Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 10:06 AM EDT

PDB ID	:	5W19
Title	:	Tryptophan indole-lyase complex with oxindolyl-L-alanine
Authors	:	Phillips, R.S.; Wood, Z.A.
Deposited on	:	2017-06-02
Resolution	:	2.10 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:

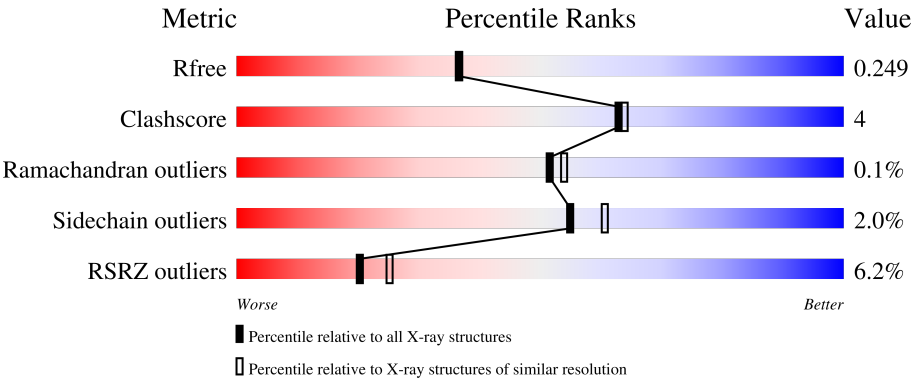
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	467	3% 88% 11%
1	B	467	4% 87% 12%
1	C	467	9% 86% 12%
1	D	467	8% 86% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15551 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.

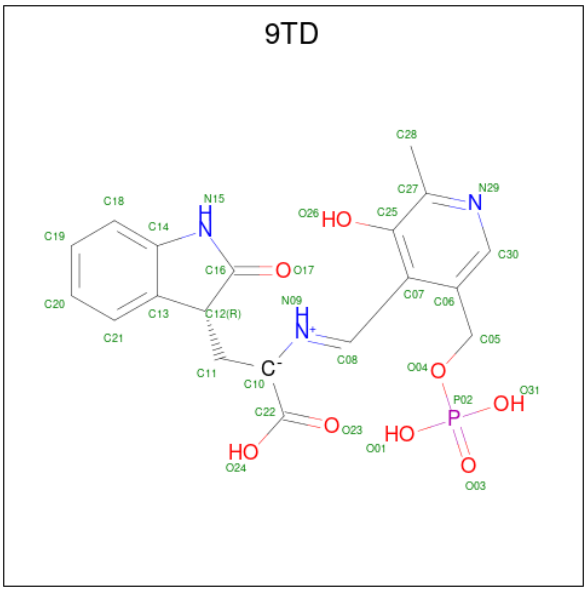
- Molecule 1 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	4	0
			3715	2373	631	692	19			
1	B	466	Total	C	N	O	S	0	3	0
			3712	2368	630	694	20			
1	C	466	Total	C	N	O	S	0	6	0
			3733	2381	639	695	18			
1	D	466	Total	C	N	O	S	0	6	0
			3726	2380	633	693	20			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	C	2	Total	K	0	0
			2	2		

- Molecule 3 is 1-carboxy-1-{[(E)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]azaniumyl}-2-[(3R)-2-oxo-2,3-dihydro-1H-indol-3-yl]ethan-1-ide (three-letter code: 9TD) (formula: $C_{19}H_{20}N_3O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	19	3	8	1		
3	B	1	Total	C	N	O	P	0	0
			31	19	3	8	1		
3	C	1	Total	C	N	O	P	0	0
			31	19	3	8	1		
3	D	1	Total	C	N	O	P	0	0
			31	19	3	8	1		

- Molecule 4 is water.

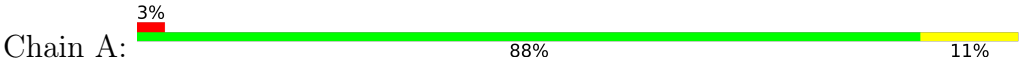
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	155	Total	O	0	0
			155	155		
4	C	143	Total	O	0	0
			143	143		
4	D	125	Total	O	0	0
			125	125		

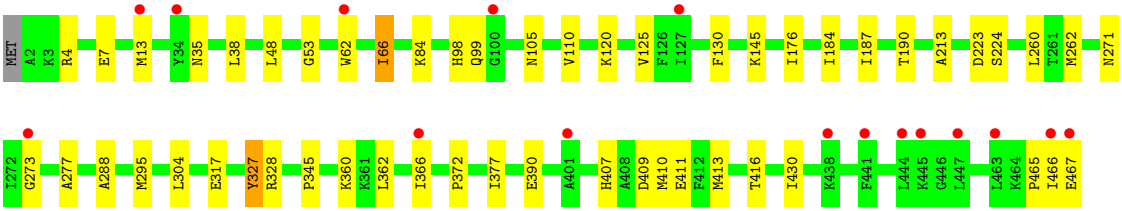
3 Residue-property plots (i)

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: Tryptophanase

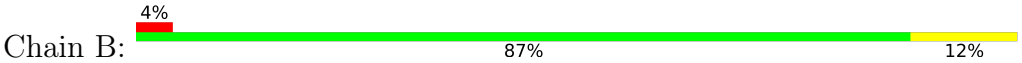
Chain A:

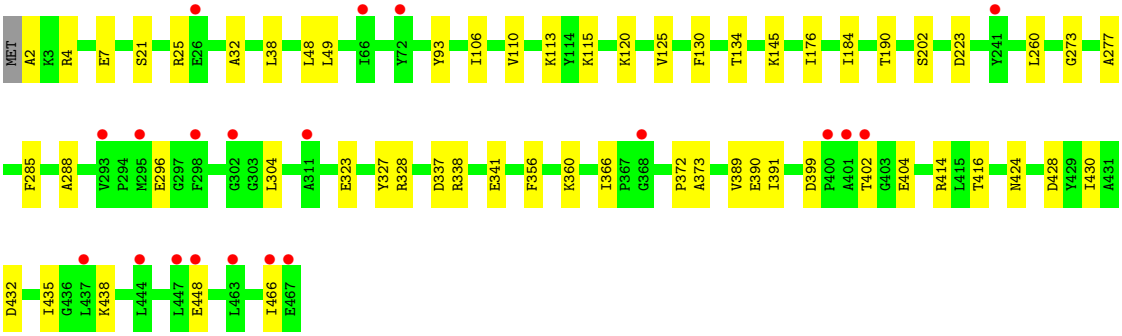




• Molecule 1: Tryptophanase

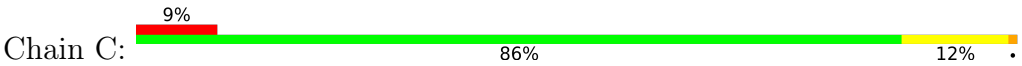
Chain B:

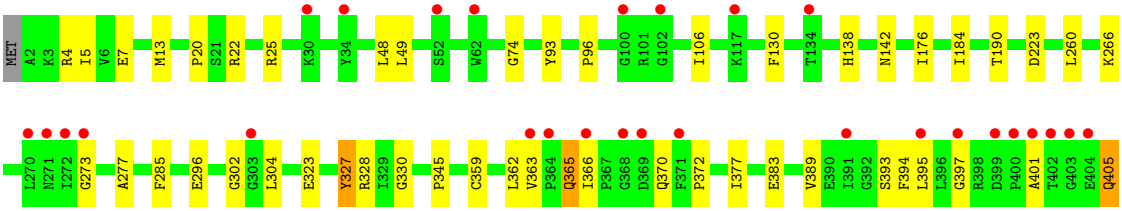


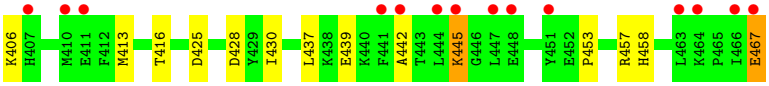


• Molecule 1: Tryptophanase

Chain C:

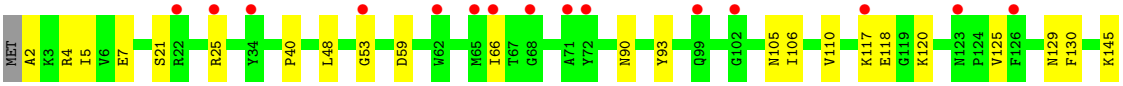






• Molecule 1: Tryptophanase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.12Å 152.08Å 211.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.10 48.11 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.11-2.10) 78.2 (48.11-2.10)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.19 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.217 , 0.244 0.222 , 0.249	Depositor DCC
R_{free} test set	5944 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15551	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 9TD

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	0.25	0/3801	0.42	0/5132
1	B	0.25	0/3791	0.42	0/5117
1	C	0.25	0/3822	0.42	0/5159
1	D	0.25	0/3821	0.42	0/5157
All	All	0.25	0/15235	0.42	0/20565

There are no bond length outliers.

There are no bond angle outliers.

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	3715	0	3695	29	0
1	B	3712	0	3682	30	0
1	C	3733	0	3713	38	0
1	D	3726	0	3713	33	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	31	0	0	1	0
3	B	31	0	0	1	0
3	C	31	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	0	1	0
4	A	114	0	0	0	0
4	B	155	0	0	1	0
4	C	143	0	0	0	0
4	D	125	0	0	1	0
All	All	15551	0	14803	128	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 4.

All (128) 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:D:4[A]:ARG:NH2	1:D:428:ASP:OD2	2.23	0.69
1:C:5:ILE:HD12	1:C:330:GLY:HA3	1.80	0.63
1:B:402:THR:HG23	1:B:404:GLU:H	1.64	0.63
1:B:360:LYS:NZ	4:B:605:HOH:O	2.31	0.62
1:C:405[A]:GLN:NE2	1:C:406:LYS:O	2.31	0.62
1:A:224:SER:HB2	1:A:262[A]:MET:HB3	1.82	0.60
1:C:48:LEU:HD11	1:C:430:ILE:HD13	1.82	0.60
1:D:106:ILE:HD11	1:D:296:GLU:HG3	1.84	0.59
1:A:48:LEU:HD11	1:A:430:ILE:HD13	1.84	0.59
1:D:5:ILE:HD12	1:D:330:GLY:HA3	1.84	0.59
1:B:448:GLU:HG3	1:B:466:ILE:HG12	1.85	0.59
1:B:106:ILE:HD11	1:B:296:GLU:HG3	1.85	0.58
1:D:366:ILE:HB	1:D:372:PRO:HB3	1.84	0.58
1:A:366:ILE:HB	1:A:372:PRO:HB3	1.85	0.57
1:C:345:PRO:HD2	1:C:362:LEU:HD21	1.86	0.57
1:C:273:GLY:HA2	1:C:304:LEU:HD21	1.86	0.57
1:D:399:ASP:HB3	1:D:402:THR:HB	1.87	0.56
1:D:152:GLU:H	1:D:152:GLU:CD	2.08	0.56
1:A:125:VAL:HG12	1:A:145:LYS:HB2	1.86	0.56
1:A:273:GLY:HA2	1:A:304:LEU:HD21	1.88	0.56
1:C:4[A]:ARG:NH2	1:C:428:ASP:OD2	2.34	0.56
1:C:359:CYS:HA	1:C:362:LEU:HB2	1.87	0.56
3:D:501:9TD:N09	3:D:501:9TD:O26	2.38	0.56
3:C:503:9TD:N09	3:C:503:9TD:O26	2.39	0.55
1:B:48:LEU:HD11	1:B:430:ILE:HD13	1.89	0.55
1:C:106:ILE:HD11	1:C:296:GLU:HG3	1.89	0.54
3:A:502:9TD:O26	3:A:502:9TD:N09	2.37	0.54
1:D:48:LEU:HD11	1:D:430:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ASP:OD2	4:D:601:HOH:O	2.18	0.53
1:A:224:SER:HB2	1:A:262[B]:MET:HB2	1.90	0.53
3:B:501:9TD:O26	3:B:501:9TD:N09	2.39	0.53
1:C:363:VAL:HG23	1:C:372:PRO:HB2	1.91	0.53
1:A:66[A]:ILE:HD11	1:D:59:ASP:O	2.09	0.52
1:C:397:GLY:HA2	1:C:457:ARG:HE	1.75	0.52
1:A:176:ILE:HA	1:A:184:ILE:HD11	1.91	0.51
1:C:439:GLU:OE1	1:C:439:GLU:N	2.42	0.51
1:D:260:LEU:HG	1:D:277:ALA:HB3	1.92	0.51
1:C:176:ILE:HA	1:C:184:ILE:HD11	1.91	0.51
1:D:393:SER:O	1:D:457:ARG:NH2	2.42	0.51
1:D:273:GLY:HA2	1:D:304:LEU:HD21	1.92	0.51
1:B:366:ILE:HB	1:B:372:PRO:HB3	1.92	0.50
1:D:125:VAL:HG12	1:D:145:LYS:HB2	1.93	0.50
1:B:125:VAL:HG12	1:B:145:LYS:HB2	1.92	0.50
1:C:393:SER:O	1:C:457:ARG:NH2	2.45	0.49
1:B:273:GLY:HA2	1:B:304:LEU:HD21	1.95	0.49
1:A:187:ILE:HD12	1:A:213:ALA:HB2	1.94	0.49
1:D:190:THR:HA	1:D:223:ASP:HB3	1.93	0.49
1:B:110:VAL:HA	1:B:113:LYS:HE3	1.94	0.48
1:C:190:THR:HA	1:C:223:ASP:HB3	1.94	0.48
1:B:4:ARG:NH2	1:B:428:ASP:OD2	2.42	0.48
1:C:366:ILE:HG23	1:C:370:GLN:HB2	1.95	0.48
1:D:163:TRP:CD2	1:D:202:SER:HB3	2.49	0.48
1:C:377:ILE:HG12	1:C:413:MET:HG3	1.96	0.48
1:D:59:ASP:N	1:D:59:ASP:OD1	2.46	0.48
1:C:377:ILE:HG12	1:C:413:MET:HE3	1.96	0.48
1:B:49:LEU:HD12	1:B:389:VAL:HB	1.96	0.47
1:D:2:ALA:N	1:D:341:GLU:OE2	2.48	0.47
1:D:7:GLU:HG3	1:D:327:TYR:CE1	2.50	0.47
1:D:53:GLY:HA2	1:D:271:ASN:HA	1.97	0.47
1:A:7:GLU:HG3	1:A:327:TYR:CE1	2.50	0.47
1:A:105:ASN:HD21	1:A:295:MET:HE2	1.80	0.47
1:B:424:ASN:ND2	1:D:425:ASP:OD2	2.37	0.47
1:A:360:LYS:HG3	1:A:411:GLU:HB2	1.97	0.47
1:D:345:PRO:HD2	1:D:362:LEU:HD13	1.96	0.47
1:A:377:ILE:HG12	1:A:413:MET:HE3	1.96	0.47
1:D:176:ILE:HA	1:D:184:ILE:HD11	1.96	0.46
1:A:4:ARG:NH1	1:C:425:ASP:OD1	2.48	0.46
1:B:323:GLU:H	1:B:323:GLU:CD	2.18	0.46
1:B:260:LEU:HG	1:B:277:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:HIS:O	1:C:142:ASN:ND2	2.44	0.46
1:B:115:LYS:HG3	1:B:120:LYS:HB2	1.98	0.45
1:C:260:LEU:HG	1:C:277:ALA:HB3	1.98	0.45
1:C:323:GLU:H	1:C:323:GLU:CD	2.19	0.45
1:C:7:GLU:HG3	1:C:327:TYR:CE1	2.51	0.45
1:C:93:TYR:HB3	1:C:285:PHE:CD1	2.52	0.45
1:A:35:ASN:HB3	1:A:38:LEU:HD23	1.98	0.45
1:B:176:ILE:HA	1:B:184:ILE:HD11	1.99	0.45
1:A:62:TRP:O	1:A:66[A]:ILE:HG23	2.17	0.45
1:A:377:ILE:HG12	1:A:413:MET:HG3	1.99	0.44
1:C:266:LYS:HZ1	3:C:503:9TD:C08	2.31	0.44
1:D:118:GLU:HB2	1:D:120:LYS:HG3	1.99	0.44
1:B:190:THR:HA	1:B:223:ASP:HB3	1.99	0.44
1:C:395:LEU:HD12	1:C:458:HIS:CE1	2.52	0.44
1:A:98:HIS:CD2	1:A:99:GLN:HG2	2.53	0.44
1:C:365:GLN:NE2	1:C:442:ALA:O	2.42	0.44
1:B:32:ALA:HB1	1:B:38:LEU:HB2	1.98	0.44
1:C:49:LEU:HD12	1:C:389:VAL:HB	2.00	0.43
1:B:7:GLU:HG3	1:B:327:TYR:CE1	2.54	0.43
1:B:337:ASP:O	1:B:341:GLU:HG3	2.18	0.43
1:A:84:LYS:NZ	1:A:317:GLU:OE1	2.41	0.43
1:C:453:PRO:HD2	1:C:457:ARG:HA	2.00	0.43
1:A:190:THR:HA	1:A:223:ASP:HB3	2.01	0.43
1:A:260:LEU:HG	1:A:277:ALA:HB3	2.01	0.43
1:D:21:SER:O	1:D:25:ARG:HG3	2.19	0.43
1:D:93:TYR:HB3	1:D:285:PHE:CD1	2.53	0.43
1:D:191:VAL:HA	1:D:192:THR:HA	1.81	0.43
1:B:435:ILE:HG23	1:B:438:LYS:HE3	2.00	0.43
1:B:399:ASP:HB3	1:B:402:THR:HG22	2.00	0.42
1:C:20:PRO:O	1:C:25:ARG:NH1	2.52	0.42
1:A:465:PRO:O	1:A:467:GLU:N	2.51	0.42
1:B:93:TYR:HB3	1:B:285:PHE:CD1	2.55	0.42
1:C:74:GLY:HA3	1:D:40:PRO:HA	2.01	0.42
1:C:96:PRO:O	1:C:302:GLY:HA3	2.19	0.42
1:C:397:GLY:HA2	1:C:457:ARG:NE	2.33	0.42
1:C:445:LYS:HG3	1:C:467:GLU:N	2.35	0.42
1:D:129:ASN:OD1	1:D:129:ASN:N	2.51	0.42
1:A:345:PRO:HD2	1:A:362:LEU:HD13	2.02	0.42
1:D:110:VAL:HG21	1:D:288:ALA:HA	2.01	0.42
1:A:407:HIS:NE2	1:A:409:ASP:OD1	2.53	0.42
1:C:405[A]:GLN:HE21	1:C:405[A]:GLN:HB2	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:VAL:HG11	1:D:414:ARG:HH21	1.84	0.42
1:B:356:PHE:HE2	1:B:391:ILE:HD12	1.85	0.41
1:C:22[A]:ARG:HE	1:C:22[A]:ARG:HB2	1.64	0.41
1:B:110:VAL:HG21	1:B:288:ALA:HA	2.02	0.41
1:B:373:ALA:HB3	1:B:390:GLU:HG2	2.01	0.41
1:D:90:ASN:HB2	1:D:251:PHE:CE1	2.55	0.41
1:B:2:ALA:N	1:B:341:GLU:OE2	2.53	0.41
1:B:338:ARG:NH2	1:B:432:ASP:OD1	2.54	0.41
1:B:21:SER:O	1:B:25:ARG:HG3	2.21	0.41
1:A:53:GLY:HA2	1:A:271:ASN:HA	2.03	0.41
1:A:120:LYS:H	1:A:120:LYS:HG2	1.75	0.40
1:A:62:TRP:CG	1:C:13:MET:HE2	2.56	0.40
1:A:110:VAL:HG21	1:A:288:ALA:HA	2.04	0.40
1:B:391:ILE:HD11	1:B:414:ARG:HD3	2.03	0.40
1:D:105:ASN:HD21	1:D:291:ARG:HH21	1.69	0.40
1:D:117:LYS:HB2	1:D:117:LYS:HE3	1.86	0.40
1:A:13:MET:HE3	1:C:13:MET:HE1	2.04	0.40
1:C:383:GLU:HG2	1:C:437:LEU:HD21	2.03	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	468/467 (100%)	451 (96%)	16 (3%)	1 (0%)	47	49
1	B	467/467 (100%)	449 (96%)	18 (4%)	0	100	100
1	C	470/467 (101%)	451 (96%)	18 (4%)	1 (0%)	47	49
1	D	470/467 (101%)	450 (96%)	20 (4%)	0	100	100
All	All	1875/1868 (100%)	1801 (96%)	72 (4%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	401	ALA
1	A	466	ILE

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	389/386 (101%)	381 (98%)	8 (2%)	53	59
1	B	388/386 (100%)	383 (99%)	5 (1%)	69	75
1	C	391/386 (101%)	381 (97%)	10 (3%)	46	50
1	D	391/386 (101%)	381 (97%)	10 (3%)	46	50
All	All	1559/1544 (101%)	1526 (98%)	33 (2%)	55	59

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66[A]	ILE
1	A	66[B]	ILE
1	A	130	PHE
1	A	327	TYR
1	A	328	ARG
1	A	390	GLU
1	A	410	MET
1	A	416	THR
1	B	130	PHE
1	B	134	THR
1	B	202	SER
1	B	328	ARG
1	B	416	THR
1	C	130	PHE
1	C	327	TYR
1	C	328	ARG
1	C	365	GLN
1	C	394	PHE
1	C	405[A]	GLN
1	C	405[B]	GLN

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Mol	Chain	Res	Type
1	C	416	THR
1	C	445	LYS
1	C	467	GLU
1	D	66	ILE
1	D	130	PHE
1	D	152	GLU
1	D	157	SER
1	D	183	ASN
1	D	327	TYR
1	D	328	ARG
1	D	369	ASP
1	D	390	GLU
1	D	416	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	B	105	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	9TD	A	502	-	31,33,33	3.07	3 (9%)	41,48,48	2.97	9 (21%)
3	9TD	C	503	-	31,33,33	3.07	2 (6%)	41,48,48	2.94	7 (17%)
3	9TD	D	501	-	31,33,33	3.06	2 (6%)	41,48,48	2.89	7 (17%)
3	9TD	B	501	-	31,33,33	3.07	3 (9%)	41,48,48	2.92	8 (19%)

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
3	9TD	A	502	-	-	4/19/31/31	0/3/3/3
3	9TD	C	503	-	-	5/19/31/31	0/3/3/3
3	9TD	D	501	-	-	5/19/31/31	0/3/3/3
3	9TD	B	501	-	-	5/19/31/31	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	9TD	C16-N15	14.66	1.47	1.35
3	A	502	9TD	C16-N15	14.65	1.47	1.35
3	B	501	9TD	C16-N15	14.62	1.47	1.35
3	D	501	9TD	C16-N15	14.61	1.47	1.35
3	A	502	9TD	C07-C08	-6.55	1.34	1.46
3	B	501	9TD	C07-C08	-6.53	1.34	1.46
3	D	501	9TD	C07-C08	-6.49	1.34	1.46
3	C	503	9TD	C07-C08	-6.45	1.34	1.46
3	A	502	9TD	C07-C06	-2.06	1.39	1.42
3	B	501	9TD	C07-C06	-2.01	1.39	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	9TD	C14-N15-C16	-13.08	104.72	111.85
3	C	503	9TD	C14-N15-C16	-13.03	104.75	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	9TD	C14-N15-C16	-12.91	104.81	111.85
3	D	501	9TD	C14-N15-C16	-12.91	104.81	111.85
3	A	502	9TD	C13-C14-N15	9.87	113.87	109.31
3	B	501	9TD	C13-C14-N15	9.78	113.83	109.31
3	C	503	9TD	C13-C14-N15	9.73	113.81	109.31
3	D	501	9TD	C13-C14-N15	9.63	113.76	109.31
3	A	502	9TD	C10-N09-C08	4.41	123.68	117.31
3	D	501	9TD	C10-N09-C08	4.35	123.58	117.31
3	C	503	9TD	C22-C10-N09	4.24	117.07	108.67
3	C	503	9TD	C10-N09-C08	4.23	123.41	117.31
3	A	502	9TD	C22-C10-N09	4.05	116.68	108.67
3	B	501	9TD	C22-C10-N09	3.89	116.38	108.67
3	B	501	9TD	C10-N09-C08	3.80	122.80	117.31
3	D	501	9TD	C22-C10-N09	3.71	116.02	108.67
3	C	503	9TD	C18-C14-N15	-2.72	125.33	130.87
3	B	501	9TD	C18-C14-N15	-2.71	125.35	130.87
3	A	502	9TD	C18-C14-N15	-2.71	125.36	130.87
3	D	501	9TD	C18-C14-N15	-2.64	125.50	130.87
3	A	502	9TD	C06-C30-N29	-2.41	119.80	123.82
3	C	503	9TD	C06-C30-N29	-2.36	119.89	123.82
3	D	501	9TD	C06-C30-N29	-2.35	119.91	123.82
3	B	501	9TD	C06-C30-N29	-2.33	119.94	123.82
3	B	501	9TD	C21-C13-C14	2.19	121.32	119.95
3	C	503	9TD	C20-C21-C13	-2.14	118.28	121.01
3	B	501	9TD	C20-C21-C13	-2.14	118.29	121.01
3	A	502	9TD	C20-C21-C13	-2.12	118.32	121.01
3	A	502	9TD	C21-C13-C14	2.05	121.23	119.95
3	A	502	9TD	C07-C08-N09	-2.05	118.46	123.01
3	D	501	9TD	C20-C21-C13	-2.01	118.45	121.01

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	9TD	C11-C10-N09-C08
3	B	501	9TD	C22-C10-C11-C12
3	B	501	9TD	C11-C10-N09-C08
3	C	503	9TD	C11-C10-N09-C08
3	D	501	9TD	C22-C10-C11-C12
3	D	501	9TD	C11-C10-N09-C08
3	A	502	9TD	C22-C10-C11-C12
3	C	503	9TD	C22-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	502	9TD	N09-C10-C11-C12
3	C	503	9TD	N09-C10-C11-C12
3	A	502	9TD	O04-C05-C06-C07
3	B	501	9TD	O04-C05-C06-C07
3	C	503	9TD	O04-C05-C06-C07
3	D	501	9TD	O04-C05-C06-C07
3	B	501	9TD	N09-C10-C11-C12
3	D	501	9TD	N09-C10-C11-C12
3	B	501	9TD	O04-C05-C06-C30
3	C	503	9TD	O04-C05-C06-C30
3	D	501	9TD	O04-C05-C06-C30

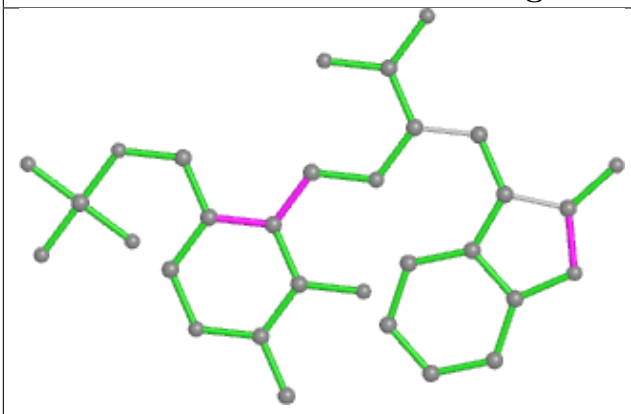
There are no ring outliers.

4 monomers are involved in 5 short contacts:

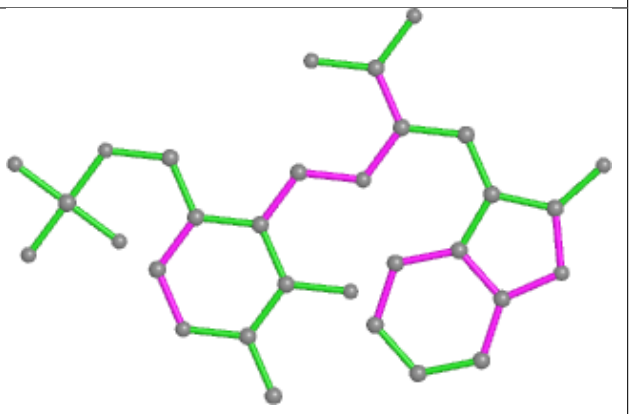
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	9TD	1	0
3	C	503	9TD	2	0
3	D	501	9TD	1	0
3	B	501	9TD	1	0

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.

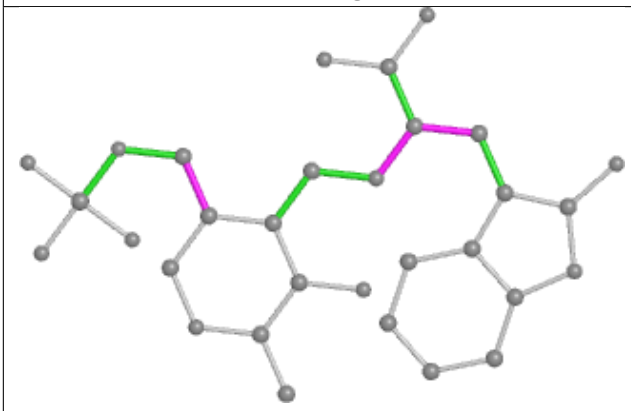
Ligand 9TD A 502



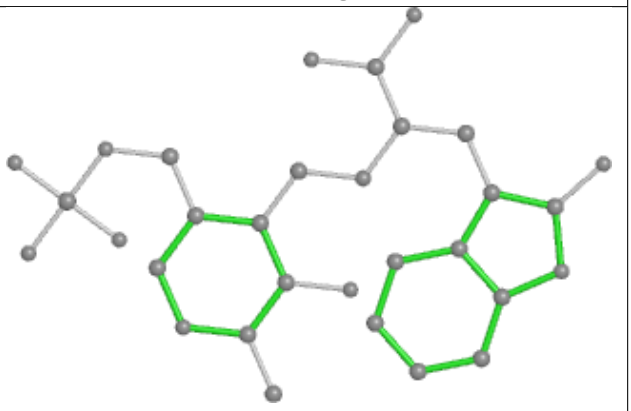
Bond lengths



Bond angles

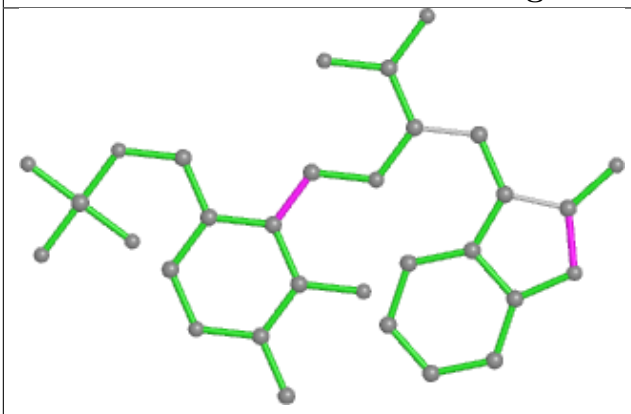


Torsions

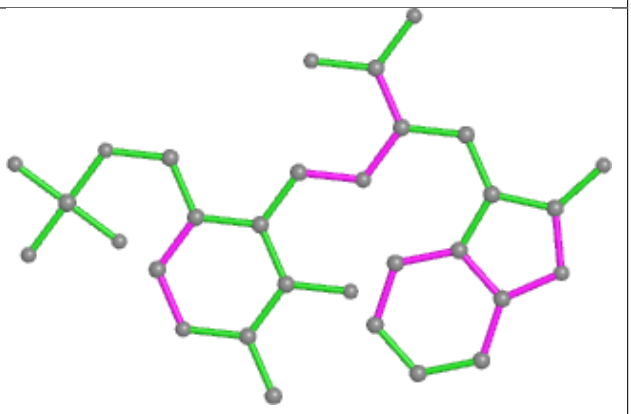


Rings

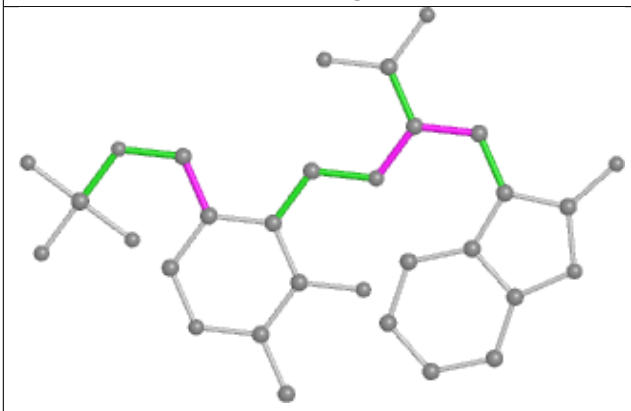
Ligand 9TD C 503



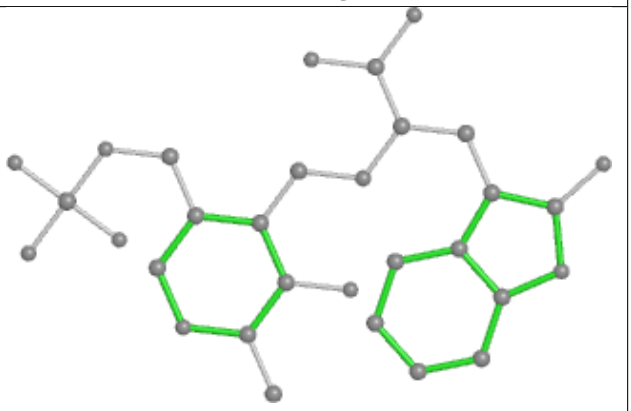
Bond lengths



Bond angles

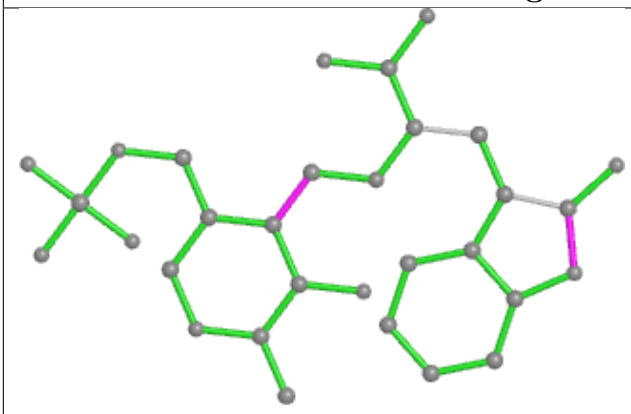


Torsions

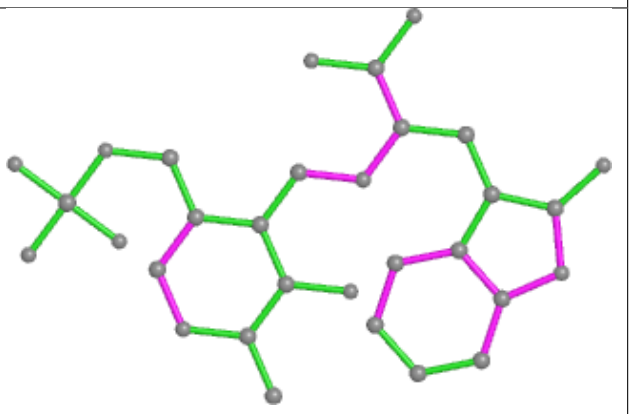


Rings

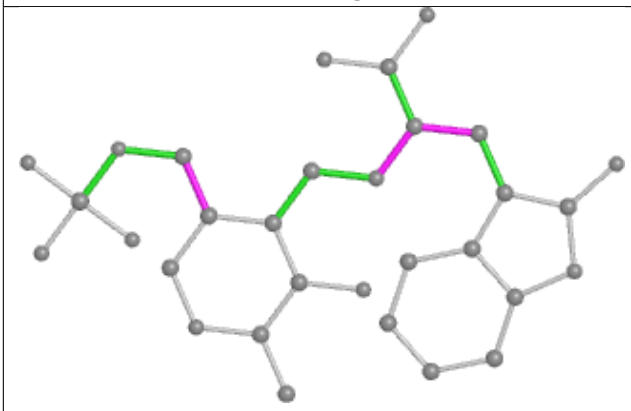
Ligand 9TD D 501



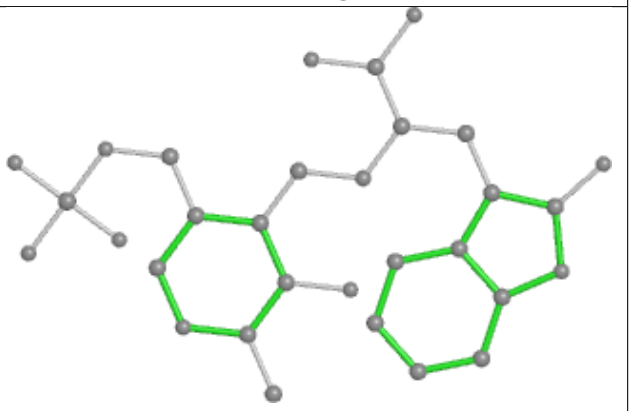
Bond lengths



Bond angles

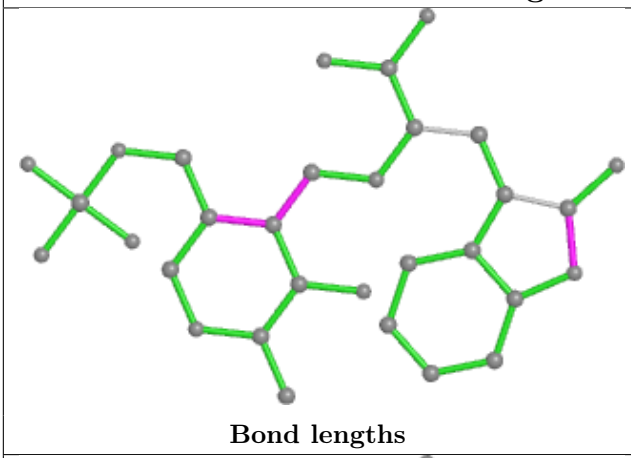


Torsions

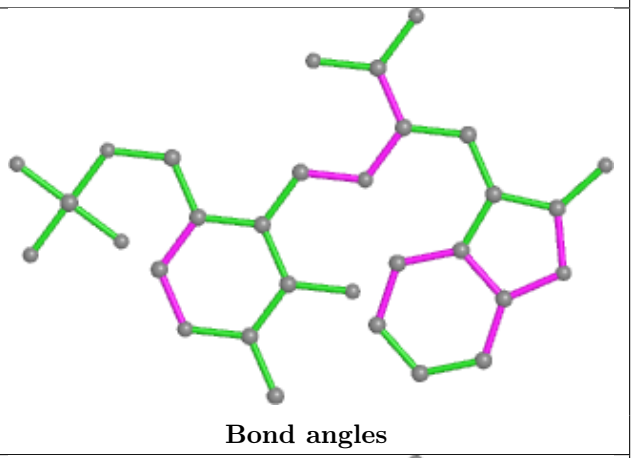


Rings

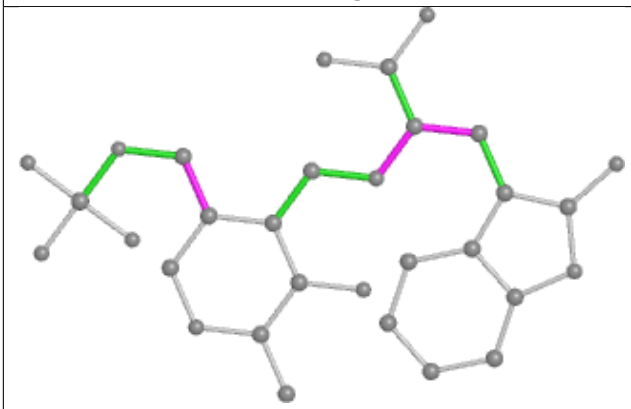
Ligand 9TD B 501



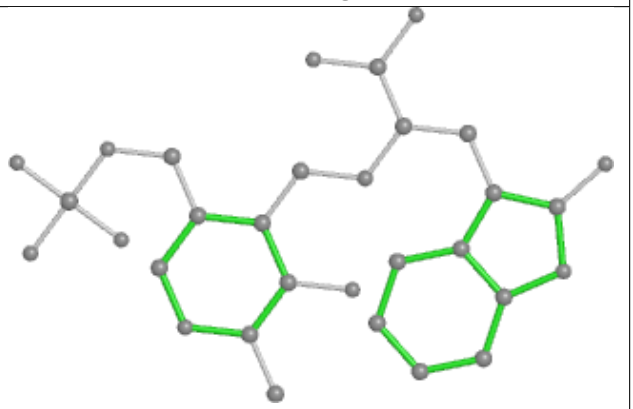
Bond lengths



Bond angles



Torsions



Rings

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	466/467 (99%)	0.32	16 (3%)	45	51	45, 71, 113, 168	0
1	B	466/467 (99%)	0.37	20 (4%)	35	41	45, 68, 106, 153	0
1	C	466/467 (99%)	0.54	42 (9%)	9	12	42, 65, 132, 234	0
1	D	466/467 (99%)	0.55	38 (8%)	11	15	46, 75, 114, 159	0
All	All	1864/1868 (99%)	0.45	116 (6%)	20	25	42, 70, 117, 234	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	401	ALA	11.7
1	B	401	ALA	8.4
1	C	463	LEU	6.5
1	C	466	ILE	6.4
1	C	444	LEU	6.1
1	D	466	ILE	6.0
1	D	444	LEU	5.9
1	C	400	PRO	5.9
1	B	467	GLU	5.7
1	C	447	LEU	5.6
1	C	464	LYS	5.5
1	B	444	LEU	4.8
1	C	467	GLU	4.7
1	D	447	LEU	4.7
1	C	441	PHE	4.6
1	D	437	LEU	4.1
1	C	402	THR	4.0
1	A	444	LEU	3.9
1	C	403	GLY	3.8
1	D	396	LEU	3.8
1	B	295	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	466	ILE	3.7
1	A	441	PHE	3.7
1	C	442	ALA	3.6
1	A	466	ILE	3.6
1	A	438	LYS	3.5
1	C	448	GLU	3.3
1	D	62	TRP	3.2
1	C	366	ILE	3.2
1	C	404	GLU	3.1
1	D	182	ASP	3.1
1	C	397	GLY	3.1
1	D	467	GLU	3.1
1	B	447	LEU	3.1
1	D	402	THR	3.0
1	D	272	ILE	3.0
1	D	72	TYR	3.0
1	C	410	MET	3.0
1	D	445	LYS	3.0
1	C	272	ILE	2.9
1	C	117	LYS	2.9
1	C	270	LEU	2.9
1	D	126	PHE	2.9
1	C	62	TRP	2.9
1	B	400	PRO	2.9
1	A	467	GLU	2.8
1	C	445	LYS	2.8
1	C	368	GLY	2.8
1	B	26	GLU	2.8
1	C	364	PRO	2.8
1	C	407	HIS	2.8
1	C	395	LEU	2.8
1	B	448	GLU	2.7
1	C	451	TYR	2.7
1	A	463	LEU	2.7
1	C	411	GLU	2.6
1	D	366	ILE	2.6
1	A	401	ALA	2.6
1	C	363	VAL	2.6
1	A	445	LYS	2.6
1	B	72	TYR	2.6
1	D	308	ASP	2.6
1	A	100	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	447	LEU	2.6
1	B	437	LEU	2.6
1	C	399	ASP	2.5
1	D	66	ILE	2.5
1	B	368	GLY	2.5
1	D	71	ALA	2.5
1	C	369	ASP	2.4
1	A	13	MET	2.4
1	B	402	THR	2.4
1	D	99	GLN	2.4
1	D	397	GLY	2.4
1	D	22	ARG	2.4
1	B	298	PHE	2.3
1	D	273	GLY	2.3
1	D	293	VAL	2.3
1	D	65[A]	MET	2.3
1	D	123	ASN	2.3
1	D	294	PRO	2.3
1	B	241	TYR	2.3
1	C	371	PHE	2.3
1	B	302	GLY	2.3
1	D	295	MET	2.2
1	C	134[A]	THR	2.2
1	A	366	ILE	2.2
1	B	66	ILE	2.2
1	C	391	ILE	2.2
1	C	303	GLY	2.2
1	D	304	LEU	2.2
1	B	293	VAL	2.2
1	C	271	ASN	2.2
1	B	463	LEU	2.2
1	D	270	LEU	2.2
1	C	30	LYS	2.2
1	D	25	ARG	2.2
1	D	301	TYR	2.2
1	C	273	GLY	2.2
1	D	53	GLY	2.2
1	A	34	TYR	2.1
1	A	127	ILE	2.1
1	D	117	LYS	2.1
1	A	62	TRP	2.1
1	C	34	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	34	TYR	2.1
1	D	381	TYR	2.1
1	D	68	GLY	2.1
1	D	296	GLU	2.1
1	C	100	GLY	2.1
1	B	311	ALA	2.1
1	C	102	GLY	2.0
1	D	418	ALA	2.0
1	C	52	SER	2.0
1	A	273	GLY	2.0
1	D	102	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

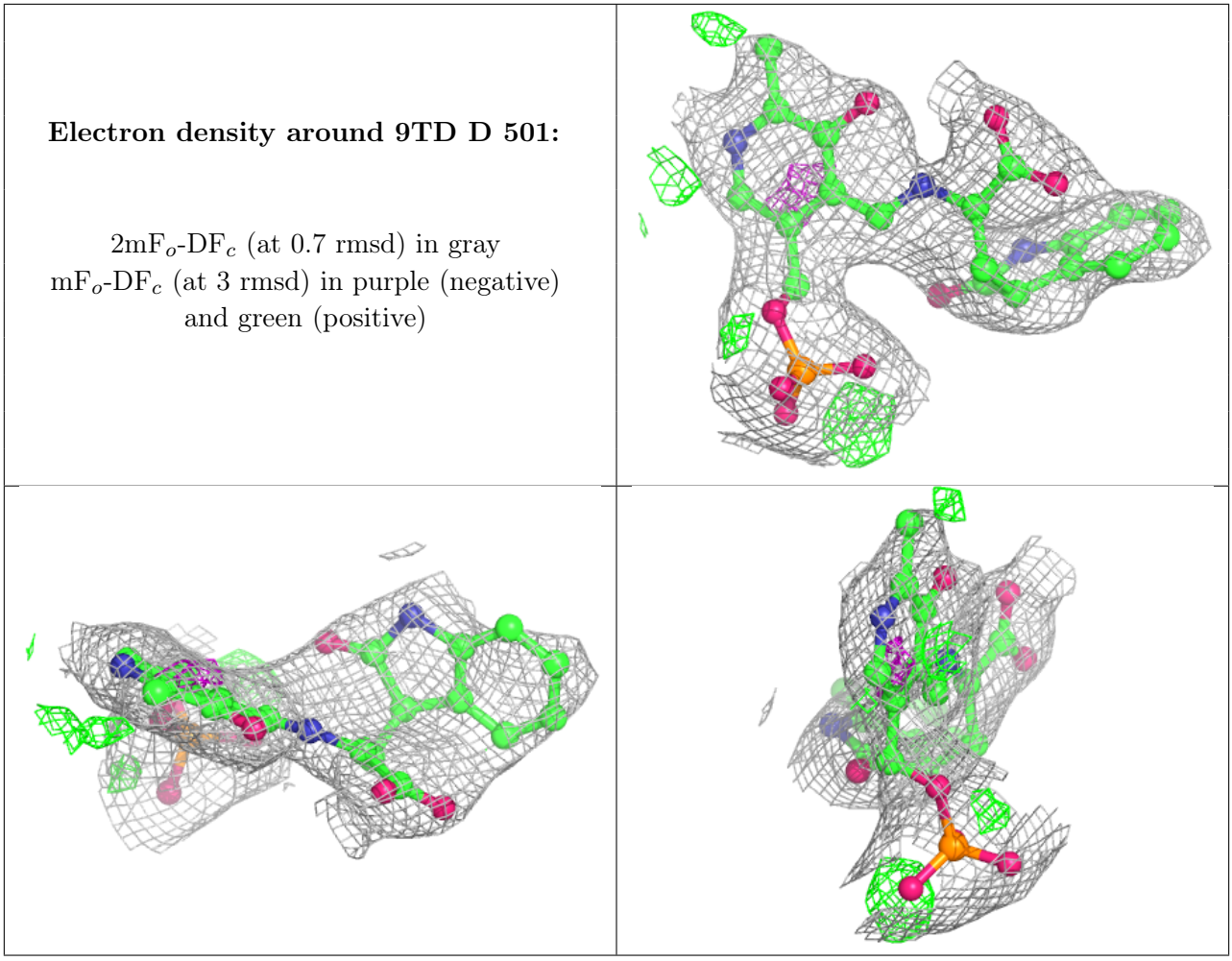
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	9TD	D	501	31/31	0.94	0.16	53,78,87,87	0
3	9TD	A	502	31/31	0.95	0.14	46,62,82,83	0
3	9TD	B	501	31/31	0.95	0.16	52,69,79,80	0
3	9TD	C	503	31/31	0.95	0.17	48,62,83,84	0
2	K	A	503	1/1	0.95	0.07	61,61,61,61	0
2	K	C	501	1/1	0.96	0.12	56,56,56,56	0
2	K	A	501	1/1	0.97	0.12	54,54,54,54	0
2	K	C	502	1/1	0.98	0.09	52,52,52,52	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.

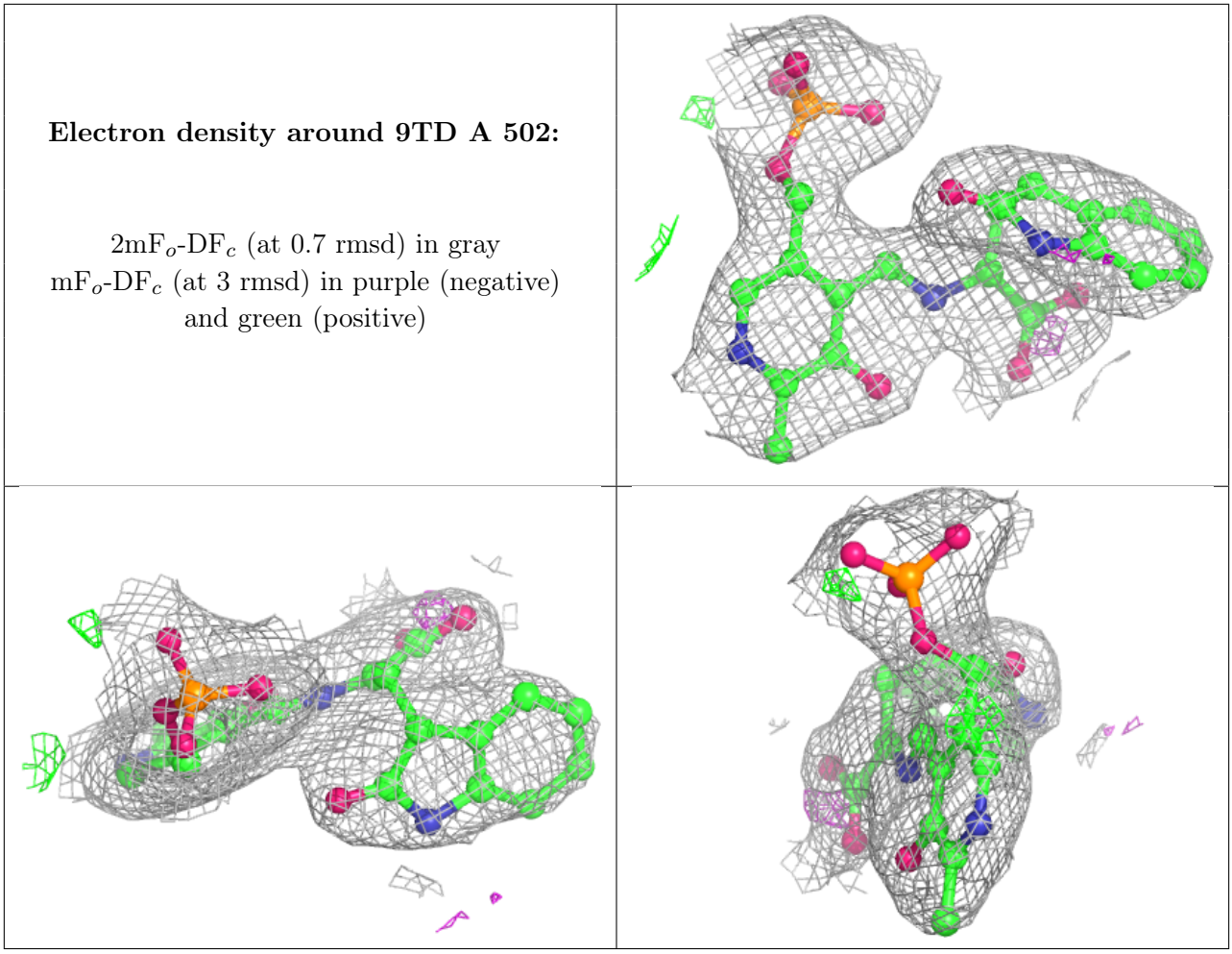
Electron density around 9TD D 501:

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



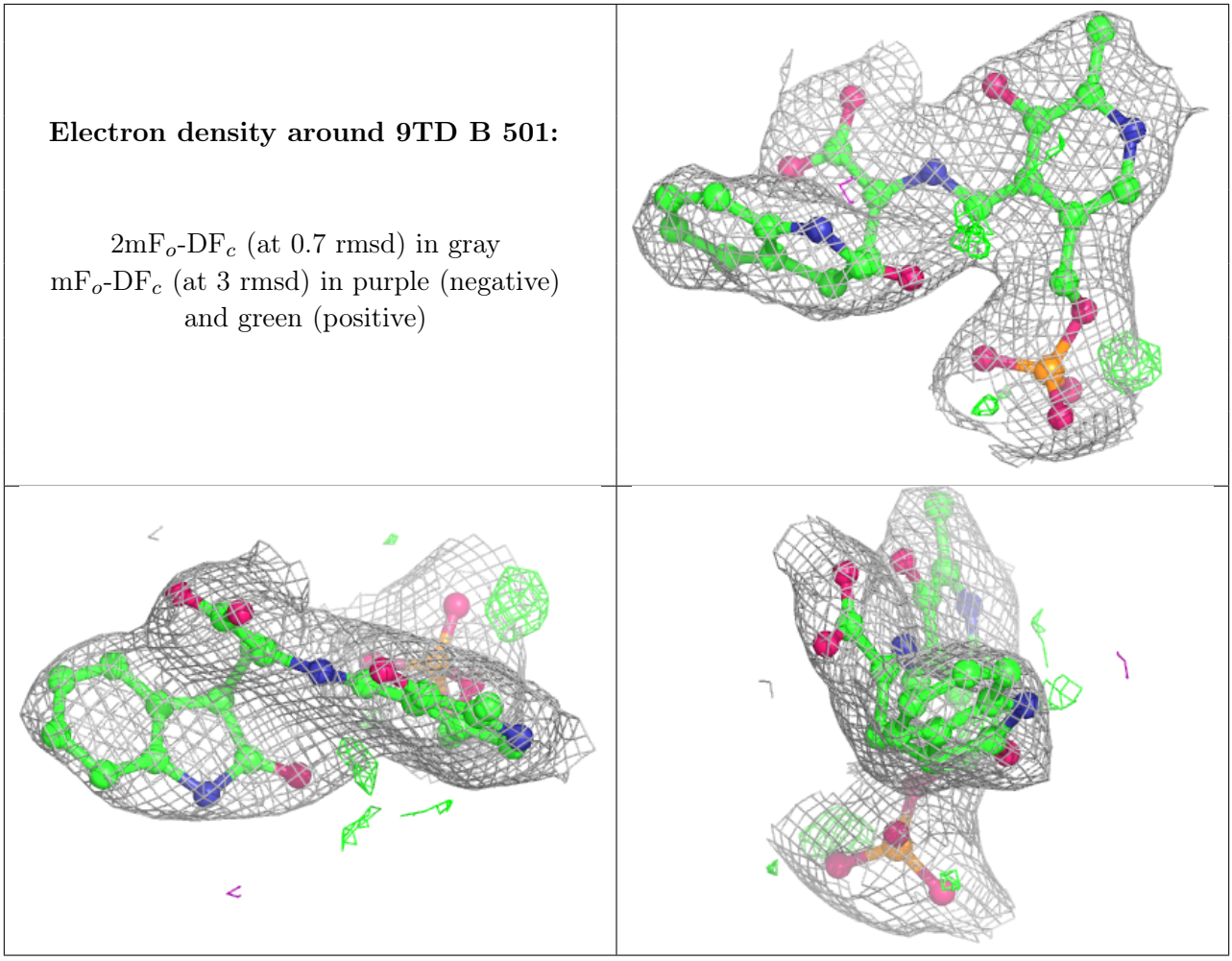
Electron density around 9TD A 502:

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



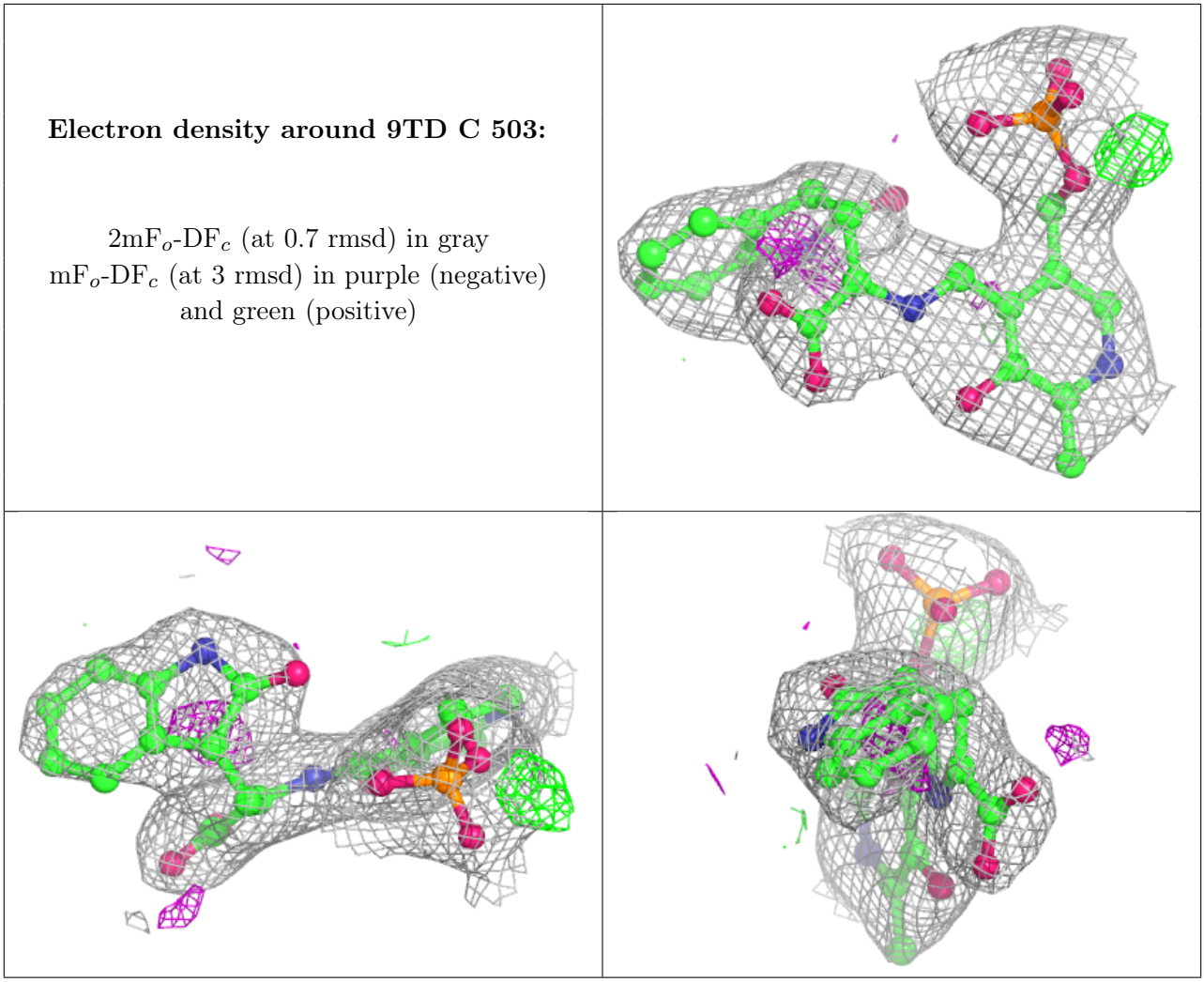
Electron density around 9TD B 501:

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



Electron density around 9TD 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

There are no such residues in this entry.