,68	0
10	ACT	D	505	4/4	0.76	0.36	67,68,69,69	0
7	K	F	512	1/1	0.77	0.33	119,119,119,119	0
10	ACT	F	506	4/4	0.77	0.28	65,67,67,68	0
3	FMT	H	508	3/3	0.78	0.34	59,59,60,61	0
7	K	B	508	1/1	0.78	0.28	84,84,84,84	0
3	FMT	E	302	3/3	0.79	0.17	73,73,73,74	0
3	FMT	F	509	3/3	0.79	0.32	80,80,80,80	0
3	FMT	E	301	3/3	0.79	0.43	71,71,72,72	0
3	FMT	C	302	3/3	0.80	0.41	64,64,65,66	0
3	FMT	D	508	3/3	0.80	0.30	71,71,72,72	0
8	EDO	G	304	4/4	0.80	0.34	55,58,61,62	0
3	FMT	H	503	3/3	0.81	0.27	60,60,61,62	0
3	FMT	H	504	3/3	0.81	0.39	70,70,72,72	0
3	FMT	D	506	3/3	0.81	0.20	71,71,72,73	0
3	FMT	D	504	3/3	0.81	0.31	56,56,58,59	0
7	K	F	513	1/1	0.82	0.29	123,123,123,123	0
8	EDO	B	510	4/4	0.83	0.21	61,64,68,71	0
7	K	D	510	1/1	0.84	0.24	101,101,101,101	0
8	EDO	F	515	4/4	0.87	0.34	59,59,60,61	0
8	EDO	D	515	4/4	0.87	0.24	60,61,61,62	0
4	MLI	A	303	7/7	0.88	0.16	58,61,61,62	0
4	MLI	F	514	7/7	0.88	0.19	50,55,58,59	0
3	FMT	F	508	3/3	0.88	0.31	57,57,59,59	0
12	NA	H	511	1/1	0.88	0.58	54,54,54,54	0
8	EDO	F	517	4/4	0.89	0.45	63,65,66,67	0
3	FMT	A	302	3/3	0.89	0.31	62,62,63,63	0
3	FMT	F	507	3/3	0.89	0.18	56,56,57,58	0
12	NA	H	512	1/1	0.89	0.22	68,68,68,68	0
10	ACT	D	509	4/4	0.90	0.37	70,71,71,72	0
8	EDO	D	514	4/4	0.90	0.24	54,54,55,56	0
3	FMT	H	506	3/3	0.91	0.15	60,60,62,62	0

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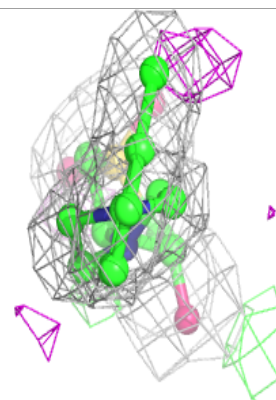
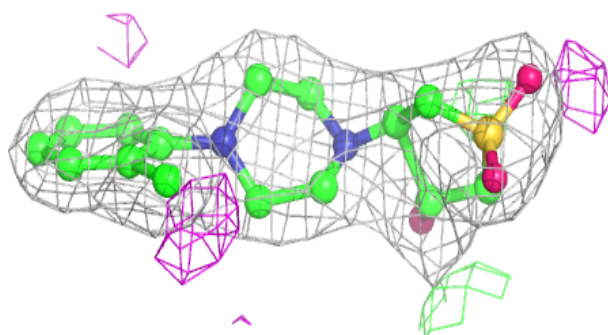
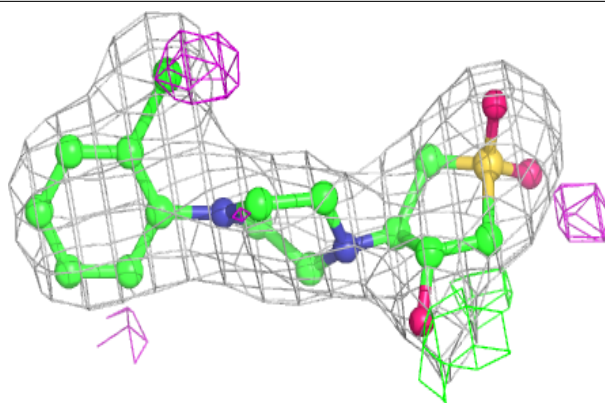
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	K	D	511	1/1	0.91	0.35	86,86,86,86	0
3	FMT	F	505	3/3	0.92	0.21	66,66,67,67	0
3	FMT	D	503	3/3	0.92	0.13	51,51,52,54	0
4	MLI	C	303	7/7	0.92	0.12	55,57,60,61	0
3	FMT	B	506	3/3	0.92	0.17	48,48,48,50	0
7	K	F	510	1/1	0.92	0.25	79,79,79,79	0
4	MLI	D	513	7/7	0.93	0.14	59,59,62,62	0
7	K	H	509	1/1	0.93	0.23	86,86,86,86	0
3	FMT	B	504	3/3	0.93	0.10	52,52,53,53	0
3	FMT	D	507	3/3	0.93	0.29	65,65,65,66	0
3	FMT	H	507	3/3	0.93	0.15	55,55,56,56	0
11	SO4	H	510	5/5	0.94	0.26	118,119,119,119	0
3	FMT	B	507	3/3	0.94	0.13	51,51,52,52	0
4	MLI	E	303	7/7	0.94	0.11	52,54,63,64	0
7	K	G	302	1/1	0.95	0.24	94,94,94,94	0
3	FMT	A	301	3/3	0.95	0.19	63,63,63,64	0
8	EDO	B	509	4/4	0.95	0.26	52,53,55,58	0
8	EDO	F	518	4/4	0.95	0.30	59,61,61,62	0
7	K	F	511	1/1	0.96	0.14	78,78,78,78	0
4	MLI	G	303	7/7	0.96	0.10	55,56,62,63	0
3	FMT	F	504	3/3	0.96	0.10	60,60,60,60	0
5	PZJ	B	501	21/21	0.97	0.14	28,37,41,47	0
5	PZJ	D	501	21/21	0.97	0.15	28,34,48,50	0
5	PZJ	F	501	21/21	0.97	0.12	36,39,46,47	0
5	PZJ	H	501	21/21	0.97	0.16	26,31,42,43	0
3	FMT	F	503	3/3	0.97	0.09	53,53,53,54	0
3	FMT	B	503	3/3	0.98	0.10	43,43,43,44	0
6	P1T	H	502	21/21	0.98	0.21	16,21,26,29	0
6	P1T	B	502	21/21	0.99	0.19	17,21,26,28	0
6	P1T	D	502	21/21	0.99	0.16	19,23,27,28	0
6	P1T	F	502	21/21	0.99	0.16	16,25,29,30	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.

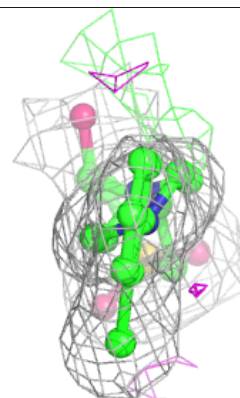
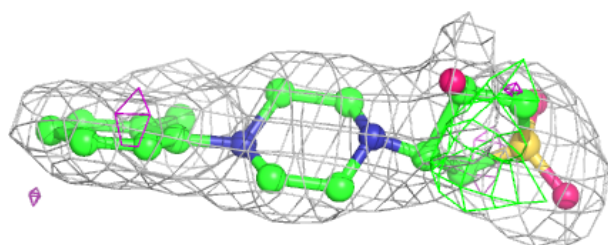
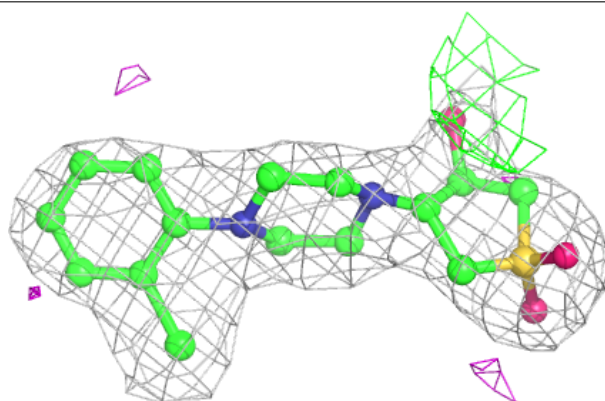


**Electron density around PZJ B 501:**

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

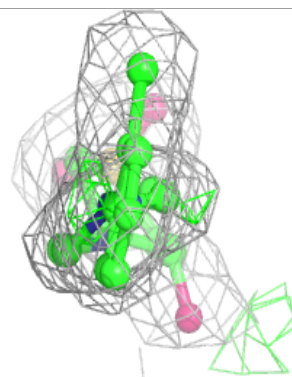
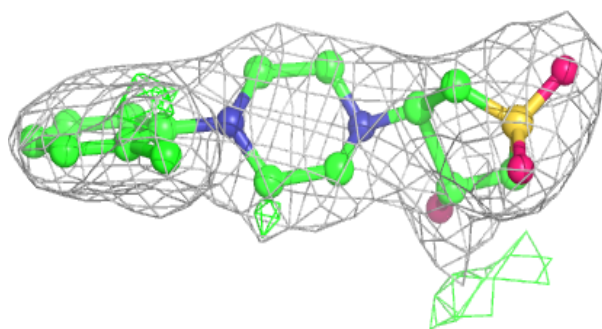
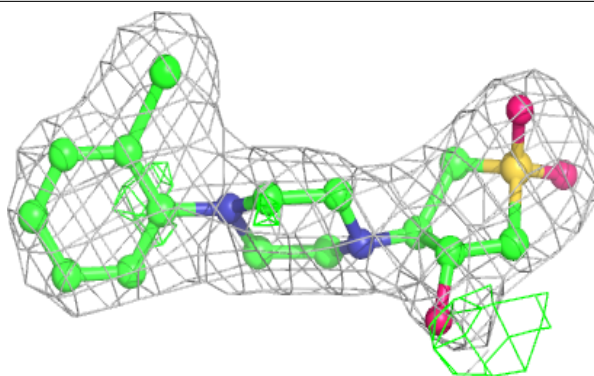
**Electron density around PZJ D 501:**

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

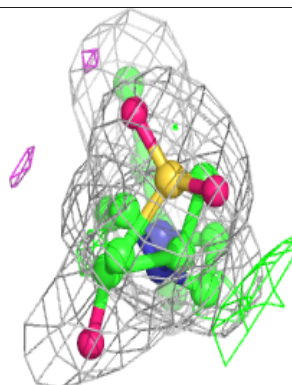
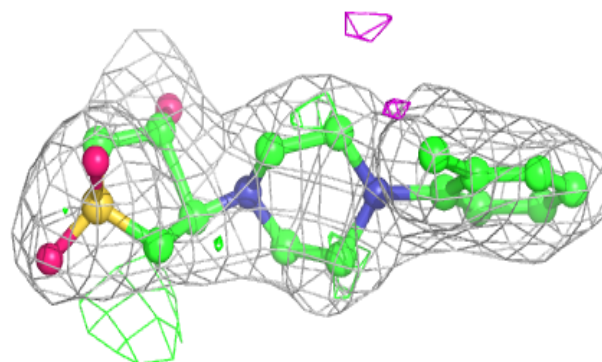
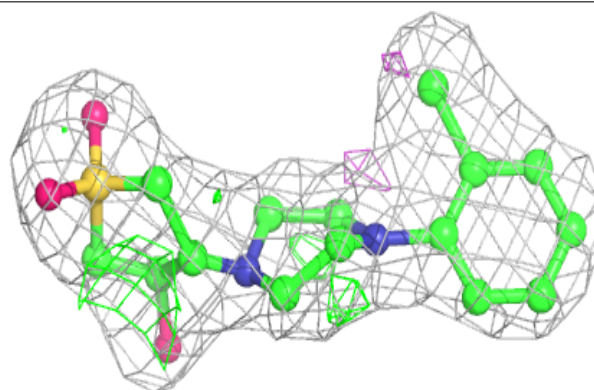


**Electron density around PZJ F 501:**

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

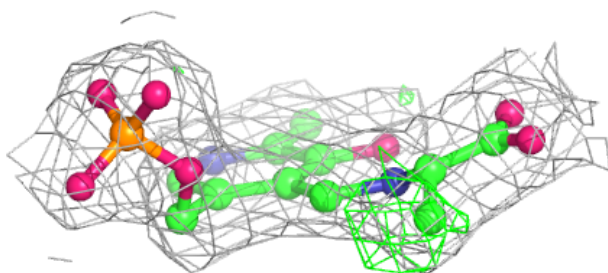
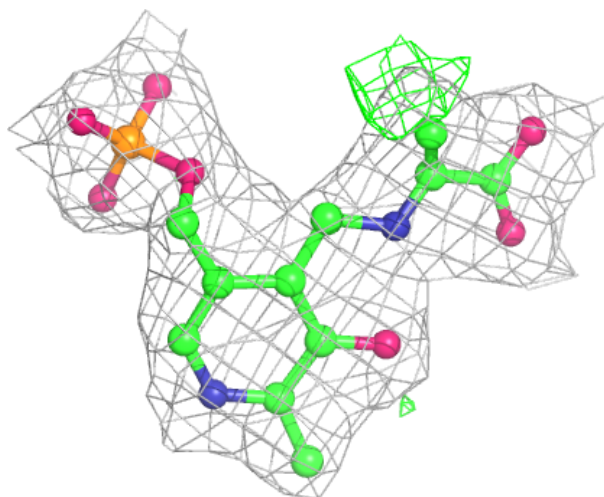
**Electron density around PZJ H 501:**

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



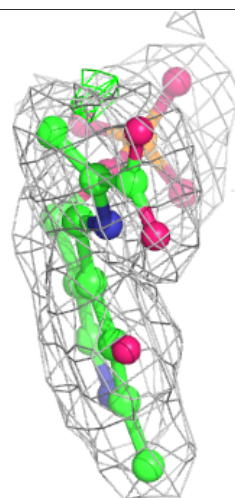
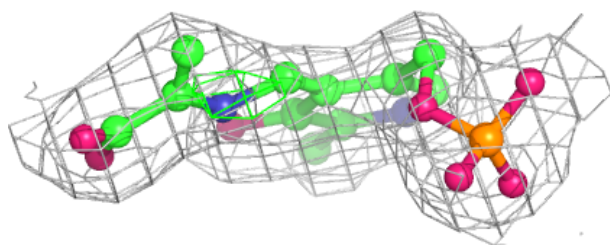
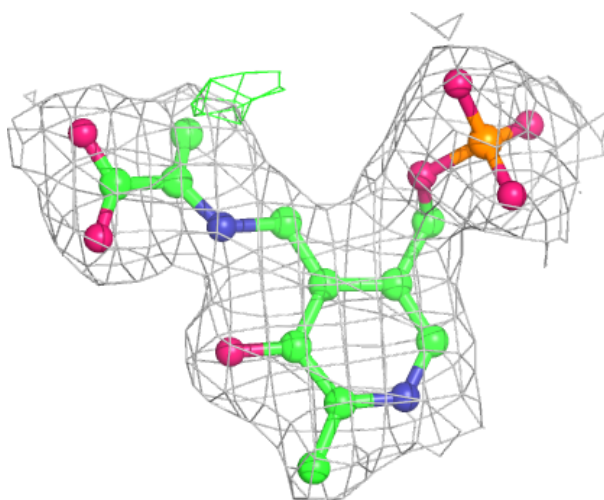
**Electron density around P1T H 502:**

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



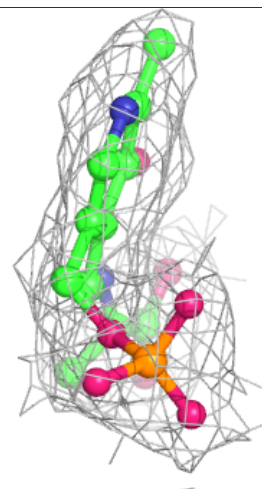
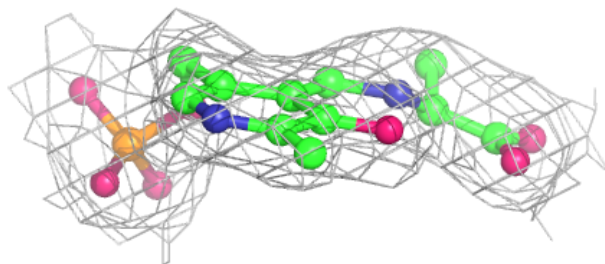
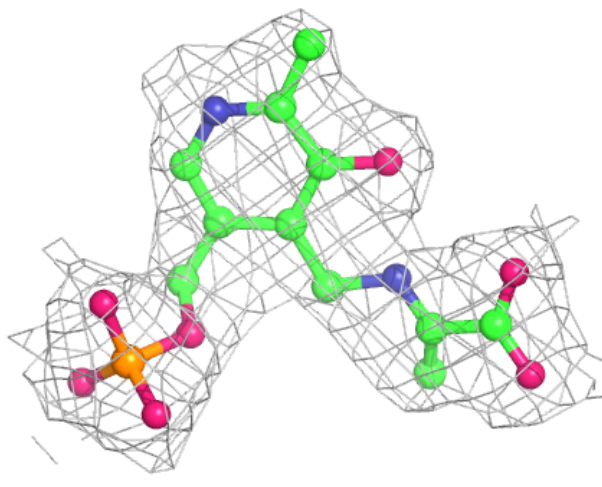
**Electron density around P1T B 502:**

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



**Electron density around P1T D 502:**

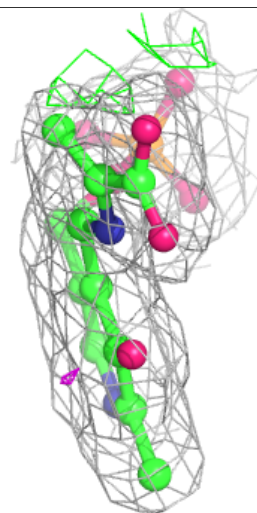
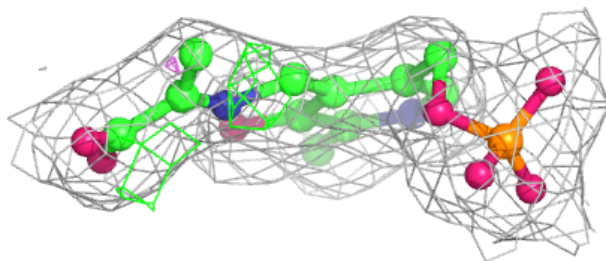
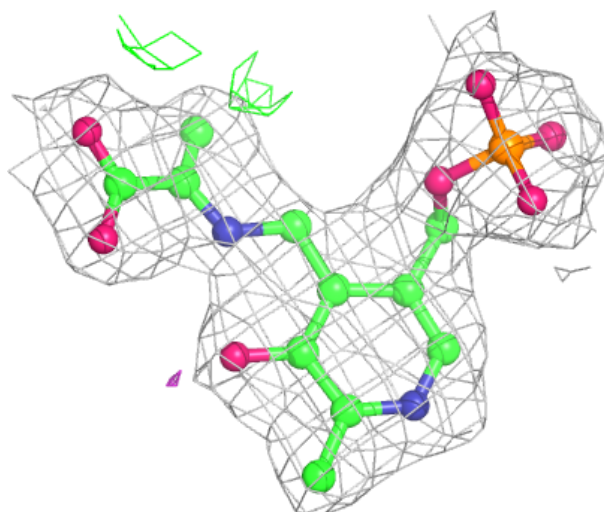
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around P1T F 502:**

$2mF_o-DF_c$  (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.