Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 PM UTC

PDB ID	:	8OWQ / pdb_00008owq
Title	:	Crystal structure of Mycobacterium smegmatis CoaB in complex with CTP and 2-(1-(3,4-dihydroxyphenyl)-5-phenyl-1H-indol-3-yl)-2-oxoacetic acid
Authors	:	Mendes, V.; Blundell, T.L.
Deposited on	:	2023-04-28
Resolution	:	2.11 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

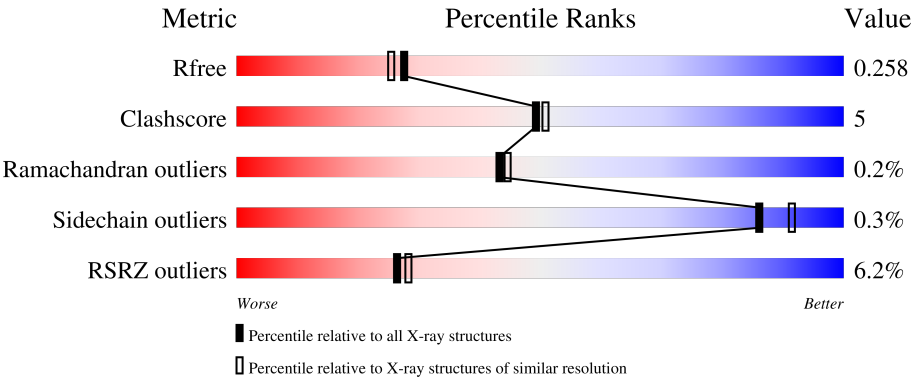
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	237	5% 78% 11% 11%
1	B	237	8% 74% 14% 12%
1	C	237	3% 79% 8% 13%
1	D	237	5% 86% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6840 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 Coenzyme A biosynthesis bifunctional protein CoaBC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1502	933	278	285	6			
1	B	209	Total	C	N	O	S	0	0	0
			1492	930	276	280	6			
1	C	207	Total	C	N	O	S	0	0	0
			1479	915	276	282	6			
1	D	227	Total	C	N	O	S	0	0	0
			1625	1007	305	307	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MET	-	initiating methionine	UNP A0QWT2
A	179	ALA	-	expression tag	UNP A0QWT2
A	180	HIS	-	expression tag	UNP A0QWT2
A	181	HIS	-	expression tag	UNP A0QWT2
A	182	HIS	-	expression tag	UNP A0QWT2
A	183	HIS	-	expression tag	UNP A0QWT2
A	184	HIS	-	expression tag	UNP A0QWT2
A	185	HIS	-	expression tag	UNP A0QWT2
B	178	MET	-	initiating methionine	UNP A0QWT2
B	179	ALA	-	expression tag	UNP A0QWT2
B	180	HIS	-	expression tag	UNP A0QWT2
B	181	HIS	-	expression tag	UNP A0QWT2
B	182	HIS	-	expression tag	UNP A0QWT2
B	183	HIS	-	expression tag	UNP A0QWT2
B	184	HIS	-	expression tag	UNP A0QWT2
B	185	HIS	-	expression tag	UNP A0QWT2
C	178	MET	-	initiating methionine	UNP A0QWT2
C	179	ALA	-	expression tag	UNP A0QWT2
C	180	HIS	-	expression tag	UNP A0QWT2
C	181	HIS	-	expression tag	UNP A0QWT2
C	182	HIS	-	expression tag	UNP A0QWT2

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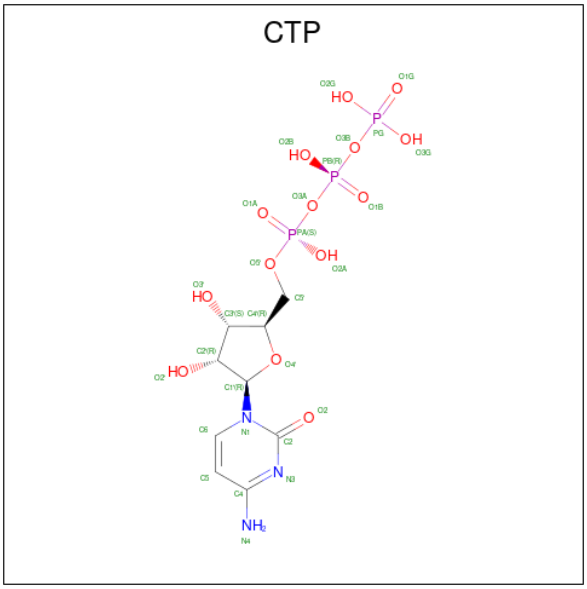
Chain	Residue	Modelled	Actual	Comment	Reference
C	183	HIS	-	expression tag	UNP A0QWT2
C	184	HIS	-	expression tag	UNP A0QWT2
C	185	HIS	-	expression tag	UNP A0QWT2
D	178	MET	-	initiating methionine	UNP A0QWT2
D	179	ALA	-	expression tag	UNP A0QWT2
D	180	HIS	-	expression tag	UNP A0QWT2
D	181	HIS	-	expression tag	UNP A0QWT2
D	182	HIS	-	expression tag	UNP A0QWT2
D	183	HIS	-	expression tag	UNP A0QWT2
D	184	HIS	-	expression tag	UNP A0QWT2
D	185	HIS	-	expression tag	UNP A0QWT2

- Molecule 2 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).

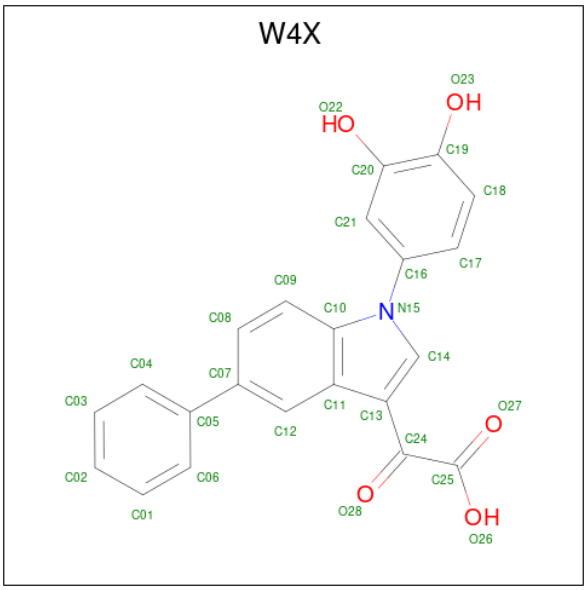


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is 2-[1-[3,4-bis(oxidanyl)phenyl]-5-phenyl-indol-3-yl]-2-oxidanylidene-ethanoic acid (CCD ID: W4X) (formula: $C_{22}H_{15}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 28 22 1 5	0	0
4	A	1	Total C N O 28 22 1 5	0	0
4	A	1	Total C N O 28 22 1 5	0	0
4	B	1	Total C N O 28 22 1 5	0	0
4	C	1	Total C N O 28 22 1 5	0	0
4	C	1	Total C N O 28 22 1 5	0	0

- Molecule 5 is water.

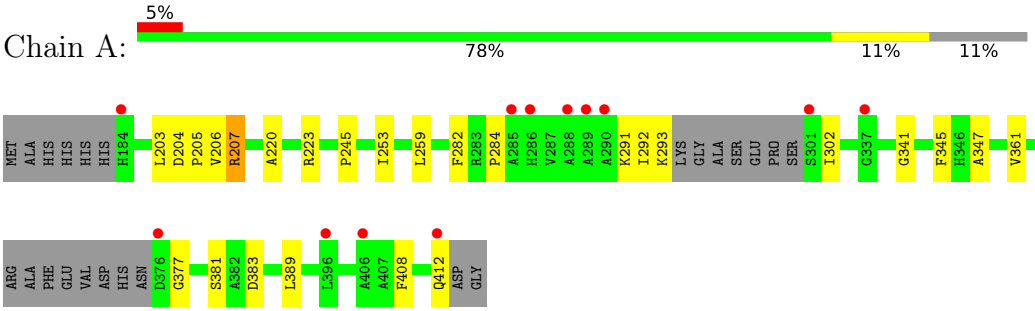
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	127	Total O 127 127	0	0
5	B	112	Total O 112 112	0	0
5	C	103	Total O 103 103	0	0
5	D	112	Total O 112 112	0	0

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.

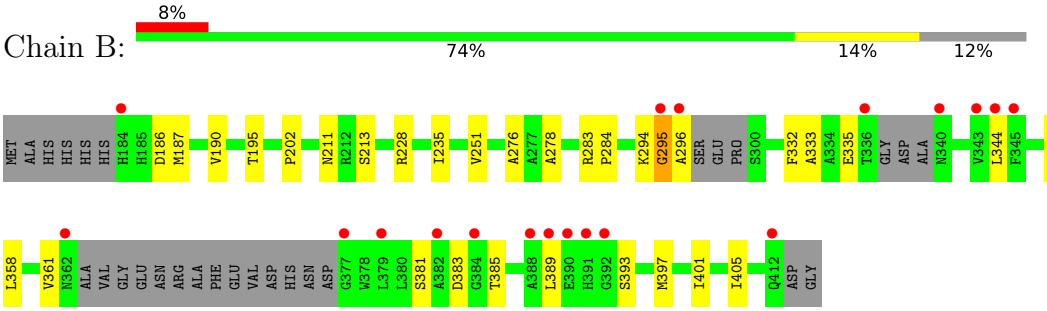
• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

Chain A:



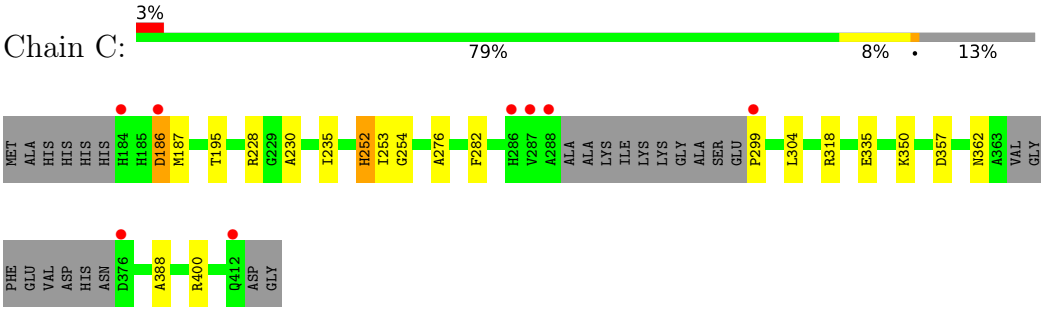
• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

Chain B:



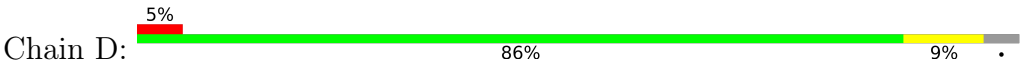
• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

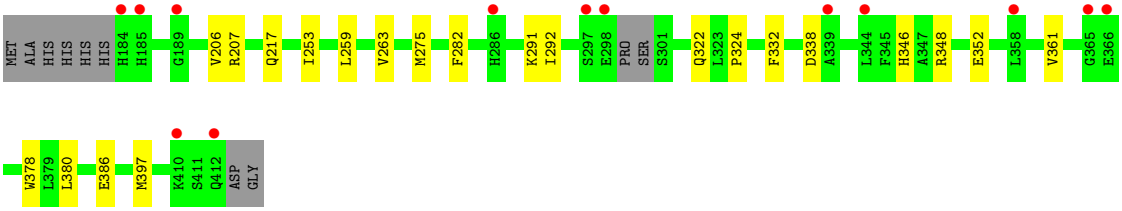
Chain C:



• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

Chain D:




MET
ALA
HIS
HIS
HIS
H184
H185
G189
V206
R207
Q217
I253
L259
V263
M275
F282
H286
K291
I292
S297
E298
PRO
SER
S301
Q322
L323
P324
F332
D338
A339
L344
F345
H346
A347
R348
E352
L358
V361
G365
E366
W378
L379
L380
E386
M397
K410
S411
Q412
ASP
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.20Å 78.47Å 150.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.35 – 2.11 69.35 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (69.35-2.11) 99.8 (69.35-2.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.207 , 0.256 0.208 , 0.258	Depositor DCC
R_{free} test set	2700 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6840	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, W4X, CTP

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	0.47	1/1519 (0.1%)	0.56	0/2061
1	B	0.36	0/1507	0.57	1/2037 (0.0%)
1	C	0.46	2/1496 (0.1%)	0.56	0/2029
1	D	0.34	0/1645	0.53	0/2230
All	All	0.41	3/6167 (0.0%)	0.55	1/8357 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	ARG	C-O	-6.66	1.15	1.23
1	C	252	HIS	C-O	-5.91	1.16	1.23
1	C	254	GLY	C-O	-5.18	1.17	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	294	LYS	N-CA-C	6.21	118.53	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1502	0	1494	21	0
1	B	1492	0	1503	21	0
1	C	1479	0	1468	12	0
1	D	1625	0	1607	12	0
2	A	29	0	12	0	0
2	B	29	0	12	2	0
2	C	29	0	12	1	0
2	D	29	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	84	0	0	6	0
4	B	28	0	0	2	0
4	C	56	0	0	3	0
5	A	127	0	0	1	0
5	B	112	0	0	1	0
5	C	103	0	0	1	0
5	D	112	0	0	0	0
All	All	6840	0	6120	67	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 5.

All (67) 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:B:389:LEU:HB3	1:B:397:MET:HE1	1.70	0.73
1:D:338:ASP:OD1	1:D:346:HIS:NE2	2.23	0.72
1:A:291:LYS:HE2	2:B:501:CTP:O1B	1.96	0.64
1:A:282:PHE:HE2	4:A:504:W4X:O27	1.82	0.62
1:B:186:ASP:OD2	1:B:228:ARG:NH1	2.24	0.61
1:B:393:SER:O	1:B:397:MET:HG2	2.01	0.61
1:D:348:ARG:O	1:D:352:GLU:HG3	2.03	0.59
1:D:253:ILE:HD13	1:D:259:LEU:HB2	1.85	0.59
1:A:408:PHE:O	1:A:412:GLN:HG2	2.04	0.58
1:B:335:GLU:OE2	1:B:350:LYS:NZ	2.26	0.56
1:B:211:ASN:HD21	1:B:278:ALA:HB3	1.71	0.56
1:B:350:LYS:HE2	1:B:353:ARG:HH21	1.71	0.55
1:C:282:PHE:HB3	1:C:304:LEU:HB3	1.90	0.54
2:B:501:CTP:O3A	4:B:503:W4X:O23	2.26	0.53
1:C:388:ALA:O	1:C:400:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:VAL:HB	1:D:378:TRP:HB2	1.92	0.51
1:D:380:LEU:HD22	1:D:386:GLU:HG2	1.92	0.51
1:B:202:PRO:O	1:B:284:PRO:HG2	2.11	0.51
1:C:335:GLU:OE1	1:C:350:LYS:NZ	2.35	0.51
1:C:195:THR:HA	1:C:235:ILE:O	2.11	0.50
1:A:220:ALA:HA	1:A:223:ARG:CZ	2.43	0.49
1:A:292:ILE:HD12	4:A:505:W4X:C17	2.43	0.49
1:A:203:LEU:HD23	1:A:284:PRO:HG3	1.95	0.49
1:D:217:GLN:NE2	1:D:397:MET:HE3	2.27	0.49
1:C:253:ILE:HD12	1:C:253:ILE:C	2.38	0.48
1:A:381:SER:HB2	1:A:383:ASP:OD1	2.14	0.48
1:B:295:GLY:O	1:B:296:ALA:HB2	2.11	0.48
1:A:203:LEU:HD23	1:A:284:PRO:CG	2.44	0.47
1:B:350:LYS:HE2	1:B:353:ARG:NH2	2.29	0.47
1:A:341:GLY:HA3	1:A:345:PHE:CD1	2.49	0.47
1:C:186:ASP:OD2	1:C:228:ARG:NH1	2.42	0.47
1:A:207:ARG:HG2	4:A:505:W4X:C05	2.45	0.46
1:A:302:ILE:HG12	4:A:505:W4X:O23	2.16	0.46
1:C:252:HIS:HD2	5:C:604:HOH:O	1.97	0.46
2:C:501:CTP:O2A	4:C:503:W4X:O23	2.33	0.46
1:D:332:PHE:O	2:D:501:CTP:H5'1	2.15	0.46
1:B:187:MET:HE3	1:B:190:VAL:HG11	1.97	0.45
1:A:203:LEU:HD22	1:A:302:ILE:HD13	1.98	0.45
1:A:293:LYS:HA	4:A:505:W4X:O26	2.16	0.45
1:B:401:ILE:O	1:B:405:ILE:HG13	2.16	0.45
1:B:211:ASN:HD21	1:B:278:ALA:CB	2.30	0.45
1:C:195:THR:O	1:C:276:ALA:HB3	2.17	0.44
1:A:347:ALA:HB1	1:A:361:VAL:HG21	1.99	0.44
5:A:645:HOH:O	1:B:296:ALA:HA	2.16	0.44
1:D:206:VAL:HG23	1:D:207:ARG:HD2	1.99	0.44
1:A:207:ARG:HG2	4:A:505:W4X:C07	2.47	0.44
1:D:263:VAL:HG21	1:D:275:MET:HE1	2.00	0.44
1:C:187:MET:HB3	1:C:230:ALA:HB2	2.00	0.43
1:A:377:GLY:C	1:A:389:LEU:HB2	2.44	0.42
1:A:253:ILE:HD13	1:A:259:LEU:HB2	2.01	0.42
1:B:235:ILE:HA	1:B:251:VAL:O	2.20	0.42
1:A:223:ARG:HG3	1:A:245:PRO:HB3	2.00	0.42
1:A:204:ASP:HB2	1:A:205:PRO:CD	2.49	0.42
1:B:383:ASP:OD1	1:B:385:THR:HG23	2.19	0.41
1:B:195:THR:HG22	1:B:235:ILE:HB	2.02	0.41
1:C:299:PRO:HB3	1:D:282:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:HG3	5:B:655:HOH:O	2.21	0.41
1:C:318:ARG:HH22	1:C:357:ASP:CG	2.28	0.41
1:D:322:GLN:C	1:D:324:PRO:HD3	2.45	0.41
1:B:333:ALA:O	1:B:361:VAL:HA	2.20	0.41
1:C:362:ASN:HB2	4:C:503:W4X:C04	2.50	0.41
4:C:504:W4X:C18	1:D:292:ILE:HD12	2.51	0.41
1:B:276:ALA:HA	1:B:332:PHE:CG	2.57	0.40
1:B:213:SER:HB2	4:B:503:W4X:O28	2.21	0.40
1:A:206:VAL:HG23	1:A:207:ARG:HD2	2.03	0.40
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.86	0.40
1:B:358:LEU:HD23	1:B:381:SER:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	205/237 (86%)	199 (97%)	6 (3%)	0	100	100
1	B	201/237 (85%)	195 (97%)	5 (2%)	1 (0%)	24	22
1	C	201/237 (85%)	193 (96%)	7 (4%)	1 (0%)	24	22
1	D	223/237 (94%)	216 (97%)	7 (3%)	0	100	100
All	All	830/948 (88%)	803 (97%)	25 (3%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	186	ASP
1	B	295	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	145/173 (84%)	145 (100%)	0	100	100
1	B	144/173 (83%)	143 (99%)	1 (1%)	76	83
1	C	144/173 (83%)	144 (100%)	0	100	100
1	D	155/173 (90%)	154 (99%)	1 (1%)	78	86
All	All	588/692 (85%)	586 (100%)	2 (0%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	344	LEU
1	D	291	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
1	A	340	ASN
1	A	412	GLN
1	B	211	ASN
1	C	217	GLN
1	C	252	HIS
1	C	325	ASN
1	C	340	ASN
1	D	217	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	W4X	C	504	3	31,31,31	1.46	5 (16%)	45,45,45	1.19	5 (11%)
4	W4X	A	505	3	31,31,31	1.47	5 (16%)	45,45,45	1.03	2 (4%)
2	CTP	C	501	3	29,30,30	1.19	2 (6%)	43,47,47	0.93	1 (2%)
4	W4X	B	503	-	31,31,31	1.57	6 (19%)	45,45,45	1.46	7 (15%)
4	W4X	A	503	-	31,31,31	1.72	6 (19%)	45,45,45	1.31	6 (13%)
2	CTP	B	501	3	29,30,30	1.30	3 (10%)	43,47,47	1.04	2 (4%)
4	W4X	A	504	3	31,31,31	1.41	5 (16%)	45,45,45	1.28	6 (13%)
4	W4X	C	503	-	31,31,31	1.55	8 (25%)	45,45,45	1.29	7 (15%)
2	CTP	D	501	3	29,30,30	1.21	4 (13%)	43,47,47	1.02	2 (4%)
2	CTP	A	501	3	29,30,30	1.31	3 (10%)	43,47,47	0.93	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	W4X	C	504	3	-	1/16/16/16	0/4/4/4
4	W4X	A	505	3	-	1/16/16/16	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTP	C	501	3	-	3/22/38/38	0/2/2/2
4	W4X	B	503	-	-	7/16/16/16	0/4/4/4
4	W4X	A	503	-	-	6/16/16/16	0/4/4/4
2	CTP	B	501	3	-	4/22/38/38	0/2/2/2
4	W4X	A	504	3	-	0/16/16/16	0/4/4/4
4	W4X	C	503	-	-	8/16/16/16	0/4/4/4
2	CTP	D	501	3	-	3/22/38/38	0/2/2/2
2	CTP	A	501	3	-	0/22/38/38	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CTP	PB-O3B	5.28	1.65	1.59
4	A	503	W4X	C13-C24	4.94	1.55	1.45
2	B	501	CTP	PB-O3B	4.49	1.64	1.59
4	B	503	W4X	C13-C24	4.16	1.54	1.45
4	C	504	W4X	C13-C24	4.05	1.53	1.45
4	A	505	W4X	C13-C24	3.86	1.53	1.45
2	C	501	CTP	PB-O3B	3.81	1.63	1.59
4	C	503	W4X	C13-C24	3.79	1.53	1.45
4	A	503	W4X	C25-C24	-3.77	1.51	1.54
4	A	504	W4X	C13-C24	3.77	1.53	1.45
4	B	503	W4X	C10-N15	-3.46	1.33	1.39
4	C	503	W4X	C10-N15	-3.34	1.33	1.39
4	A	503	W4X	C10-N15	-3.18	1.34	1.39
2	D	501	CTP	PB-O3B	3.04	1.62	1.59
4	B	503	W4X	C25-C24	-3.03	1.51	1.54
4	B	503	W4X	C14-N15	-2.87	1.31	1.39
4	A	503	W4X	C14-N15	-2.85	1.32	1.39
4	A	504	W4X	C14-N15	-2.74	1.32	1.39
2	B	501	CTP	PB-O3A	2.65	1.62	1.59
4	A	505	W4X	C11-C13	-2.65	1.41	1.45
4	C	503	W4X	C11-C13	-2.61	1.41	1.45
4	A	504	W4X	C10-N15	-2.51	1.35	1.39
4	A	505	W4X	O22-C20	2.49	1.41	1.36
2	D	501	CTP	PB-O3A	2.49	1.62	1.59
4	A	504	W4X	C11-C13	-2.48	1.41	1.45
4	A	505	W4X	C14-N15	-2.45	1.33	1.39
4	C	503	W4X	C11-C10	-2.44	1.37	1.41
4	C	504	W4X	C10-N15	-2.43	1.35	1.39
4	C	504	W4X	C14-N15	-2.42	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	W4X	O23-C19	2.33	1.41	1.36
4	A	505	W4X	C10-N15	-2.30	1.35	1.39
4	A	503	W4X	C11-C10	-2.29	1.38	1.41
4	A	503	W4X	O22-C20	2.28	1.40	1.36
2	A	501	CTP	C4-N3	2.27	1.39	1.34
4	C	503	W4X	C14-N15	-2.27	1.33	1.39
4	B	503	W4X	O22-C20	2.27	1.40	1.36
2	C	501	CTP	C4-N3	2.24	1.39	1.34
4	C	504	W4X	O22-C20	2.24	1.40	1.36
4	C	503	W4X	O22-C20	2.21	1.40	1.36
4	A	504	W4X	O23-C19	2.20	1.40	1.36
2	D	501	CTP	PA-O3A	2.19	1.61	1.59
2	B	501	CTP	C6-C5	2.15	1.40	1.35
4	C	504	W4X	C11-C13	-2.15	1.41	1.45
2	A	501	CTP	C6-C5	2.12	1.40	1.35
4	B	503	W4X	C11-C10	-2.11	1.38	1.41
4	C	503	W4X	O28-C24	-2.06	1.18	1.23
2	D	501	CTP	C4-N3	2.04	1.38	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	W4X	C17-C16-N15	4.82	126.10	119.89
4	B	503	W4X	C10-N15-C14	4.55	111.54	107.98
4	C	503	W4X	C17-C16-N15	4.31	125.44	119.89
2	B	501	CTP	O2B-PB-O3B	4.04	118.19	107.27
2	C	501	CTP	O2A-PA-O3A	3.10	115.66	107.27
4	B	503	W4X	C08-C07-C05	-3.00	116.08	121.25
4	C	504	W4X	O26-C25-C24	3.00	121.35	112.94
2	A	501	CTP	O2B-PB-O3B	2.82	114.89	107.27
4	A	504	W4X	O26-C25-C24	2.67	120.42	112.94
4	A	503	W4X	C21-C16-N15	-2.63	114.73	119.26
4	B	503	W4X	C11-C13-C24	2.63	129.46	126.09
4	C	503	W4X	C16-N15-C10	-2.58	123.77	127.88
4	C	503	W4X	C21-C16-N15	-2.57	114.83	119.26
4	B	503	W4X	C08-C07-C12	2.53	121.71	118.23
4	A	504	W4X	C16-N15-C14	-2.46	121.37	124.78
4	C	504	W4X	C21-C16-N15	2.46	123.49	119.26
4	C	504	W4X	C09-C10-C11	-2.44	119.23	121.95
4	B	503	W4X	C16-C21-C20	-2.41	119.19	121.29
4	A	505	W4X	C09-C10-C11	-2.36	119.31	121.95
4	A	504	W4X	O26-C25-O27	-2.34	118.32	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	CTP	O2B-PB-O3B	2.33	113.57	107.27
4	C	503	W4X	C11-C10-N15	2.27	109.26	107.58
4	C	503	W4X	C08-C07-C12	2.26	121.34	118.23
4	A	503	W4X	C08-C07-C05	-2.26	117.35	121.25
4	A	503	W4X	O26-C25-C24	2.26	119.28	112.94
4	A	504	W4X	C11-C13-C24	2.25	128.97	126.09
4	A	503	W4X	C11-C10-N15	2.21	109.22	107.58
4	B	503	W4X	C16-N15-C10	-2.21	124.37	127.88
4	A	504	W4X	C06-C05-C04	2.17	121.56	117.68
2	B	501	CTP	O3A-PA-O1A	-2.17	104.18	110.70
4	A	504	W4X	C08-C07-C12	2.15	121.19	118.23
4	A	505	W4X	C06-C05-C04	2.12	121.48	117.68
2	A	501	CTP	O2G-PG-O3B	2.11	111.73	104.64
4	C	503	W4X	C10-N15-C14	2.09	109.62	107.98
2	D	501	CTP	O2B-PB-O3A	2.08	112.91	107.27
4	C	504	W4X	C13-C24-C25	2.07	122.09	118.83
4	C	504	W4X	C10-N15-C14	2.06	109.59	107.98
4	B	503	W4X	O26-C25-C24	2.06	118.71	112.94
4	A	503	W4X	C11-C13-C24	2.04	128.71	126.09
4	C	503	W4X	O26-C25-C24	2.03	118.64	112.94

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	CTP	PB-O3B-PG-O3G
4	C	503	W4X	O28-C24-C25-O26
4	C	503	W4X	C17-C16-N15-C14
4	A	503	W4X	C17-C16-N15-C14
4	A	503	W4X	C21-C16-N15-C14
4	B	503	W4X	C17-C16-N15-C14
4	B	503	W4X	C21-C16-N15-C14
4	C	503	W4X	C21-C16-N15-C14
4	A	503	W4X	C21-C16-N15-C10
4	B	503	W4X	C17-C16-N15-C10
4	A	503	W4X	C17-C16-N15-C10
4	B	503	W4X	C21-C16-N15-C10
4	C	503	W4X	C17-C16-N15-C10
4	C	503	W4X	C13-C24-C25-O26
4	C	504	W4X	C13-C24-C25-O27
4	C	503	W4X	C21-C16-N15-C10
2	B	501	CTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	C	501	CTP	PB-O3A-PA-O2A
2	D	501	CTP	PB-O3A-PA-O1A
2	B	501	CTP	C5'-O5'-PA-O1A
2	C	501	CTP	PB-O3B-PG-O1G
2	B	501	CTP	O4'-C4'-C5'-O5'
4	A	505	W4X	C13-C24-C25-O26
2	B	501	CTP	PA-O3A-PB-O1B
2	D	501	CTP	PA-O3A-PB-O1B
4	A	503	W4X	C11-C13-C24-O28
4	B	503	W4X	C11-C13-C24-O28
4	C	503	W4X	C11-C13-C24-O28
4	A	503	W4X	C14-C13-C24-O28
4	B	503	W4X	C14-C13-C24-O28
4	C	503	W4X	C14-C13-C24-O28
4	B	503	W4X	C14-C13-C24-C25
2	C	501	CTP	PG-O3B-PB-O2B

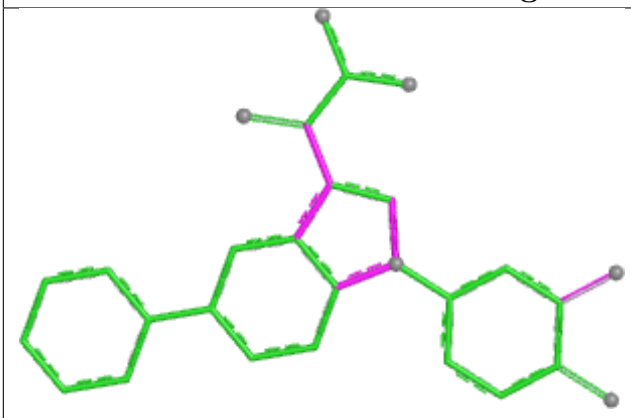
There are no ring outliers.

8 monomers are involved in 13 short contacts:

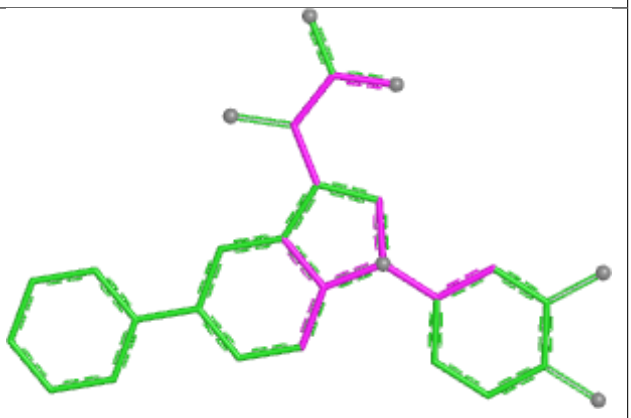
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	W4X	1	0
4	A	505	W4X	5	0
2	C	501	CTP	1	0
4	B	503	W4X	2	0
2	B	501	CTP	2	0
4	A	504	W4X	1	0
4	C	503	W4X	2	0
2	D	501	CTP	1	0

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 then 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.

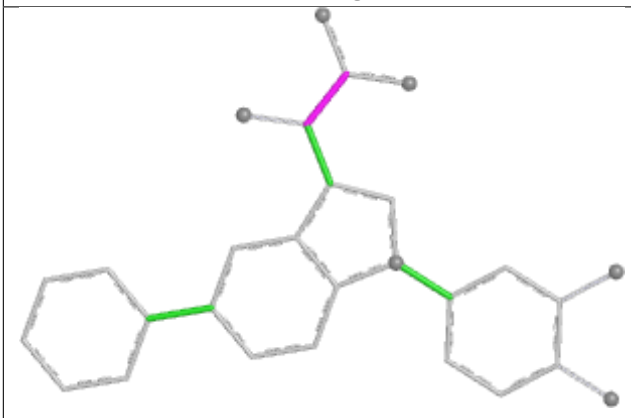
Ligand W4X C 504



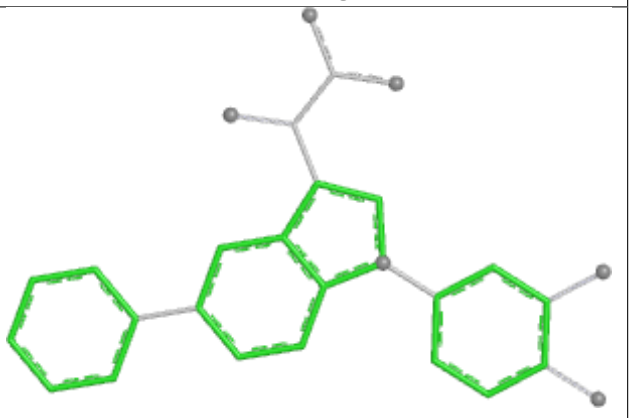
Bond lengths



Bond angles

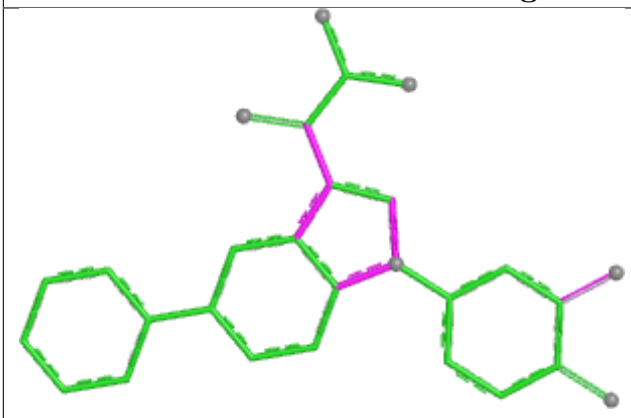


Torsions



Rings

Ligand W4X A 505



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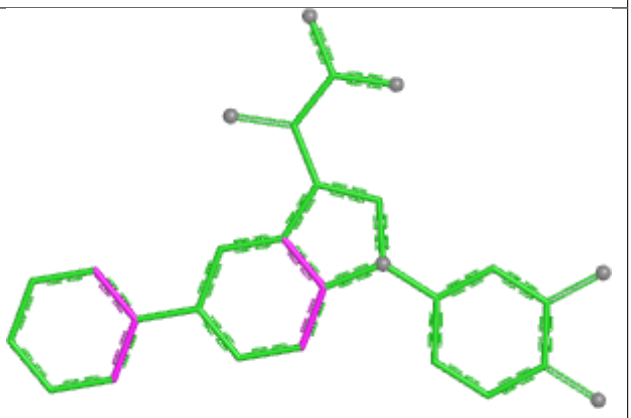
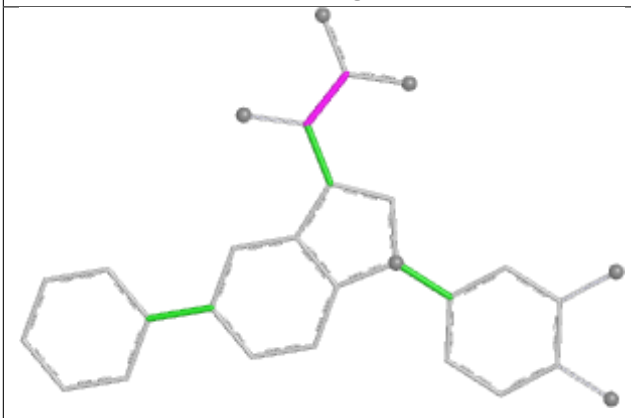
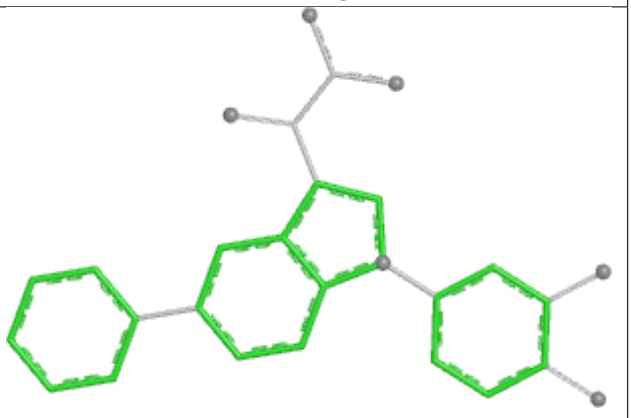


Bond angles

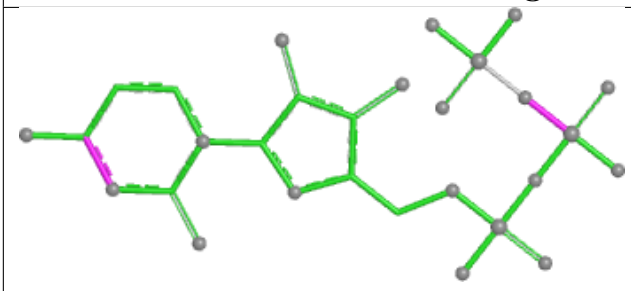


Torsions

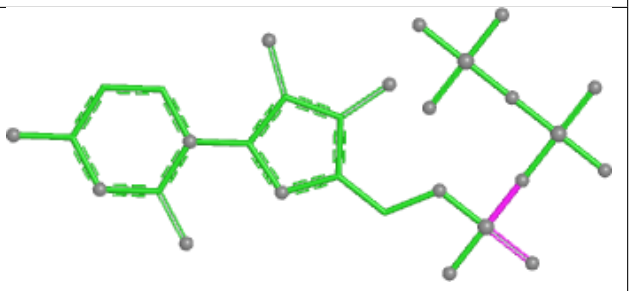


Rings

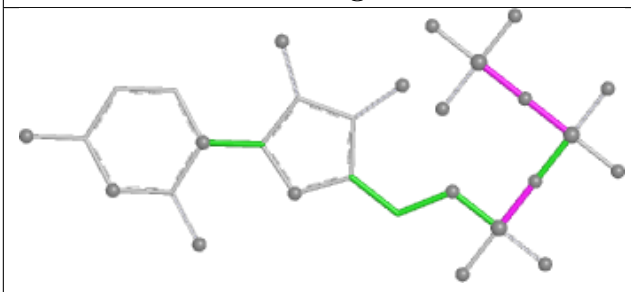
Ligand CTP C 501



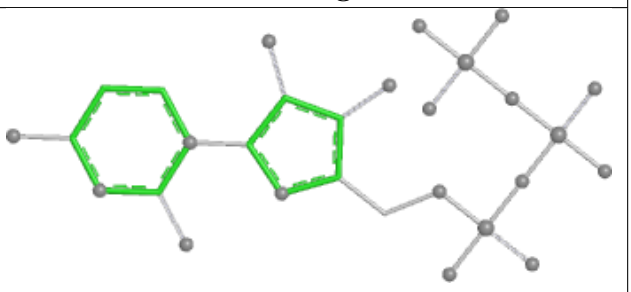
Bond lengths



Bond angles

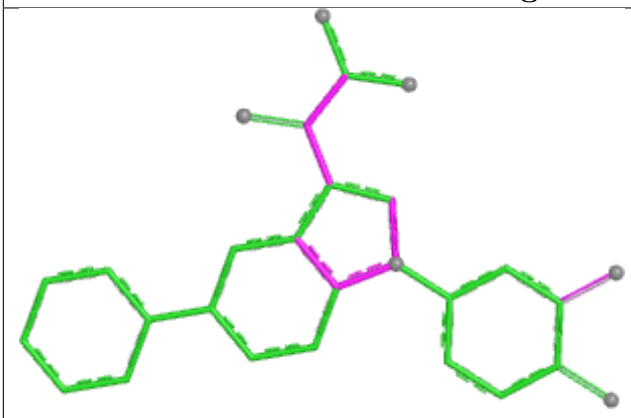


Torsions

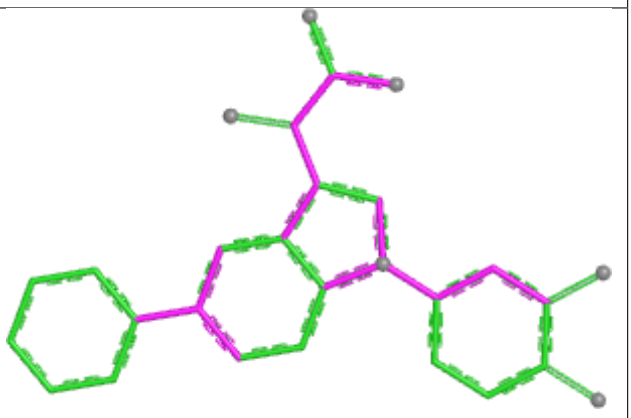


Rings

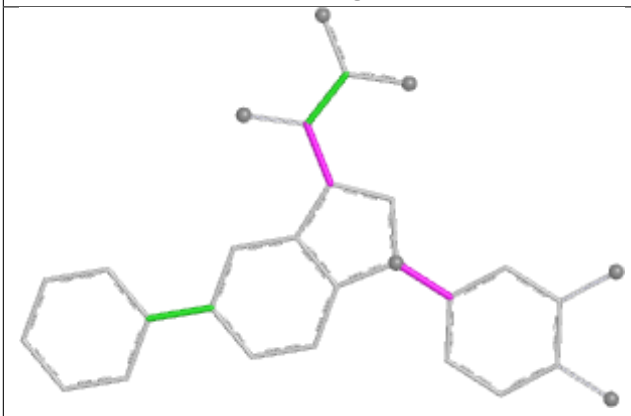
Ligand W4X B 503



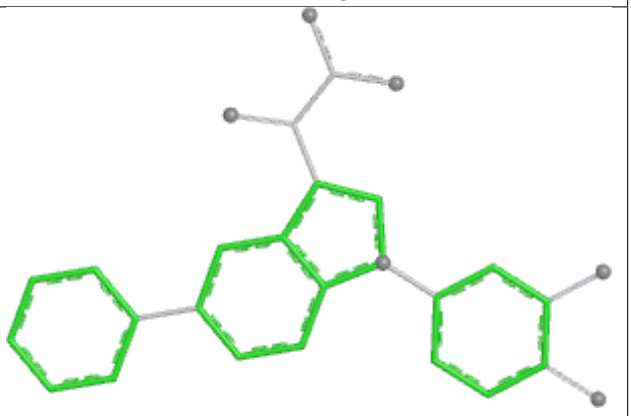
Bond lengths



Bond angles

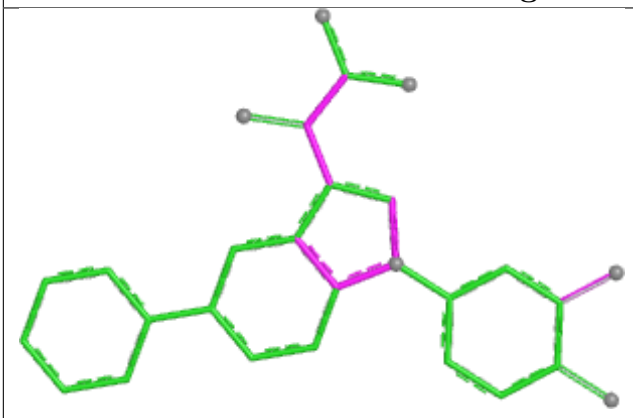


Torsions

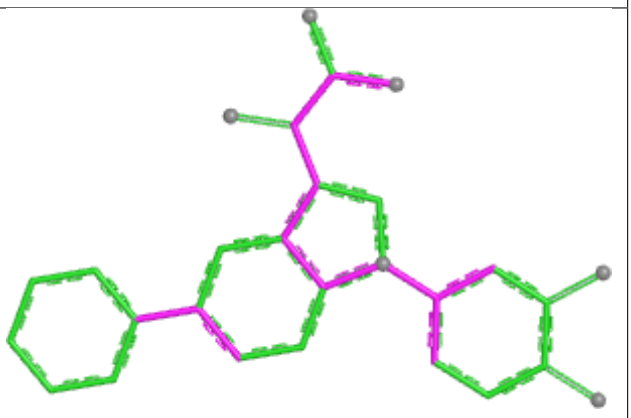


Rings

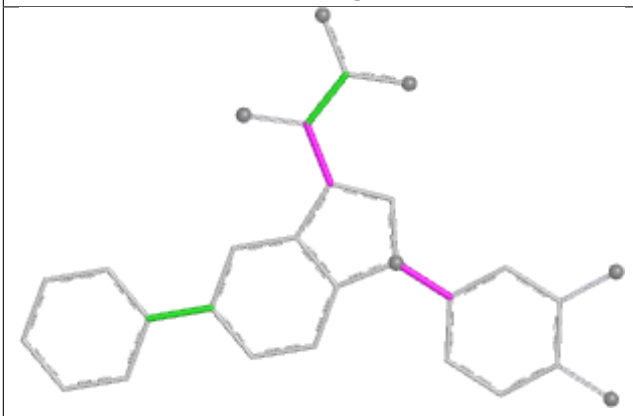
Ligand W4X A 503



Bond lengths



Bond angles



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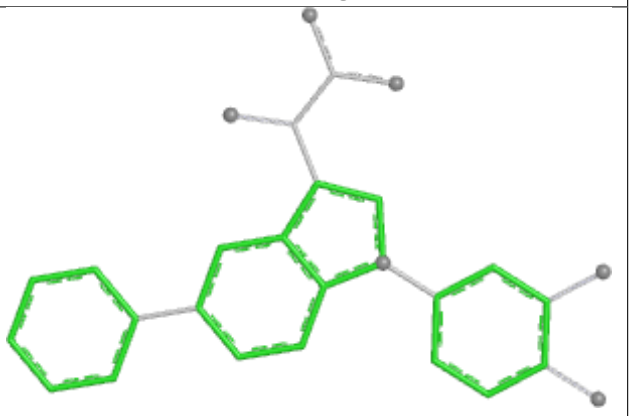
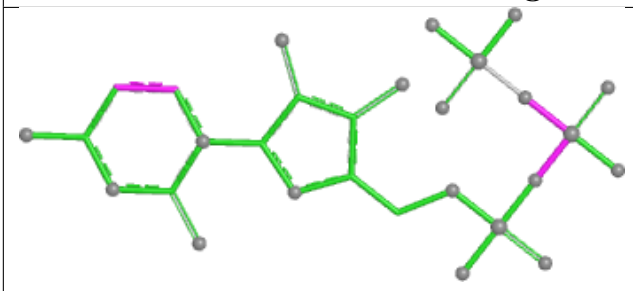
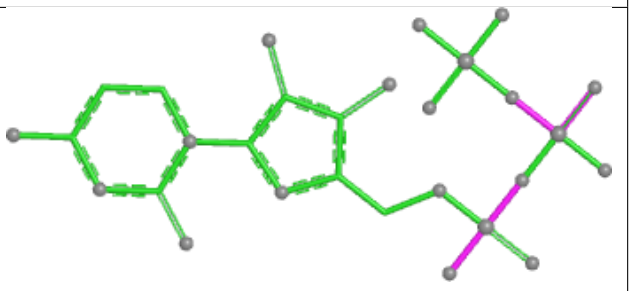


Rings

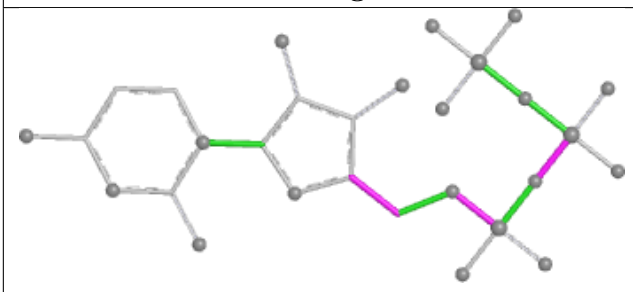
Ligand CTP B 501



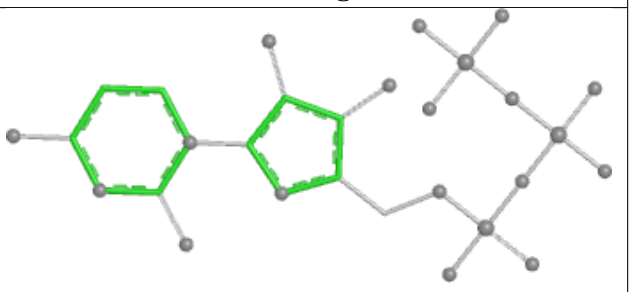
Bond lengths



Bond angles

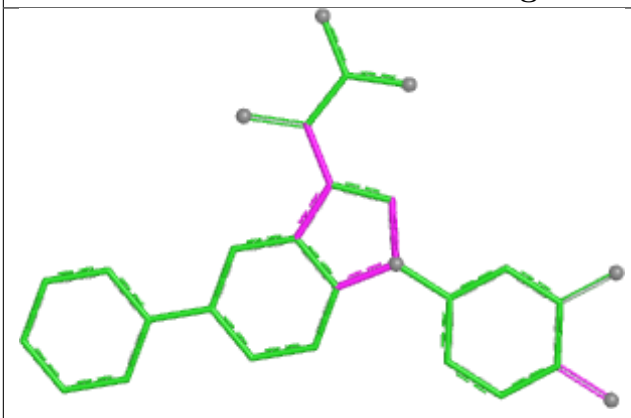


Torsions



Rings

Ligand W4X A 504



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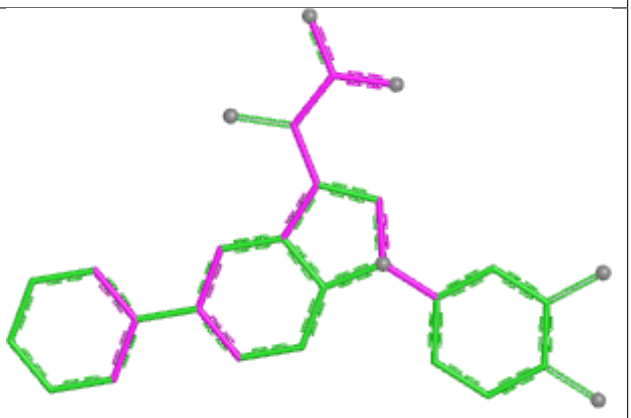
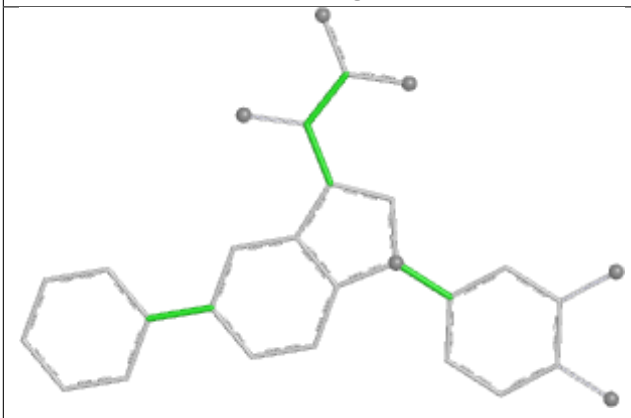


Bond angles



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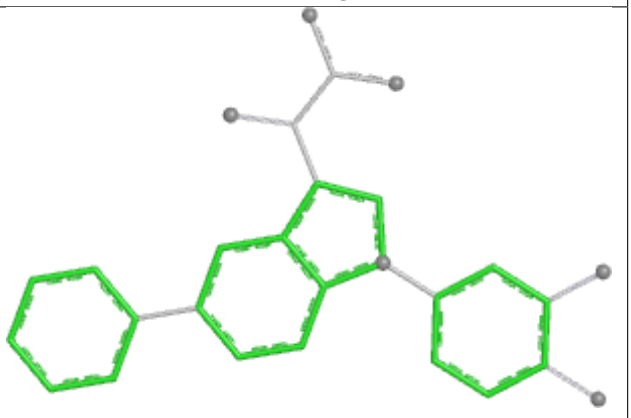
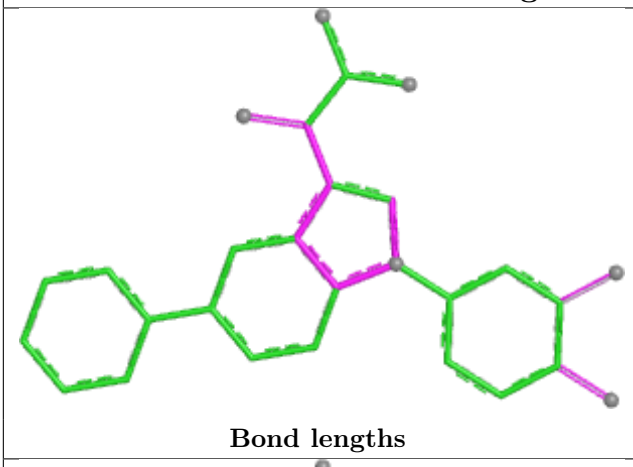


Rings

Ligand W4X C 503



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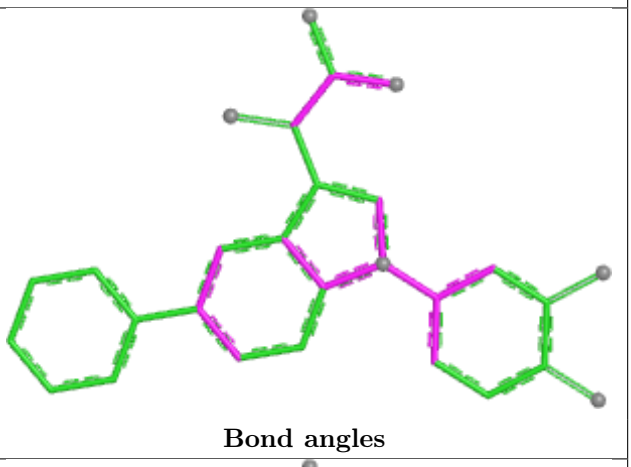
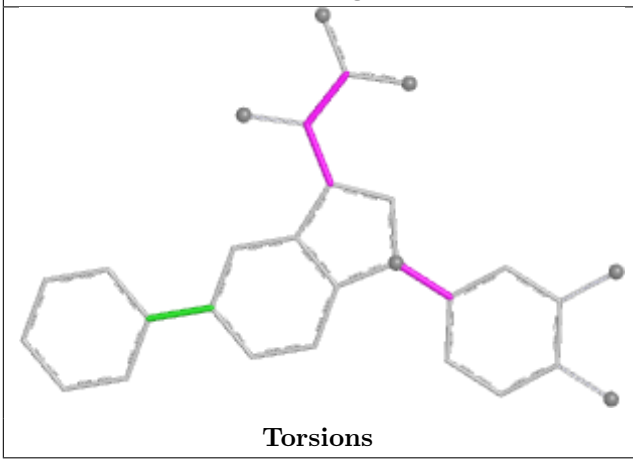
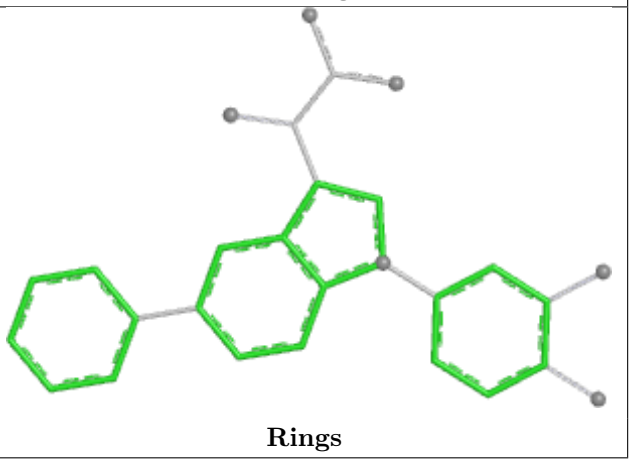


Bond angles

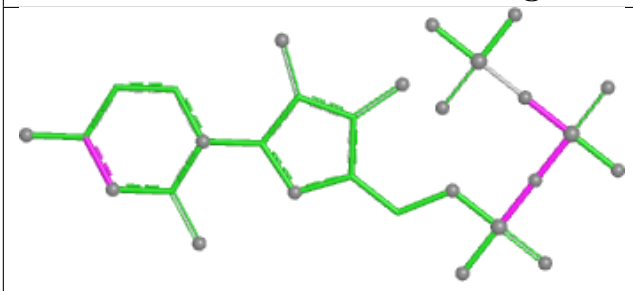


Torsions

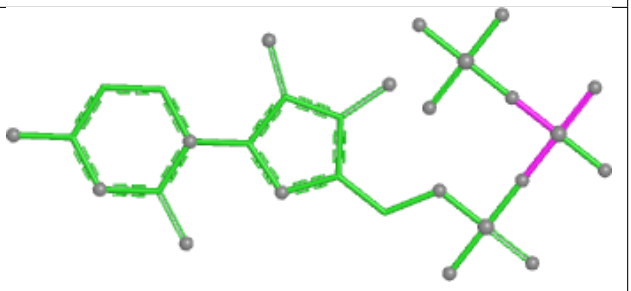


Rings

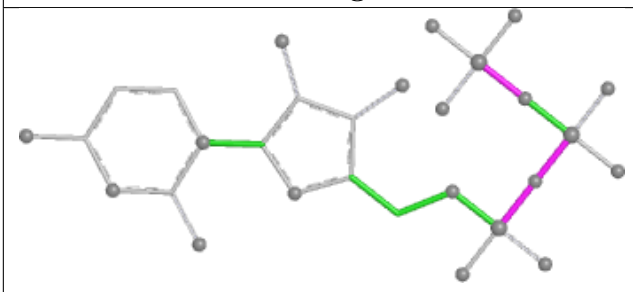
Ligand CTP D 501



Bond lengths



Bond angles



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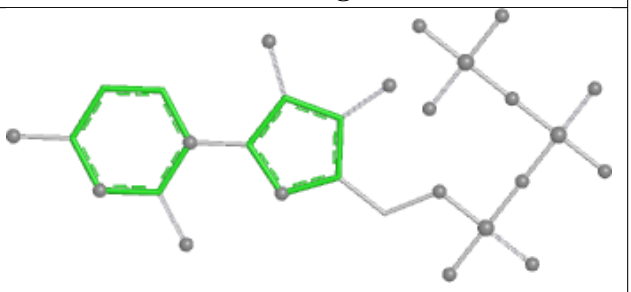
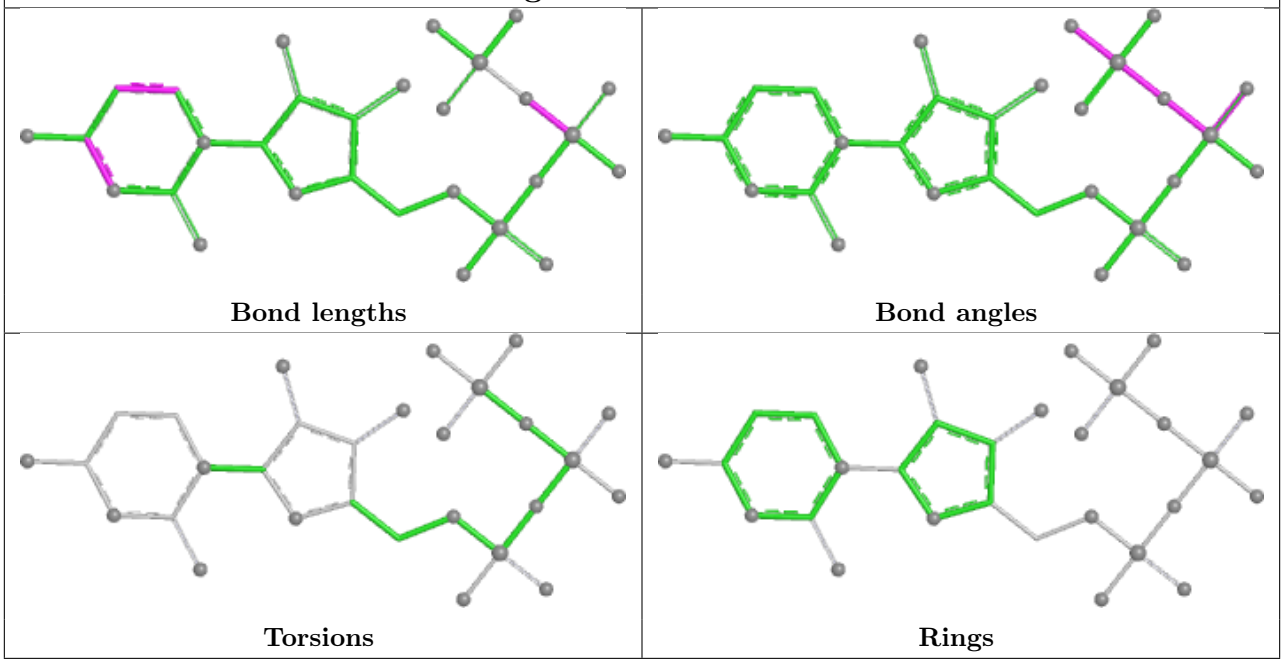


Rings

Ligand CTP A 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	211/237 (89%)	0.23	13 (6%)	26	28	19, 29, 56, 71	0
1	B	209/237 (88%)	0.48	19 (9%)	15	15	20, 32, 74, 102	0
1	C	207/237 (87%)	0.25	8 (3%)	43	45	20, 31, 58, 79	0
1	D	227/237 (95%)	0.43	13 (5%)	29	31	20, 36, 63, 76	0
All	All	854/948 (90%)	0.35	53 (6%)	26	28	19, 32, 63, 102	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	ALA	4.9
1	D	297	SER	4.8
1	B	391	HIS	4.7
1	C	184	HIS	4.7
1	B	340	ASN	4.6
1	B	184	HIS	4.6
1	C	286	HIS	4.5
1	D	184	HIS	4.2
1	B	389	LEU	4.1
1	B	392	GLY	4.0
1	B	343	VAL	4.0
1	C	376	ASP	4.0
1	C	288	ALA	3.7
1	C	299	PRO	3.7
1	B	345	PHE	3.6
1	B	379	LEU	3.4
1	B	382	ALA	3.3
1	B	336	THR	3.2
1	A	376	ASP	3.1
1	D	365	GLY	3.0
1	A	285	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	412	GLN	2.9
1	D	358	LEU	2.9
1	A	286	HIS	2.9
1	B	344	LEU	2.9
1	A	184	HIS	2.9
1	B	384	GLY	2.9
1	A	288	ALA	2.6
1	D	185	HIS	2.6
1	D	189	GLY	2.6
1	A	289	ALA	2.5
1	D	344	LEU	2.5
1	B	390	GLU	2.5
1	A	412	GLN	2.4
1	A	364	VAL	2.4
1	B	295	GLY	2.4
1	C	287	VAL	2.3
1	A	337	GLY	2.3
1	C	186	ASP	2.3
1	D	410	LYS	2.2
1	B	388	ALA	2.2
1	D	412	GLN	2.2
1	D	298	GLU	2.2
1	B	377	GLY	2.1
1	A	406	ALA	2.1
1	C	412	GLN	2.1
1	D	339	ALA	2.1
1	A	301	SER	2.1
1	A	290	ALA	2.1
1	D	366	GLU	2.0
1	A	396	LEU	2.0
1	B	362	ASN	2.0
1	D	286	HIS	2.0

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 oligosaccharides in this entry.

6.4 Ligands (i)

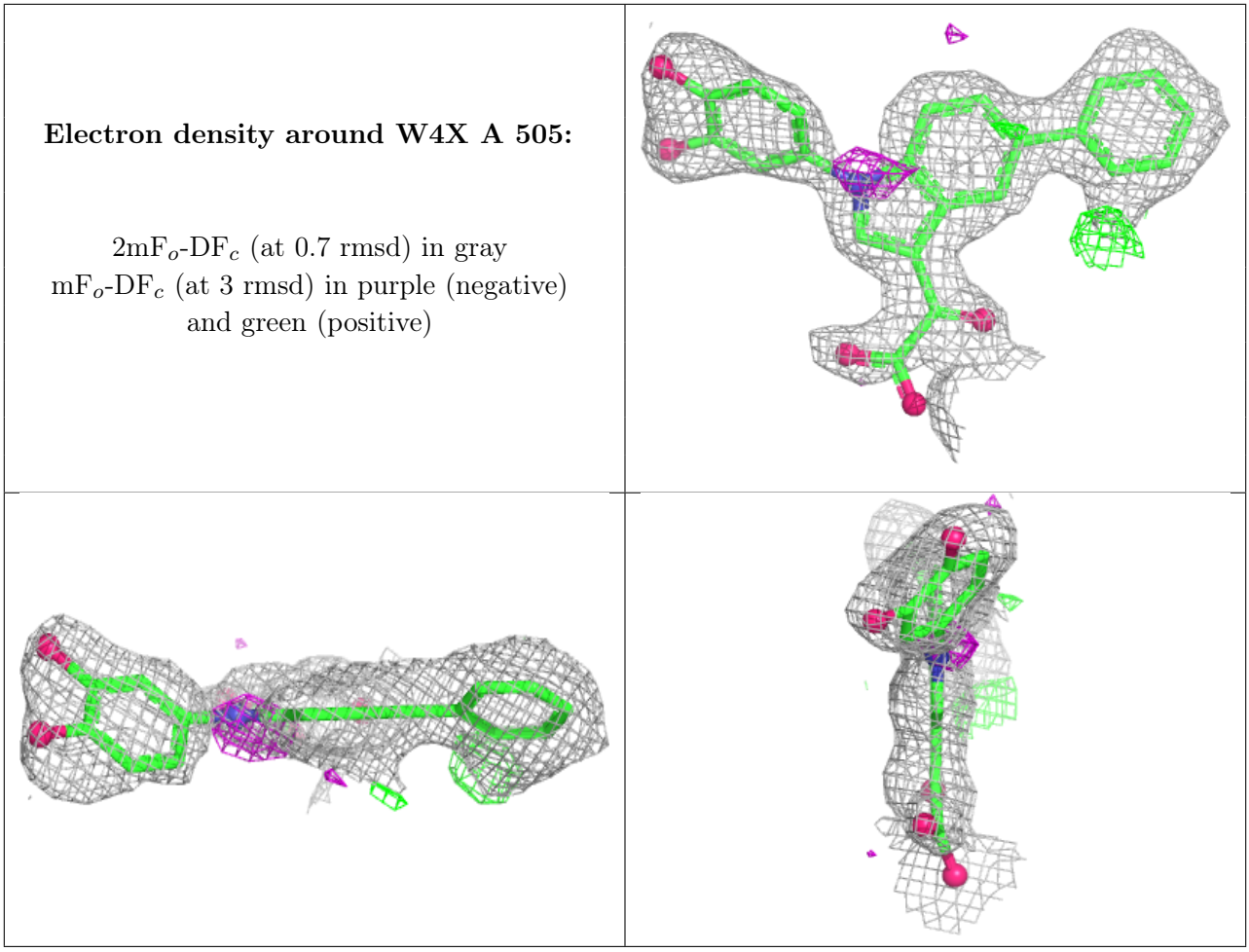
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	W4X	A	505	28/28	0.83	0.13	34,59,72,77	0
4	W4X	C	504	28/28	0.88	0.10	24,38,45,47	0
2	CTP	B	501	29/29	0.90	0.08	20,32,60,65	0
4	W4X	B	503	28/28	0.90	0.09	25,37,51,54	0
4	W4X	A	504	28/28	0.90	0.11	21,41,53,59	0
2	CTP	C	501	29/29	0.92	0.08	16,27,54,59	0
4	W4X	C	503	28/28	0.93	0.07	20,29,35,40	0
4	W4X	A	503	28/28	0.94	0.08	22,26,33,43	0
2	CTP	D	501	29/29	0.94	0.07	22,29,49,50	0
3	CA	C	502	1/1	0.94	0.07	50,50,50,50	0
3	CA	B	502	1/1	0.95	0.07	48,48,48,48	0
2	CTP	A	501	29/29	0.95	0.08	12,23,52,56	0
3	CA	D	502	1/1	0.95	0.07	55,55,55,55	0
3	CA	A	502	1/1	0.97	0.05	35,35,35,35	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.

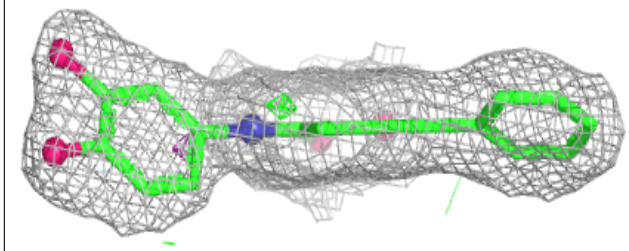
Electron density around W4X A 505:

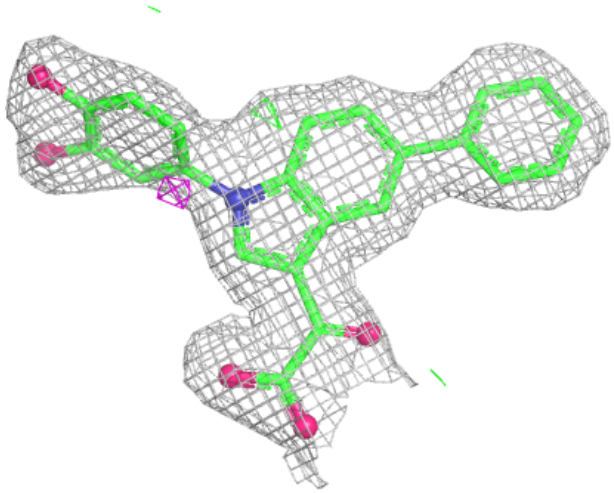
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

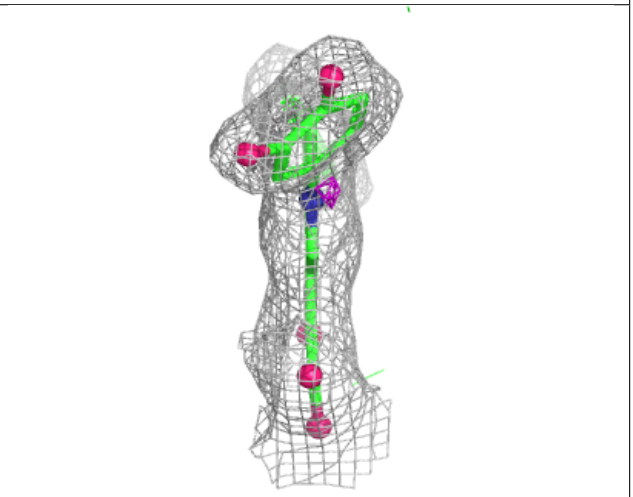


Electron density around W4X C 504:

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

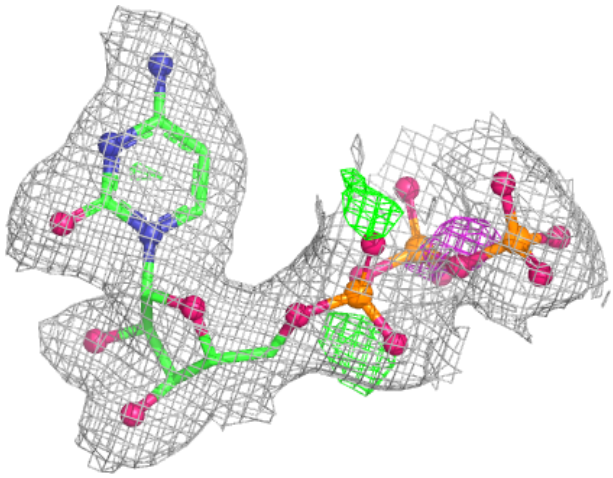


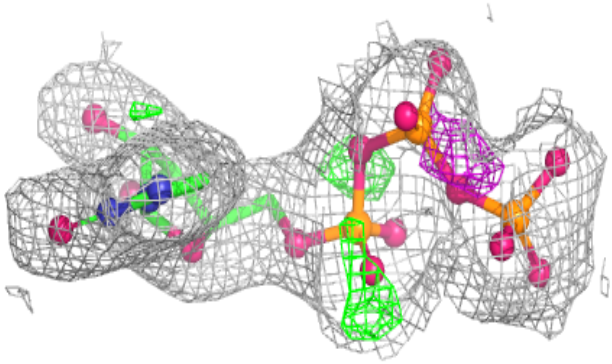


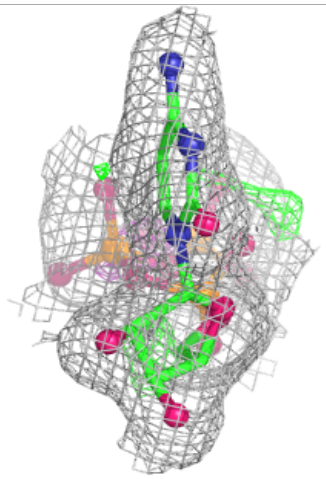


Electron density around CTP B 501:

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

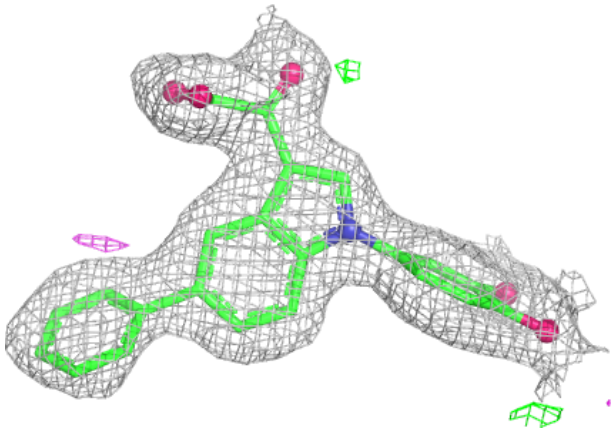


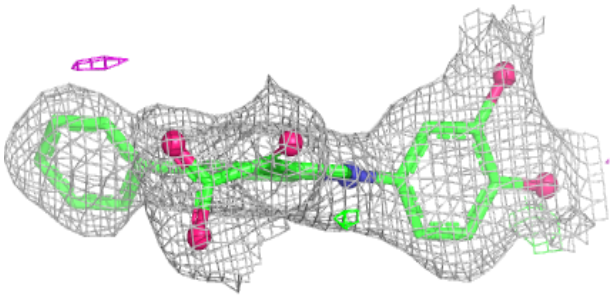


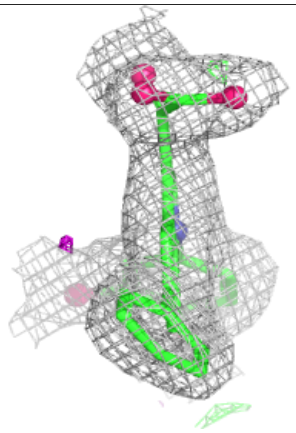


Electron density around W4X B 503:

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

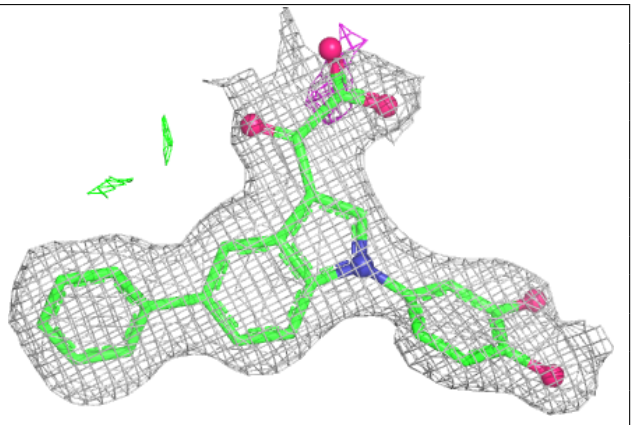


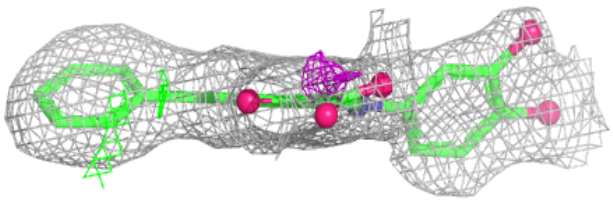


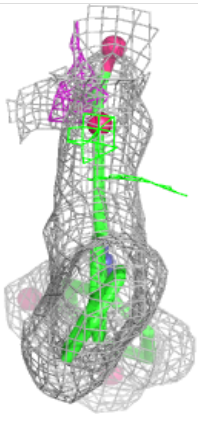


Electron density around W4X A 504:

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

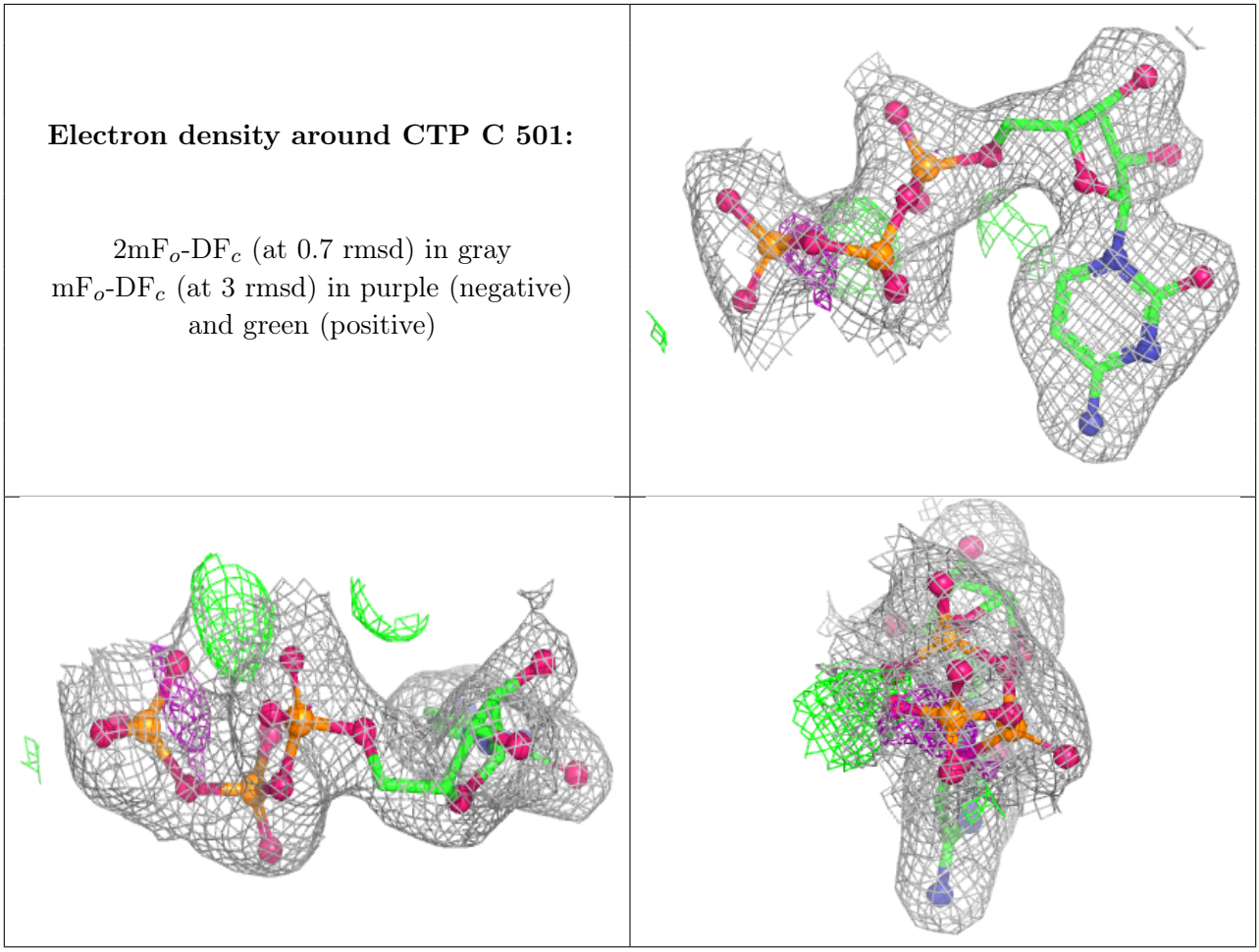






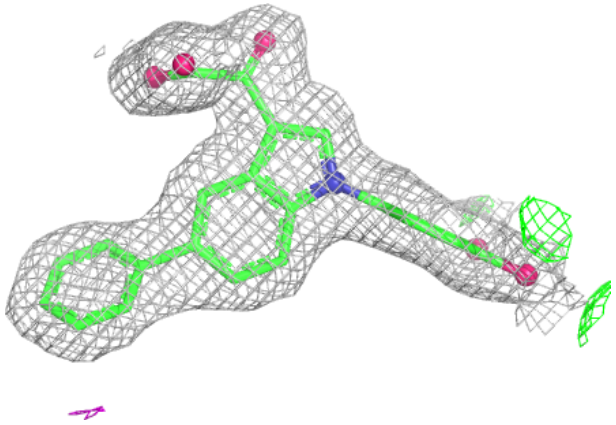
Electron density around CTP C 501:

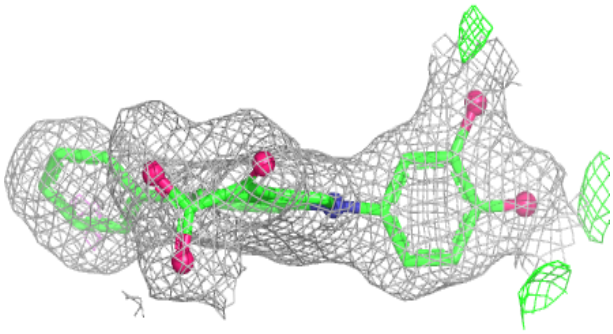
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

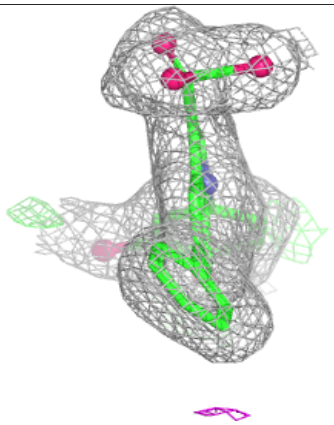


Electron density around W4X C 503:

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

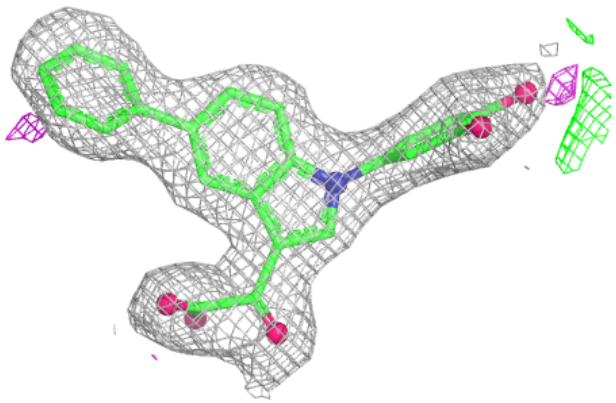


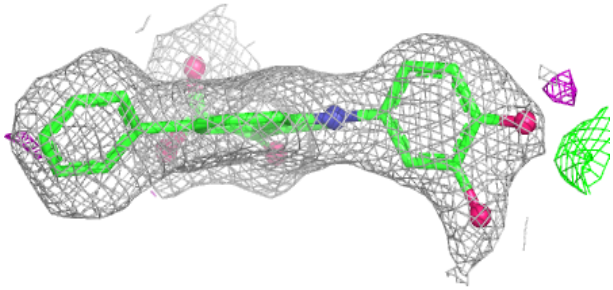




Electron density around W4X A 503:

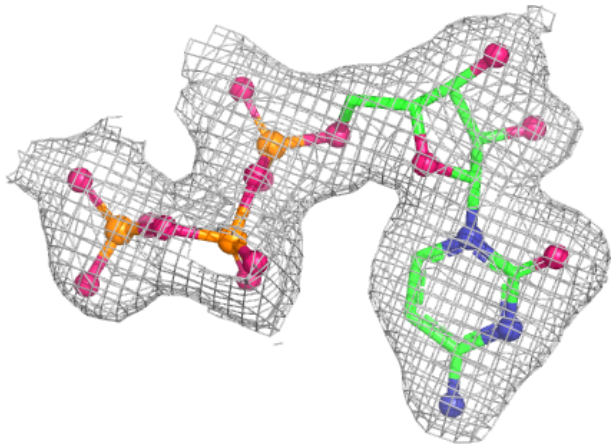
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

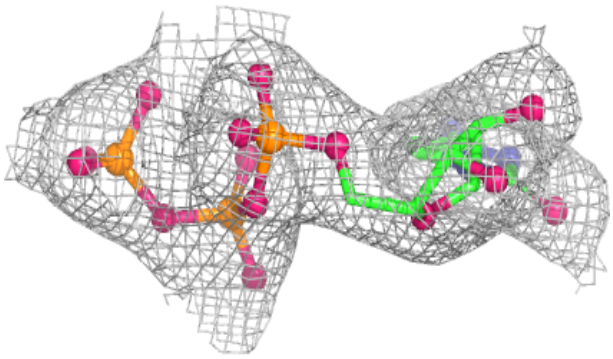


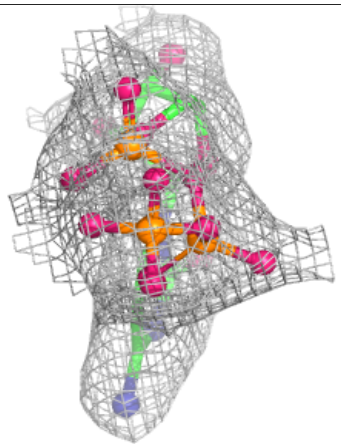


Electron density around CTP D 501:

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

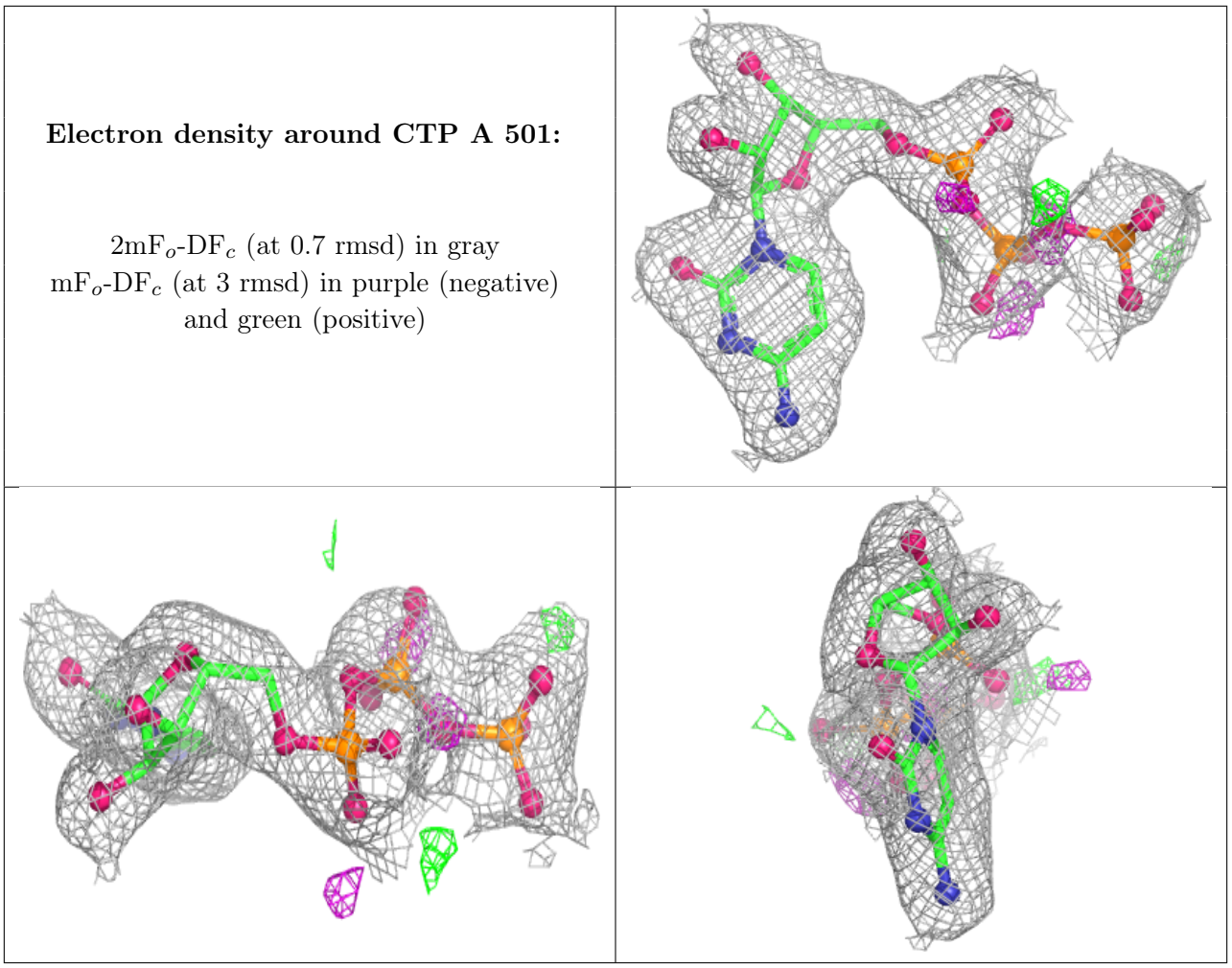






Electron density around CTP A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.