Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:26 AM UTC

PDB ID	:	8OWP / pdb_00008owp
Title	:	Crystal structure of Mycobacterium smegmatis CoaB in complex with CTP and 2-(1-(4-hydroxyphenyl)-5-phenyl-1H-indol-3-yl)-2-oxoacetic acid
Authors	:	Mendes, V.; Blundell, T.L.
Deposited on	:	2023-04-28
Resolution	:	1.99 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:

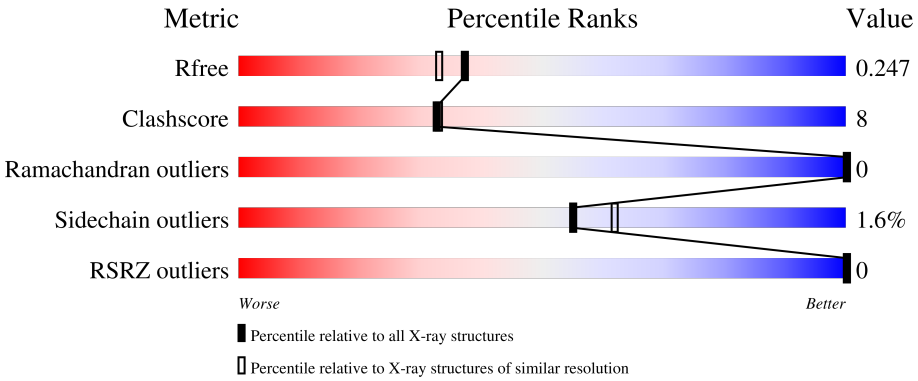
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	74% 16% 10%
1	B	237	74% 14% 12%
1	C	237	71% 16% • 12%
1	D	237	76% 16% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6533 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	214	Total	C	N	O	S	0	0	0
			1519	940	283	290	6			
1	B	209	Total	C	N	O	S	0	0	0
			1478	921	278	273	6			
1	C	208	Total	C	N	O	S	0	0	0
			1466	906	272	282	6			
1	D	217	Total	C	N	O	S	0	0	0
			1525	944	284	291	6			

There are 32 discrepancies between the modelled and reference sequences:

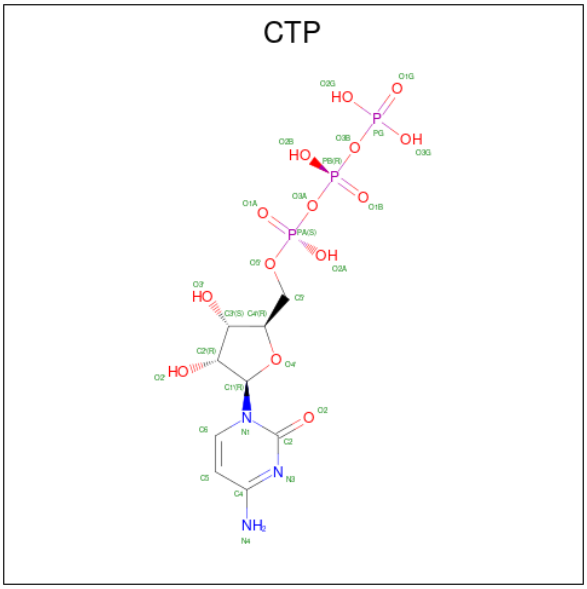
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MET	-	initiating methionine	UNP A0QWT2
A	179	ALA	-	expression tag	UNP A0QWT2
A	180	HIS	-	expression tag	UNP A0QWT2
A	181	HIS	-	expression tag	UNP A0QWT2
A	182	HIS	-	expression tag	UNP A0QWT2
A	183	HIS	-	expression tag	UNP A0QWT2
A	184	HIS	-	expression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

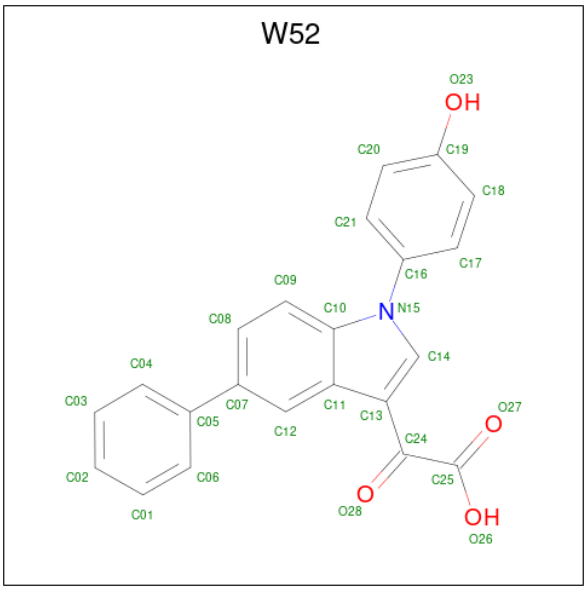


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

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

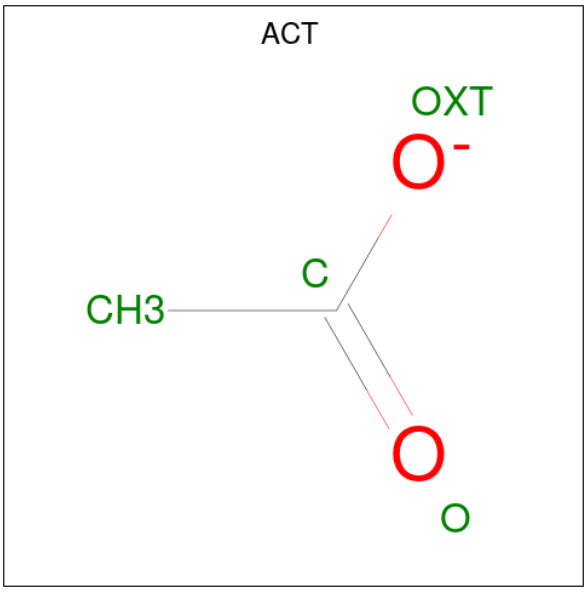
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is 2-[1-(4-hydroxyphenyl)-5-phenyl-indol-3-yl]-2-oxidanylidene-ethanoic acid (CCD ID: W52) (formula: $C_{22}H_{15}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 27 22 1 4	0	0
4	A	1	Total C N O 27 22 1 4	0	0
4	C	1	Total C N O 27 22 1 4	0	0

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	104	Total O 104 104	0	0
6	B	87	Total O 87 87	0	0
6	C	63	Total O 63 63	0	0
6	D	86	Total O 86 86	0	0

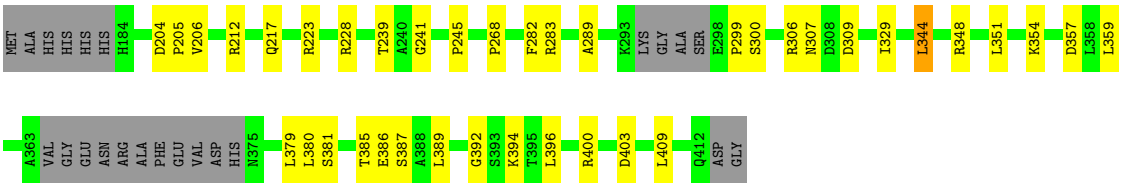
3 Residue-property plots (i)

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:

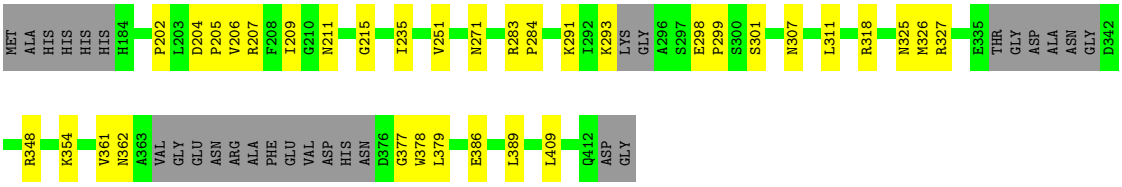




• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

Chain B:

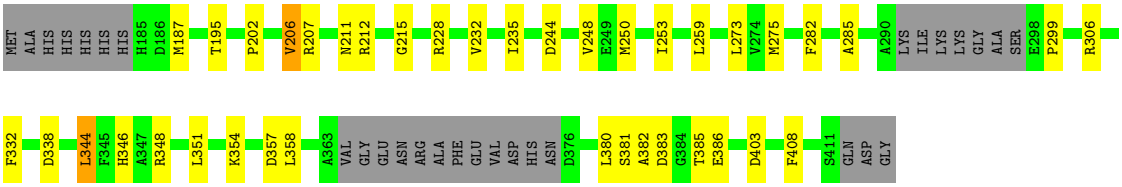




• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

Chain C:

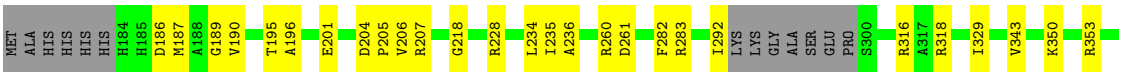




• Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

Chain D:






D357
L358
A363
VAL
GLY
GLU
ASN
R368
D376
G377
W378
L379
L380
S381
E386
S387
A388
L389
G392
S411
GLN
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	75.82Å 76.41Å 143.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.82 – 1.99 53.82 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.0 (53.82-1.99) 91.9 (53.82-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.00Å)	Xtriage
Refinement program	PHENIX (dev_2947: ???)	Depositor
R, R_{free}	0.199 , 0.254 0.197 , 0.247	Depositor DCC
R_{free} test set	2753 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.126 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6533	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: W52, CA, CTP, 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	0.50	1/1537 (0.1%)	0.65	1/2088 (0.0%)
1	B	0.48	0/1493	0.67	1/2022 (0.0%)
1	C	0.51	0/1483	0.67	0/2015
1	D	0.70	2/1540 (0.1%)	0.69	0/2090
All	All	0.56	3/6053 (0.0%)	0.67	2/8215 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	392	GLY	C-O	-6.76	1.19	1.23
1	A	299	PRO	CA-C	-5.66	1.46	1.52
1	D	389	LEU	CA-C	-5.43	1.46	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	PRO	N-CA-C	6.96	121.30	110.80
1	B	301	SER	N-CA-C	-5.96	100.91	110.14

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	1519	0	1494	25	0
1	B	1478	0	1488	20	0
1	C	1466	0	1433	30	0
1	D	1525	0	1491	24	0
2	A	29	0	12	1	0
2	B	29	0	12	2	0
2	C	29	0	12	3	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
3	D	1	0	0	0	0
4	A	54	0	0	1	0
4	C	27	0	0	1	0
5	C	4	0	3	1	0
6	A	104	0	0	2	0
6	B	87	0	0	1	0
6	C	63	0	0	2	0
6	D	86	0	0	3	0
All	All	6533	0	5957	96	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 8.

All (96) 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:C:380:LEU:HD22	1:C:386:GLU:HG2	1.67	0.76
1:A:392:GLY:HA3	1:A:396:LEU:HD23	1.67	0.76
1:A:380:LEU:HD22	1:A:386:GLU:HG2	1.72	0.70
1:D:187:MET:O	1:D:190:VAL:HG12	1.96	0.64
1:A:381:SER:HB3	1:A:385:THR:HB	1.77	0.64
1:D:358:LEU:HD23	1:D:381:SER:HA	1.79	0.64
1:A:204:ASP:HB2	1:A:205:PRO:HD2	1.79	0.63
1:C:232:VAL:HB	1:C:248:VAL:HG22	1.79	0.63
1:C:282:PHE:CE2	1:C:306:ARG:HG2	2.35	0.62
1:C:273:LEU:HD21	1:C:275:MET:HE3	1.82	0.62
1:D:343:VAL:HG21	1:D:376:ASP:HB2	1.79	0.62
1:B:318:ARG:HD3	1:B:326:MET:HB3	1.80	0.61
1:C:244:ASP:HB3	1:C:250:MET:HG3	1.82	0.61
1:C:228:ARG:NH1	1:C:403:ASP:OD2	2.34	0.60
2:C:501:CTP:O1A	4:C:503:W52:O23	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:NH1	1:A:403:ASP:OD1	2.36	0.58
1:D:318:ARG:HH22	1:D:357:ASP:CG	2.12	0.58
1:A:212:ARG:HG3	1:B:206:VAL:O	2.03	0.57
1:B:327:ARG:NH2	1:B:409:LEU:O	2.38	0.57
1:C:211:ASN:ND2	5:C:504:ACT:OXT	2.35	0.57
1:C:215:GLY:HA2	6:C:623:HOH:O	2.03	0.57
1:C:195:THR:HG22	1:C:235:ILE:HB	1.86	0.56
1:B:362:ASN:HB2	1:B:377:GLY:HA2	1.87	0.56
1:C:282:PHE:HE2	1:C:306:ARG:HG2	1.70	0.55
1:A:223:ARG:HG3	1:A:245:PRO:HB3	1.87	0.55
1:D:207:ARG:NH2	6:D:605:HOH:O	2.38	0.55
1:D:186:ASP:OD2	1:D:228:ARG:NH1	2.32	0.54
1:B:311:LEU:HD23	1:B:354:LYS:HD2	1.90	0.54
2:B:501:CTP:H6	2:B:501:CTP:H5'2	1.73	0.54
1:A:282:PHE:CE1	1:A:306:ARG:HG2	2.44	0.53
1:B:379:LEU:HG	1:B:389:LEU:HG	1.92	0.52
1:C:206:VAL:HG12	1:C:207:ARG:HG3	1.92	0.52
1:A:329:ILE:N	1:A:357:ASP:OD2	2.33	0.52
1:A:289:ALA:HB3	1:C:285:ALA:HA	1.92	0.51
1:C:344:LEU:HD13	1:C:348:ARG:CZ	2.41	0.51
1:D:350:LYS:HG3	1:D:353:ARG:NH2	2.25	0.50
1:A:309:ASP:OD2	1:A:354:LYS:NZ	2.33	0.50
1:C:253:ILE:HD13	1:C:259:LEU:HB2	1.94	0.49
1:D:260:ARG:NH1	1:D:261:ASP:OD1	2.32	0.49
4:A:504:W52:O26	1:B:293:LYS:C	2.56	0.49
1:D:378:TRP:HA	1:D:388:ALA:HA	1.96	0.48
1:A:354:LYS:HE3	2:A:501:CTP:H5'2	1.96	0.47
1:A:396:LEU:HD21	1:A:400:ARG:NH1	2.28	0.47
1:B:361:VAL:CG1	1:B:378:TRP:HB2	2.43	0.47
1:C:195:THR:HA	1:C:235:ILE:O	2.14	0.47
1:C:212:ARG:HG3	1:D:206:VAL:O	2.15	0.47
1:C:299:PRO:HB3	1:D:282:PHE:CE2	2.48	0.47
1:D:195:THR:HA	1:D:235:ILE:O	2.15	0.47
1:C:351:LEU:HD22	1:C:380:LEU:HB3	1.95	0.47
1:C:358:LEU:HD12	1:C:380:LEU:O	2.15	0.47
1:A:228:ARG:HD2	6:A:653:HOH:O	2.15	0.46
1:B:283:ARG:HD3	1:B:307:ASN:OD1	2.15	0.46
1:D:329:ILE:N	1:D:357:ASP:OD1	2.37	0.46
1:D:204:ASP:HB2	1:D:205:PRO:CD	2.46	0.46
1:C:381:SER:HB3	1:C:383:ASP:OD2	2.15	0.46
1:C:354:LYS:HE3	2:C:501:CTP:H5'2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLN:OE1	1:A:394:LYS:HD2	2.16	0.46
1:A:283:ARG:HD3	1:A:307:ASN:OD1	2.15	0.46
1:D:201:GLU:HB3	1:D:283:ARG:HB2	1.98	0.46
1:D:187:MET:HE3	1:D:190:VAL:HG11	1.98	0.46
1:D:186:ASP:OD1	1:D:228:ARG:HB3	2.16	0.46
1:C:357:ASP:HB3	1:C:408:PHE:CZ	2.52	0.45
1:D:204:ASP:OD2	1:D:292:ILE:HD12	2.17	0.45
1:D:353:ARG:NH2	6:D:602:HOH:O	2.49	0.45
1:C:338:ASP:CG	1:C:346:HIS:HE1	2.25	0.45
1:D:234:LEU:HD22	1:D:236:ALA:HB2	2.00	0.44
1:C:357:ASP:O	1:C:382:ALA:N	2.45	0.44
1:A:268:PRO:HB3	6:A:650:HOH:O	2.16	0.44
1:A:389:LEU:HD12	1:A:389:LEU:HA	1.84	0.43
1:C:244:ASP:CB	1:C:250:MET:HG3	2.48	0.43
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.73	0.43
1:A:344:LEU:HD13	1:A:348:ARG:CZ	2.49	0.43
1:B:271:ASN:HA	1:B:325:ASN:O	2.18	0.43
1:D:379:LEU:HD21	1:D:389:LEU:HG	2.01	0.43
1:C:332:PHE:O	2:C:501:CTP:H5'1	2.19	0.42
1:D:189:GLY:N	6:D:610:HOH:O	2.47	0.42
1:B:202:PRO:O	1:B:284:PRO:HG2	2.19	0.42
1:B:215:GLY:HA2	6:B:617:HOH:O	2.18	0.42
1:A:351:LEU:HD13	1:A:359:LEU:HB2	2.01	0.42
1:B:298:GLU:HA	1:B:299:PRO:HD2	1.78	0.42
1:C:357:ASP:HB3	1:C:408:PHE:CE1	2.55	0.42
1:B:348:ARG:HH21	1:B:386:GLU:CG	2.33	0.42
1:B:204:ASP:HB2	1:B:205:PRO:CD	2.50	0.41
1:C:211:ASN:HA	1:D:206:VAL:O	2.20	0.41
1:B:235:ILE:HA	1:B:251:VAL:O	2.20	0.41
1:A:206:VAL:O	1:B:211:ASN:HA	2.21	0.41
1:A:379:LEU:HB2	1:A:387:SER:HB2	2.02	0.41
1:A:239:THR:C	1:A:241:GLY:H	2.29	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.84	0.41
1:B:207:ARG:HH22	1:B:291:LYS:HE3	1.85	0.41
1:B:361:VAL:HG13	1:B:378:TRP:HB2	2.02	0.40
1:B:209:ILE:HD12	1:B:284:PRO:HD3	2.04	0.40
1:C:202:PRO:HD2	6:C:635:HOH:O	2.22	0.40
1:D:196:ALA:HB2	1:D:218:GLY:HA3	2.03	0.40
2:B:501:CTP:H5'2	2:B:501:CTP:C6	2.53	0.40
1:C:381:SER:HB2	1:C:385:THR:HB	2.02	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	208/237 (88%)	203 (98%)	5 (2%)	0	100	100
1	B	201/237 (85%)	195 (97%)	6 (3%)	0	100	100
1	C	202/237 (85%)	196 (97%)	6 (3%)	0	100	100
1	D	211/237 (89%)	205 (97%)	6 (3%)	0	100	100
All	All	822/948 (87%)	799 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	146/173 (84%)	144 (99%)	2 (1%)	59	66
1	B	140/173 (81%)	140 (100%)	0	100	100
1	C	139/173 (80%)	136 (98%)	3 (2%)	45	50
1	D	142/173 (82%)	138 (97%)	4 (3%)	38	41
All	All	567/692 (82%)	558 (98%)	9 (2%)	55	62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	SER
1	A	344	LEU

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Mol	Chain	Res	Type
1	C	187	MET
1	C	206	VAL
1	C	344	LEU
1	D	316	ARG
1	D	386	GLU
1	D	389	LEU
1	D	411	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	252	HIS
1	C	185	HIS
1	C	252	HIS
1	C	271	ASN
1	D	227	GLN
1	D	375	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	W52	A	503	-	30,30,30	1.74	8 (26%)	43,43,43	1.59	7 (16%)
4	W52	A	504	-	30,30,30	1.56	5 (16%)	43,43,43	1.48	6 (13%)
2	CTP	C	501	3	29,30,30	1.05	1 (3%)	43,47,47	0.99	4 (9%)
2	CTP	B	501	3	29,30,30	1.15	2 (6%)	43,47,47	0.97	4 (9%)
5	ACT	C	504	-	3,3,3	0.80	0	3,3,3	1.77	1 (33%)
4	W52	C	503	-	30,30,30	1.48	3 (10%)	43,43,43	1.29	4 (9%)
2	CTP	A	501	3	29,30,30	1.19	2 (6%)	43,47,47	1.25	6 (13%)
2	CTP	D	501	3	29,30,30	1.16	2 (6%)	43,47,47	1.13	4 (9%)

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	W52	A	503	-	-	8/16/16/16	0/4/4/4
4	W52	A	504	-	-	2/16/16/16	0/4/4/4
2	CTP	C	501	3	-	3/22/38/38	0/2/2/2
2	CTP	B	501	3	-	3/22/38/38	0/2/2/2
4	W52	C	503	-	-	8/16/16/16	0/4/4/4
2	CTP	A	501	3	-	1/22/38/38	0/2/2/2
2	CTP	D	501	3	-	7/22/38/38	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	W52	C13-C24	4.48	1.54	1.45
4	A	504	W52	C13-C24	4.21	1.54	1.45
4	C	503	W52	C10-N15	-3.90	1.32	1.39
4	A	503	W52	C10-N15	-3.90	1.32	1.39
4	A	503	W52	C25-C24	-3.68	1.51	1.54
2	D	501	CTP	PB-O3B	3.53	1.63	1.59
4	A	503	W52	C14-N15	-3.45	1.30	1.39
4	A	503	W52	C13-C24	3.35	1.52	1.45
2	B	501	CTP	PB-O3B	3.11	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	W52	C16-N15	3.04	1.49	1.43
4	A	503	W52	C11-C13	-3.01	1.40	1.45
4	A	503	W52	O28-C24	-2.94	1.16	1.23
4	C	503	W52	C14-N15	-2.79	1.32	1.39
4	A	504	W52	C10-N15	-2.66	1.35	1.39
2	A	501	CTP	C6-N1	-2.57	1.32	1.38
4	A	503	W52	C11-C10	-2.44	1.37	1.41
2	B	501	CTP	PA-O3A	2.32	1.62	1.59
2	C	501	CTP	PA-O3A	2.21	1.61	1.59
2	A	501	CTP	PG-O2G	-2.21	1.46	1.54
4	A	504	W52	O28-C24	-2.15	1.18	1.23
4	A	503	W52	O26-C25	-2.07	1.24	1.30
4	A	504	W52	O23-C19	2.02	1.41	1.37
2	D	501	CTP	C4-N3	2.01	1.38	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	W52	C17-C16-N15	-4.38	114.25	119.89
4	A	503	W52	C10-N15-C14	4.29	111.34	107.98
4	C	503	W52	C10-N15-C14	3.96	111.08	107.98
4	A	504	W52	C13-C24-C25	3.76	124.75	118.83
2	D	501	CTP	O2A-PA-O3A	3.54	116.84	107.27
4	A	503	W52	C21-C16-N15	3.53	124.44	119.89
4	A	504	W52	C11-C10-N15	3.28	110.01	107.58
4	C	503	W52	C11-C13-C24	3.03	129.97	126.09
4	A	504	W52	C08-C07-C05	-2.87	116.31	121.25
2	A	501	CTP	O3'-C3'-C4'	-2.84	102.93	111.08
4	A	504	W52	O26-C25-C24	2.82	120.84	112.94
2	C	501	CTP	O3G-PG-O3B	2.55	113.19	104.64
2	A	501	CTP	O3B-PG-O1G	-2.52	97.76	111.04
4	C	503	W52	O26-C25-C24	2.43	119.75	112.94
4	A	503	W52	C11-C13-C24	2.42	129.19	126.09
2	C	501	CTP	O2A-PA-O3A	2.42	113.80	107.27
2	A	501	CTP	C5-C6-N1	-2.38	117.98	121.84
4	A	503	W52	C08-C07-C12	2.37	121.50	118.23
2	D	501	CTP	O2G-PG-O3B	2.36	112.55	104.64
2	B	501	CTP	O2A-PA-O3A	2.33	113.58	107.27
4	A	504	W52	C21-C16-N15	2.32	122.89	119.89
5	C	504	ACT	O-C-CH3	-2.27	113.24	122.53
4	C	503	W52	C16-N15-C10	-2.23	124.33	127.88
4	A	503	W52	C13-C24-C25	2.22	122.33	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	W52	C18-C17-C16	2.22	123.11	120.30
2	C	501	CTP	C5-C6-N1	-2.21	118.24	121.84
2	A	501	CTP	O3G-PG-O2G	2.21	116.10	107.80
2	A	501	CTP	C2'-C3'-C4'	2.17	106.81	102.61
2	C	501	CTP	O2B-PB-O3A	2.17	113.13	107.27
2	D	501	CTP	O2B-PB-O3B	2.16	113.12	107.27
2	A	501	CTP	O2B-PB-O3A	2.16	113.12	107.27
2	B	501	CTP	O5'-C5'-C4'	2.16	116.35	108.99
4	A	503	W52	O26-C25-C24	2.11	118.84	112.94
2	B	501	CTP	O2-C2-N3	-2.09	119.04	122.33
2	D	501	CTP	O3G-PG-O3B	2.05	111.51	104.64
2	B	501	CTP	O3'-C3'-C2'	-2.01	105.38	111.82

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	CTP	C5'-O5'-PA-O1A
4	C	503	W52	O28-C24-C25-O26
4	A	503	W52	C21-C16-N15-C14
2	B	501	CTP	O4'-C4'-C5'-O5'
2	D	501	CTP	C3'-C4'-C5'-O5'
2	D	501	CTP	O4'-C4'-C5'-O5'
4	A	503	W52	C17-C16-N15-C14
4	C	503	W52	C17-C16-N15-C14
4	C	503	W52	C21-C16-N15-C14
4	A	503	W52	C17-C16-N15-C10
4	A	503	W52	C21-C16-N15-C10
4	C	503	W52	C21-C16-N15-C10
4	C	503	W52	C13-C24-C25-O26
4	A	504	W52	C13-C24-C25-O27
4	C	503	W52	C17-C16-N15-C10
2	B	501	CTP	PB-O3A-PA-O2A
2	D	501	CTP	C5'-O5'-PA-O2A
2	D	501	CTP	C5'-O5'-PA-O3A
4	A	503	W52	O28-C24-C25-O26
2	C	501	CTP	PA-O3A-PB-O1B
2	C	501	CTP	PA-O3A-PB-O2B
2	D	501	CTP	PB-O3A-PA-O2A
4	A	503	W52	C13-C24-C25-O26
4	A	503	W52	C11-C13-C24-O28
4	C	503	W52	C11-C13-C24-O28

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Mol	Chain	Res	Type	Atoms
4	A	504	W52	O28-C24-C25-O27
4	A	503	W52	C14-C13-C24-O28
4	C	503	W52	C14-C13-C24-O28
2	A	501	CTP	PB-O3A-PA-O1A
2	B	501	CTP	PB-O3A-PA-O1A
2	C	501	CTP	PB-O3A-PA-O2A
2	D	501	CTP	PG-O3B-PB-O2B

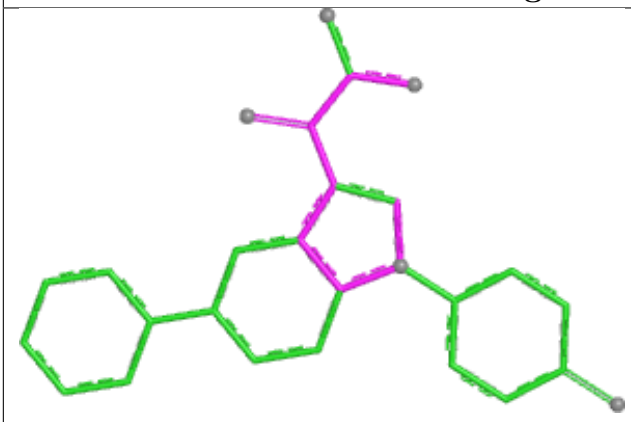
There are no ring outliers.

6 monomers are involved in 8 short contacts:

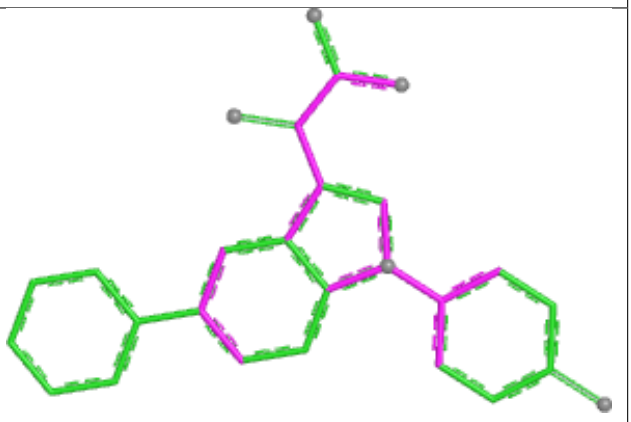
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	W52	1	0
2	C	501	CTP	3	0
2	B	501	CTP	2	0
5	C	504	ACT	1	0
4	C	503	W52	1	0
2	A	501	CTP	1	0

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.

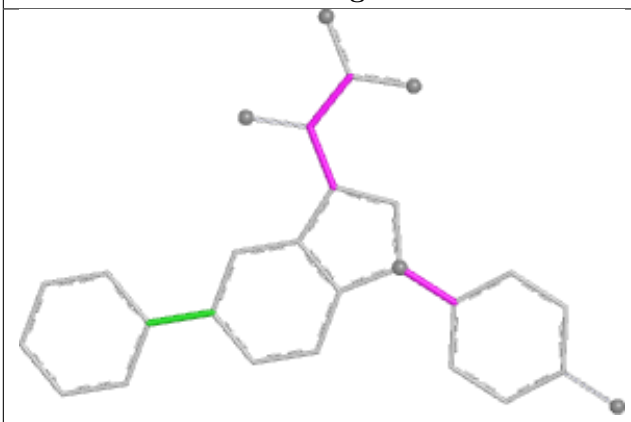
Ligand W52 A 503



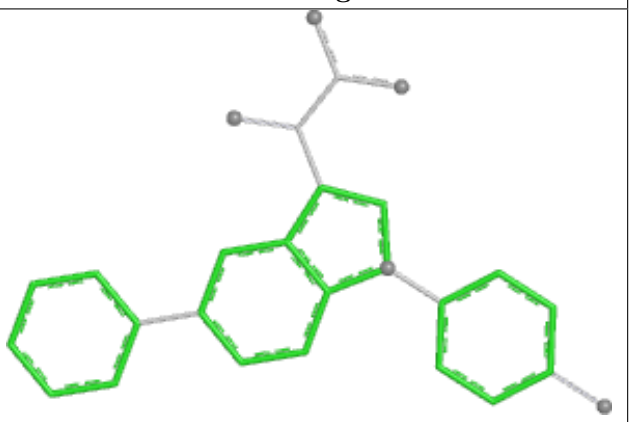
Bond lengths



Bond angles

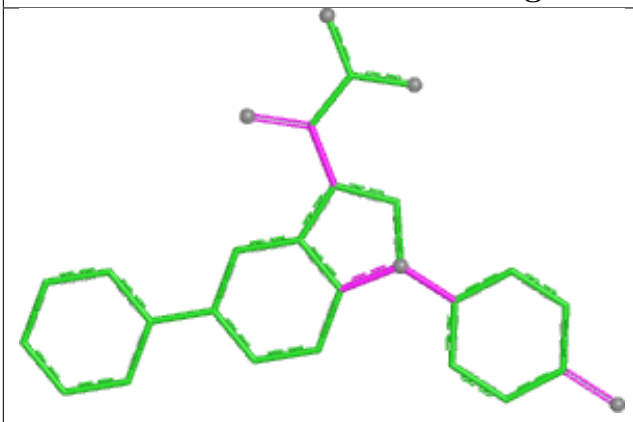


Torsions

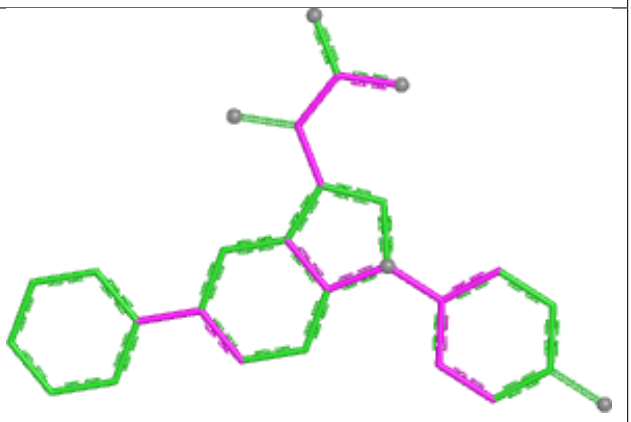


Rings

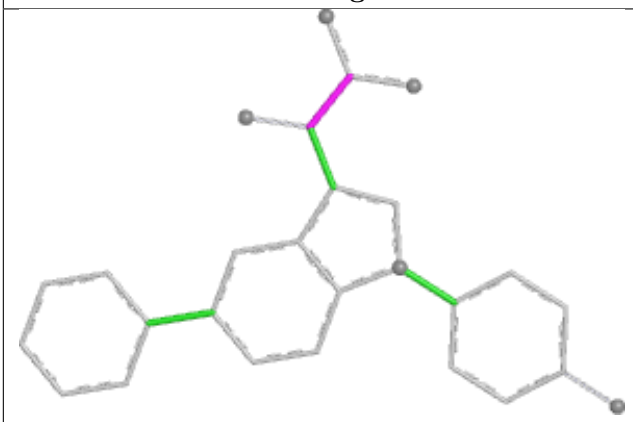
Ligand W52 A 504



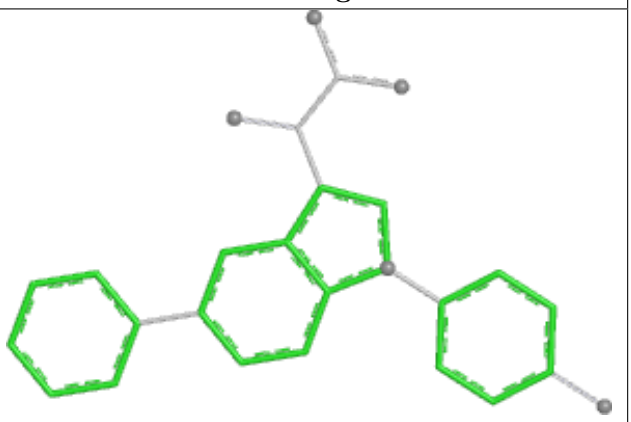
Bond lengths



Bond angles

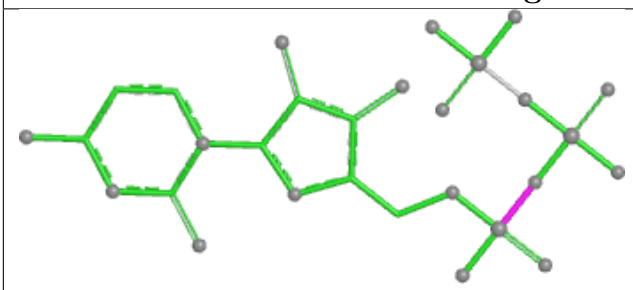


Torsions

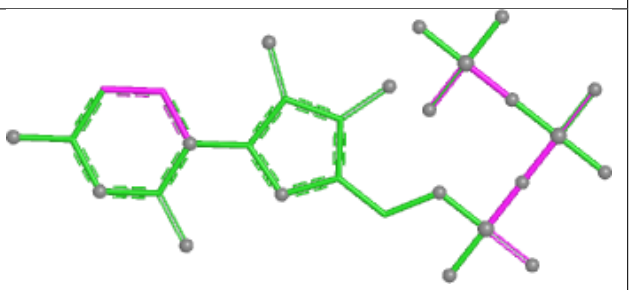


Rings

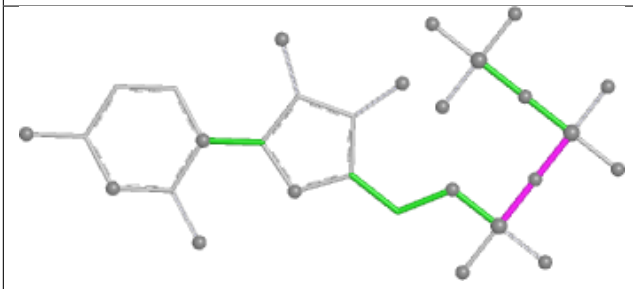
Ligand CTP C 501



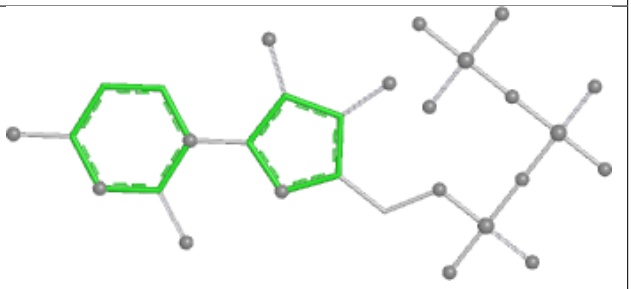
Bond lengths



Bond angles

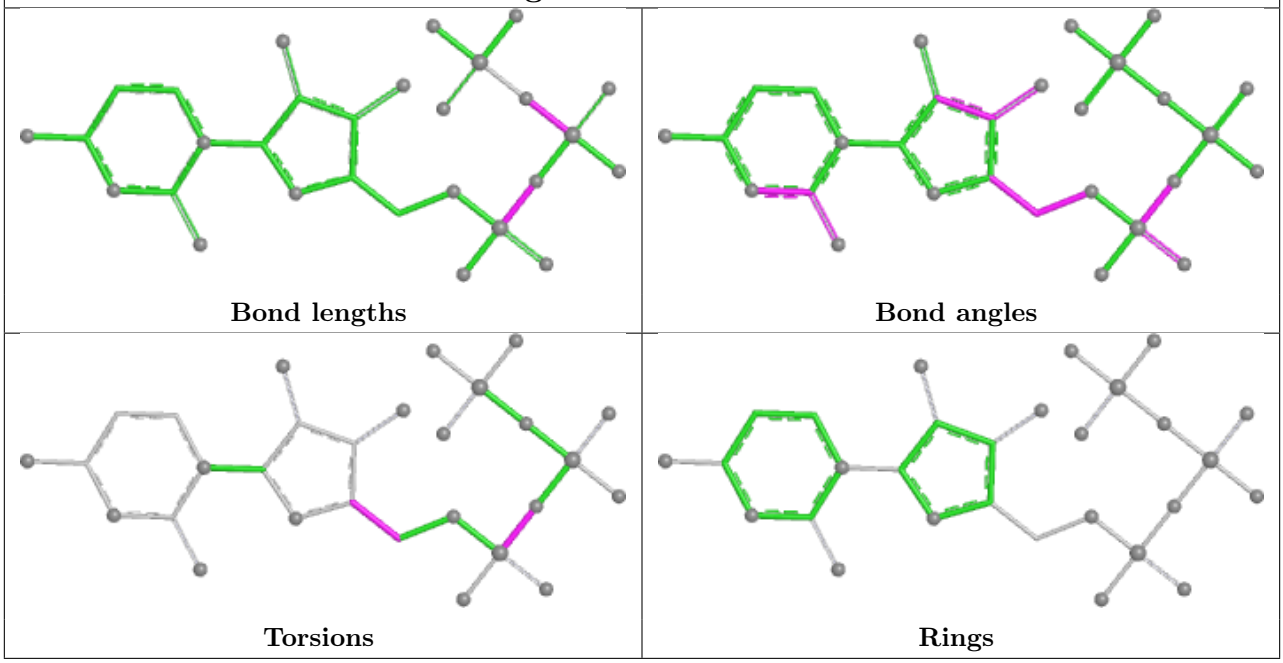


Torsions

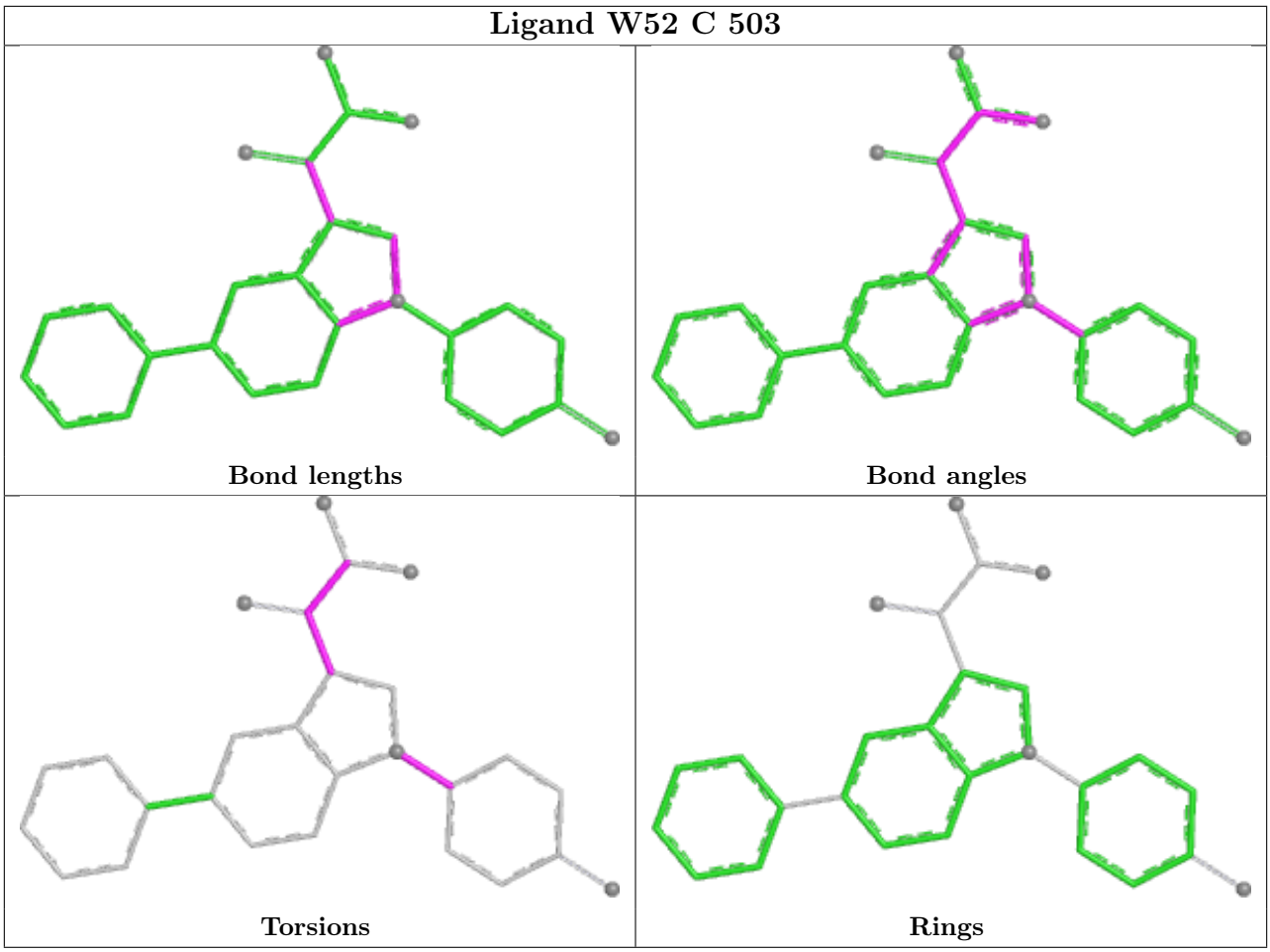


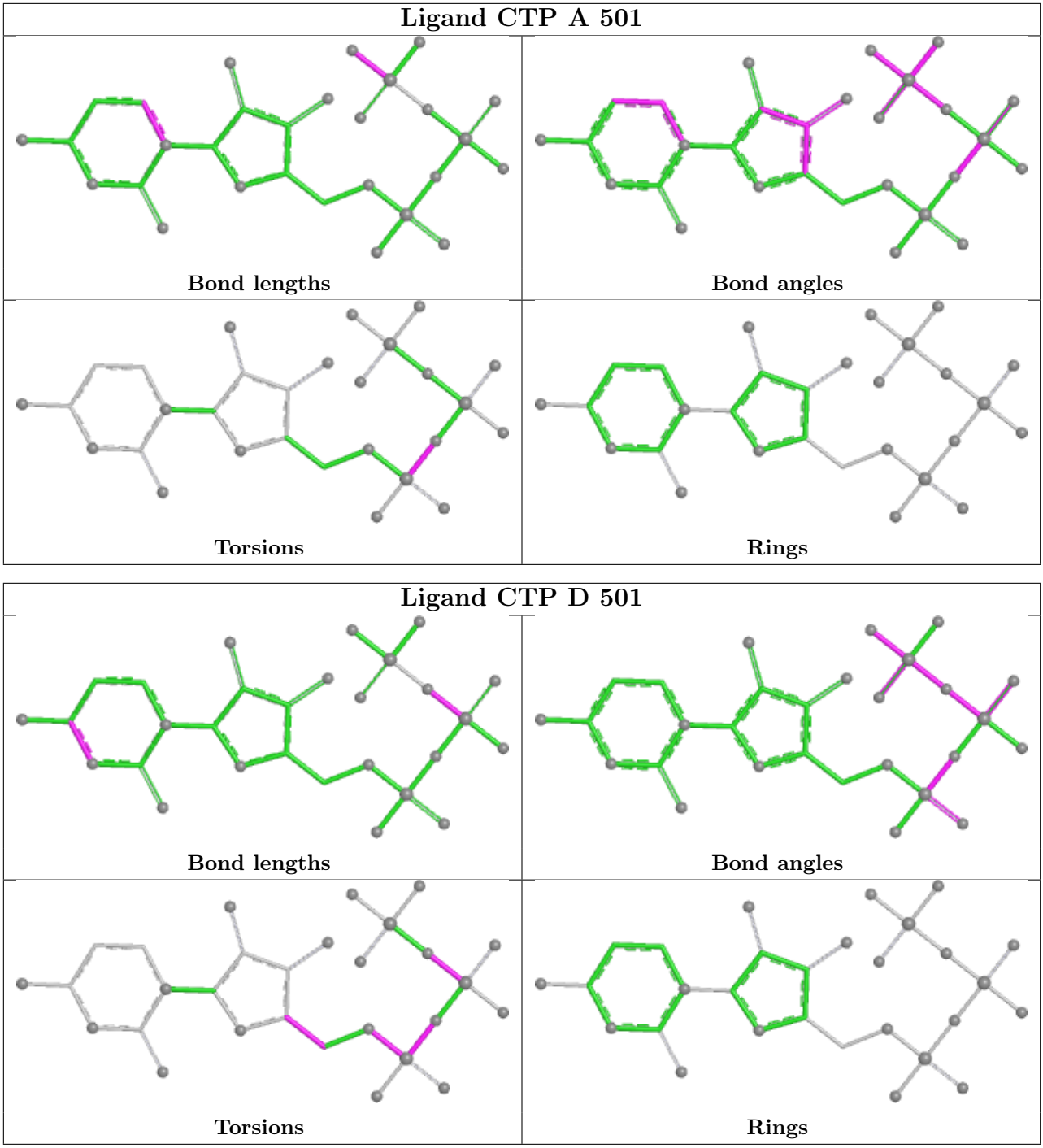
Rings

Ligand CTP B 501



Ligand W52 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, 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	214/237 (90%)	-1.16	0	100	100	23, 33, 59, 92	0
1	B	209/237 (88%)	-1.03	0	100	100	25, 37, 80, 102	0
1	C	208/237 (87%)	-0.99	0	100	100	25, 40, 73, 101	0
1	D	217/237 (91%)	-0.98	0	100	100	25, 41, 72, 101	0
All	All	848/948 (89%)	-1.04	0	100	100	23, 38, 74, 102	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	W52	A	504	27/27	0.98	0.05	30,42,52,54	0
2	CTP	B	501	29/29	0.99	0.03	22,31,69,71	0
2	CTP	C	501	29/29	0.99	0.03	18,32,59,65	0
2	CTP	D	501	29/29	0.99	0.03	25,37,50,55	0

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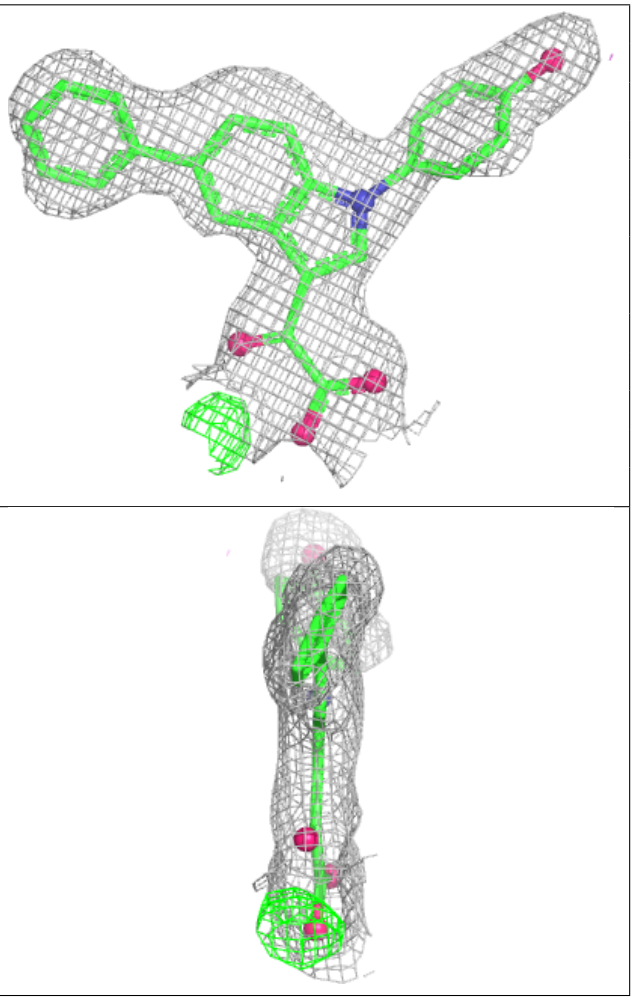
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	A	502	1/1	0.99	0.03	50,50,50,50	0
3	CA	B	502	1/1	0.99	0.02	54,54,54,54	0
4	W52	A	503	27/27	0.99	0.03	27,32,42,50	0
2	CTP	A	501	29/29	0.99	0.03	18,26,46,48	0
4	W52	C	503	27/27	0.99	0.04	38,49,61,64	0
5	ACT	C	504	4/4	0.99	0.04	32,32,35,37	0
3	CA	C	502	1/1	1.00	0.03	63,63,63,63	0
3	CA	D	502	1/1	1.00	0.02	38,38,38,38	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.

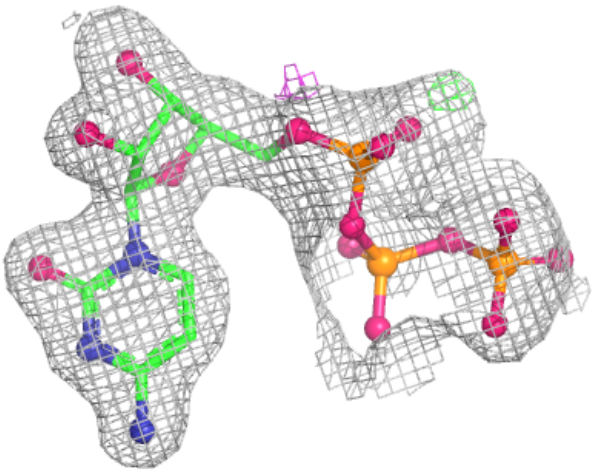
Electron density around W52 A 504:

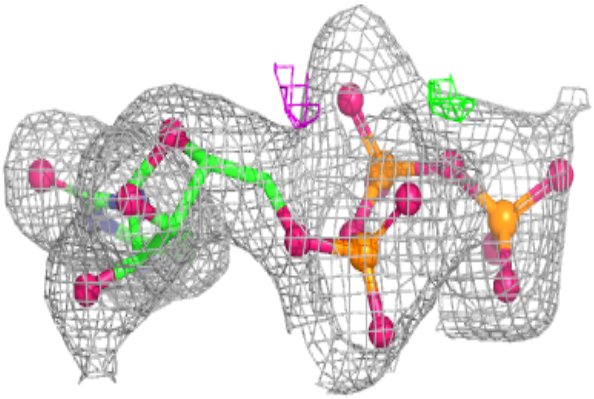
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

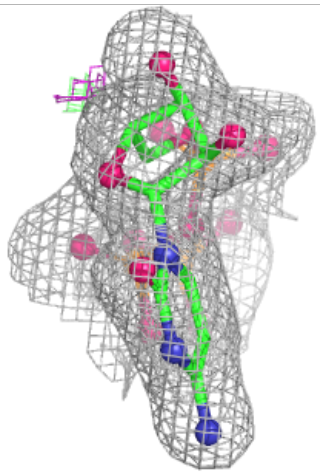


Electron density around CTP B 501:

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

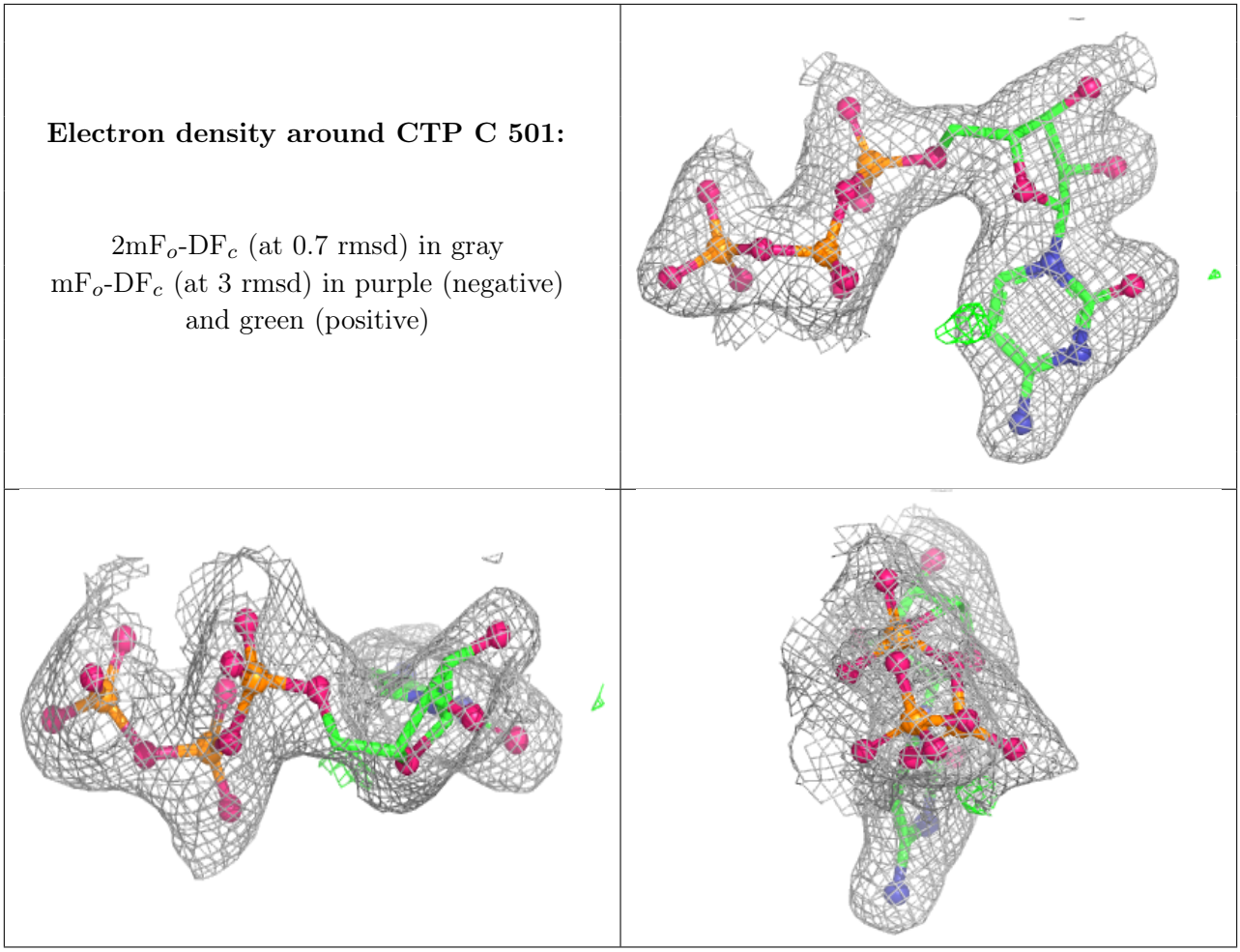






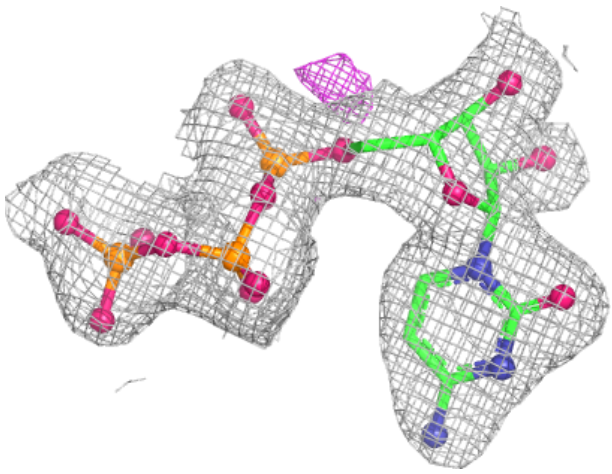
Electron density around CTP C 501:

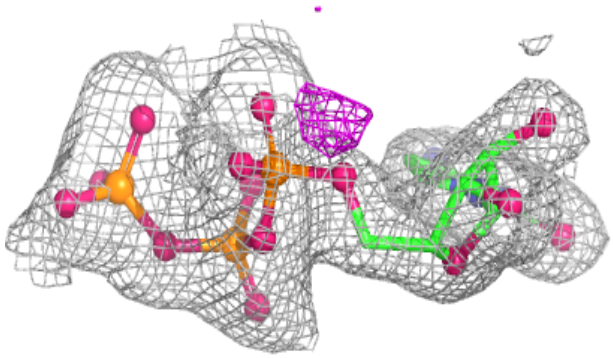
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

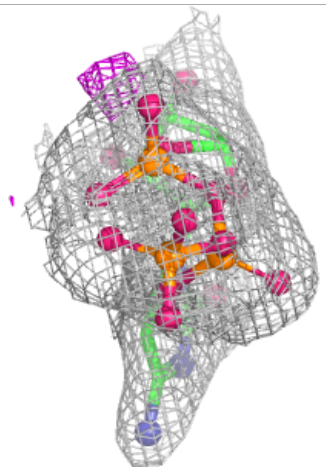


Electron density around CTP D 501:

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

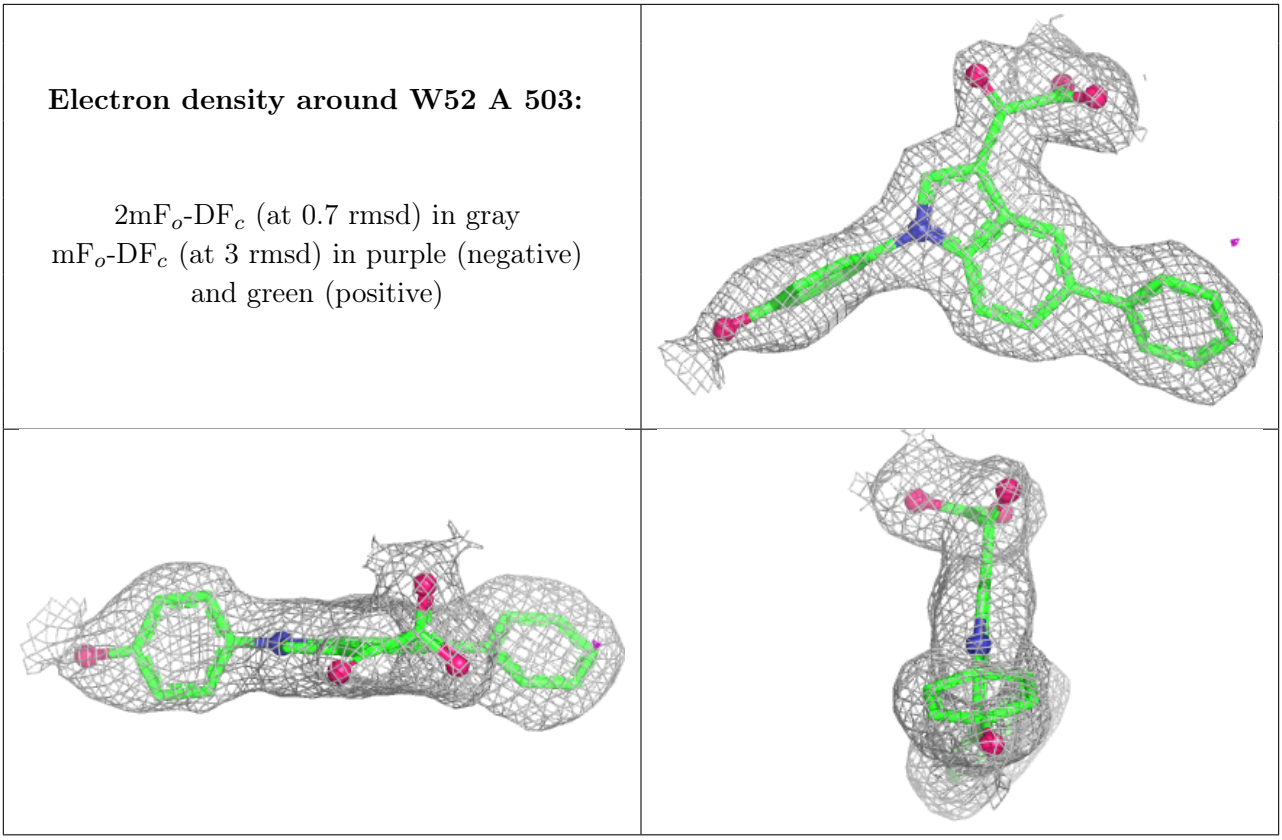






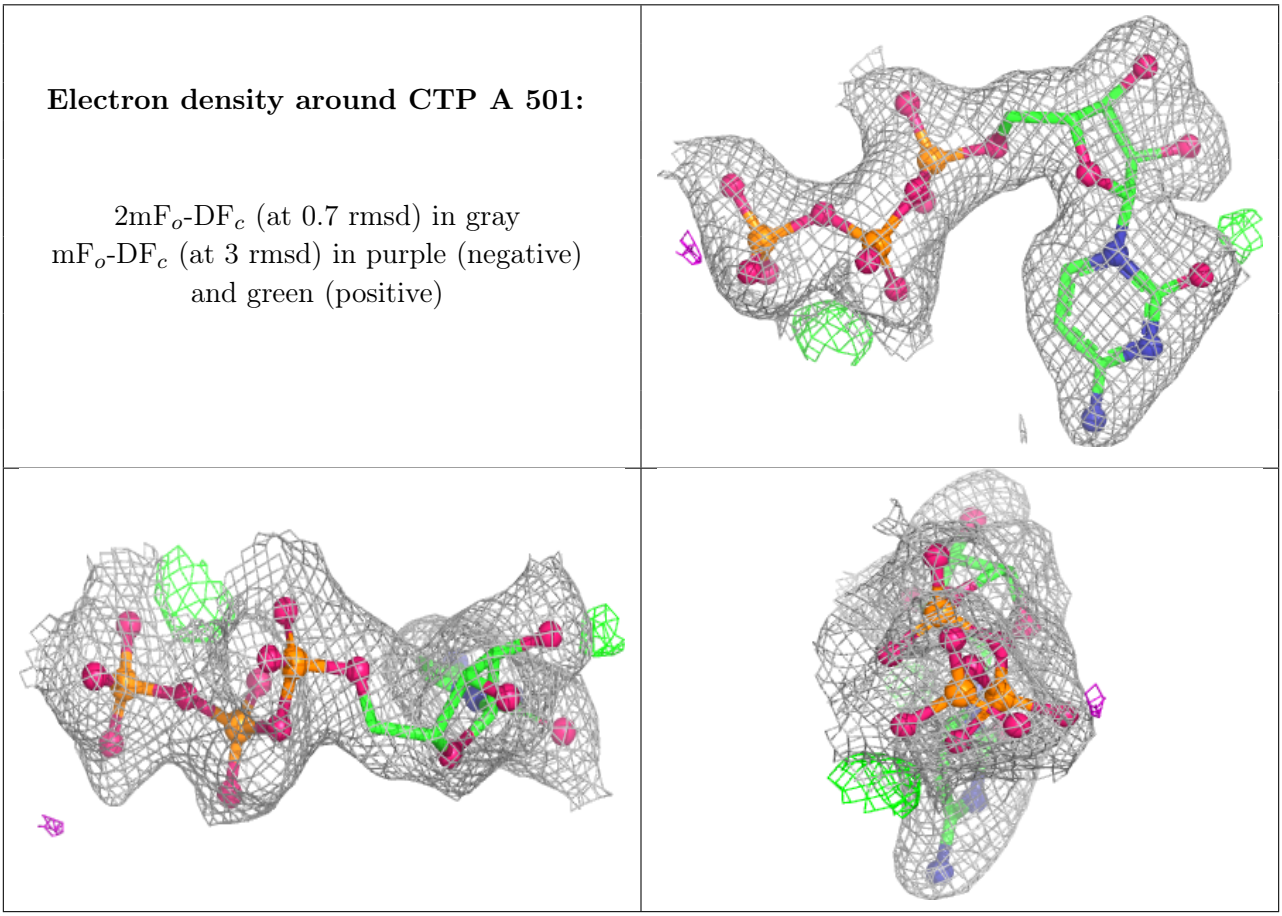
Electron density around W52 A 503:

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



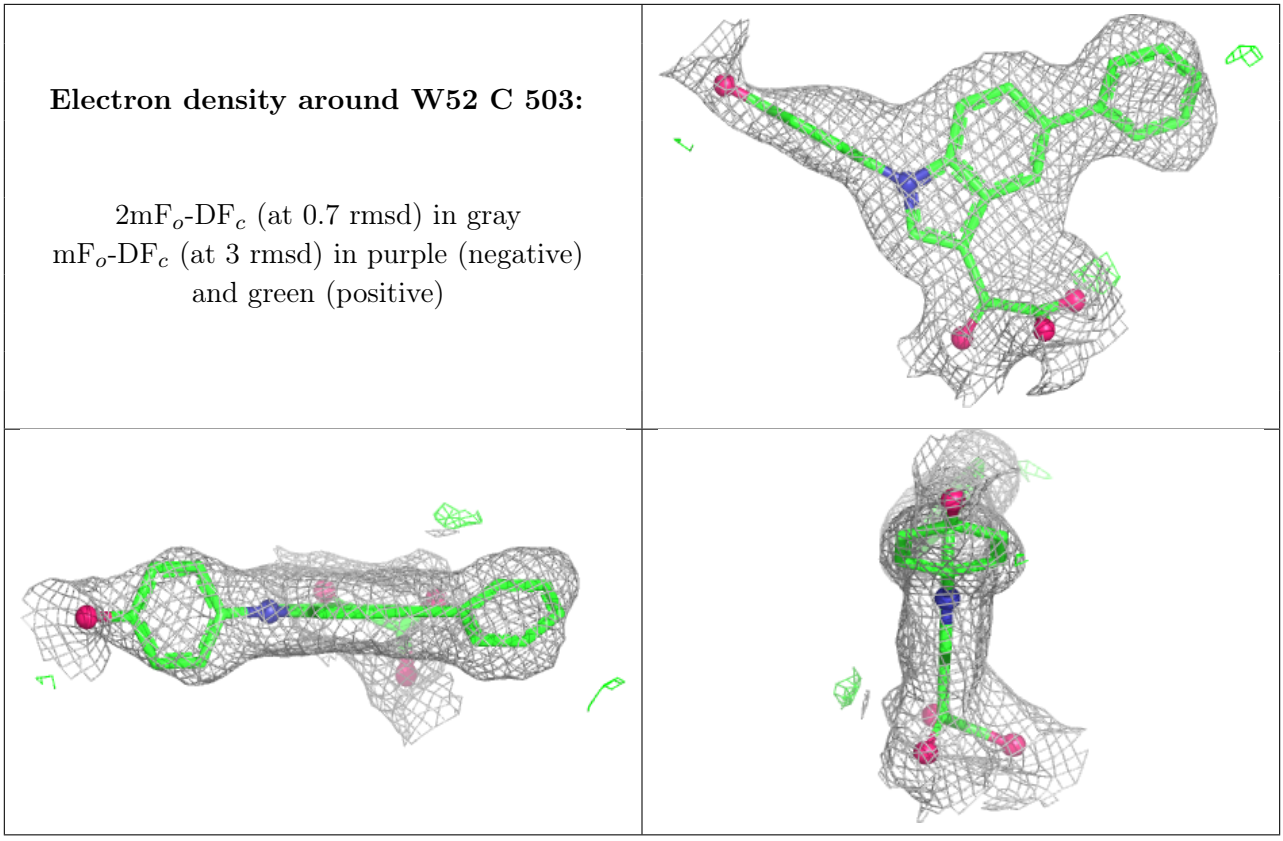
Electron density around CTP A 501:

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



Electron density around W52 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)



6.5 Other polymers (i)

There are no such residues in this entry.