



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:23 PM UTC

PDB ID : 8OWB / pdb_00008owb
Title : Crystal structure of Mycobacterium smegmatis CoaB in complex with CTP and 2-(5-bromo-1-(4-hydroxyphenyl)-1H-indol-3-yl)-2-oxoacetic acid
Authors : Mendes, V.; Blundell, T.L.
Deposited on : 2023-04-27
Resolution : 2.25 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

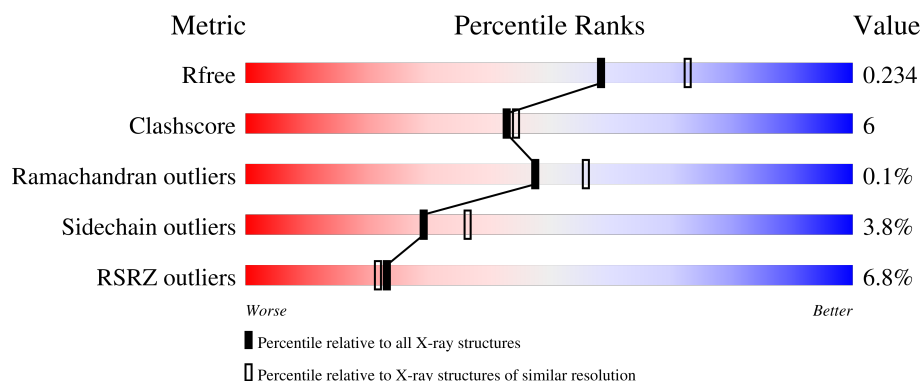
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	 3% 74% 14% • 10%
1	B	237	 11% 81% 13% • 5%
1	C	237	 3% 75% 13% • 11%
1	D	237	 8% 78% 17% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6739 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	213	Total	C	N	O	S	0	0	0
			1520	940	284	290	6			
1	B	224	Total	C	N	O	S	0	0	0
			1608	997	304	301	6			
1	C	210	Total	C	N	O	S	0	0	0
			1495	925	277	287	6			
1	D	227	Total	C	N	O	S	0	0	0
			1627	1006	307	308	6			

There are 32 discrepancies between the modelled and reference sequences:

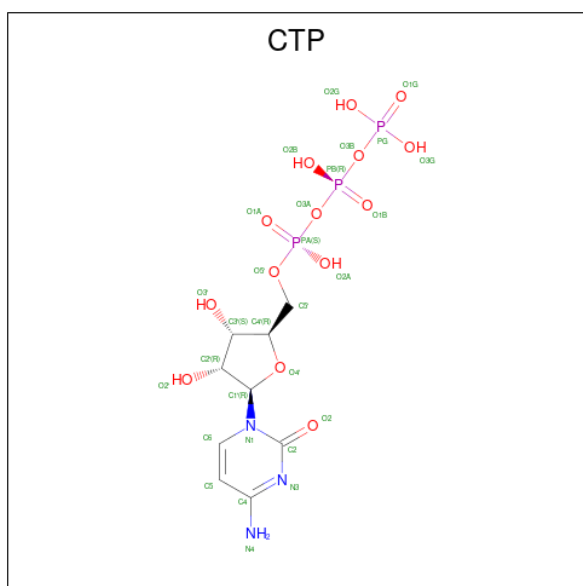
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	MET	-	initiating methionine	UNP A0QWT2
A	179	ALA	-	expression tag	UNP A0QWT2
A	180	HIS	-	expression tag	UNP A0QWT2
A	181	HIS	-	expression tag	UNP A0QWT2
A	182	HIS	-	expression tag	UNP A0QWT2
A	183	HIS	-	expression tag	UNP A0QWT2
A	184	HIS	-	expression 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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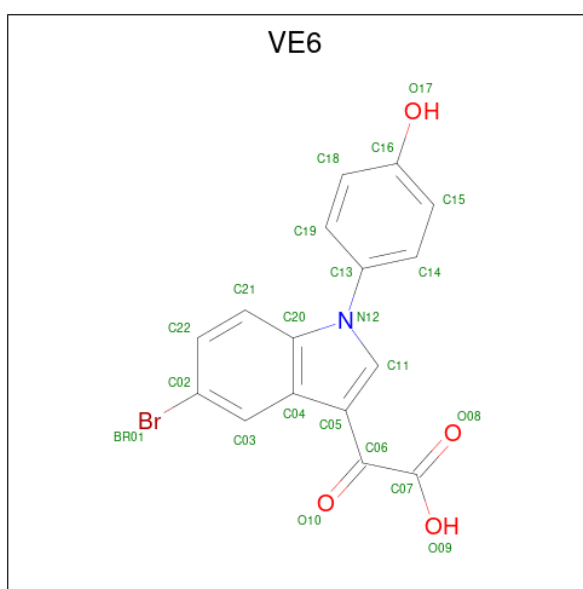
Chain	Residue	Modelled	Actual	Comment	Reference
C	183	HIS	-	expression tag	UNP A0QWT2
C	184	HIS	-	expression tag	UNP A0QWT2
C	185	HIS	-	expression tag	UNP A0QWT2
D	178	MET	-	initiating methionine	UNP A0QWT2
D	179	ALA	-	expression tag	UNP A0QWT2
D	180	HIS	-	expression tag	UNP A0QWT2
D	181	HIS	-	expression 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 2-[5-bromanyl-1-(4-hydroxyphenyl)indol-3-yl]-2-oxidanylidene-ethanoic acid (CCD ID: VE6) (formula: C₁₆H₁₀BrNO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Br C N O 22 1 16 1 4	0	0
4	C	1	Total Br C N O 22 1 16 1 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	73	Total O 73 73	0	0
5	B	80	Total O 80 80	0	0
5	C	93	Total O 93 93	0	0

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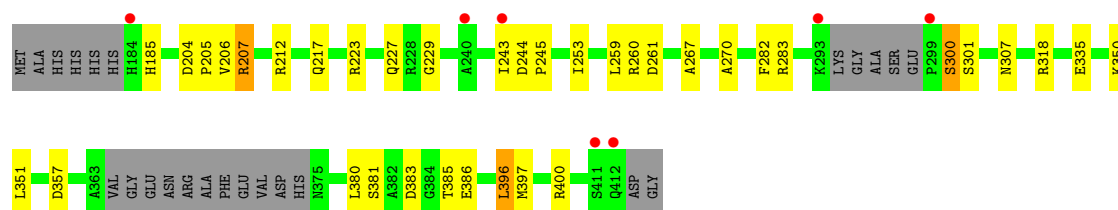
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	79	Total	O	0	0
			79	79		

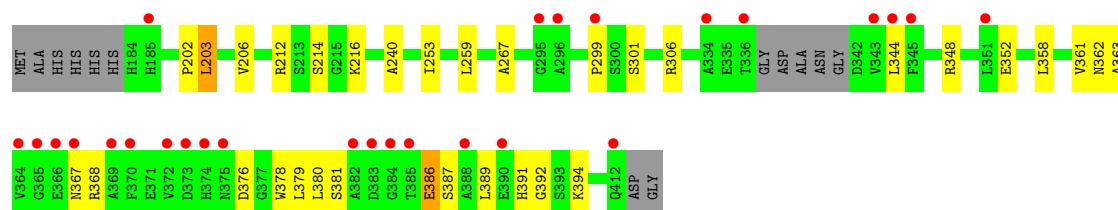
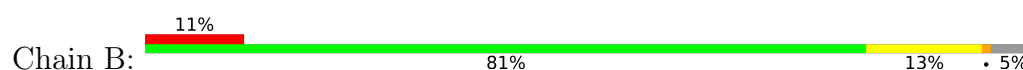
3 Residue-property plots [i](#)

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.

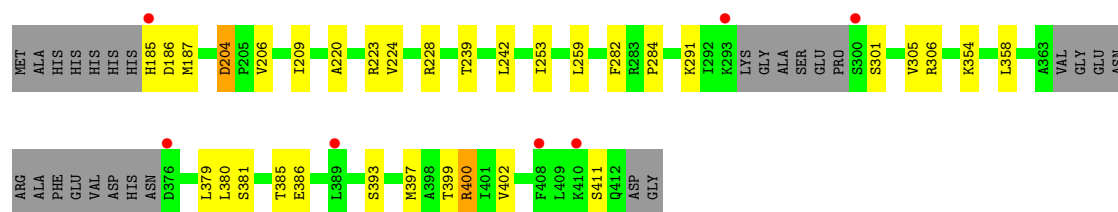
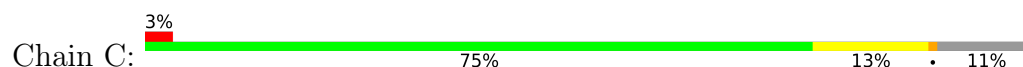
- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



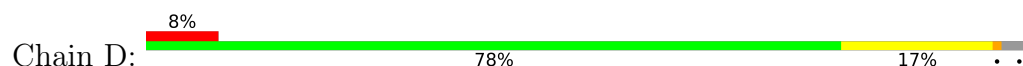
- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC

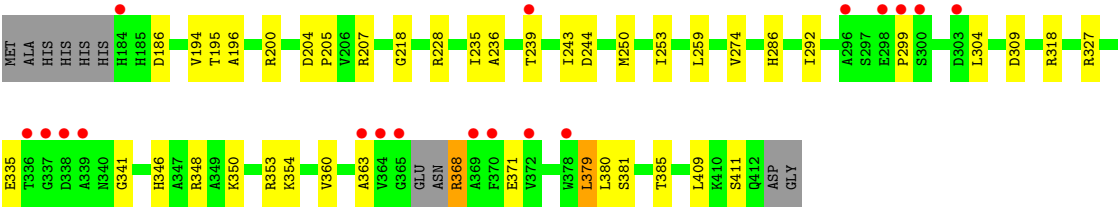


- Molecule 1: Coenzyme A biosynthesis bifunctional protein CoaBC



- 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	75.88Å 76.83Å 144.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.16 – 2.25 72.16 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (72.16-2.25) 98.3 (72.16-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.25Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.207 , 0.246 (Not available) , 0.234	Depositor DCC
R_{free} test set	1939 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.077 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6739	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 4.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VE6, CA, CTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	2/1538 (0.1%)	0.76	2/2087 (0.1%)
1	B	0.73	2/1629 (0.1%)	0.76	6/2210 (0.3%)
1	C	0.59	0/1511	0.68	1/2050 (0.0%)
1	D	0.52	0/1648	0.62	2/2235 (0.1%)
All	All	0.67	4/6326 (0.1%)	0.71	11/8582 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	363	ALA	CA-CB	-5.81	1.45	1.52
1	A	300	SER	CA-C	-5.49	1.46	1.52
1	A	267	ALA	C-O	-5.20	1.19	1.24
1	B	362	ASN	CA-C	-5.08	1.47	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	SER	N-CA-C	-10.94	99.67	113.23
1	B	203	LEU	N-CA-C	-8.65	102.31	113.12
1	A	270	ALA	N-CA-C	8.03	122.88	110.20
1	B	240	ALA	N-CA-C	7.37	119.31	111.28
1	B	363	ALA	N-CA-C	-6.24	100.26	109.62
1	D	236	ALA	N-CA-C	6.21	119.07	109.07
1	B	202	PRO	N-CA-C	6.11	120.78	111.19
1	B	212	ARG	N-CA-C	5.82	120.07	113.15
1	A	229	GLY	N-CA-C	5.47	122.30	114.64
1	B	267	ALA	N-CA-C	5.15	121.20	109.81
1	D	304	LEU	N-CA-C	5.05	117.98	109.95

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	1520	0	1502	20	0
1	B	1608	0	1600	20	0
1	C	1495	0	1483	16	0
1	D	1627	0	1615	27	0
2	A	29	0	12	0	0
2	B	29	0	12	0	0
2	C	29	0	12	0	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	22	0	0	1	0
4	C	22	0	0	0	0
5	A	73	0	0	1	0
5	B	80	0	0	2	0
5	C	93	0	0	2	0
5	D	79	0	0	3	0
All	All	6739	0	6248	79	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 (79) 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:223:ARG:HG3	1:A:245:PRO:HB3	1.62	0.81
1:B:380:LEU:HD21	1:B:386:GLU:HG3	1.63	0.78
1:D:207:ARG:NH2	1:D:292:ILE:O	2.28	0.67
1:A:260:ARG:NH1	1:A:261:ASP:OD1	2.28	0.65
1:B:348:ARG:NH1	1:B:352:GLU:HG3	2.15	0.62
1:C:223:ARG:NH1	5:C:602:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:CD2	1:B:386:GLU:HG3	2.32	0.60
1:D:186:ASP:OD2	1:D:228:ARG:NH2	2.29	0.60
1:A:380:LEU:HD22	1:A:386:GLU:HG2	1.85	0.59
1:A:396:LEU:HD13	1:A:400:ARG:HD3	1.84	0.58
1:B:376:ASP:O	1:B:378:TRP:HD1	1.86	0.58
1:C:204:ASP:OD2	1:C:291:LYS:HA	2.03	0.58
1:A:397:MET:HA	1:A:400:ARG:HG2	1.87	0.57
1:A:206:VAL:HG23	1:A:207:ARG:HG2	1.86	0.56
1:C:393:SER:O	1:C:397:MET:HG3	2.04	0.56
1:D:200:ARG:NH1	5:D:603:HOH:O	2.38	0.56
1:B:376:ASP:OD1	1:B:391:HIS:NE2	2.35	0.55
1:A:253:ILE:HD13	1:A:259:LEU:HB2	1.89	0.54
1:C:253:ILE:HD13	1:C:259:LEU:HB2	1.88	0.54
1:A:204:ASP:HB2	1:A:205:PRO:HD2	1.90	0.53
1:D:253:ILE:HD13	1:D:259:LEU:HB2	1.90	0.53
1:D:204:ASP:HB2	1:D:205:PRO:HD2	1.92	0.52
1:B:367:ASN:HD22	1:B:392:GLY:HA2	1.75	0.51
1:D:335:GLU:OE2	1:D:350:LYS:HD2	2.11	0.51
1:D:350:LYS:HE3	1:D:353:ARG:NH1	2.26	0.51
1:D:341:GLY:O	1:D:346:HIS:HE1	1.93	0.51
1:C:380:LEU:HD22	1:C:386:GLU:HG2	1.92	0.50
1:C:381:SER:HB2	1:C:385:THR:HB	1.93	0.50
1:D:350:LYS:HE3	1:D:353:ARG:HH12	1.76	0.50
1:B:394:LYS:H	1:B:394:LYS:CE	2.25	0.50
1:A:282:PHE:CE1	1:B:299:PRO:HB3	2.46	0.50
1:B:214:SER:OG	1:B:216:LYS:HG3	2.12	0.50
1:B:368:ARG:NH2	5:B:606:HOH:O	2.45	0.49
1:C:228:ARG:HH22	1:C:399:THR:HG23	1.78	0.49
1:D:348:ARG:HD3	1:D:380:LEU:HD23	1.94	0.49
1:B:216:LYS:NZ	5:B:609:HOH:O	2.46	0.48
1:D:327:ARG:NH2	1:D:409:LEU:HB3	2.29	0.48
1:D:368:ARG:HG3	1:D:371:GLU:OE1	2.14	0.48
1:D:327:ARG:HH22	1:D:409:LEU:HB3	1.79	0.47
1:B:379:LEU:HG	1:B:389:LEU:HD13	1.96	0.47
1:A:385:THR:HG22	5:A:636:HOH:O	2.14	0.47
1:C:239:THR:HB	1:C:242:LEU:HG	1.96	0.47
1:C:354:LYS:HA	1:C:354:LYS:HD3	1.50	0.47
1:B:253:ILE:HD13	1:B:259:LEU:HB2	1.97	0.46
1:C:282:PHE:CE1	1:D:299:PRO:HB3	2.50	0.46
1:A:212:ARG:HG3	1:B:206:VAL:O	2.15	0.46
1:D:286:HIS:CE1	5:D:646:HOH:O	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:VAL:HG12	1:C:402:VAL:HG21	1.98	0.46
1:D:309:ASP:OD2	1:D:354:LYS:NZ	2.43	0.46
1:B:394:LYS:H	1:B:394:LYS:HE2	1.81	0.46
1:A:243:ILE:HD12	1:A:244:ASP:H	1.80	0.46
1:B:344:LEU:HD21	1:B:378:TRP:CE2	2.51	0.45
1:C:381:SER:HB3	5:C:623:HOH:O	2.15	0.45
1:D:195:THR:HG22	1:D:235:ILE:HB	1.99	0.45
1:A:351:LEU:HD22	1:A:380:LEU:HB3	1.99	0.45
1:A:318:ARG:HH22	1:A:357:ASP:CG	2.25	0.44
1:D:194:VAL:HG22	1:D:274:VAL:HB	2.00	0.44
1:A:283:ARG:HD3	1:A:307:ASN:OD1	2.18	0.44
1:D:341:GLY:C	1:D:346:HIS:HE1	2.26	0.43
1:C:220:ALA:O	1:C:224:VAL:HG23	2.18	0.43
1:D:381:SER:HB3	1:D:385:THR:HB	1.99	0.43
1:A:217:GLN:H	4:A:503:VE6:C07	2.31	0.43
1:D:244:ASP:OD1	1:D:250:MET:HE2	2.19	0.43
1:A:301:SER:HB3	1:B:301:SER:HB3	2.01	0.42
1:D:379:LEU:HD12	1:D:379:LEU:HA	1.90	0.42
1:B:389:LEU:HA	1:B:389:LEU:HD12	1.77	0.42
1:C:400:ARG:O	1:C:400:ARG:HD2	2.20	0.42
1:A:381:SER:HB2	1:A:383:ASP:OD2	2.19	0.42
1:C:358:LEU:HD11	1:C:379:LEU:HB3	2.02	0.41
1:B:358:LEU:HD12	1:B:381:SER:HA	2.03	0.41
1:A:243:ILE:HD12	1:A:244:ASP:N	2.35	0.41
1:C:209:ILE:HD12	1:C:284:PRO:HD3	2.02	0.41
1:A:335:GLU:OE2	1:A:350:LYS:NZ	2.51	0.41
1:D:196:ALA:HB2	1:D:218:GLY:HA3	2.03	0.41
1:D:350:LYS:O	1:D:354:LYS:HG2	2.20	0.41
1:D:360:VAL:HG12	1:D:363:ALA:HB2	2.02	0.41
1:D:318:ARG:HD3	5:D:634:HOH:O	2.21	0.41
1:D:244:ASP:CG	1:D:250:MET:HG3	2.46	0.40
1:B:344:LEU:HD13	1:B:344:LEU:HA	1.92	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	207/237 (87%)	202 (98%)	5 (2%)	0	100	100
1	B	220/237 (93%)	214 (97%)	6 (3%)	0	100	100
1	C	204/237 (86%)	198 (97%)	5 (2%)	1 (0%)	24	24
1	D	223/237 (94%)	217 (97%)	6 (3%)	0	100	100
All	All	854/948 (90%)	831 (97%)	22 (3%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	MET

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	40
1	B	156/173 (90%)	151 (97%)	5 (3%)	34	43
1	C	145/173 (84%)	137 (94%)	8 (6%)	19	20
1	D	158/173 (91%)	153 (97%)	5 (3%)	34	43
All	All	606/692 (88%)	583 (96%)	23 (4%)	29	36

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	207	ARG
1	A	227	GLN
1	A	300	SER
1	A	396	LEU

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Mol	Chain	Res	Type
1	B	203	LEU
1	B	306	ARG
1	B	361	VAL
1	B	386	GLU
1	B	387	SER
1	C	185	HIS
1	C	186	ASP
1	C	204	ASP
1	C	206	VAL
1	C	301	SER
1	C	305	VAL
1	C	306	ARG
1	C	400	ARG
1	D	239	THR
1	D	243	ILE
1	D	368	ARG
1	D	379	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	238	ASN
1	A	252	HIS
1	A	286	HIS
1	B	362	ASN
1	C	238	ASN
1	C	252	HIS
1	C	322	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	A	501	3	29,30,30	0.94	1 (3%)	43,47,47	0.94	1 (2%)
4	VE6	C	503	-	24,24,24	1.39	4 (16%)	35,35,35	1.30	5 (14%)
4	VE6	A	503	-	24,24,24	1.44	4 (16%)	35,35,35	1.39	4 (11%)
2	CTP	B	501	3	29,30,30	1.07	2 (6%)	43,47,47	1.10	2 (4%)
2	CTP	D	501	3	29,30,30	1.07	2 (6%)	43,47,47	1.09	2 (4%)
2	CTP	C	501	3	29,30,30	1.00	1 (3%)	43,47,47	0.98	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTP	A	501	3	-	1/22/38/38	0/2/2/2
4	VE6	C	503	-	-	0/12/12/12	0/3/3/3
4	VE6	A	503	-	-	9/12/12/12	0/3/3/3
2	CTP	B	501	3	-	3/22/38/38	0/2/2/2
2	CTP	D	501	3	-	2/22/38/38	0/2/2/2
2	CTP	C	501	3	-	4/22/38/38	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	VE6	C05-C06	3.56	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	VE6	C05-C06	3.21	1.52	1.45
2	B	501	CTP	PB-O3B	2.92	1.62	1.59
4	A	503	VE6	C20-N12	-2.83	1.34	1.39
2	D	501	CTP	PB-O3B	2.74	1.62	1.59
4	A	503	VE6	C11-N12	-2.64	1.32	1.39
4	C	503	VE6	C11-N12	-2.62	1.32	1.39
4	C	503	VE6	C20-N12	-2.50	1.35	1.39
4	A	503	VE6	C07-C06	-2.25	1.52	1.54
2	D	501	CTP	C6-N1	-2.20	1.32	1.38
2	C	501	CTP	PB-O3B	2.17	1.61	1.59
4	C	503	VE6	O08-C07	2.14	1.27	1.22
2	A	501	CTP	C4-N3	2.03	1.38	1.34
2	B	501	CTP	C6-N1	-2.01	1.33	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	VE6	C20-N12-C11	3.60	110.79	107.98
4	C	503	VE6	C20-N12-C11	3.51	110.73	107.98
4	A	503	VE6	C05-C06-C07	3.43	124.23	118.83
4	A	503	VE6	O09-C07-C06	3.42	122.52	112.94
2	C	501	CTP	C5-C6-N1	-3.00	116.97	121.84
4	C	503	VE6	C04-C05-C06	2.81	129.69	126.09
4	C	503	VE6	O09-C07-C06	2.52	120.01	112.94
2	B	501	CTP	C2'-C3'-C4'	2.38	107.21	102.61
4	C	503	VE6	C13-N12-C11	-2.35	121.53	124.78
4	A	503	VE6	C21-C20-C04	-2.35	119.33	121.95
2	B	501	CTP	O3A-PA-O1A	-2.28	103.84	110.70
2	D	501	CTP	O3A-PB-O1B	-2.21	104.07	110.70
2	A	501	CTP	O2-C2-N3	-2.16	118.93	122.33
2	D	501	CTP	O2B-PB-O3B	2.15	113.09	107.27
2	C	501	CTP	O3'-C3'-C4'	-2.12	105.00	111.08
4	C	503	VE6	O10-C06-C07	2.07	122.84	117.79

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	VE6	C04-C05-C06-C07
4	A	503	VE6	C04-C05-C06-O10
4	A	503	VE6	C11-C05-C06-C07
4	A	503	VE6	C11-C05-C06-O10

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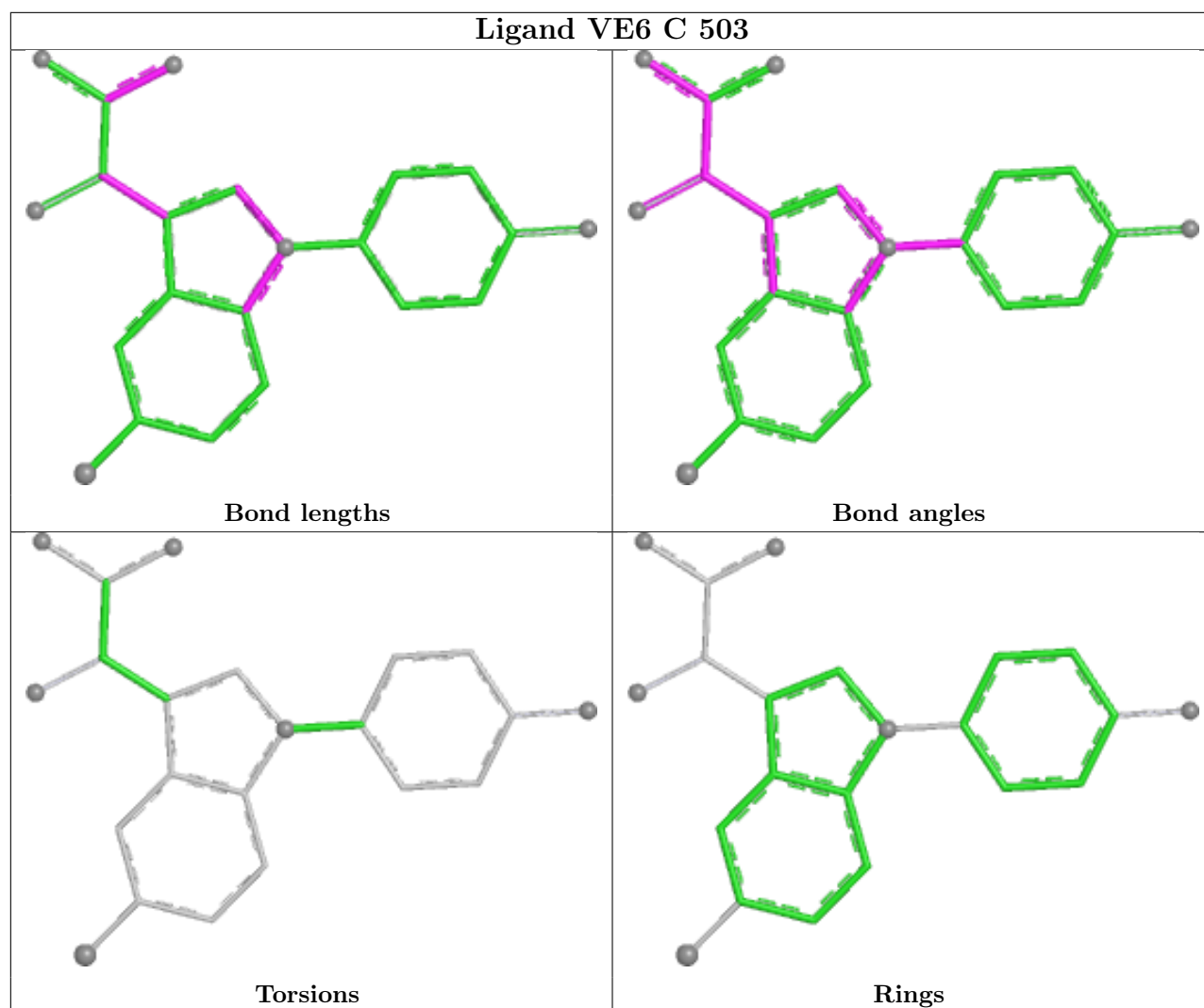
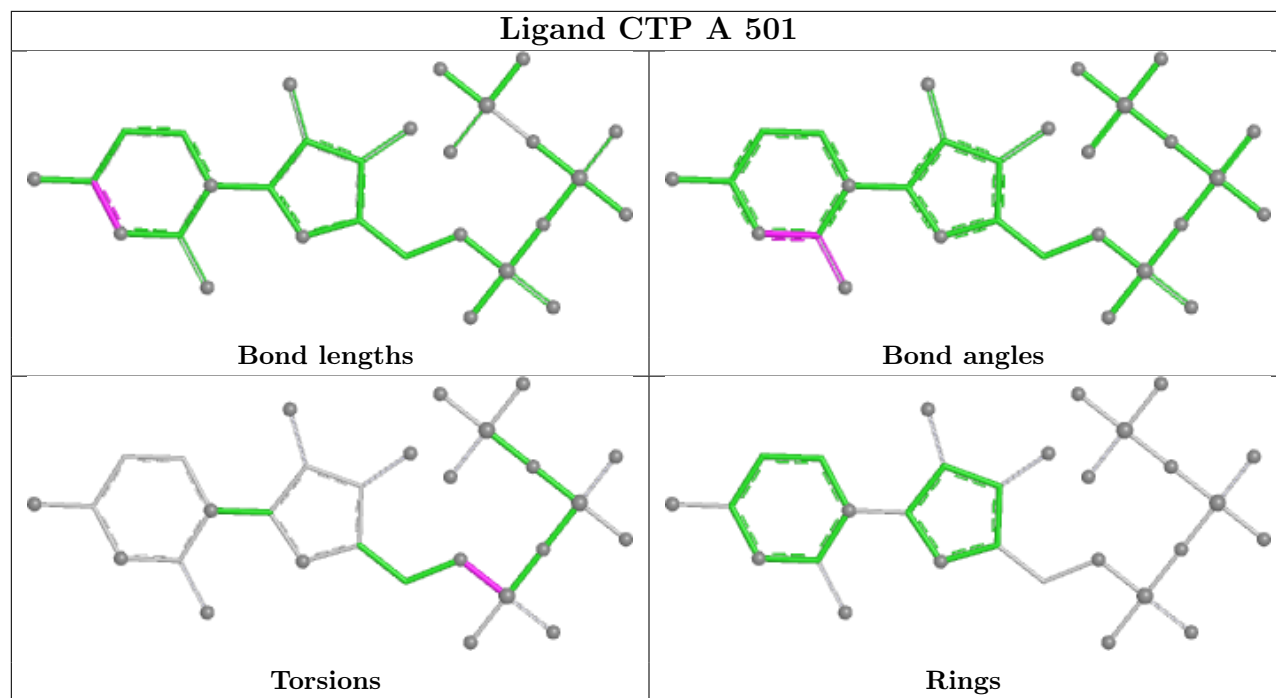
Mol	Chain	Res	Type	Atoms
4	A	503	VE6	C05-C06-C07-O08
2	C	501	CTP	PB-O3B-PG-O2G
2	C	501	CTP	PA-O3A-PB-O2B
2	D	501	CTP	PB-O3A-PA-O2A
2	A	501	CTP	C5'-O5'-PA-O1A
4	A	503	VE6	O10-C06-C07-O09
2	B	501	CTP	PB-O3A-PA-O1A
4	A	503	VE6	C19-C13-N12-C11
2	D	501	CTP	PB-O3A-PA-O1A
2	C	501	CTP	PB-O3B-PG-O1G
4	A	503	VE6	O10-C06-C07-O08
2	B	501	CTP	PB-O3A-PA-O2A
2	B	501	CTP	PG-O3B-PB-O2B
2	C	501	CTP	PA-O3A-PB-O1B
4	A	503	VE6	C14-C13-N12-C11

There are no ring outliers.

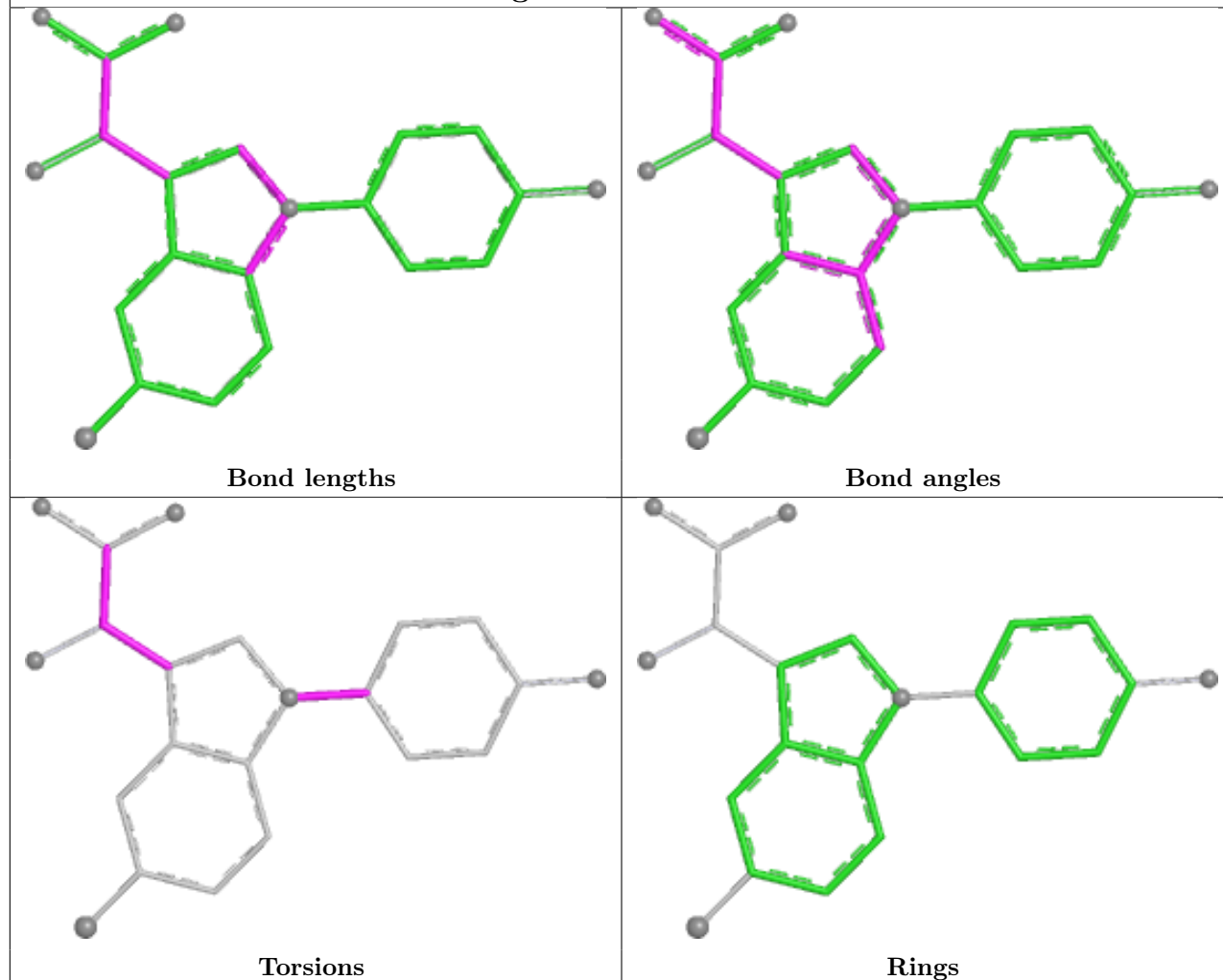
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	VE6	1	0

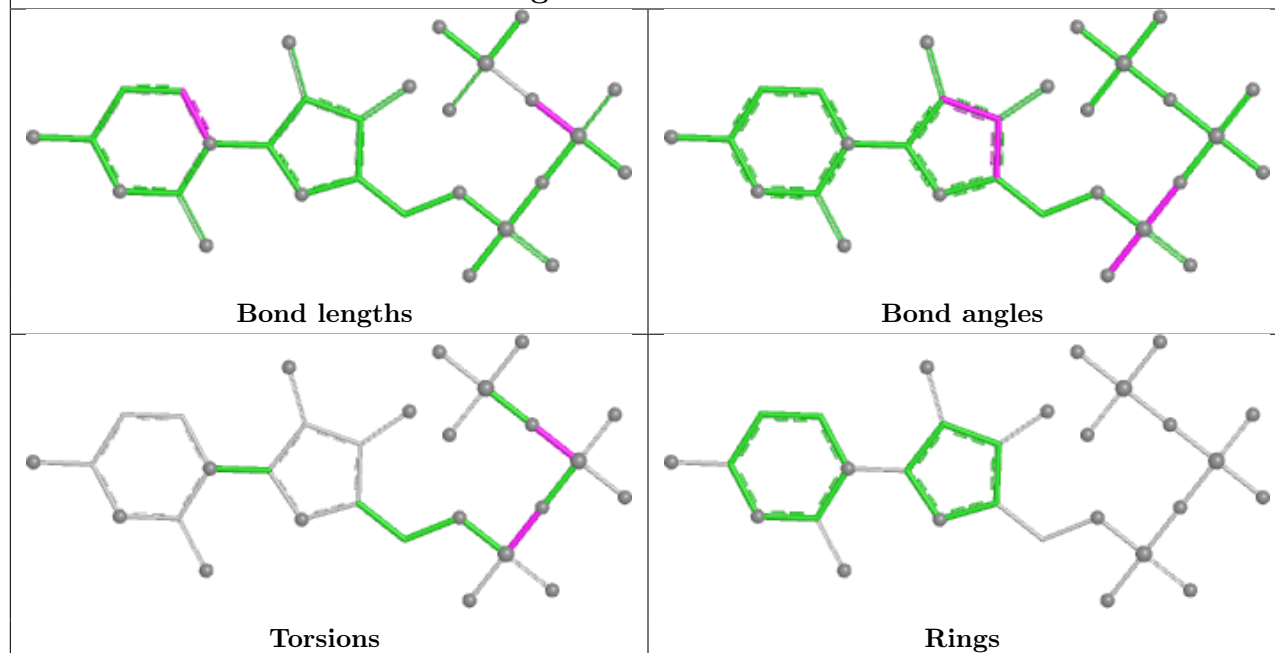
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

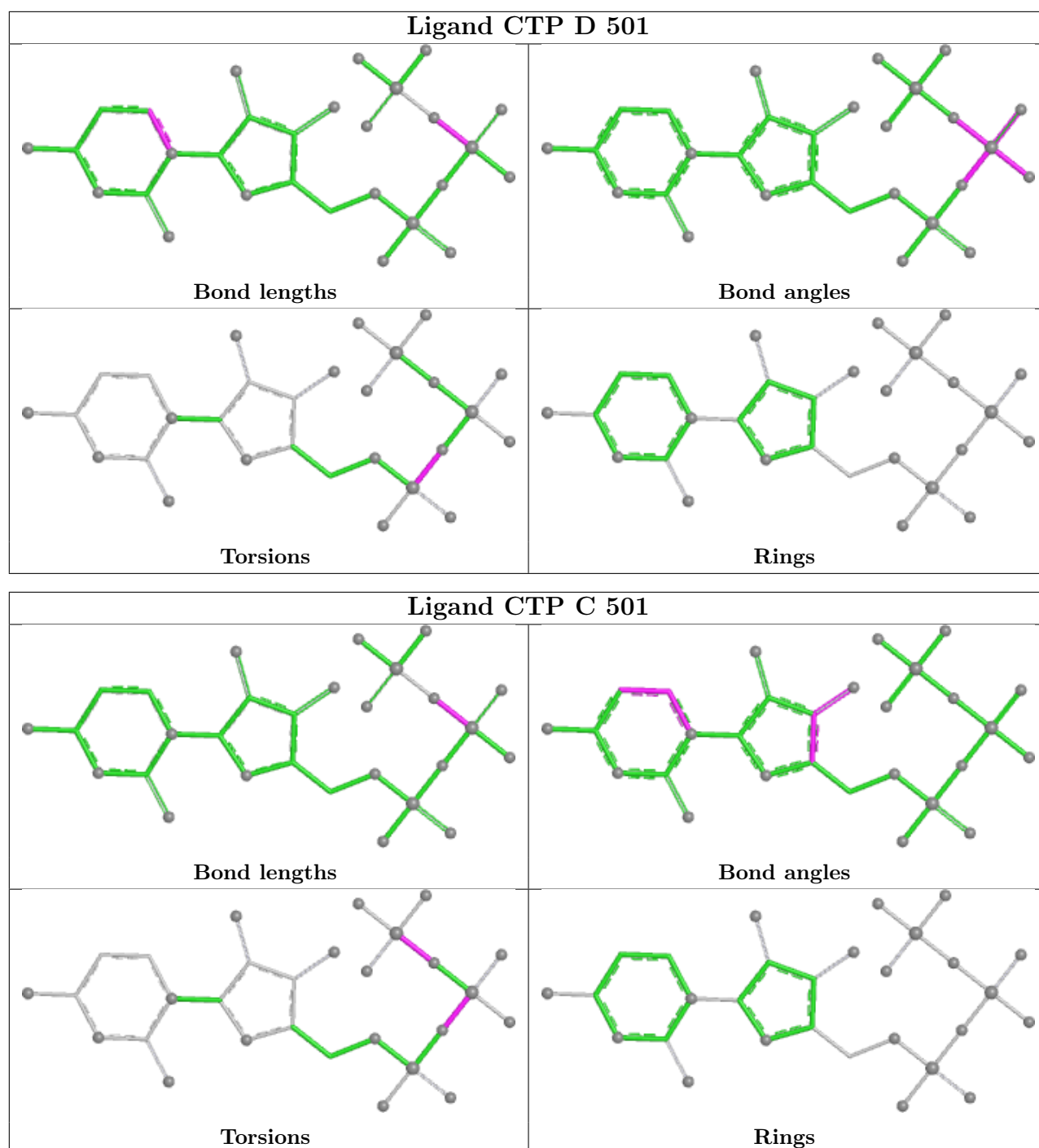


Ligand VE6 A 503



Ligand CTP B 501





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	213/237 (89%)	0.17	7 (3%) 49 49	27, 36, 56, 77	0
1	B	224/237 (94%)	0.57	27 (12%) 8 8	28, 38, 86, 114	0
1	C	210/237 (88%)	0.20	7 (3%) 49 49	26, 35, 63, 80	0
1	D	227/237 (95%)	0.51	18 (7%) 18 17	26, 39, 78, 94	0
All	All	874/948 (92%)	0.37	59 (6%) 23 22	26, 37, 75, 114	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	364	VAL	4.4
1	A	299	PRO	4.2
1	B	372	VAL	3.8
1	B	366	GLU	3.7
1	A	411	SER	3.5
1	B	296	ALA	3.4
1	D	339	ALA	3.2
1	B	299	PRO	3.1
1	B	383	ASP	3.1
1	A	184	HIS	3.1
1	D	378	TRP	3.0
1	B	345	PHE	3.0
1	B	351	LEU	3.0
1	B	364	VAL	2.9
1	D	336	THR	2.9
1	B	344	LEU	2.9
1	D	363	ALA	2.8
1	B	343	VAL	2.8
1	B	385	THR	2.8
1	B	412	GLN	2.8
1	B	336	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	239	THR	2.8
1	C	300	SER	2.8
1	B	334	ALA	2.8
1	B	365	GLY	2.7
1	D	184	HIS	2.7
1	D	298	GLU	2.7
1	D	372	VAL	2.7
1	A	293	LYS	2.6
1	B	370	PHE	2.6
1	D	365	GLY	2.6
1	D	370	PHE	2.6
1	A	240	ALA	2.5
1	B	388	ALA	2.5
1	D	337	GLY	2.5
1	B	295	GLY	2.5
1	B	369	ALA	2.5
1	D	299	PRO	2.5
1	B	382	ALA	2.4
1	D	296	ALA	2.4
1	D	300	SER	2.3
1	A	412	GLN	2.3
1	B	384	GLY	2.3
1	D	338	ASP	2.3
1	B	373	ASP	2.2
1	D	303	ASP	2.1
1	C	293	LYS	2.1
1	B	185	HIS	2.1
1	D	369	ALA	2.1
1	C	410	LYS	2.1
1	B	390	GLU	2.1
1	C	408	PHE	2.1
1	B	374	HIS	2.0
1	C	185	HIS	2.0
1	B	367	ASN	2.0
1	C	389	LEU	2.0
1	B	375	ASN	2.0
1	C	376	ASP	2.0
1	A	243	ILE	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](#)

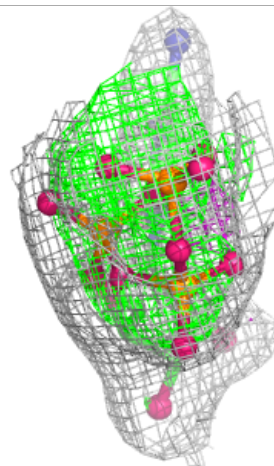
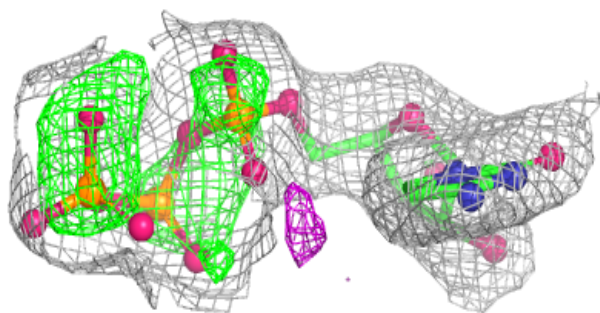
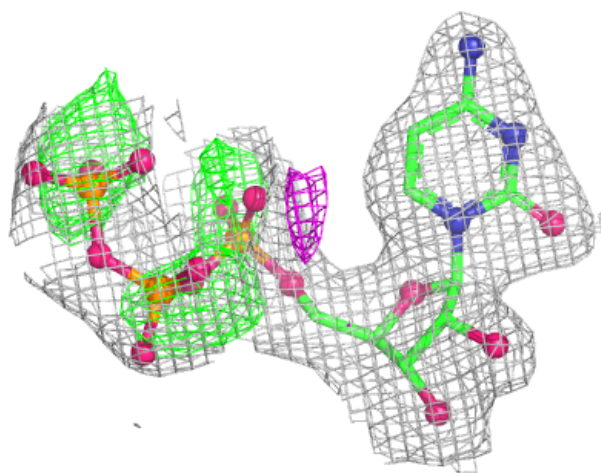
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.81	0.20	31,41,173,177	0
2	CTP	B	501	29/29	0.87	0.10	30,39,60,89	0
3	CA	B	502	1/1	0.90	0.09	49,49,49,49	0
3	CA	A	502	1/1	0.93	0.07	48,48,48,48	0
2	CTP	A	501	29/29	0.94	0.07	27,31,46,49	0
4	VE6	C	503	22/22	0.94	0.09	33,37,39,55	0
4	VE6	A	503	22/22	0.95	0.08	31,35,42,50	0
2	CTP	C	501	29/29	0.95	0.07	27,32,47,52	0
3	CA	C	502	1/1	0.98	0.04	45,45,45,45	0
3	CA	D	502	1/1	0.99	0.09	68,68,68,68	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.

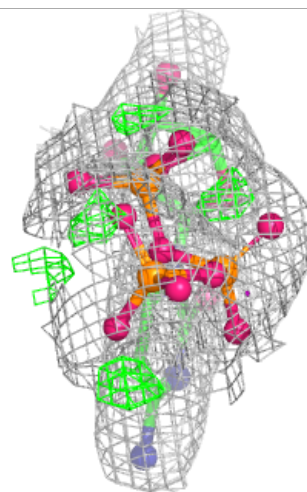
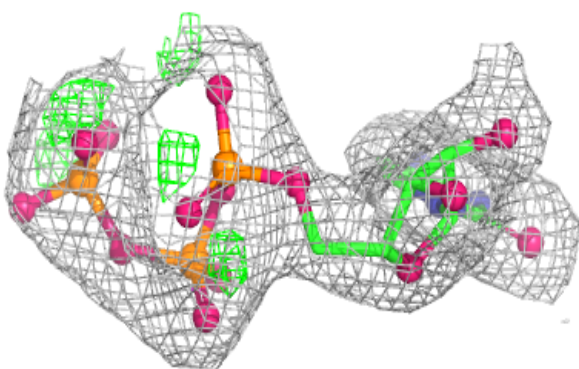
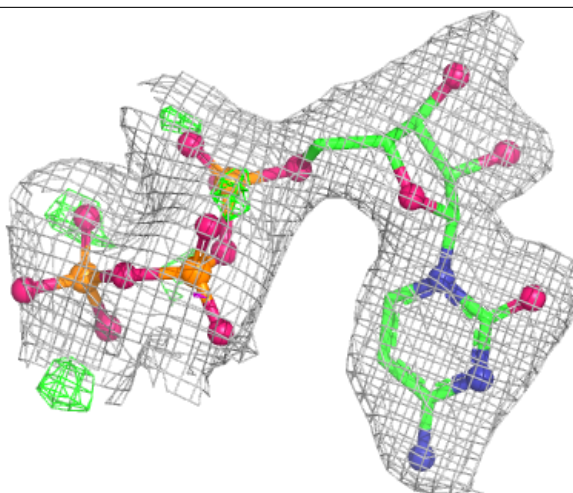
Electron density around CTP D 501:

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



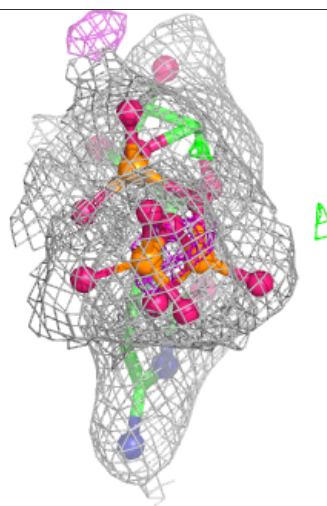
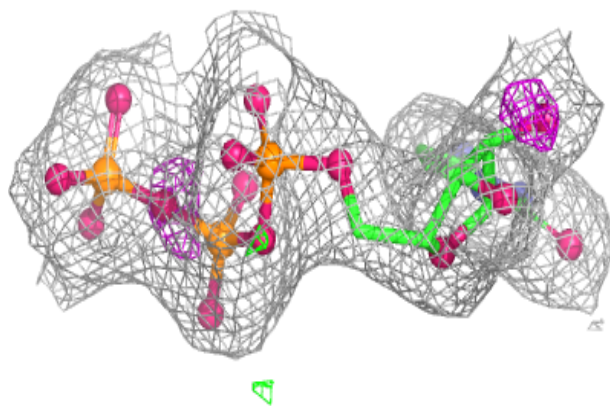
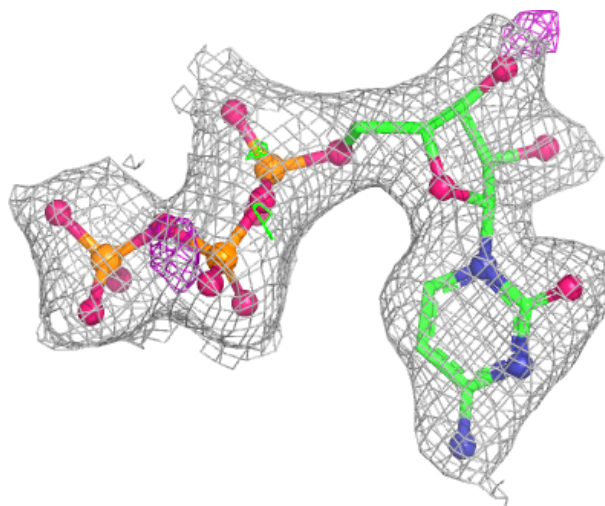
Electron density around CTP B 501:

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



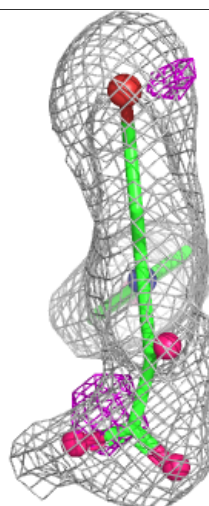
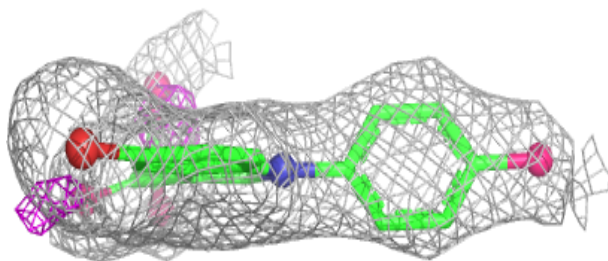
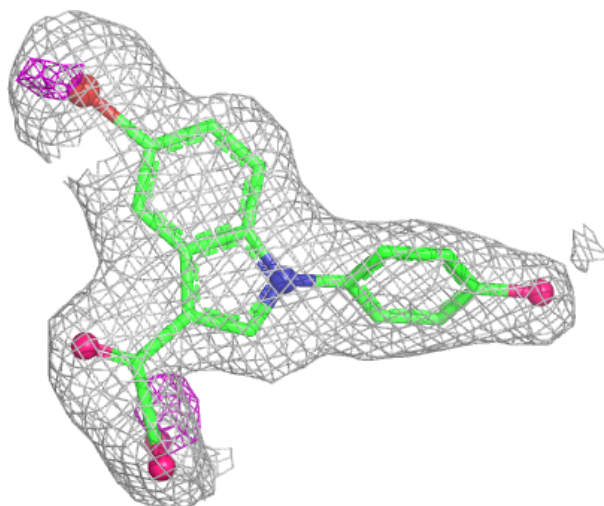
Electron density around CTP A 501:

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



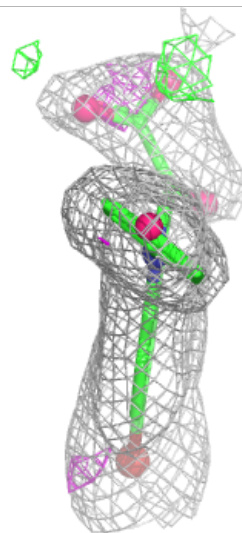
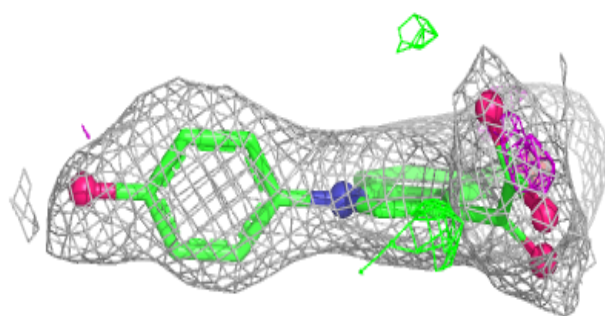
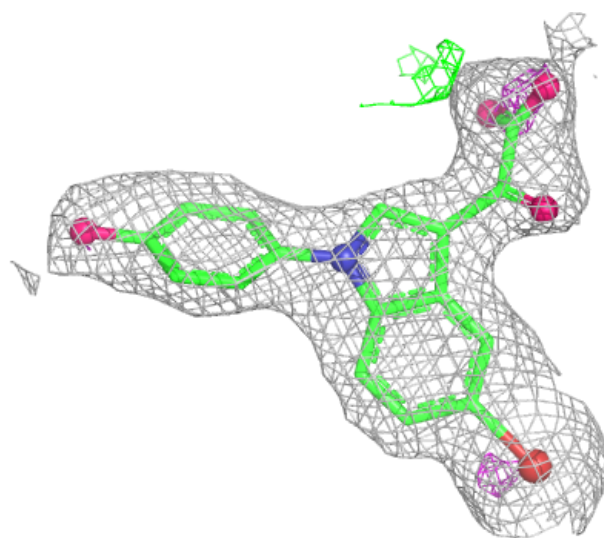
Electron density around VE6 C 503:

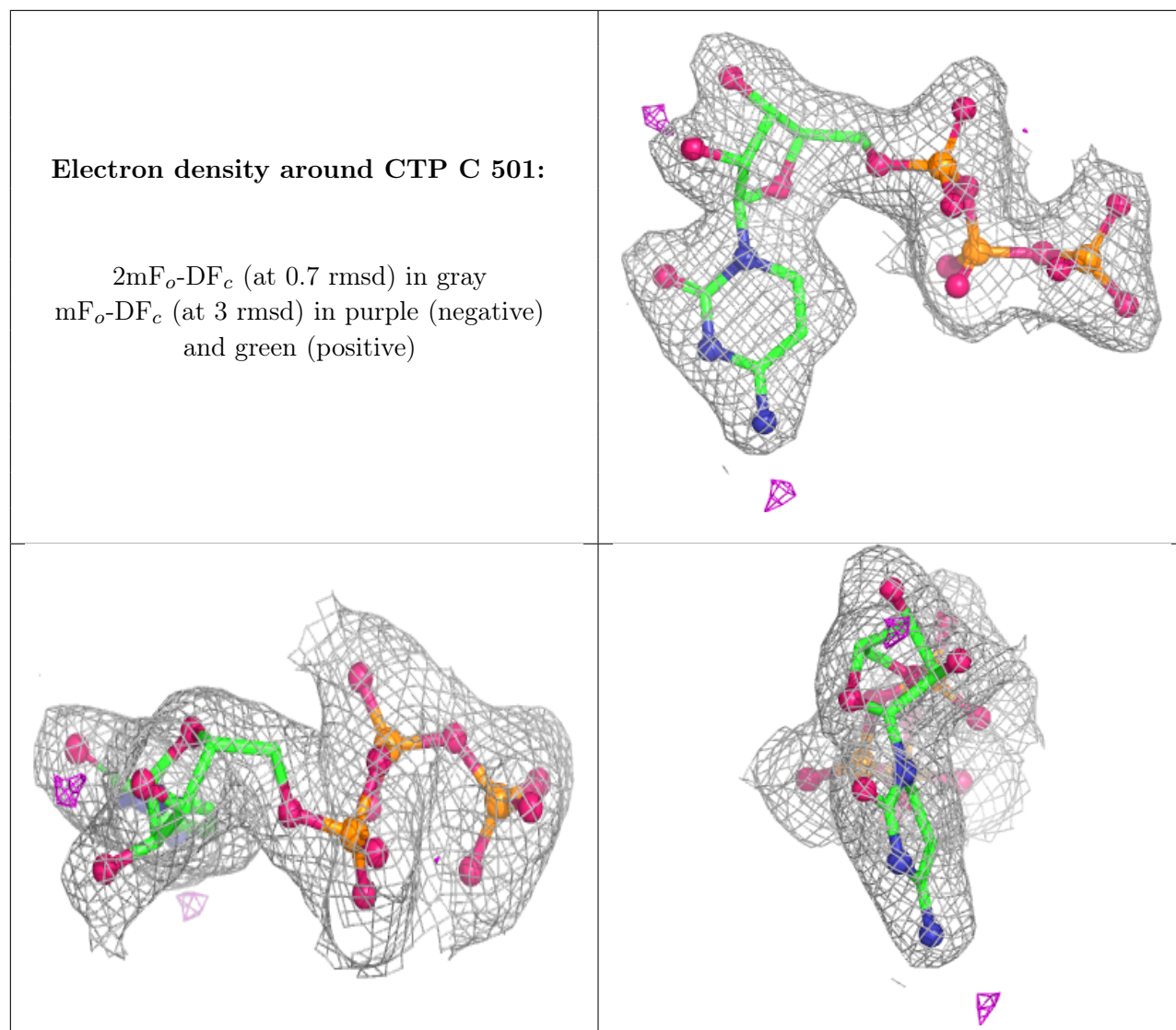
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VE6 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.