



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:14 AM UTC

PDB ID : 6THC / pdb_00006thc
Title : Crystal structure of Mycobacterium smegmatis CoaB in complex with CTP and (4-hydroxyphenyl)(2,3,4-trihydroxyphenyl)methanone
Authors : Mendes, V.; Blaszczyk, M.; Bryant, O.; Cory-Wright, J.; Blundell, T.L.
Deposited on : 2019-11-19
Resolution : 2.03 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

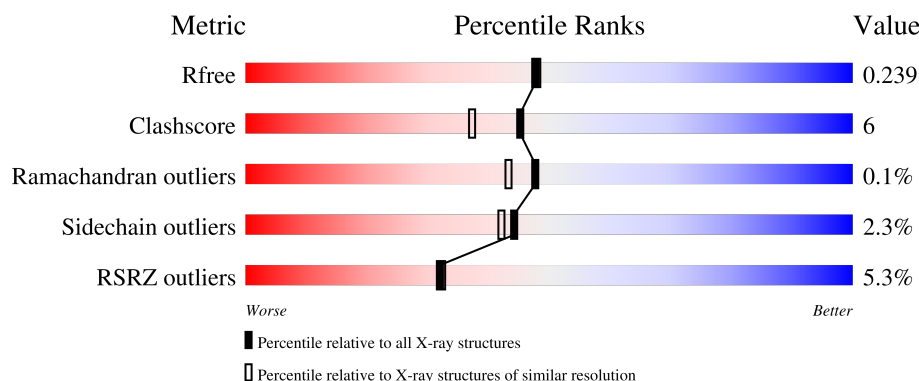
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	5% 81% 8% 10%
1	B	237	7% 81% 12% 6%
1	C	237	3% 83% 6% 10%
1	D	237	5% 83% 11% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6752 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
			1528	950	282	290	6			
1	B	223	Total	C	N	O	S	0	0	0
			1588	990	296	296	6			
1	C	213	Total	C	N	O	S	0	0	0
			1509	935	281	287	6			
1	D	224	Total	C	N	O	S	0	0	0
			1595	992	295	302	6			

There are 32 discrepancies between the modelled and reference sequences:

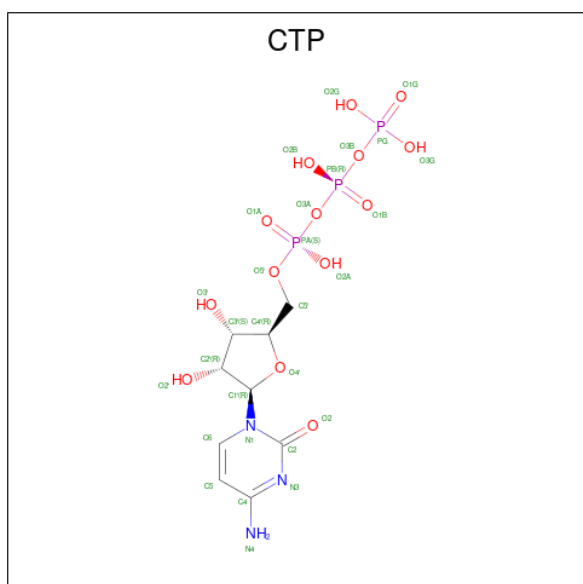
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MET	-	initiating methionine	UNP A0QWT2
A	179	ALA	-	expression tag	UNP A0QWT2
A	180	HIS	-	expression tag	UNP A0QWT2
A	181	HIS	-	expression tag	UNP A0QWT2
A	182	HIS	-	expression tag	UNP A0QWT2
A	183	HIS	-	expression tag	UNP A0QWT2
A	184	HIS	-	expression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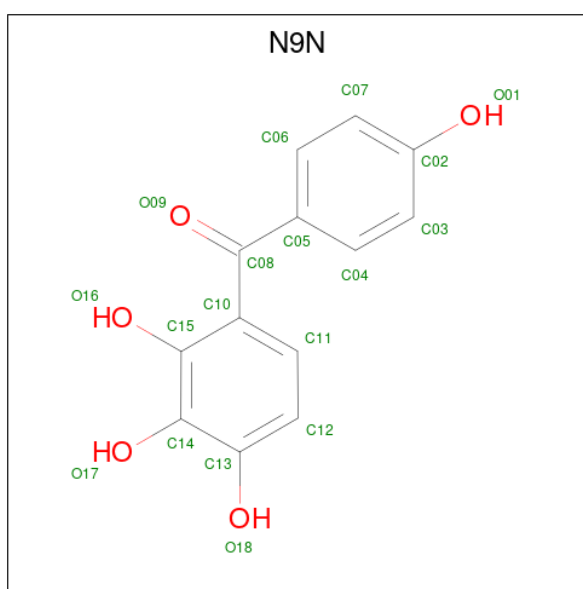
Chain	Residue	Modelled	Actual	Comment	Reference
C	183	HIS	-	expression tag	UNP A0QWT2
C	184	HIS	-	expression tag	UNP A0QWT2
C	185	HIS	-	expression tag	UNP A0QWT2
D	178	MET	-	initiating methionine	UNP A0QWT2
D	179	ALA	-	expression tag	UNP A0QWT2
D	180	HIS	-	expression tag	UNP A0QWT2
D	181	HIS	-	expression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



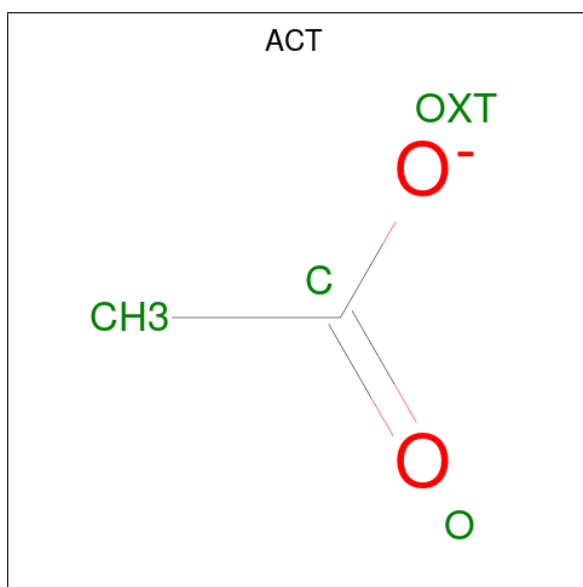
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is (4-hydroxyphenyl)-[2,3,4-tris(oxidanyl)phenyl]methanone (CCD ID: N9N) (formula: C₁₃H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 18 13 5	0	0
4	B	1	Total C O 18 13 5	0	0
4	B	1	Total C O 18 13 5	0	0
4	C	1	Total C O 18 13 5	0	0
4	D	1	Total C O 18 13 5	0	0
4	D	1	Total C O 18 13 5	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

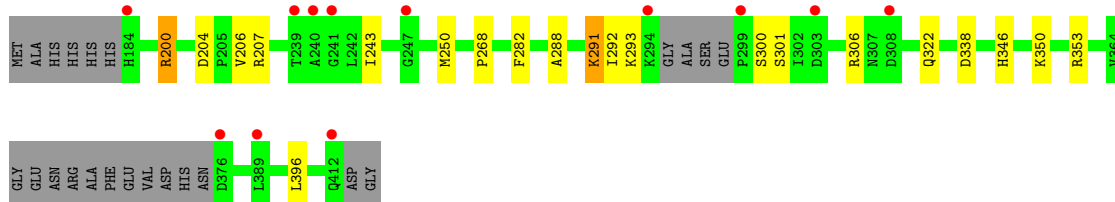


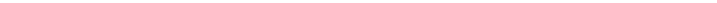
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

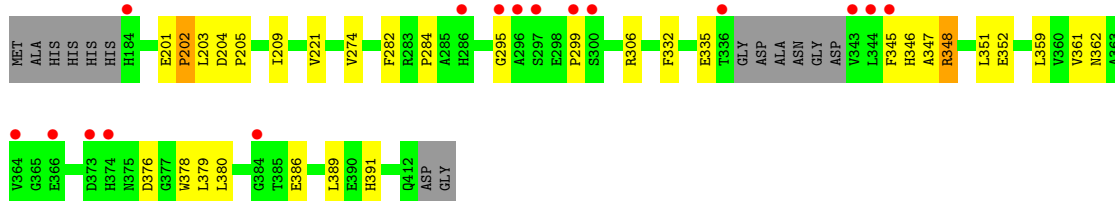
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total	O	0	0
			60	60		
6	B	70	Total	O	0	0
			70	70		
6	C	77	Total	O	0	0
			77	77		
6	D	85	Total	O	0	0
			85	85		

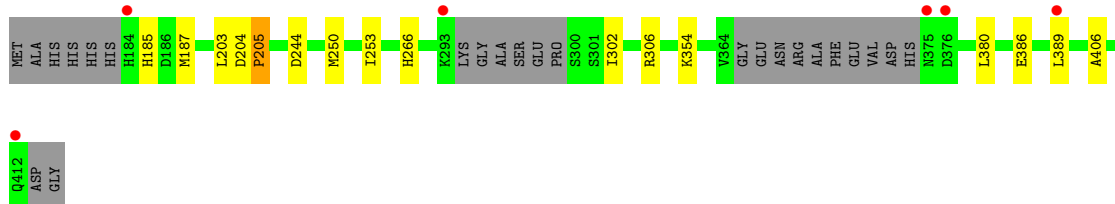
- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



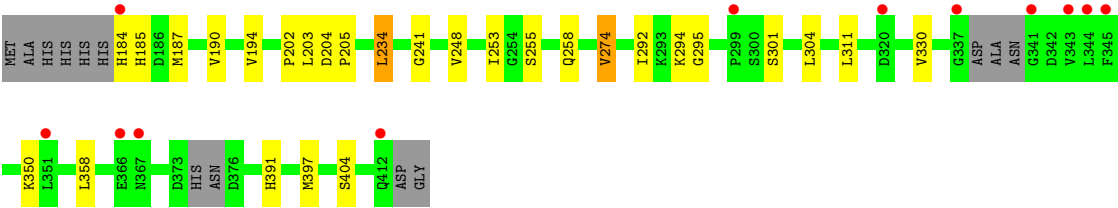
Chain B:  7% 81% 12% 6%



Chain C:  3% 83% 6% 10%



Chain D:  5% 83% 11% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.01Å 77.37Å 144.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.18 – 2.03 72.18 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.18-2.03) 99.9 (72.18-2.03)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.184 , 0.241 0.187 , 0.239	Depositor DCC
R_{free} test set	2793 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.078 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6752	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 5.00% 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, ACT, CA, N9N

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	0.55	1/1546 (0.1%)	0.69	0/2096
1	B	0.50	1/1608 (0.1%)	0.60	1/2181 (0.0%)
1	C	0.42	1/1525 (0.1%)	0.57	1/2070 (0.0%)
1	D	0.55	1/1614 (0.1%)	0.64	1/2187 (0.0%)
All	All	0.51	4/6293 (0.1%)	0.63	3/8534 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	PRO	C-O	-6.37	1.16	1.23
1	B	202	PRO	C-O	-5.81	1.17	1.23
1	A	268	PRO	C-O	-5.34	1.17	1.24
1	C	205	PRO	C-O	-5.32	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	LEU	N-CA-C	-6.34	105.19	113.12
1	C	203	LEU	N-CA-C	-6.18	105.76	113.55
1	B	203	LEU	N-CA-C	-5.61	106.10	113.12

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	1528	0	1519	16	0
1	B	1588	0	1586	30	0
1	C	1509	0	1492	12	0
1	D	1595	0	1584	21	0
2	A	29	0	12	0	0
2	B	29	0	12	1	0
2	C	29	0	12	1	0
2	D	29	0	12	2	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	B	54	0	0	0	0
4	C	18	0	0	1	0
4	D	36	0	0	0	0
5	B	4	0	3	0	0
5	C	8	0	6	0	0
6	A	60	0	0	2	0
6	B	70	0	0	0	0
6	C	77	0	0	1	0
6	D	85	0	0	2	0
All	All	6752	0	6238	75	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 6.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HH21	1:A:200:ARG:HG3	1.41	0.83
1:A:200:ARG:HG3	1:A:200:ARG:NH2	2.00	0.73
1:D:187:MET:O	1:D:190:VAL:HG12	1.91	0.69
1:B:351:LEU:HD13	1:B:351:LEU:C	2.18	0.69
1:D:204:ASP:HB2	1:D:205:PRO:CD	2.23	0.69
1:A:206:VAL:HG23	1:A:207:ARG:HG3	1.76	0.68
1:C:306:ARG:NH2	1:D:295:GLY:O	2.26	0.67
1:B:362:ASN:ND2	1:B:376:ASP:HB3	2.11	0.66
1:C:204:ASP:HB2	1:C:205:PRO:CD	2.26	0.66
1:B:348:ARG:HH12	1:B:386:GLU:CD	2.05	0.65
1:A:306:ARG:NH2	1:B:295:GLY:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ASP:HB2	1:C:205:PRO:HD3	1.81	0.63
1:B:204:ASP:HB2	1:B:205:PRO:CD	2.31	0.61
1:A:350:LYS:HD2	1:A:353:ARG:NH2	2.15	0.61
1:D:253:ILE:C	1:D:253:ILE:HD12	2.26	0.61
1:B:348:ARG:HH11	1:B:348:ARG:CG	2.15	0.60
4:C:503:N9N:C04	1:D:292:ILE:HD13	2.32	0.59
1:D:255:SER:H	1:D:258:GLN:HE21	1.51	0.58
1:B:362:ASN:HD22	1:B:376:ASP:HB3	1.67	0.58
1:D:204:ASP:HB3	1:D:292:ILE:HD12	1.87	0.57
1:B:348:ARG:HH11	1:B:348:ARG:HG3	1.70	0.57
1:B:332:PHE:O	2:B:501:CTP:H5'1	2.05	0.56
1:B:380:LEU:HD22	1:B:386:GLU:HG3	1.86	0.56
1:A:282:PHE:CE2	1:B:299:PRO:HB3	2.41	0.55
1:B:361:VAL:CG2	1:B:378:TRP:HB2	2.37	0.55
1:B:209:ILE:HD12	1:B:284:PRO:HD3	1.87	0.55
1:D:204:ASP:HB2	1:D:205:PRO:HD2	1.88	0.54
1:D:184:HIS:N	6:D:603:HOH:O	2.41	0.54
1:A:207:ARG:HH22	1:A:291:LYS:HD3	1.72	0.53
1:A:346:HIS:HD2	6:A:658:HOH:O	1.92	0.53
1:B:282:PHE:CE2	1:B:306:ARG:HG2	2.43	0.53
1:A:322:GLN:NE2	6:A:604:HOH:O	2.41	0.52
1:B:379:LEU:HG	1:B:389:LEU:HG	1.93	0.51
1:D:187:MET:HE3	1:D:190:VAL:HG11	1.94	0.50
1:C:204:ASP:CB	1:C:205:PRO:CD	2.90	0.50
1:C:354:LYS:HE3	2:C:501:CTP:H5'2	1.94	0.50
1:B:376:ASP:H	1:B:391:HIS:HE1	1.60	0.49
1:D:255:SER:H	1:D:258:GLN:NE2	2.10	0.49
1:A:200:ARG:HH21	1:A:200:ARG:CG	2.13	0.49
1:A:204:ASP:HB3	1:A:292:ILE:HD13	1.95	0.48
1:B:351:LEU:C	1:B:351:LEU:CD1	2.85	0.48
1:B:202:PRO:O	1:B:284:PRO:HG2	2.14	0.48
1:B:348:ARG:CG	1:B:348:ARG:NH1	2.73	0.48
1:B:201:GLU:HB3	1:B:284:PRO:HD2	1.95	0.48
1:C:187:MET:CE	1:C:406:ALA:HB2	2.45	0.47
1:D:204:ASP:CB	1:D:205:PRO:CD	2.91	0.47
1:B:348:ARG:HH12	1:B:386:GLU:CG	2.27	0.47
1:A:288:ALA:HB3	1:A:292:ILE:HD11	1.97	0.46
1:C:244:ASP:CG	1:C:250:MET:HG3	2.41	0.46
1:D:253:ILE:HD12	1:D:253:ILE:O	2.15	0.46
1:B:204:ASP:HB2	1:B:205:PRO:HD3	1.97	0.46
1:C:302:ILE:HG13	1:D:304:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:LEU:HD22	1:C:386:GLU:HG2	1.97	0.45
1:B:347:ALA:HB1	1:B:361:VAL:HG11	1.99	0.45
1:D:204:ASP:HB2	1:D:205:PRO:HD3	1.98	0.45
1:B:351:LEU:HD23	1:B:359:LEU:HB2	2.00	0.44
1:D:350:LYS:NZ	2:D:501:CTP:O2A	2.41	0.44
1:D:194:VAL:HG22	1:D:274:VAL:HG13	2.00	0.44
1:A:250:MET:HE3	1:A:250:MET:HB3	1.90	0.44
1:B:204:ASP:CB	1:B:205:PRO:CD	2.95	0.43
1:C:253:ILE:HD12	1:C:253:ILE:C	2.44	0.43
1:B:345:PHE:CG	1:B:346:HIS:N	2.86	0.43
1:D:241:GLY:HA3	6:D:676:HOH:O	2.19	0.42
1:A:293:LYS:NZ	1:B:335:GLU:OE1	2.53	0.42
1:B:221:VAL:HG11	1:B:274:VAL:HG11	2.02	0.42
1:C:266:HIS:HE1	6:C:632:HOH:O	2.02	0.41
1:A:338:ASP:OD1	1:A:346:HIS:HE1	2.03	0.41
1:C:389:LEU:HD23	1:C:389:LEU:HA	1.96	0.41
1:D:391:HIS:HA	1:D:397:MET:HE3	2.03	0.41
1:B:351:LEU:HD12	1:B:352:GLU:HG3	2.02	0.41
1:D:234:LEU:HB2	1:D:248:VAL:CG1	2.51	0.41
2:D:501:CTP:H6	2:D:501:CTP:H5'1	1.85	0.41
1:A:288:ALA:CB	1:A:292:ILE:HD11	2.51	0.40
1:D:330:VAL:HG22	1:D:358:LEU:HD13	2.03	0.40
1:B:348:ARG:NH2	1:B:386:GLU:OE2	2.54	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%)	202 (97%)	5 (2%)	1 (0%)	24	16
1	B	219/237 (92%)	215 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	207/237 (87%)	203 (98%)	4 (2%)	0	100	100
1	D	218/237 (92%)	211 (97%)	7 (3%)	0	100	100
All	All	852/948 (90%)	831 (98%)	20 (2%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	147/173 (85%)	142 (97%)	5 (3%)	32	27
1	B	152/173 (88%)	151 (99%)	1 (1%)	76	80
1	C	144/173 (83%)	143 (99%)	1 (1%)	76	80
1	D	153/173 (88%)	146 (95%)	7 (5%)	24	18
All	All	596/692 (86%)	582 (98%)	14 (2%)	44	42

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	243	ILE
1	A	291	LYS
1	A	301	SER
1	A	396	LEU
1	B	348	ARG
1	C	185	HIS
1	D	185	HIS
1	D	234	LEU
1	D	274	VAL
1	D	294	LYS

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Mol	Chain	Res	Type
1	D	301	SER
1	D	311	LEU
1	D	404	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	238	ASN
1	A	286	HIS
1	A	340	ASN
1	A	346	HIS
1	B	185	HIS
1	B	322	GLN
1	B	374	HIS
1	C	252	HIS
1	C	322	GLN
1	D	217	GLN
1	D	258	GLN
1	D	367	ASN
1	D	391	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
2	CTP	B	501	3	29,30,30	0.86	1 (3%)	43,47,47	0.72	0
5	ACT	B	506	-	3,3,3	0.86	0	3,3,3	1.25	0
4	N9N	D	503	-	19,19,19	1.15	3 (15%)	27,27,27	0.62	0
2	CTP	A	501	3	29,30,30	1.36	5 (17%)	43,47,47	0.60	1 (2%)
5	ACT	C	504	-	3,3,3	0.79	0	3,3,3	1.39	0
4	N9N	C	503	-	19,19,19	1.30	2 (10%)	27,27,27	0.79	0
5	ACT	C	505	-	3,3,3	0.72	0	3,3,3	1.32	0
4	N9N	B	504	-	19,19,19	1.20	2 (10%)	27,27,27	0.60	0
2	CTP	C	501	3	29,30,30	1.43	4 (13%)	43,47,47	0.92	3 (6%)
4	N9N	D	504	-	19,19,19	1.23	3 (15%)	27,27,27	0.91	1 (3%)
2	CTP	D	501	3	29,30,30	1.20	2 (6%)	43,47,47	0.72	0
4	N9N	B	505	-	19,19,19	1.21	3 (15%)	27,27,27	0.87	1 (3%)
4	N9N	B	503	-	19,19,19	1.27	3 (15%)	27,27,27	1.04	1 (3%)

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	B	501	3	-	5/22/38/38	0/2/2/2
4	N9N	D	503	-	-	4/8/8/8	0/2/2/2
2	CTP	A	501	3	-	1/22/38/38	0/2/2/2
4	N9N	C	503	-	-	4/8/8/8	0/2/2/2
4	N9N	B	504	-	-	4/8/8/8	0/2/2/2
2	CTP	C	501	3	-	2/22/38/38	0/2/2/2
4	N9N	D	504	-	-	0/8/8/8	0/2/2/2
2	CTP	D	501	3	-	3/22/38/38	0/2/2/2
4	N9N	B	505	-	-	0/8/8/8	0/2/2/2
4	N9N	B	503	-	-	4/8/8/8	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	CTP	PG-O3G	-4.13	1.39	1.54
2	D	501	CTP	PA-O3A	-3.73	1.55	1.59
2	A	501	CTP	PG-O2G	-3.35	1.42	1.54
2	C	501	CTP	PB-O2B	-2.71	1.42	1.55
2	C	501	CTP	PG-O2G	-2.64	1.45	1.54
2	A	501	CTP	PA-O3A	-2.64	1.56	1.59
4	C	503	N9N	C05-C08	2.61	1.53	1.49
2	D	501	CTP	PB-O3A	-2.56	1.56	1.59
2	A	501	CTP	PG-O3G	-2.52	1.45	1.54
4	D	504	N9N	C05-C08	2.47	1.53	1.49
4	B	503	N9N	C05-C08	2.46	1.53	1.49
4	B	504	N9N	O09-C08	-2.36	1.18	1.22
4	B	503	N9N	O09-C08	-2.29	1.18	1.22
2	A	501	CTP	PB-O1B	-2.29	1.42	1.50
2	C	501	CTP	PA-O2A	-2.27	1.44	1.55
4	B	505	N9N	C05-C08	2.27	1.53	1.49
4	B	504	N9N	C05-C08	2.24	1.53	1.49
4	B	505	N9N	O18-C13	2.23	1.40	1.36
2	A	501	CTP	PB-O2B	-2.21	1.45	1.55
4	C	503	N9N	O09-C08	-2.16	1.19	1.22
4	D	504	N9N	O09-C08	-2.16	1.19	1.22
4	D	503	N9N	O09-C08	-2.14	1.19	1.22
4	D	504	N9N	O18-C13	2.13	1.40	1.36
4	D	503	N9N	O18-C13	2.10	1.40	1.36
4	D	503	N9N	C05-C08	2.10	1.53	1.49
4	B	503	N9N	O18-C13	2.09	1.40	1.36
4	B	505	N9N	O09-C08	-2.08	1.19	1.22
2	B	501	CTP	PG-O3G	-2.00	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	N9N	C10-C08-C05	3.51	125.17	119.56
2	C	501	CTP	O2A-PA-O3A	2.90	115.10	107.27
4	D	504	N9N	C10-C08-C05	2.38	123.37	119.56
4	B	505	N9N	C10-C08-C05	2.16	123.02	119.56
2	C	501	CTP	O3G-PG-O3B	2.15	111.85	104.64
2	C	501	CTP	O3'-C3'-C4'	-2.05	105.19	111.08
2	A	501	CTP	O2G-PG-O3B	2.03	111.44	104.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	CTP	C5'-O5'-PA-O3A
4	D	503	N9N	C06-C05-C08-O09
4	D	503	N9N	C04-C05-C08-C10
4	D	503	N9N	C06-C05-C08-C10
4	B	503	N9N	C04-C05-C08-O09
4	B	504	N9N	C04-C05-C08-O09
4	D	503	N9N	C04-C05-C08-O09
4	B	504	N9N	C04-C05-C08-C10
4	B	504	N9N	C06-C05-C08-O09
4	C	503	N9N	C06-C05-C08-O09
4	B	504	N9N	C06-C05-C08-C10
4	B	503	N9N	C04-C05-C08-C10
4	B	503	N9N	C06-C05-C08-O09
4	C	503	N9N	C04-C05-C08-O09
4	C	503	N9N	C04-C05-C08-C10
4	C	503	N9N	C06-C05-C08-C10
4	B	503	N9N	C06-C05-C08-C10
2	D	501	CTP	C3'-C4'-C5'-O5'
2	D	501	CTP	O4'-C4'-C5'-O5'
2	A	501	CTP	PB-O3B-PG-O1G
2	C	501	CTP	PA-O3A-PB-O2B
2	B	501	CTP	C5'-O5'-PA-O1A
2	B	501	CTP	PB-O3B-PG-O1G
2	B	501	CTP	PB-O3A-PA-O1A
2	B	501	CTP	PB-O3A-PA-O2A
2	C	501	CTP	PA-O3A-PB-O1B
2	D	501	CTP	PA-O3A-PB-O2B

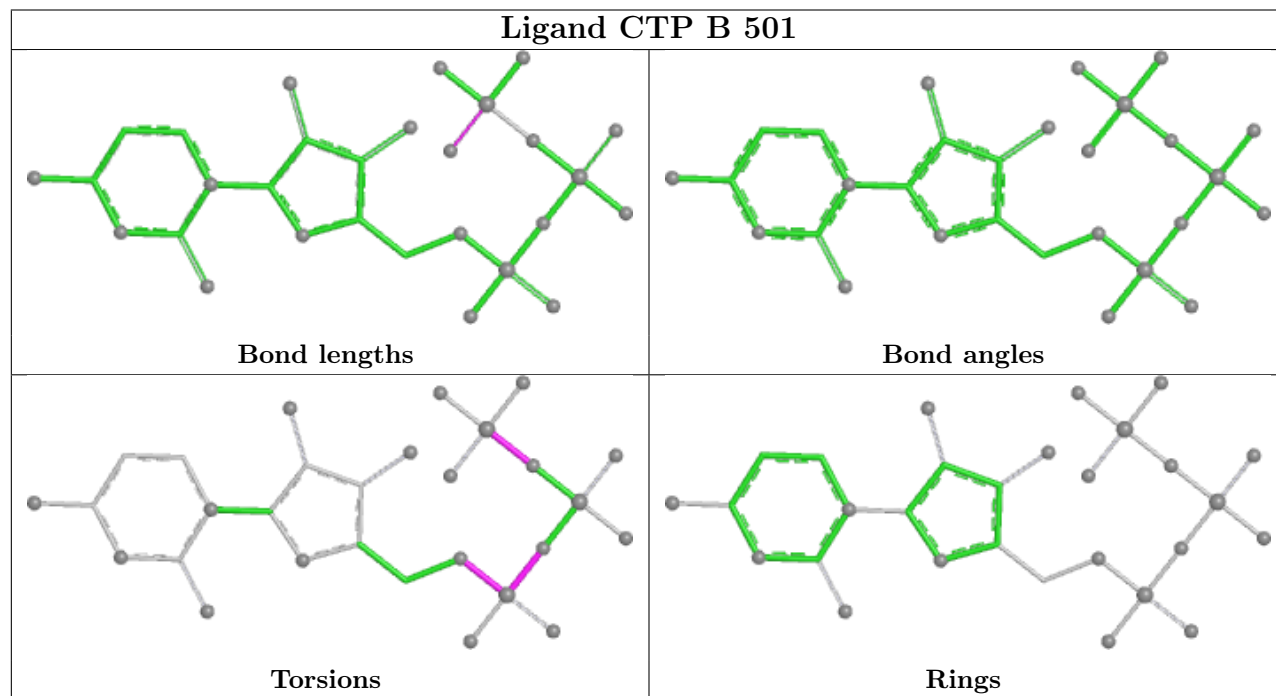
There are no ring outliers.

4 monomers are involved in 5 short contacts:

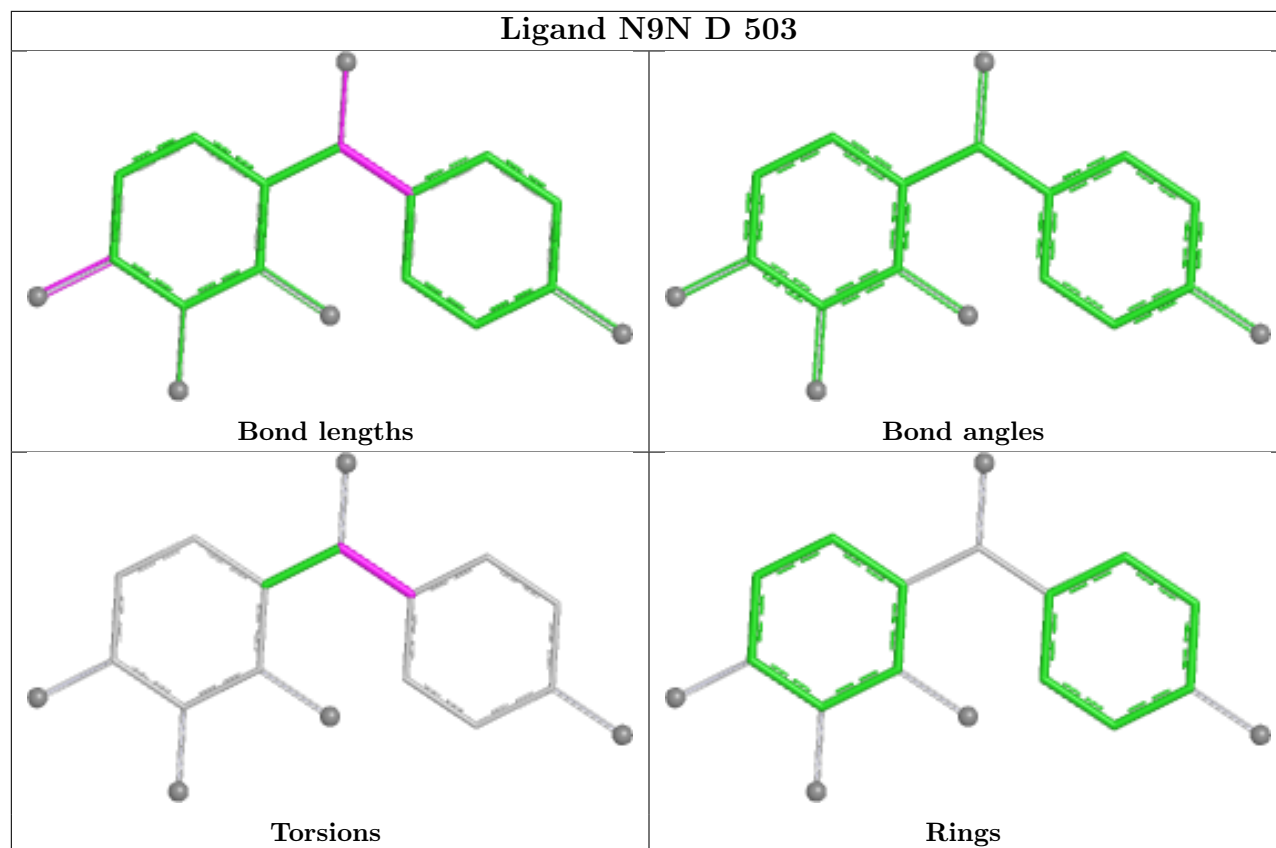
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	CTP	1	0
4	C	503	N9N	1	0
2	C	501	CTP	1	0
2	D	501	CTP	2	0

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

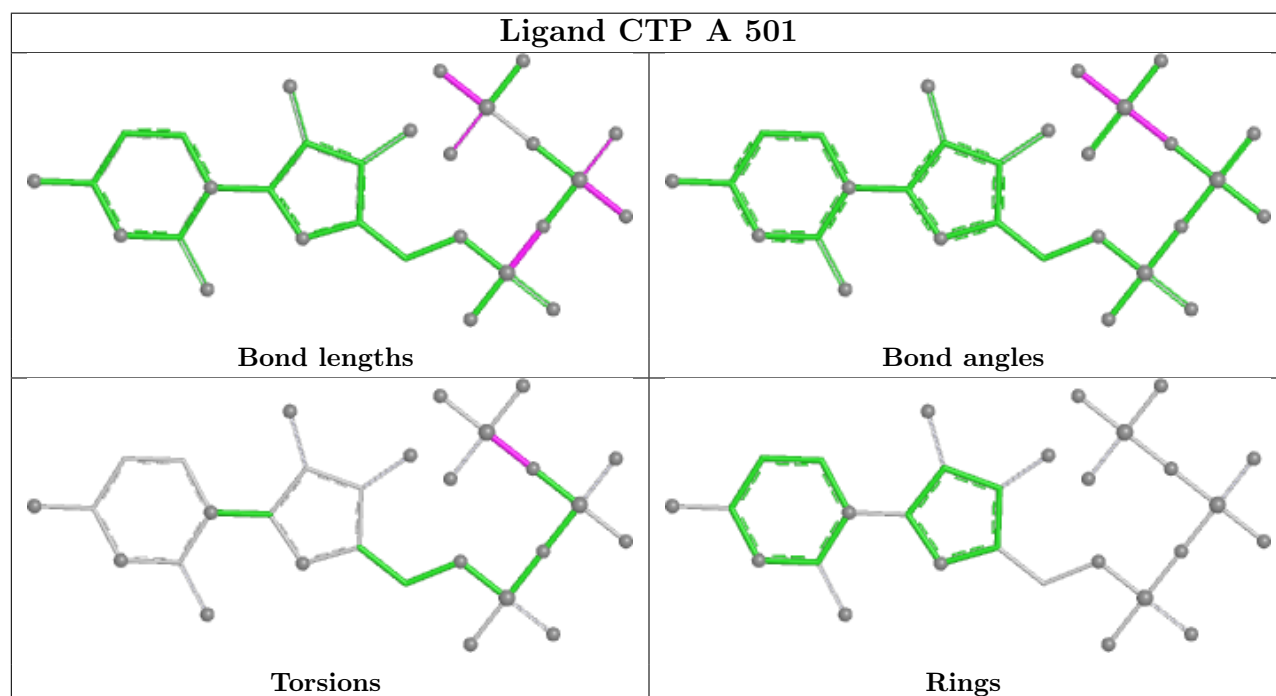
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



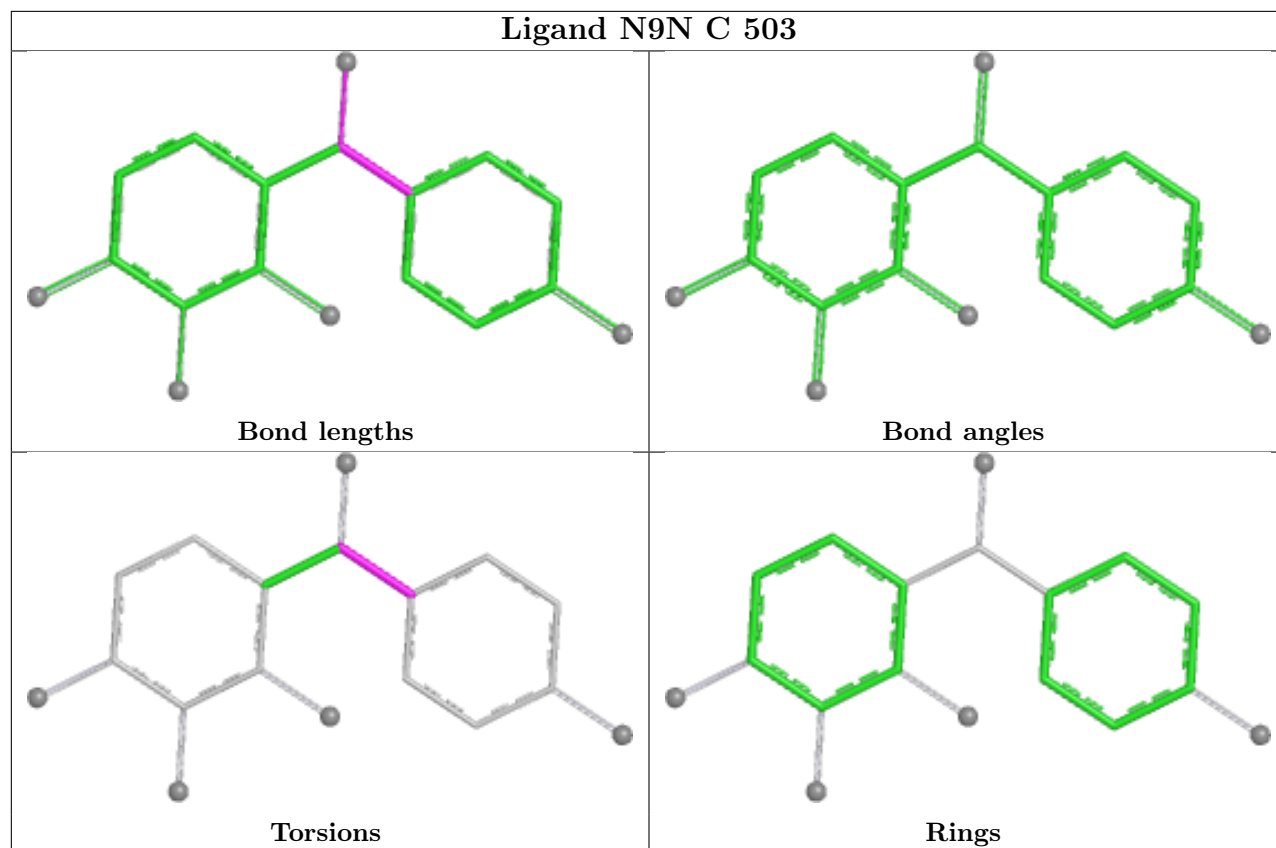
Ligand N9N D 503



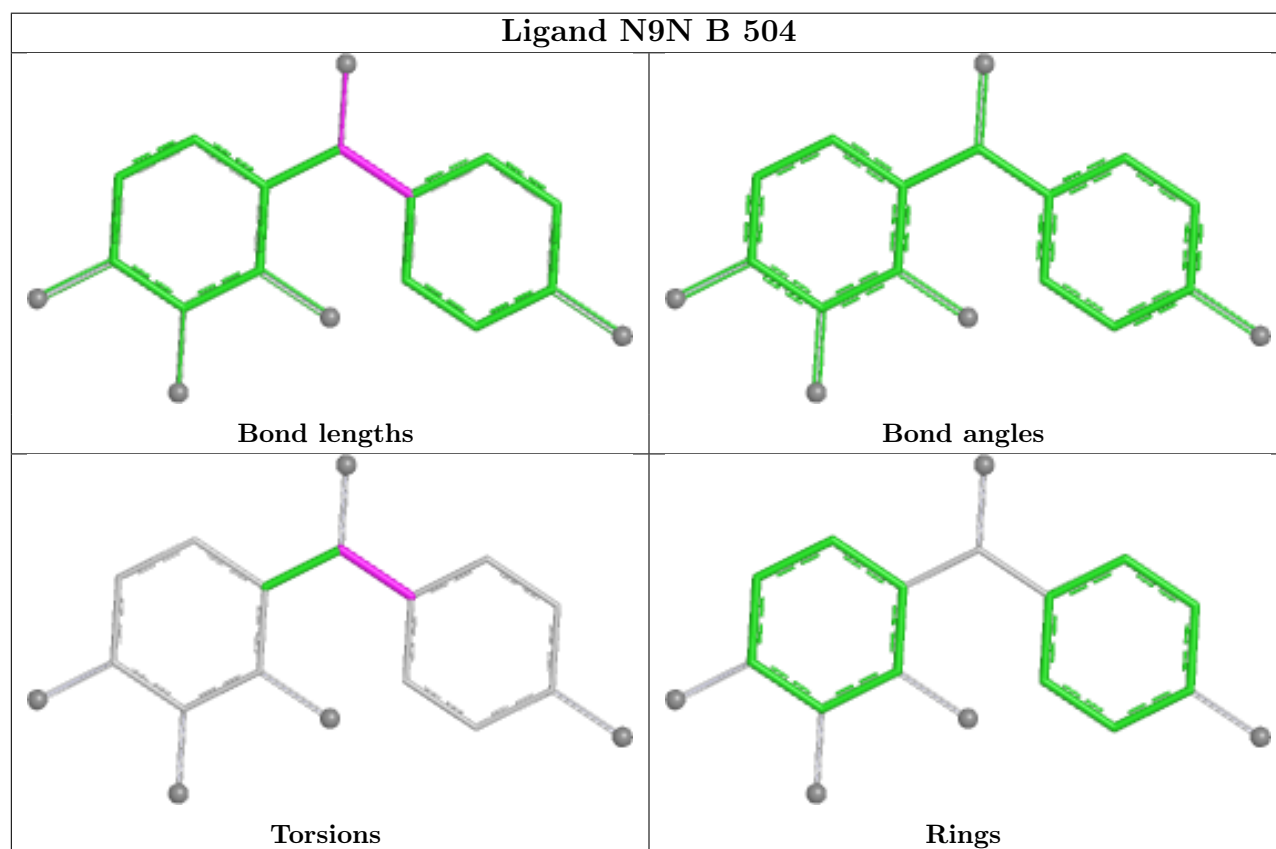
Ligand CTP A 501



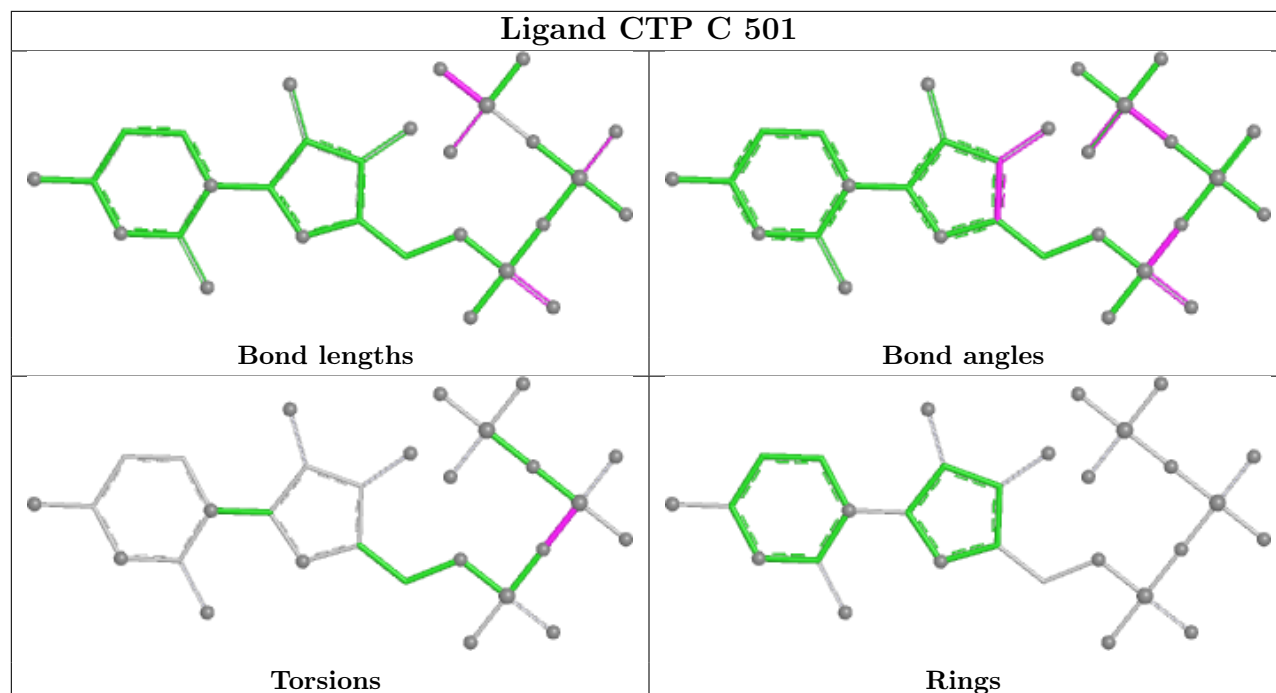
Ligand N9N C 503



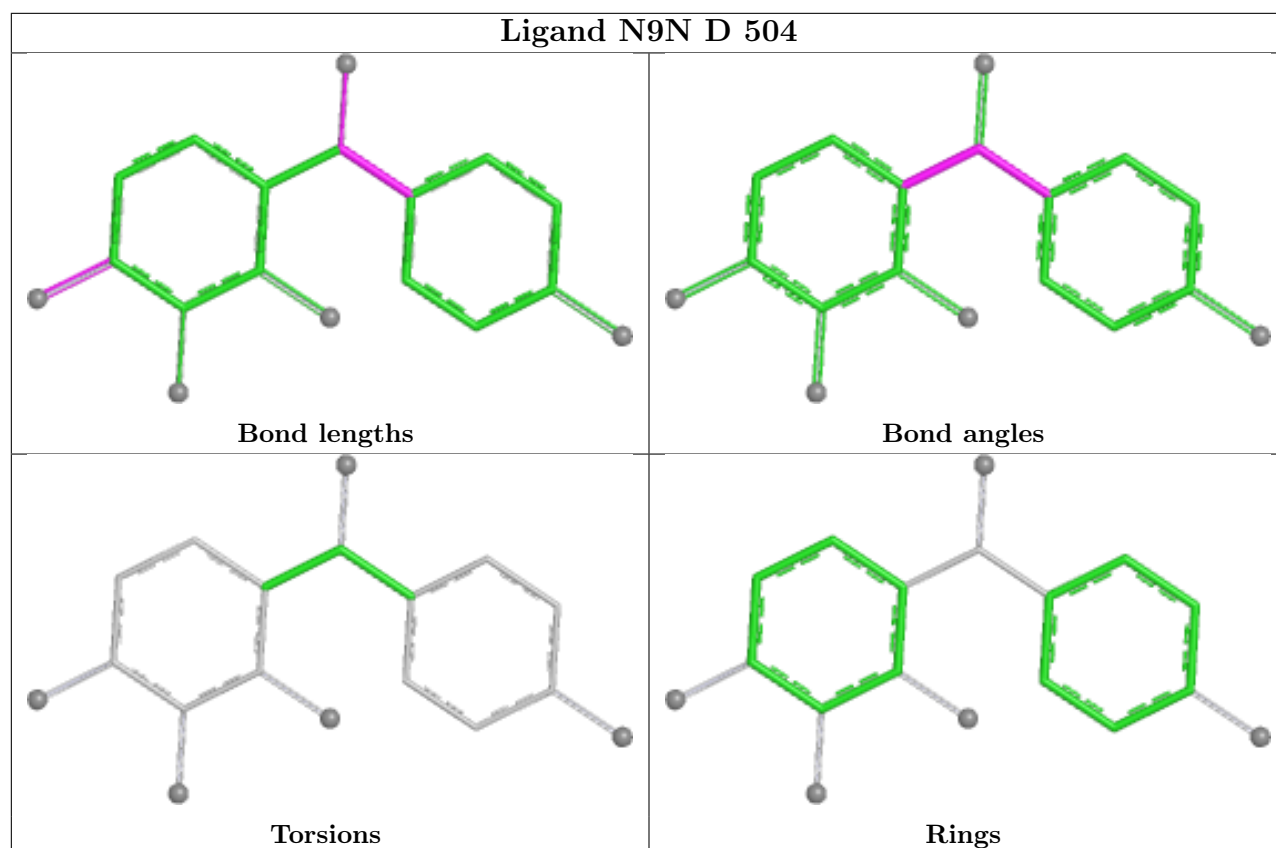
Ligand N9N B 504



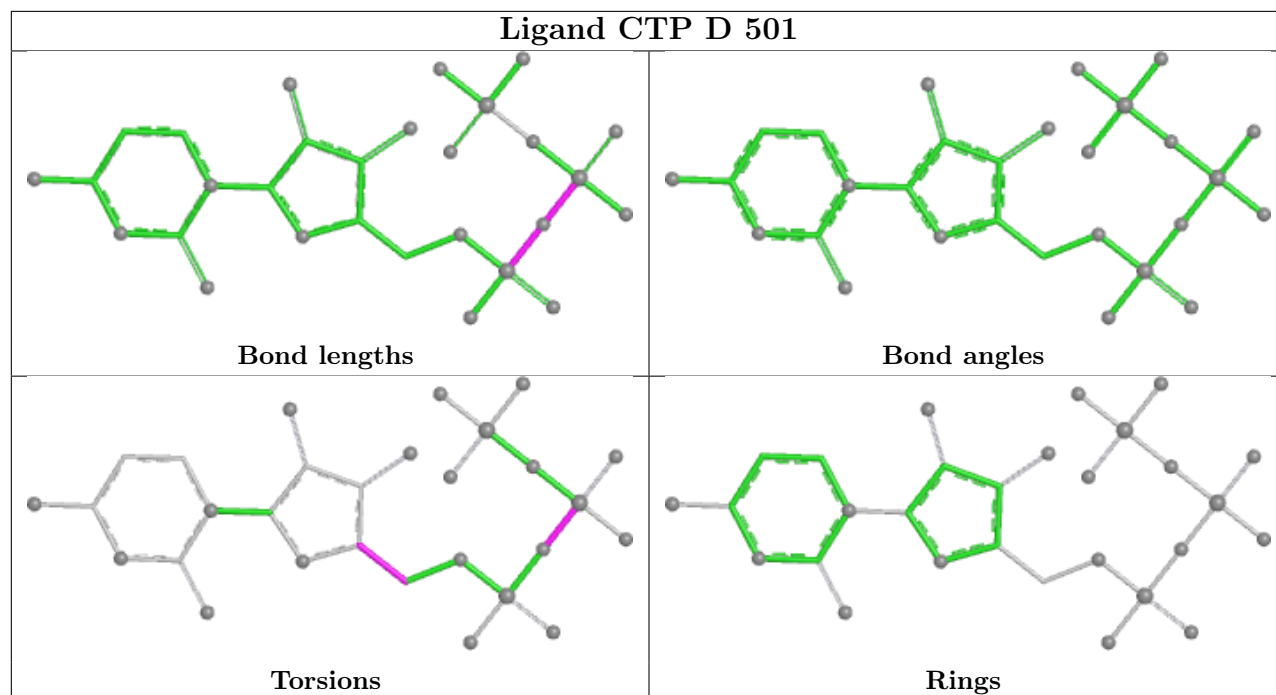
Ligand CTP C 501



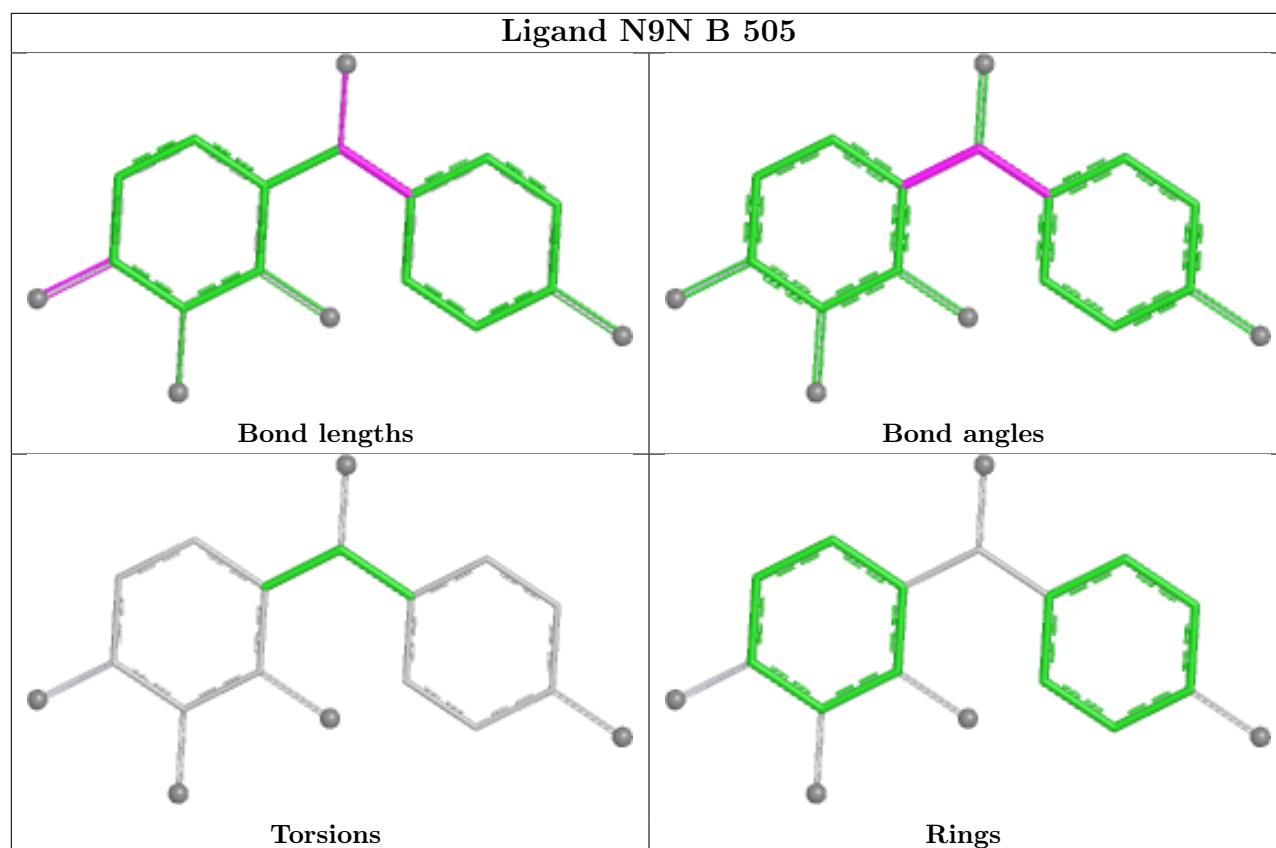
Ligand N9N D 504

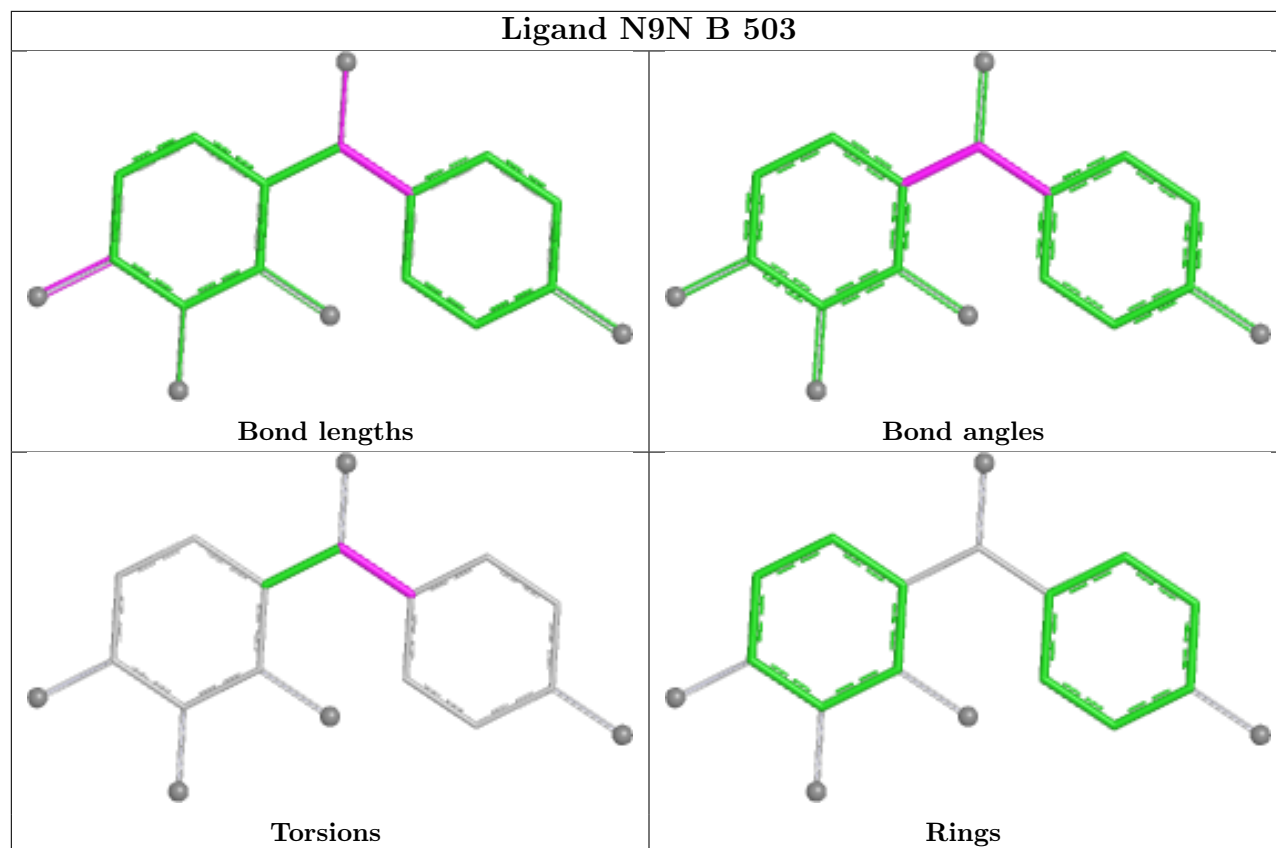


Ligand CTP D 501



Ligand N9N B 505





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	214/237 (90%)	0.21	12 (5%) 30 30	27, 44, 80, 105	0
1	B	223/237 (94%)	0.41	16 (7%) 21 21	28, 46, 105, 129	0
1	C	213/237 (89%)	-0.02	6 (2%) 55 57	24, 37, 78, 121	0
1	D	224/237 (94%)	0.29	12 (5%) 31 31	26, 42, 86, 115	0
All	All	874/948 (92%)	0.22	46 (5%) 32 32	24, 42, 91, 129	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	THR	3.8
1	C	389	LEU	3.8
1	D	299	PRO	3.7
1	B	344	LEU	3.7
1	A	240	ALA	3.6
1	B	366	GLU	3.5
1	D	184	HIS	3.5
1	B	184	HIS	3.4
1	A	184	HIS	3.4
1	D	341	GLY	3.3
1	D	366	GLU	3.3
1	A	299	PRO	3.2
1	B	299	PRO	3.2
1	C	412	GLN	3.1
1	C	375	ASN	3.1
1	B	345	PHE	3.0
1	D	320	ASP	2.7
1	D	412	GLN	2.7
1	B	300	SER	2.7
1	A	389	LEU	2.6
1	B	364	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	294	LYS	2.5
1	B	336	THR	2.5
1	C	376	ASP	2.5
1	B	296	ALA	2.4
1	C	184	HIS	2.4
1	D	344	LEU	2.4
1	B	297	SER	2.3
1	A	412	GLN	2.3
1	D	345	PHE	2.2
1	C	293	LYS	2.2
1	A	247	GLY	2.2
1	D	337	GLY	2.1
1	B	384	GLY	2.1
1	B	343	VAL	2.1
1	D	351	LEU	2.1
1	B	373	ASP	2.1
1	D	343	VAL	2.1
1	A	303	ASP	2.0
1	A	241	GLY	2.0
1	B	295	GLY	2.0
1	D	367	ASN	2.0
1	A	308	ASP	2.0
1	A	376	ASP	2.0
1	B	286	HIS	2.0
1	B	374	HIS	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 ⓘ

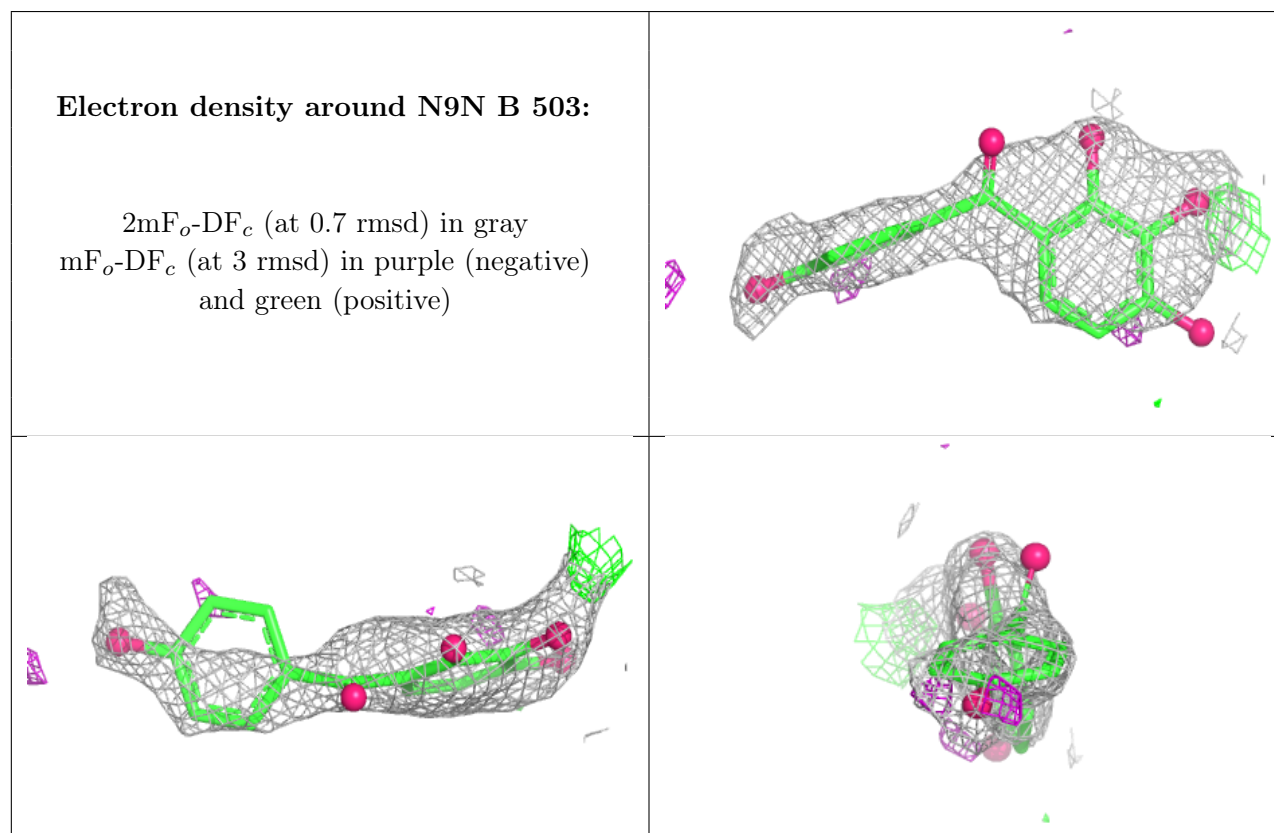
There are no oligosaccharides in this entry.

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, 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.

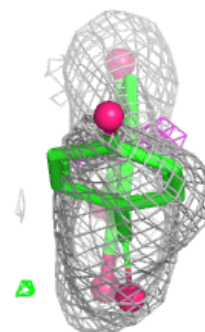
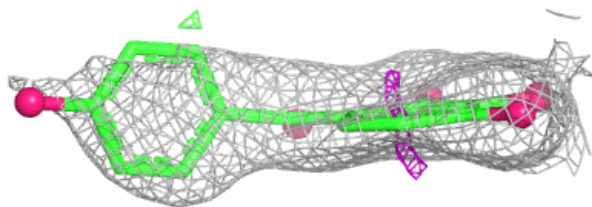
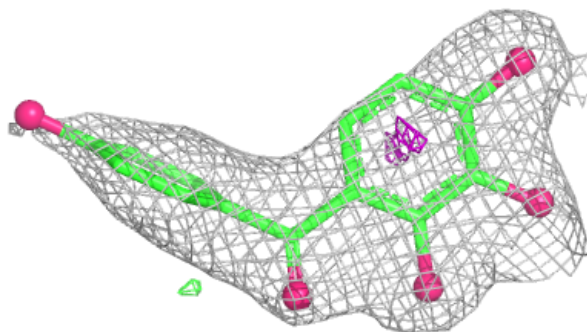
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	N9N	B	503	18/18	0.81	0.17	84,92,102,103	0
5	ACT	B	506	4/4	0.84	0.14	56,62,62,63	0
4	N9N	D	503	18/18	0.88	0.12	42,61,83,87	0
4	N9N	B	504	18/18	0.88	0.12	59,72,101,102	0
4	N9N	D	504	18/18	0.89	0.09	47,58,67,68	0
5	ACT	C	504	4/4	0.89	0.14	51,56,58,63	0
4	N9N	C	503	18/18	0.91	0.11	37,44,69,71	0
5	ACT	C	505	4/4	0.91	0.11	42,43,49,49	0
4	N9N	B	505	18/18	0.92	0.08	44,51,66,68	0
2	CTP	D	501	29/29	0.93	0.08	29,35,86,90	0
2	CTP	B	501	29/29	0.93	0.08	30,37,99,104	0
3	CA	B	502	1/1	0.95	0.06	59,59,59,59	0
2	CTP	A	501	29/29	0.96	0.06	24,33,49,53	0
3	CA	A	502	1/1	0.97	0.04	45,45,45,45	0
2	CTP	C	501	29/29	0.97	0.05	18,27,47,50	0
3	CA	D	502	1/1	0.97	0.04	50,50,50,50	0
3	CA	C	502	1/1	0.98	0.07	40,40,40,40	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.

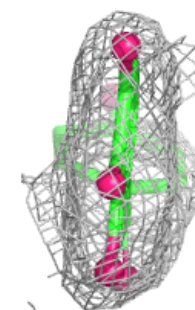
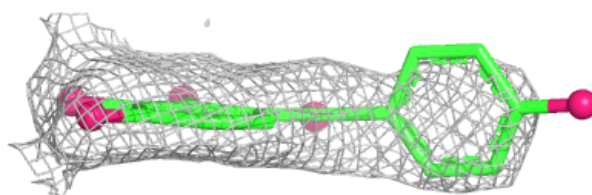
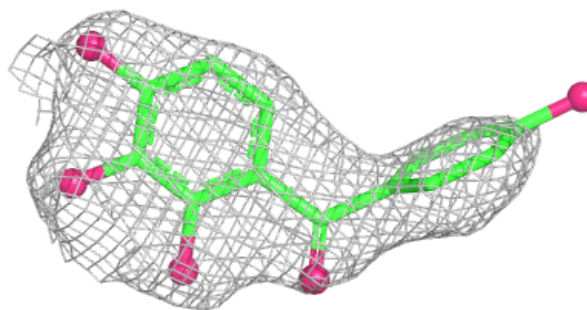


Electron density around N9N D 503:

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

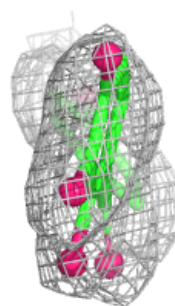
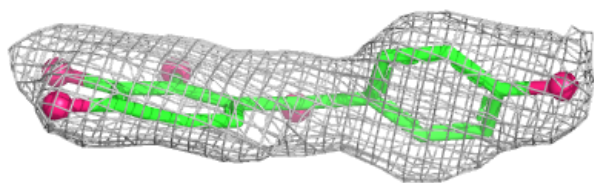
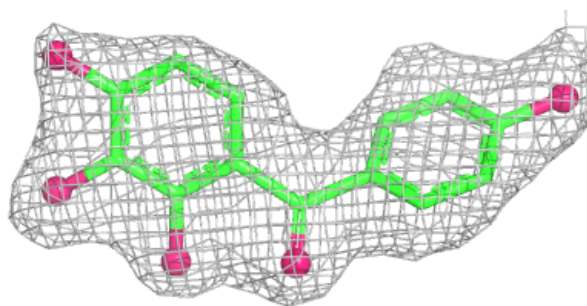
**Electron density around N9N B 504:**

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

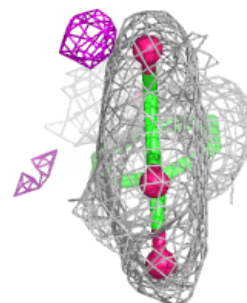
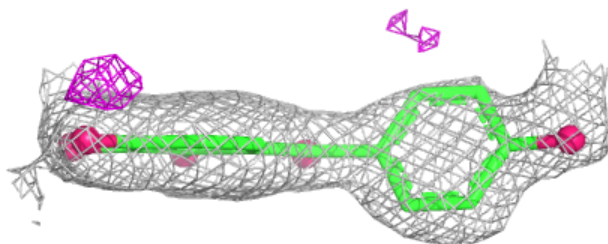
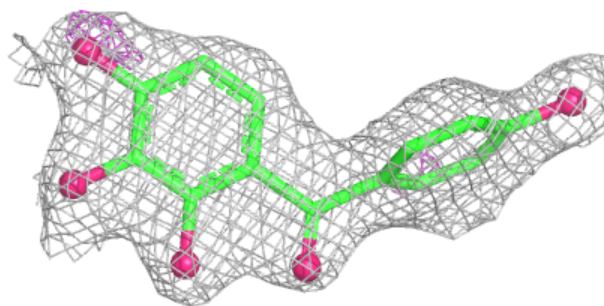


Electron density around N9N D 504:

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

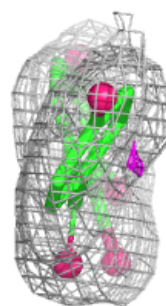
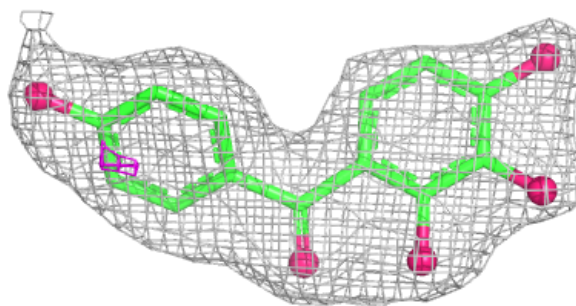
**Electron density around N9N C 503:**

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



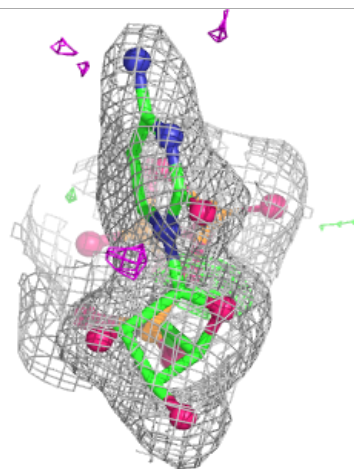
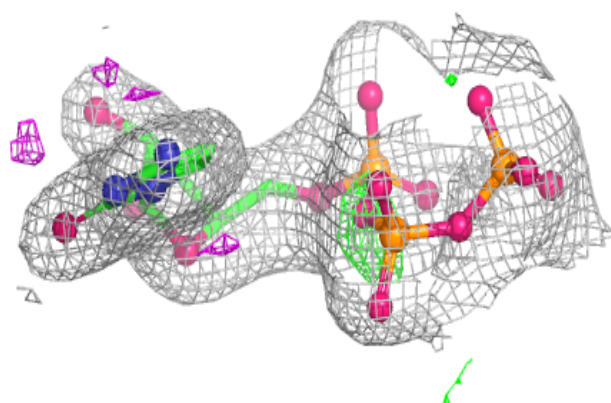
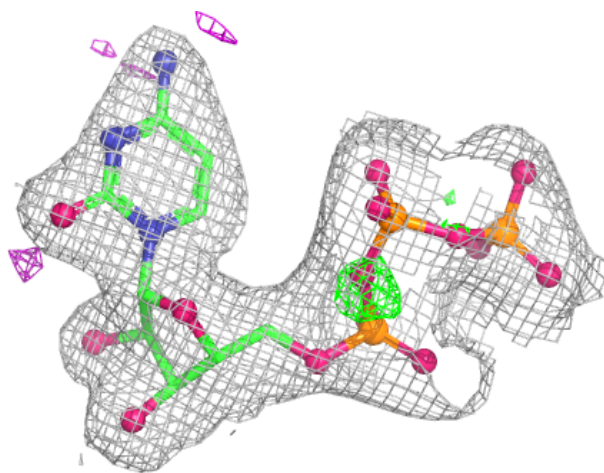
Electron density around N9N B 505:

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



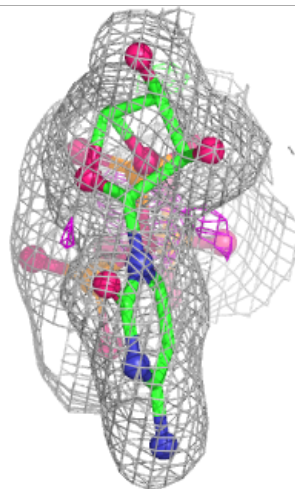
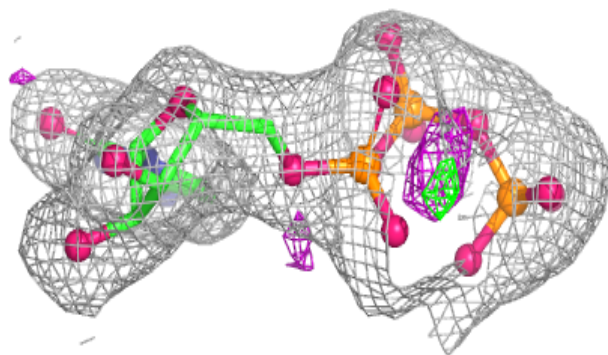
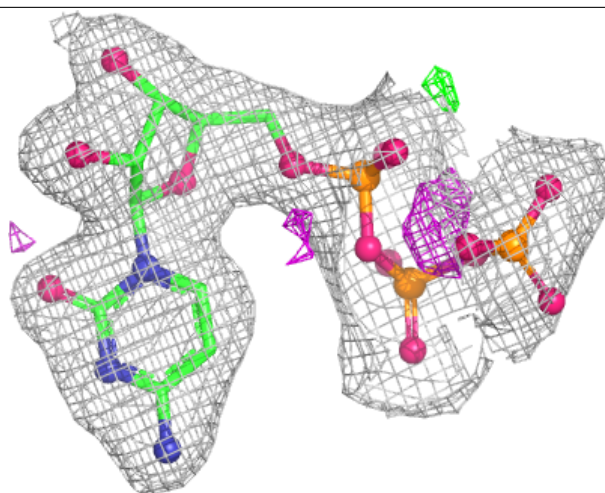
Electron density around CTP D 501:

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



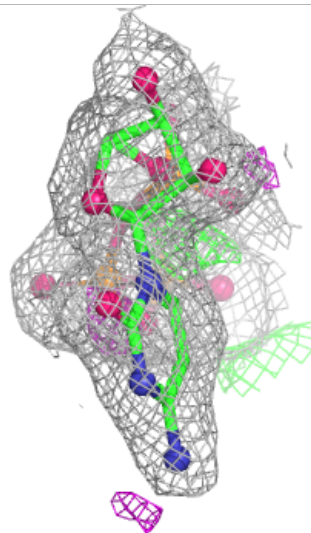
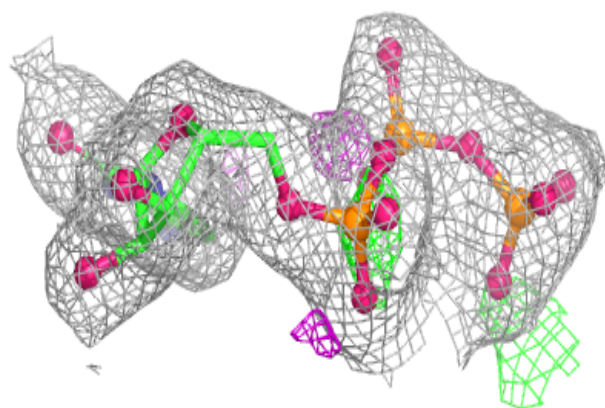
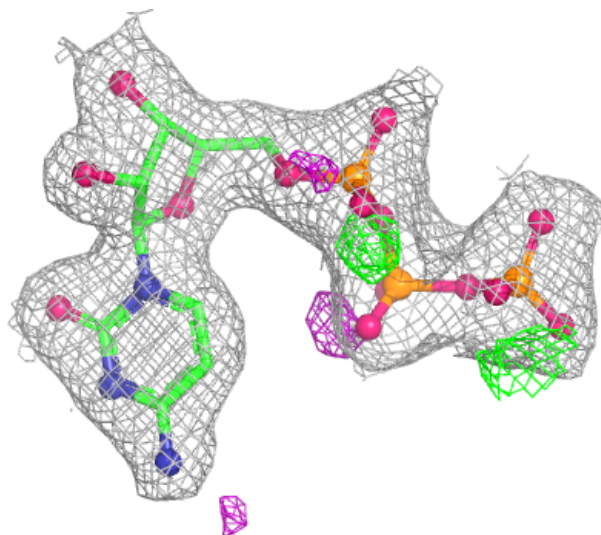
Electron density around CTP B 501:

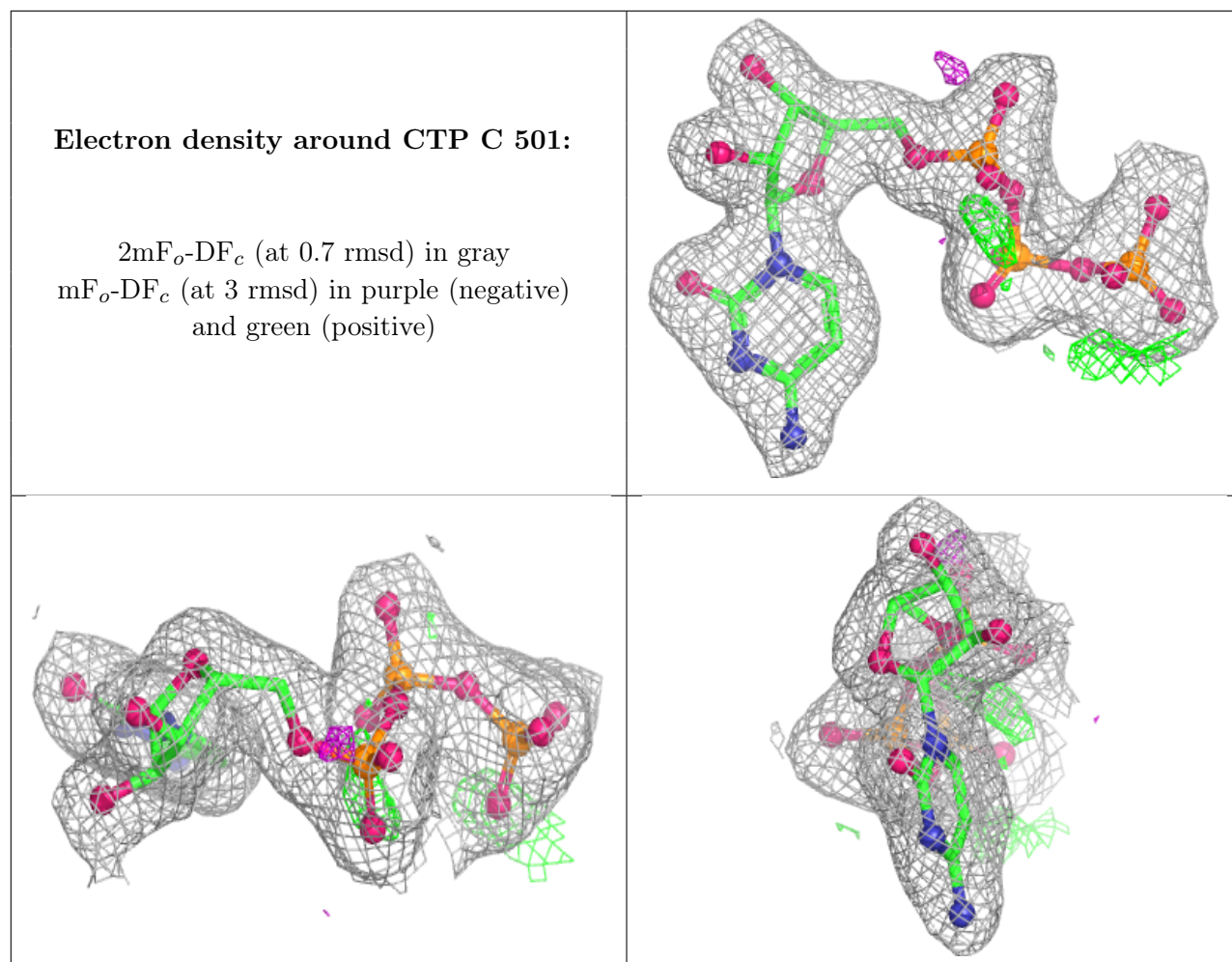
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.