



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 AM UTC

PDB ID : 8OWR / pdb_00008owr
Title : Crystal structure of Mycobacterium smegmatis CoaB in complex with CTP and 2-(1-(3,4-dihydroxyphenyl)-5-(3-hydroxyphenyl)-1H-indol-3-yl)-2-oxoacetic acid
Authors : Mendes, V.; Blundell, T.L.
Deposited on : 2023-04-28
Resolution : 2.44 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

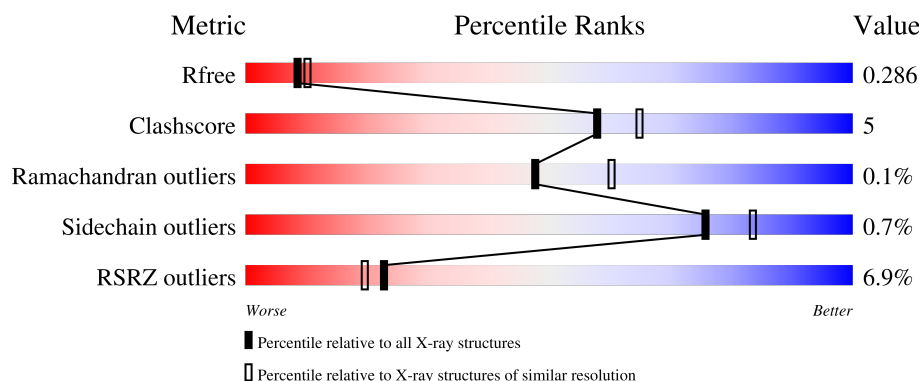
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	6% 77% 12% 11%
1	B	237	5% 86% 10% .
1	C	237	4% 81% 6% 13%
1	D	237	10% 80% 8% 11%

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
5	ACT	D	503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6499 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	212	Total	C	N	O	S	0	0	0
			1506	936	278	286	6			
1	B	229	Total	C	N	O	S	0	0	0
			1646	1017	311	312	6			
1	C	206	Total	C	N	O	S	0	0	0
			1477	913	275	283	6			
1	D	211	Total	C	N	O	S	0	0	0
			1478	916	280	276	6			

There are 32 discrepancies between the modelled and reference sequences:

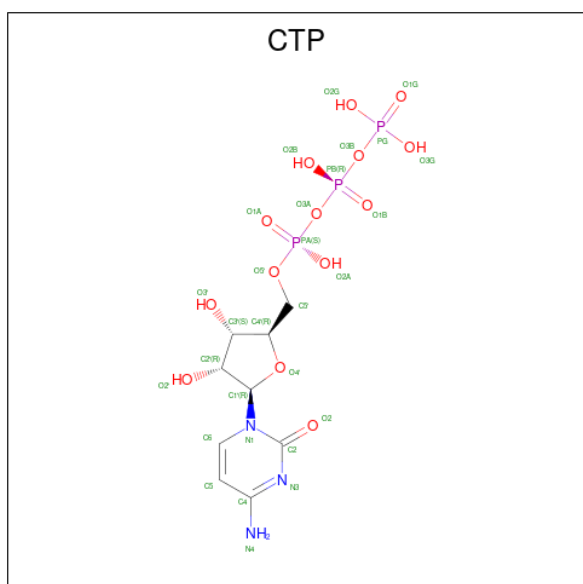
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MET	-	initiating methionine	UNP A0QWT2
A	179	ALA	-	expression tag	UNP A0QWT2
A	180	HIS	-	expression tag	UNP A0QWT2
A	181	HIS	-	expression tag	UNP A0QWT2
A	182	HIS	-	expression tag	UNP A0QWT2
A	183	HIS	-	expression tag	UNP A0QWT2
A	184	HIS	-	expression 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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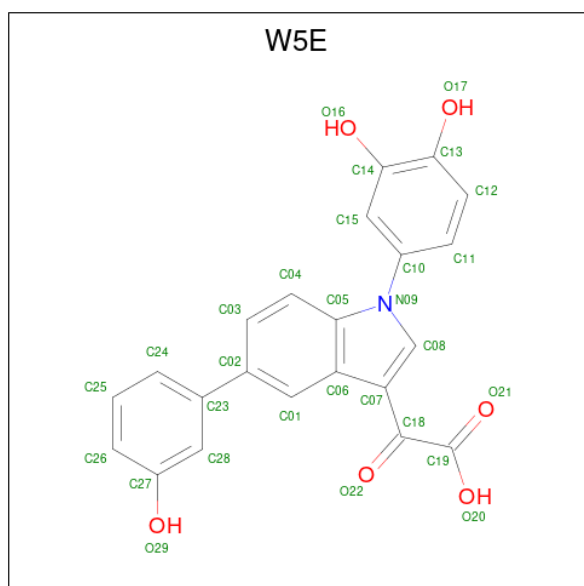
Chain	Residue	Modelled	Actual	Comment	Reference
C	183	HIS	-	expression tag	UNP A0QWT2
C	184	HIS	-	expression tag	UNP A0QWT2
C	185	HIS	-	expression tag	UNP A0QWT2
D	178	MET	-	initiating methionine	UNP A0QWT2
D	179	ALA	-	expression tag	UNP A0QWT2
D	180	HIS	-	expression tag	UNP A0QWT2
D	181	HIS	-	expression 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: $C_9H_{16}N_3O_{14}P_3$).



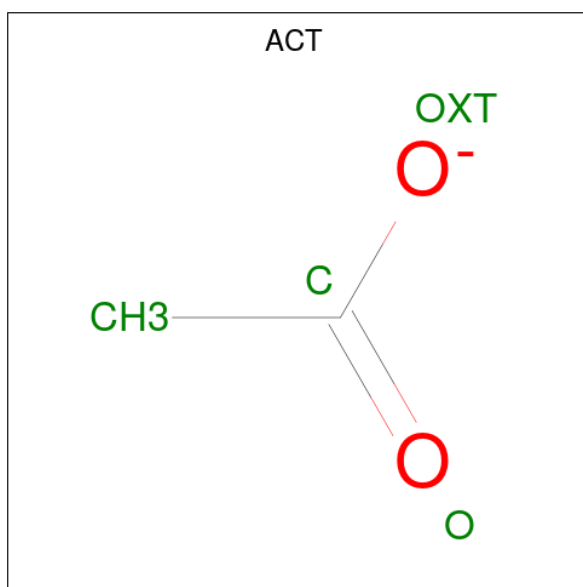
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is 2-[1-[3,4-bis(oxidanyl)phenyl]-5-(3-hydroxyphenyl)indol-3-yl]-2-oxidanylidene-ethanoic acid (CCD ID: W5E) (formula: $C_{22}H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 29 22 1 6	0	0
4	C	1	Total C N O 29 22 1 6	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

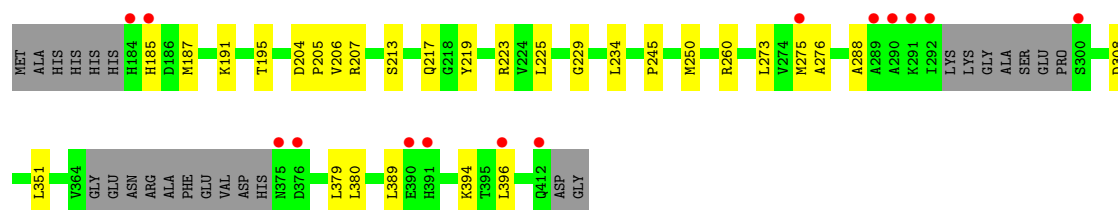
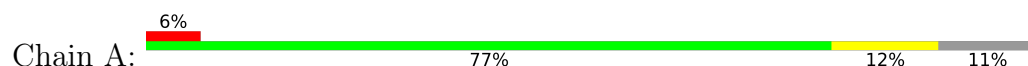
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		
6	B	64	Total	O	0	0
			64	64		
6	C	45	Total	O	0	0
			45	45		
6	D	39	Total	O	0	0
			39	39		

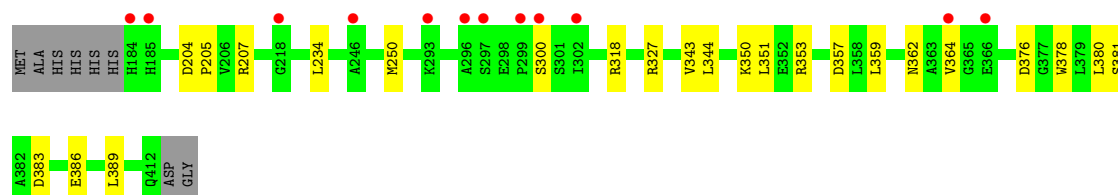
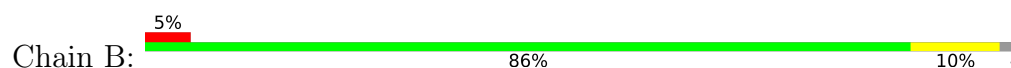
3 Residue-property plots [i](#)

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.

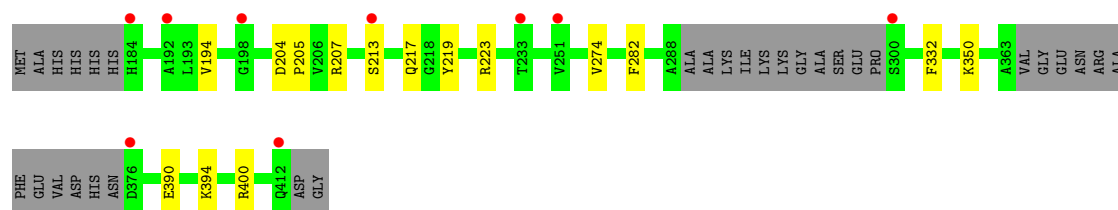
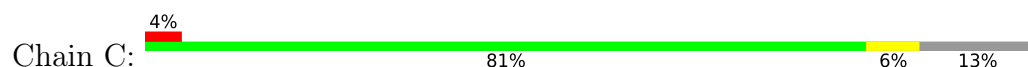
- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



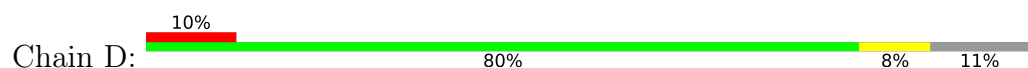
- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

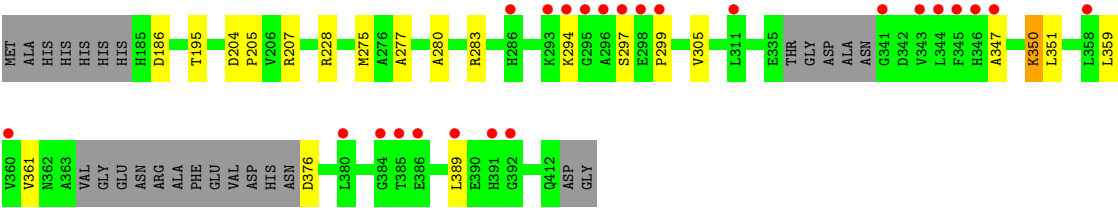


- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.55Å 77.17Å 149.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.59 – 2.44 74.59 – 2.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.59-2.44) 100.0 (74.59-2.44)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.45Å)	Xtriage
Refinement program	PHENIX (dev_2947: ???)	Depositor
R, R_{free}	0.214 , 0.284 0.220 , 0.286	Depositor DCC
R_{free} test set	1763 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.073 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CTP, W5E, CA, 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	0.36	0/1522	0.57	0/2064
1	B	0.36	0/1668	0.61	0/2263
1	C	0.36	0/1494	0.58	0/2026
1	D	0.46	0/1495	0.66	1/2029 (0.0%)
All	All	0.39	0/6179	0.61	1/8382 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294	LYS	N-CA-C	-5.94	98.15	110.80

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	1506	0	1498	18	0
1	B	1646	0	1634	15	0
1	C	1477	0	1465	9	0
1	D	1478	0	1463	15	0
2	A	29	0	12	0	0
2	B	29	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	29	0	12	2	0
2	D	29	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	29	0	0	0	0
4	C	29	0	0	0	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
5	D	8	0	6	3	0
6	A	51	0	0	1	0
6	B	64	0	0	1	0
6	C	45	0	0	0	0
6	D	39	0	0	0	0
All	All	6499	0	6120	56	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 (56) 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:380:LEU:HD22	1:B:386:GLU:HG2	1.61	0.81
1:D:195:THR:HG22	1:D:275:MET:HA	1.76	0.68
1:D:195:THR:CG2	1:D:275:MET:HA	2.30	0.62
1:B:362:ASN:O	1:B:364:VAL:HG12	2.00	0.60
1:C:282:PHE:CE2	1:D:299:PRO:HB3	2.37	0.60
1:B:327:ARG:NH1	6:B:604:HOH:O	2.36	0.58
5:A:504:ACT:O	1:B:207:ARG:NH2	2.36	0.58
1:A:379:LEU:HD11	1:A:389:LEU:HD13	1.86	0.58
1:A:217:GLN:OE1	1:A:394:LYS:HD3	2.03	0.58
1:B:234:LEU:HD23	1:B:250:MET:SD	2.44	0.58
1:A:223:ARG:HG2	1:A:245:PRO:HB3	1.85	0.57
1:A:204:ASP:HB3	1:A:288:ALA:HB3	1.85	0.57
1:A:219:TYR:O	1:A:223:ARG:HG3	2.05	0.56
1:D:280:ALA:HB2	5:D:503:ACT:H3	1.87	0.56
1:B:318:ARG:HH22	1:B:357:ASP:CG	2.13	0.56
1:A:185:HIS:CE1	1:A:229:GLY:CA	2.89	0.55
1:D:186:ASP:OD2	1:D:228:ARG:NH1	2.37	0.54
1:A:185:HIS:CE1	1:A:229:GLY:HA3	2.42	0.54
1:B:343:VAL:HG11	1:B:376:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LYS:NZ	2:B:501:CTP:O1A	2.37	0.52
1:C:217:GLN:OE1	1:C:394:LYS:HD3	2.09	0.52
1:A:191:LYS:HG2	6:A:641:HOH:O	2.08	0.52
1:B:380:LEU:CD2	1:B:386:GLU:HG2	2.37	0.51
1:D:195:THR:HG23	1:D:277:ALA:H	1.76	0.50
1:D:207:ARG:HD3	5:D:502:ACT:C	2.43	0.49
1:D:195:THR:HG21	1:D:275:MET:SD	2.53	0.48
1:C:219:TYR:O	1:C:223:ARG:HG3	2.13	0.48
1:D:376:ASP:N	1:D:376:ASP:OD1	2.46	0.48
1:D:350:LYS:HE2	1:D:350:LYS:HB2	1.45	0.46
1:A:185:HIS:CE1	1:A:229:GLY:HA2	2.51	0.45
1:A:260:ARG:NH2	1:A:308:ASP:OD2	2.43	0.45
1:A:206:VAL:HG23	1:A:207:ARG:HG3	1.97	0.45
1:C:204:ASP:HB2	1:C:205:PRO:CD	2.47	0.45
1:A:396:LEU:O	1:A:396:LEU:HD13	2.16	0.44
1:C:207:ARG:HD2	5:D:503:ACT:O	2.17	0.44
1:B:389:LEU:HD12	1:B:389:LEU:HA	1.81	0.44
1:D:347:ALA:HB1	1:D:361:VAL:HG21	2.00	0.43
1:B:351:LEU:HD13	1:B:359:LEU:HB2	2.00	0.43
1:C:390:GLU:O	1:C:400:ARG:NH1	2.50	0.43
1:B:204:ASP:HB2	1:B:205:PRO:CD	2.49	0.43
1:A:204:ASP:HB2	1:A:205:PRO:CD	2.48	0.43
1:D:351:LEU:HD13	1:D:359:LEU:HB2	2.00	0.43
1:B:353:ARG:NH2	2:B:501:CTP:O2B	2.47	0.43
1:A:234:LEU:HD23	1:A:250:MET:SD	2.58	0.43
1:C:194:VAL:HG22	1:C:274:VAL:HB	2.02	0.42
1:C:350:LYS:NZ	2:C:501:CTP:O1G	2.53	0.42
1:A:351:LEU:HD22	1:A:380:LEU:HB3	2.01	0.42
1:B:344:LEU:HD11	1:B:378:TRP:CZ2	2.55	0.42
1:A:273:LEU:HD11	1:A:275:MET:SD	2.60	0.41
1:D:204:ASP:HB2	1:D:205:PRO:CD	2.50	0.41
1:A:187:MET:HE2	1:A:225:LEU:CD2	2.50	0.41
1:B:381:SER:HB2	1:B:383:ASP:OD1	2.21	0.41
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.96	0.41
1:A:195:THR:O	1:A:276:ALA:HB3	2.21	0.40
1:C:332:PHE:O	2:C:501:CTP:H5'1	2.21	0.40
1:D:283:ARG:N	1:D:305:VAL:O	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	206/237 (87%)	202 (98%)	4 (2%)	0	100	100
1	B	227/237 (96%)	221 (97%)	5 (2%)	1 (0%)	30	36
1	C	200/237 (84%)	197 (98%)	3 (2%)	0	100	100
1	D	205/237 (86%)	197 (96%)	8 (4%)	0	100	100
All	All	838/948 (88%)	817 (98%)	20 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	SER

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	144/173 (83%)	143 (99%)	1 (1%)	76	83
1	B	160/173 (92%)	160 (100%)	0	100	100
1	C	145/173 (84%)	144 (99%)	1 (1%)	76	83
1	D	139/173 (80%)	137 (99%)	2 (1%)	59	70
All	All	588/692 (85%)	584 (99%)	4 (1%)	76	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	SER
1	C	213	SER
1	D	297	SER
1	D	350	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	238	ASN
1	C	238	ASN
1	C	412	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 13 ligands modelled in this entry, 3 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	$\# Z > 2$
5	ACT	D	503	-	3,3,3	1.15	0	3,3,3	1.58	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	B	503	-	3,3,3	1.23	0	3,3,3	1.32	0
2	CTP	D	501	-	29,30,30	1.12	3 (10%)	43,47,47	0.82	0
2	CTP	B	501	3	29,30,30	1.09	3 (10%)	43,47,47	0.94	2 (4%)
5	ACT	D	502	-	3,3,3	1.91	1 (33%)	3,3,3	1.36	0
4	W5E	C	503	-	32,32,32	1.65	9 (28%)	47,47,47	1.39	6 (12%)
4	W5E	A	503	-	32,32,32	1.63	6 (18%)	47,47,47	1.30	6 (12%)
5	ACT	A	504	-	3,3,3	1.78	1 (33%)	3,3,3	1.49	0
2	CTP	A	501	3	29,30,30	1.19	3 (10%)	43,47,47	1.02	2 (4%)
2	CTP	C	501	3	29,30,30	1.34	4 (13%)	43,47,47	0.95	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTP	D	501	-	-	7/22/38/38	0/2/2/2
2	CTP	B	501	3	-	7/22/38/38	0/2/2/2
4	W5E	C	503	-	-	8/16/16/16	0/4/4/4
4	W5E	A	503	-	-	9/16/16/16	0/4/4/4
2	CTP	A	501	3	-	0/22/38/38	0/2/2/2
2	CTP	C	501	3	-	7/22/38/38	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	W5E	C07-C18	4.06	1.53	1.45
4	C	503	W5E	C19-C18	-3.74	1.51	1.54
4	A	503	W5E	C05-N09	-3.44	1.33	1.39
4	C	503	W5E	C05-N09	-3.43	1.33	1.39
4	C	503	W5E	C07-C18	3.32	1.52	1.45
2	C	501	CTP	PA-O3A	3.23	1.63	1.59
4	A	503	W5E	C19-C18	-3.18	1.51	1.54
5	D	502	ACT	CH3-C	2.91	1.60	1.49
5	A	504	ACT	CH3-C	2.89	1.60	1.49
4	A	503	W5E	C08-N09	-2.86	1.32	1.39
4	C	503	W5E	C08-N09	-2.85	1.32	1.39
2	C	501	CTP	PB-O3A	2.78	1.62	1.59
2	C	501	CTP	PB-O3B	2.77	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	CTP	PB-O3B	2.69	1.62	1.59
2	A	501	CTP	PA-O3A	2.59	1.62	1.59
2	B	501	CTP	PA-O3A	2.54	1.62	1.59
4	C	503	W5E	C06-C07	-2.49	1.41	1.45
2	A	501	CTP	PB-O3B	2.47	1.62	1.59
4	A	503	W5E	C06-C07	-2.45	1.41	1.45
4	A	503	W5E	O16-C14	2.33	1.41	1.36
4	C	503	W5E	O22-C18	-2.30	1.18	1.23
4	C	503	W5E	O17-C13	2.29	1.40	1.36
2	A	501	CTP	C5-C4	-2.25	1.37	1.42
4	C	503	W5E	O16-C14	2.23	1.40	1.36
4	C	503	W5E	C06-C05	-2.22	1.38	1.41
2	D	501	CTP	PB-O3A	2.10	1.61	1.59
2	C	501	CTP	C5-C4	-2.06	1.38	1.42
2	B	501	CTP	PB-O3A	2.02	1.61	1.59
2	D	501	CTP	C4-N3	2.02	1.38	1.34
2	B	501	CTP	C6-C5	2.01	1.39	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	W5E	C11-C10-N09	4.38	125.53	119.89
4	C	503	W5E	C11-C10-N09	4.23	125.34	119.89
4	C	503	W5E	C15-C10-N09	-3.04	114.03	119.26
4	C	503	W5E	C05-N09-C08	2.99	110.32	107.98
4	A	503	W5E	C15-C10-N09	-2.94	114.20	119.26
2	A	501	CTP	O2B-PB-O3B	2.88	115.06	107.27
2	C	501	CTP	O3G-PG-O3B	2.82	114.10	104.64
4	C	503	W5E	C10-N09-C05	-2.79	123.45	127.88
2	A	501	CTP	O3'-C3'-C4'	-2.76	103.14	111.08
4	A	503	W5E	C05-N09-C08	2.59	110.01	107.98
4	A	503	W5E	C28-C23-C02	-2.38	116.84	120.84
2	B	501	CTP	O3'-C3'-C4'	-2.36	104.31	111.08
4	C	503	W5E	O20-C19-C18	2.28	119.34	112.94
4	A	503	W5E	O20-C19-C18	2.24	119.21	112.94
4	C	503	W5E	C06-C05-N09	2.23	109.23	107.58
4	A	503	W5E	C10-N09-C05	-2.14	124.48	127.88
5	D	503	ACT	O-C-CH3	-2.05	114.12	122.53
2	B	501	CTP	C2'-C1'-N1	-2.01	107.67	113.25

There are no chirality outliers.

All (38) torsion outliers are listed below:

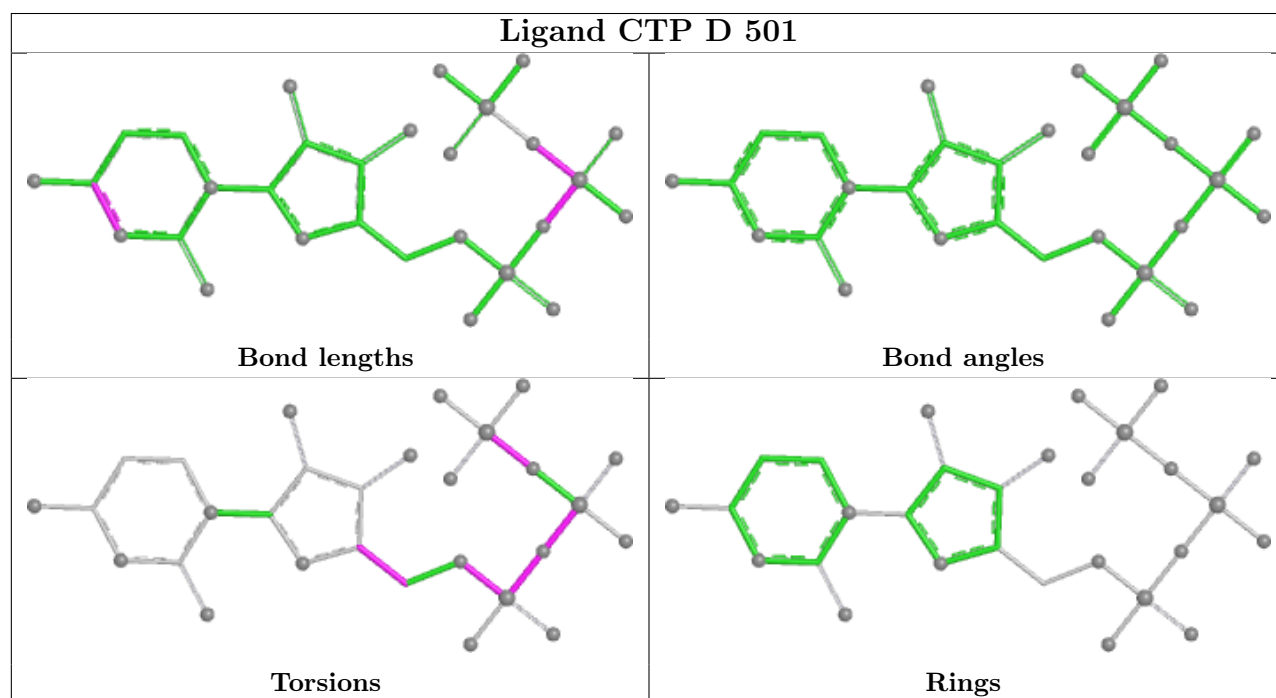
Mol	Chain	Res	Type	Atoms
2	C	501	CTP	PB-O3B-PG-O3G
2	D	501	CTP	O4'-C4'-C5'-O5'
2	D	501	CTP	C5'-O5'-PA-O1A
2	D	501	CTP	C5'-O5'-PA-O3A
2	D	501	CTP	PB-O3B-PG-O3G
2	B	501	CTP	C3'-C4'-C5'-O5'
2	D	501	CTP	C3'-C4'-C5'-O5'
2	B	501	CTP	O4'-C4'-C5'-O5'
4	C	503	W5E	C15-C10-N09-C08
4	A	503	W5E	C15-C10-N09-C08
4	A	503	W5E	C11-C10-N09-C08
4	C	503	W5E	C11-C10-N09-C08
2	D	501	CTP	PA-O3A-PB-O1B
4	A	503	W5E	C15-C10-N09-C05
4	C	503	W5E	C15-C10-N09-C05
4	A	503	W5E	C11-C10-N09-C05
4	C	503	W5E	C11-C10-N09-C05
2	B	501	CTP	C5'-O5'-PA-O1A
2	B	501	CTP	C5'-O5'-PA-O2A
2	B	501	CTP	C5'-O5'-PA-O3A
2	C	501	CTP	C5'-O5'-PA-O1A
4	C	503	W5E	O22-C18-C19-O20
2	B	501	CTP	PG-O3B-PB-O1B
2	C	501	CTP	PG-O3B-PB-O1B
4	A	503	W5E	C03-C02-C23-C28
2	C	501	CTP	PB-O3B-PG-O2G
4	A	503	W5E	C06-C07-C18-O22
4	C	503	W5E	C06-C07-C18-O22
4	A	503	W5E	C08-C07-C18-O22
4	C	503	W5E	C08-C07-C18-O22
2	C	501	CTP	PB-O3A-PA-O1A
2	C	501	CTP	PB-O3A-PA-O2A
2	C	501	CTP	PG-O3B-PB-O2B
4	A	503	W5E	C01-C02-C23-C28
4	C	503	W5E	C03-C02-C23-C28
4	A	503	W5E	C03-C02-C23-C24
2	B	501	CTP	PB-O3A-PA-O2A
2	D	501	CTP	PB-O3A-PA-O2A

There are no ring outliers.

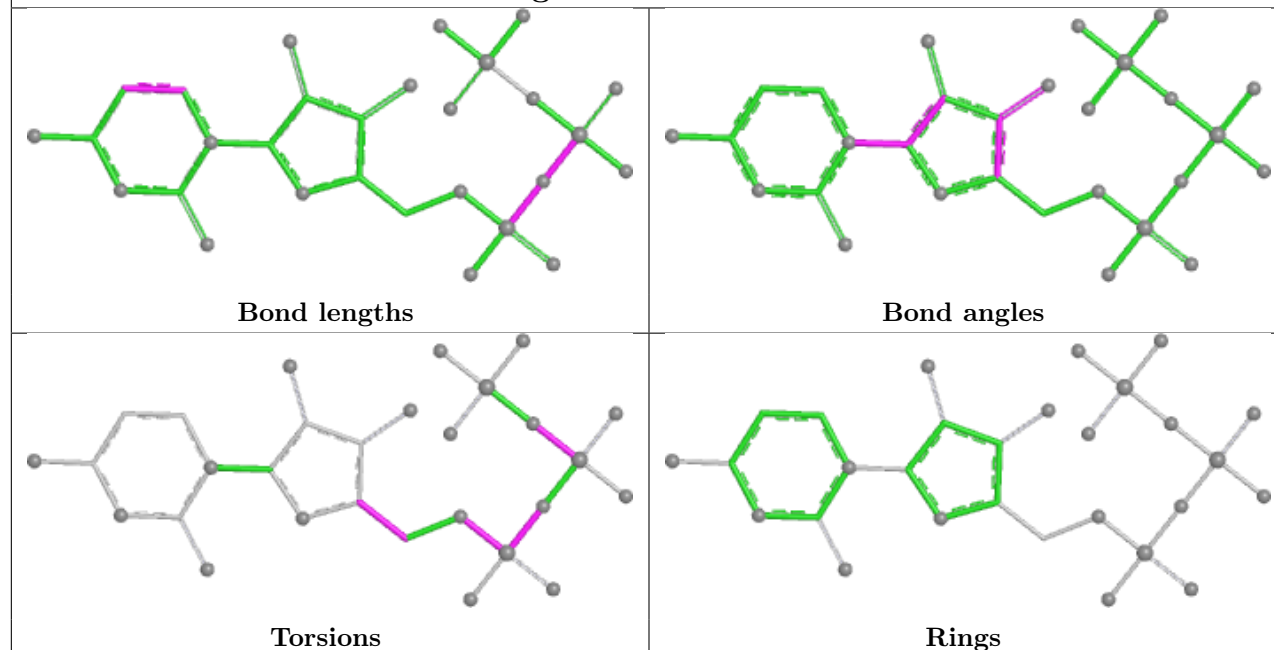
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	503	ACT	2	0
2	B	501	CTP	2	0
5	D	502	ACT	1	0
5	A	504	ACT	1	0
2	C	501	CTP	2	0

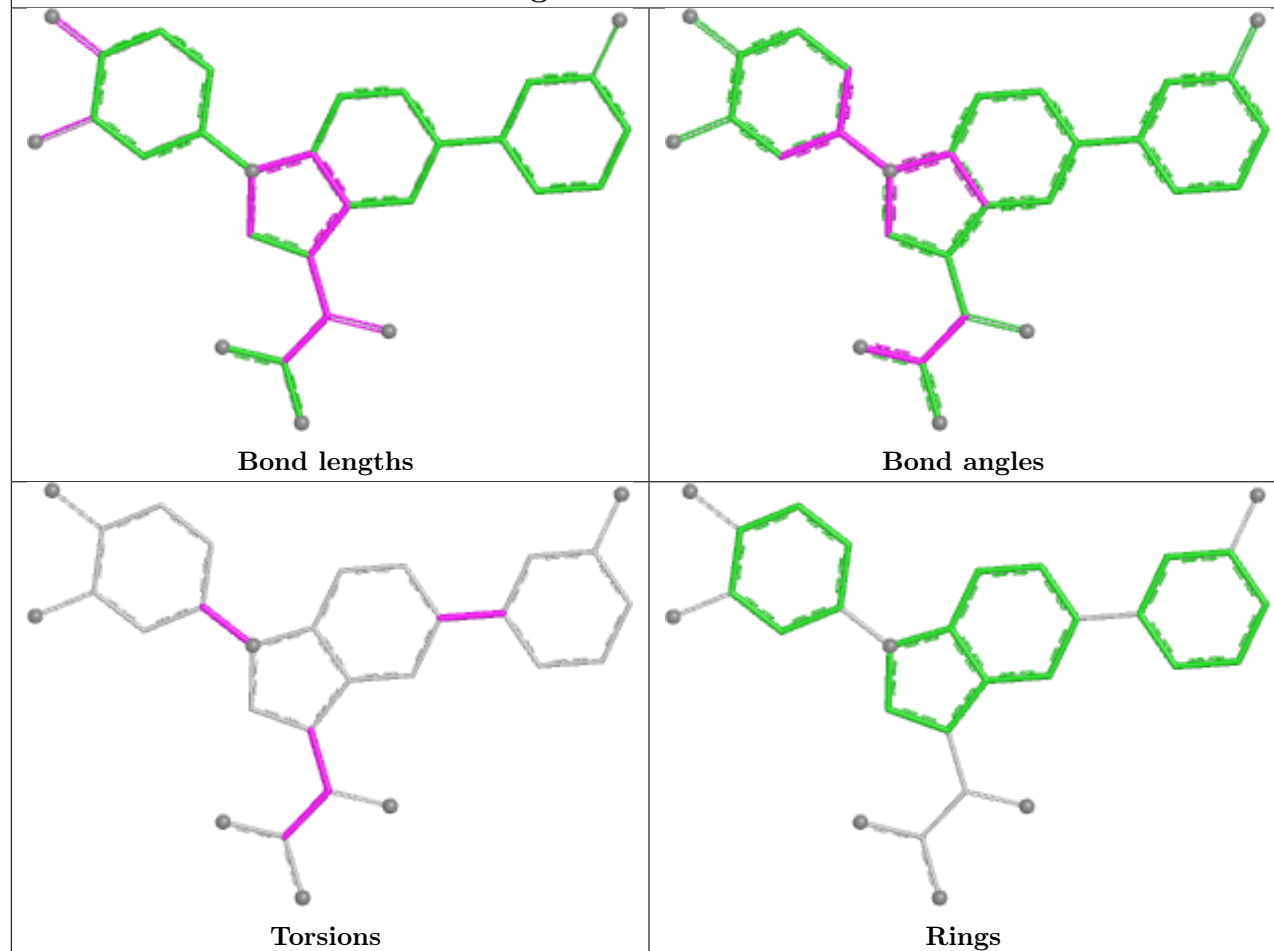
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

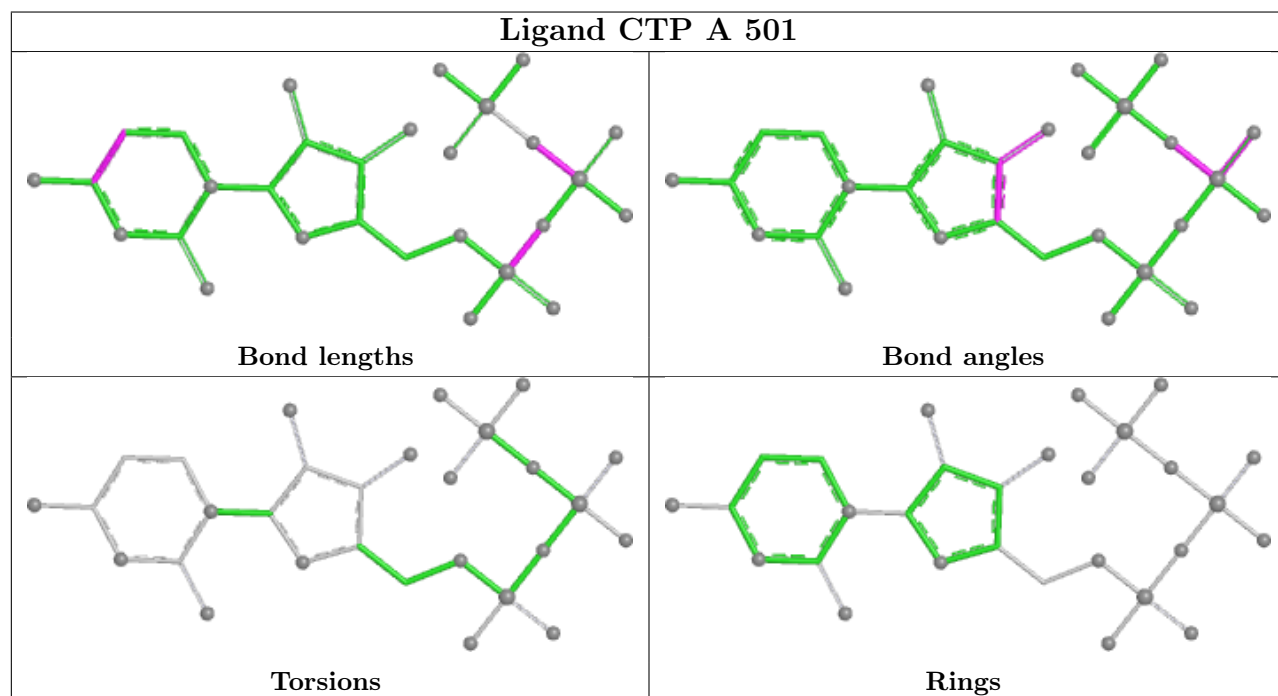
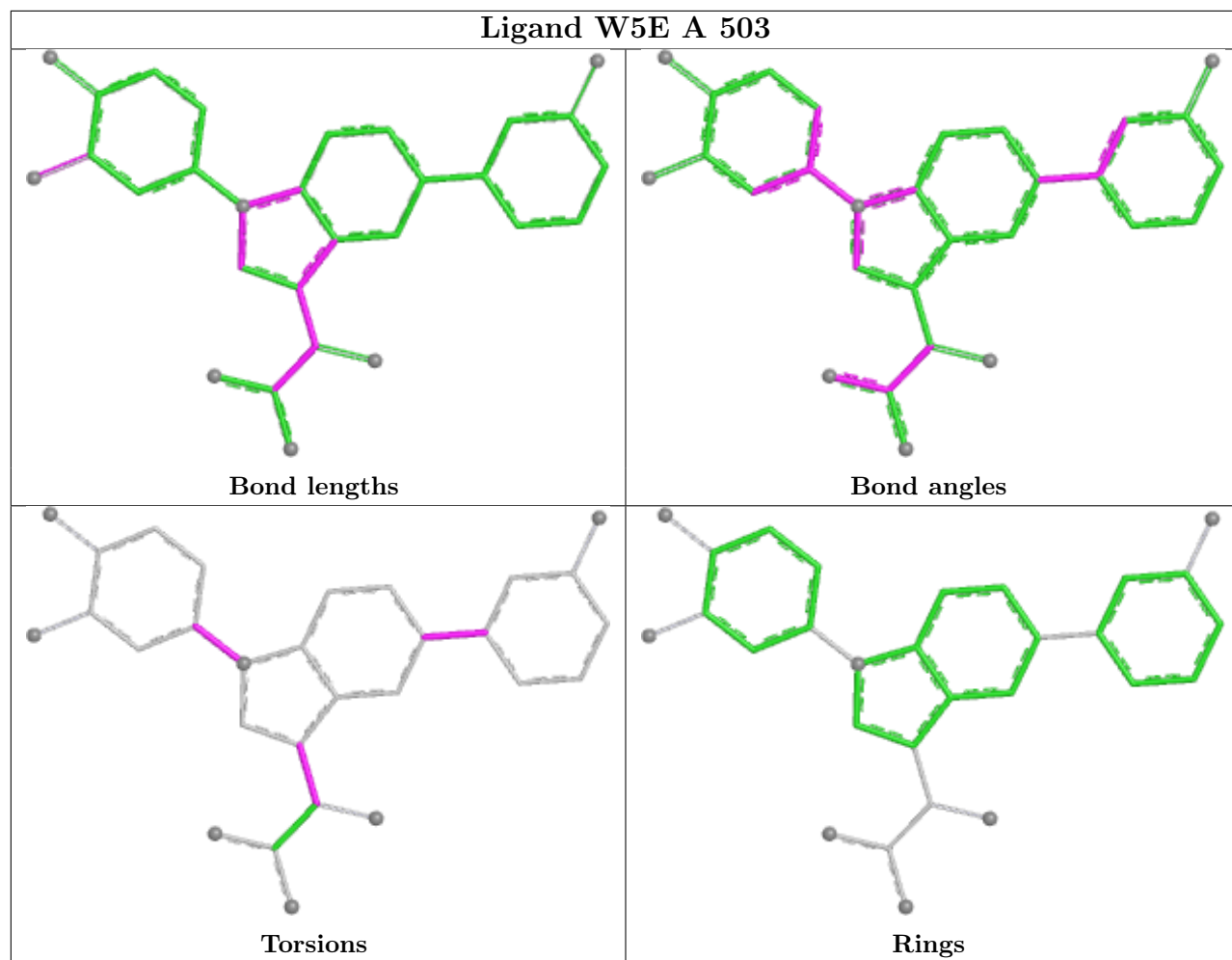


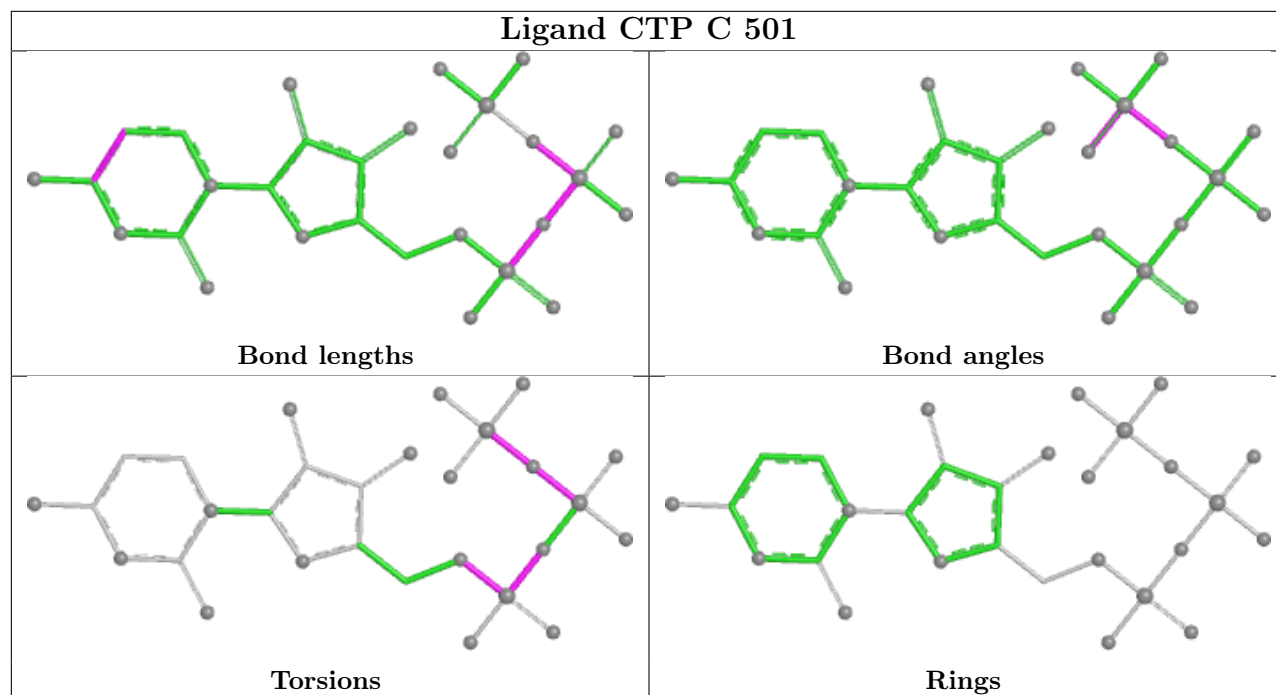
Ligand CTP B 501



Ligand W5E C 503







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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	212/237 (89%)	0.40	14 (6%) 24 21	27, 42, 74, 109	0
1	B	229/237 (96%)	0.36	12 (5%) 33 29	25, 44, 79, 104	0
1	C	206/237 (86%)	0.32	9 (4%) 39 36	27, 42, 71, 100	0
1	D	211/237 (89%)	0.58	24 (11%) 10 8	27, 48, 104, 134	0
All	All	858/948 (90%)	0.42	59 (6%) 23 19	25, 44, 86, 134	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	GLY	5.7
1	A	376	ASP	5.0
1	A	375	ASN	4.7
1	A	184	HIS	4.1
1	A	289	ALA	3.8
1	D	344	LEU	3.8
1	A	291	LYS	3.7
1	B	364	VAL	3.6
1	C	412	GLN	3.6
1	A	396	LEU	3.4
1	B	297	SER	3.2
1	B	218	GLY	3.2
1	D	299	PRO	3.2
1	D	295	GLY	3.1
1	B	300	SER	3.0
1	D	385	THR	3.0
1	A	290	ALA	3.0
1	D	297	SER	3.0
1	D	346	HIS	2.9
1	D	360	VAL	2.8
1	B	296	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	311	LEU	2.8
1	A	185	HIS	2.8
1	D	386	GLU	2.7
1	B	299	PRO	2.7
1	B	246	ALA	2.7
1	A	292	ILE	2.6
1	D	347	ALA	2.6
1	C	184	HIS	2.6
1	C	198	GLY	2.6
1	D	343	VAL	2.6
1	C	213	SER	2.5
1	C	376	ASP	2.5
1	D	380	LEU	2.5
1	B	366	GLU	2.5
1	D	384	GLY	2.5
1	C	300	SER	2.4
1	D	358	LEU	2.4
1	D	286	HIS	2.4
1	A	391	HIS	2.4
1	D	294	LYS	2.4
1	C	192	ALA	2.3
1	B	185	HIS	2.3
1	D	293	LYS	2.3
1	C	251	VAL	2.3
1	B	293	LYS	2.3
1	A	412	GLN	2.2
1	B	302	ILE	2.2
1	A	390	GLU	2.2
1	D	345	PHE	2.2
1	D	392	GLY	2.1
1	C	233	THR	2.1
1	D	389	LEU	2.1
1	D	296	ALA	2.1
1	D	298	GLU	2.0
1	A	275	MET	2.0
1	B	184	HIS	2.0
1	D	391	HIS	2.0
1	A	300	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

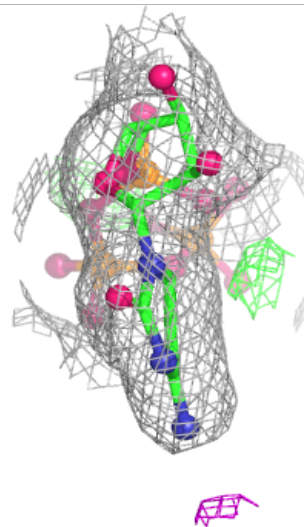
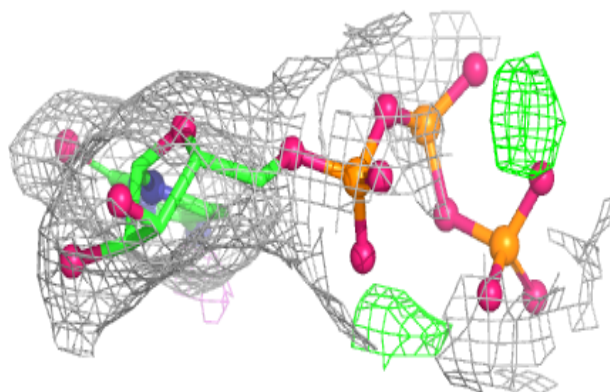
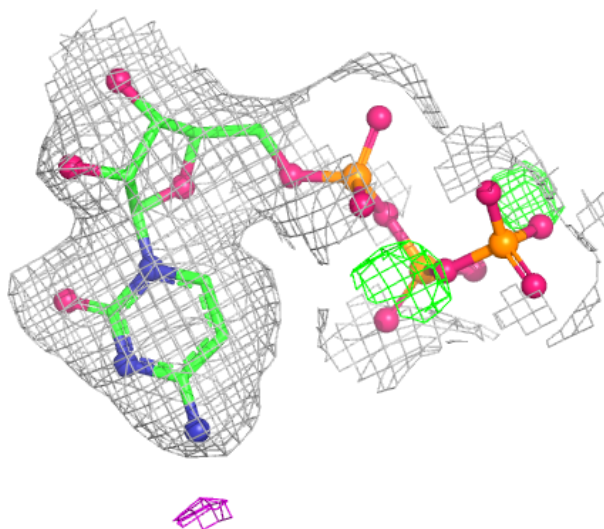
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CTP	D	501	29/29	0.84	0.10	27,42,102,104	0
4	W5E	A	503	29/29	0.85	0.13	53,62,69,72	0
4	W5E	C	503	29/29	0.85	0.13	51,58,66,69	0
5	ACT	D	502	4/4	0.87	0.10	27,41,42,47	0
5	ACT	D	503	4/4	0.88	0.14	52,54,54,66	0
3	CA	C	502	1/1	0.90	0.07	74,74,74,74	0
5	ACT	B	503	4/4	0.90	0.13	48,57,60,68	0
2	CTP	B	501	29/29	0.91	0.08	30,45,65,68	0
5	ACT	A	504	4/4	0.92	0.11	23,31,33,43	0
2	CTP	A	501	29/29	0.92	0.08	24,39,62,69	0
3	CA	A	502	1/1	0.93	0.05	61,61,61,61	0
2	CTP	C	501	29/29	0.94	0.07	27,38,63,73	0
3	CA	B	502	1/1	0.98	0.10	61,61,61,61	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.

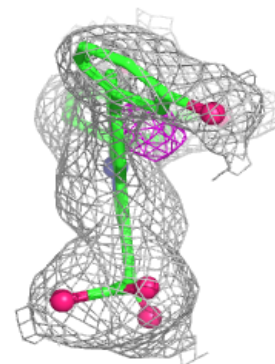
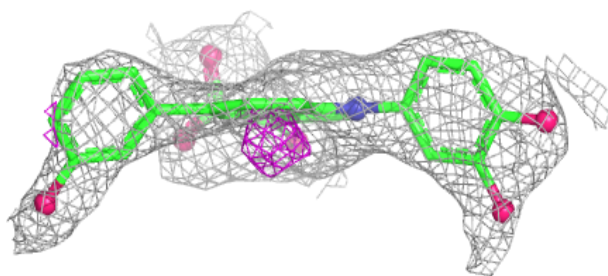
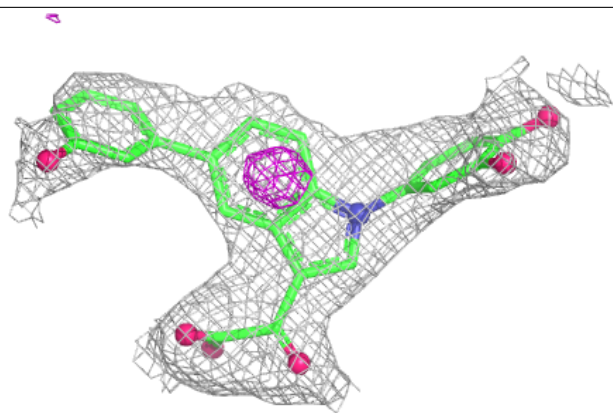
Electron density around CTP D 501:

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



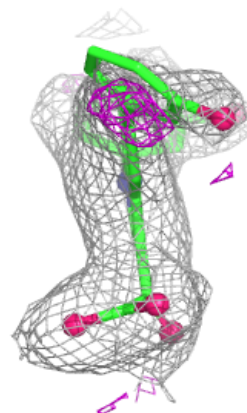
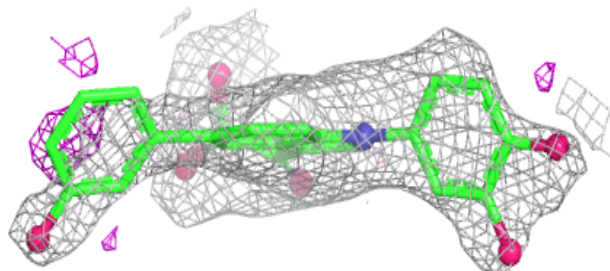
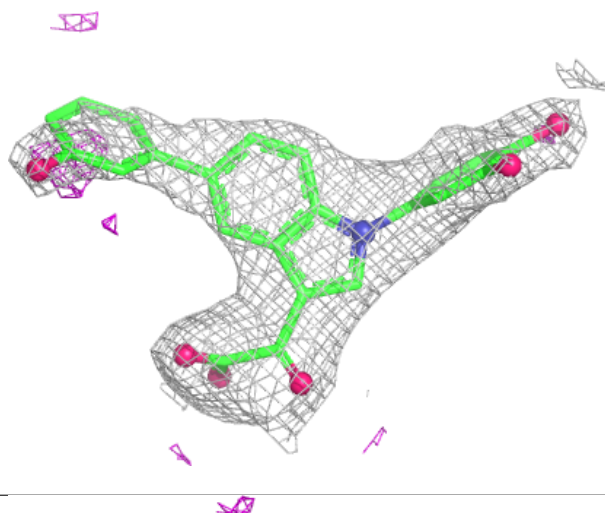
Electron density around W5E A 503:

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



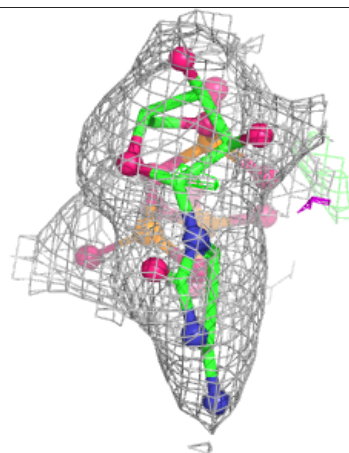
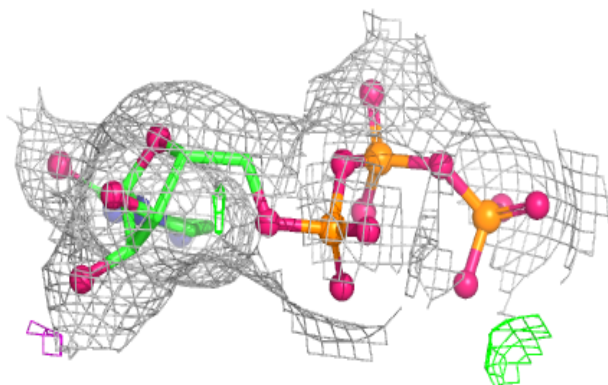
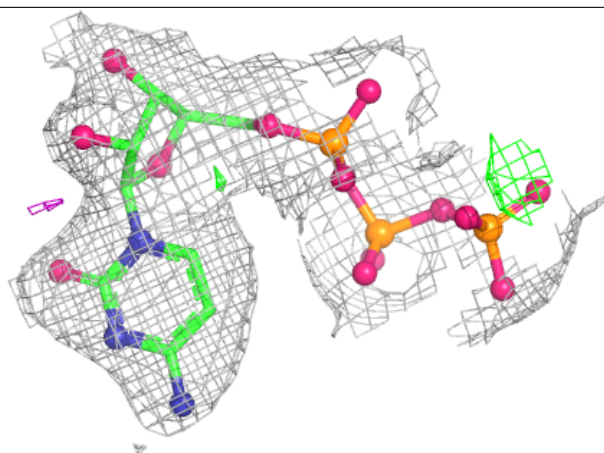
Electron density around W5E C 503:

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



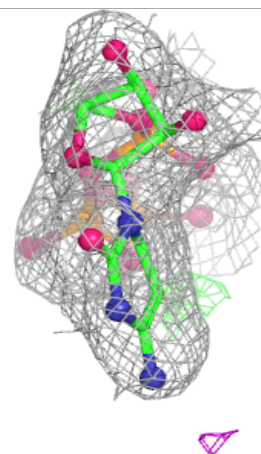
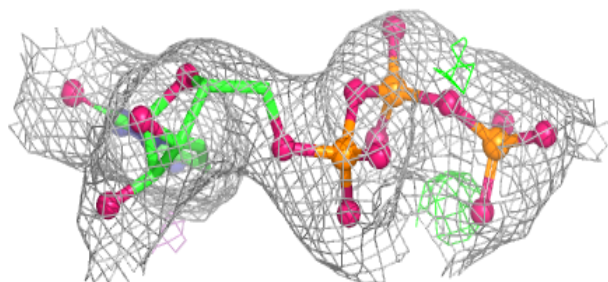
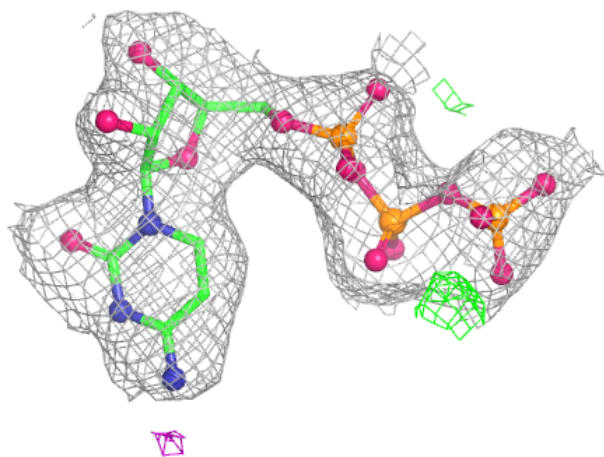
Electron density around CTP B 501:

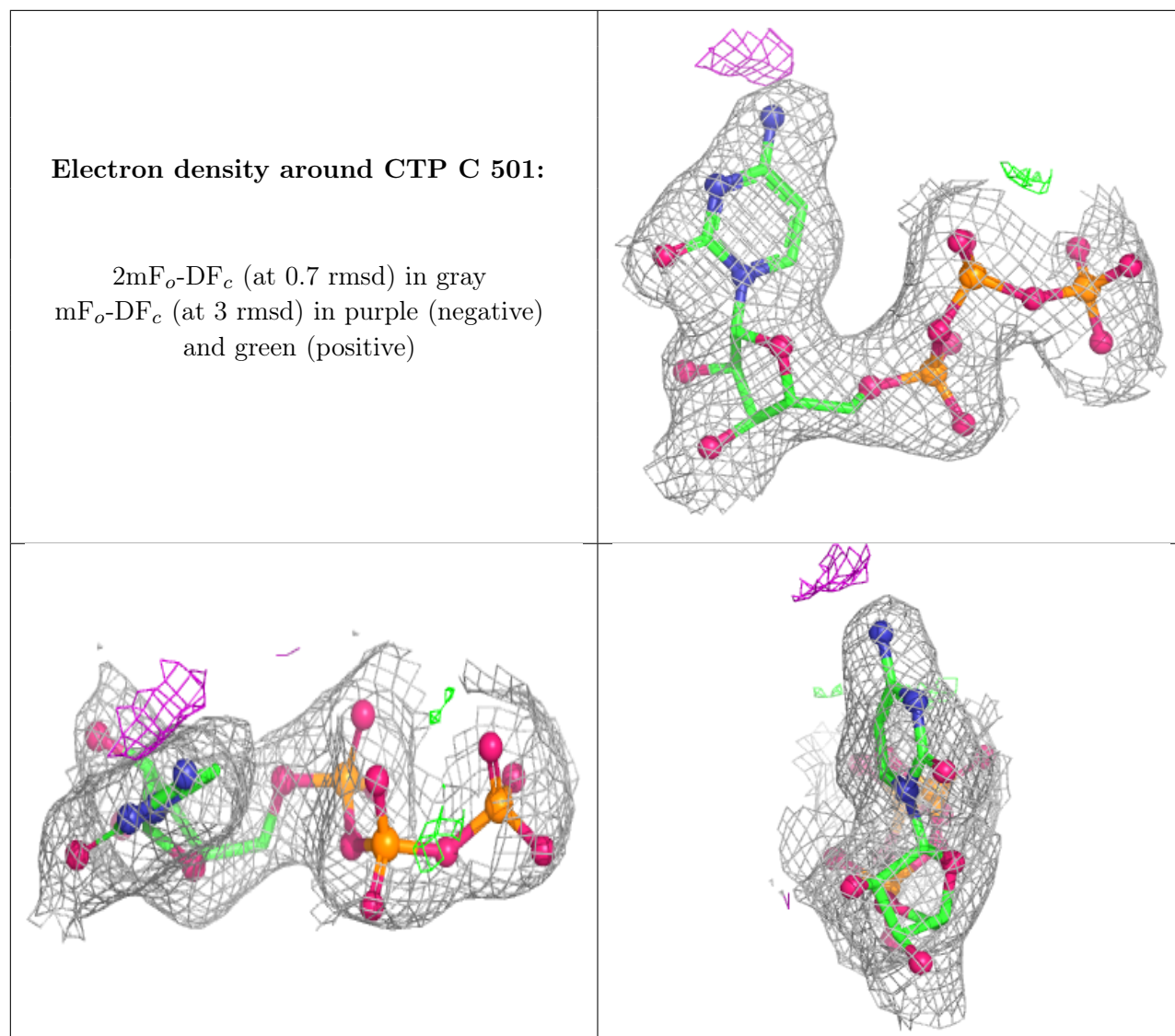
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.