Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 03:35 AM EDT

PDB ID	:	7TEV
Title	:	Human Ornithine Aminotransferase cocrystallized with its inhibitor, (3S,4R)-3-amino-4-(difluoromethyl)cyclopent-1-ene-1-carboxylate
Authors	:	Butrin, A.; Zhu, W.; Silverman, R.; Liu, D.
Deposited on	:	2022-01-05
Resolution	:	1.91 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:

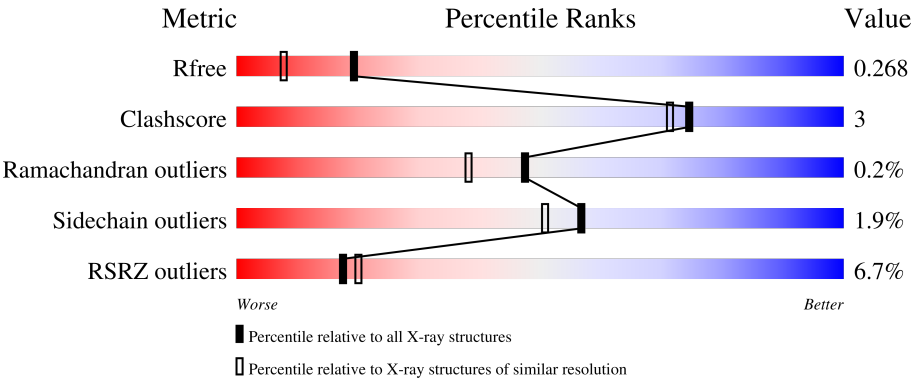
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	404	9% 91% 8%
1	B	404	8% 90% 9%
1	C	404	3% 91% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	I1T	B	501	X	-	-	-
2	I1T	C	501	X	-	-	-

2 Entry composition

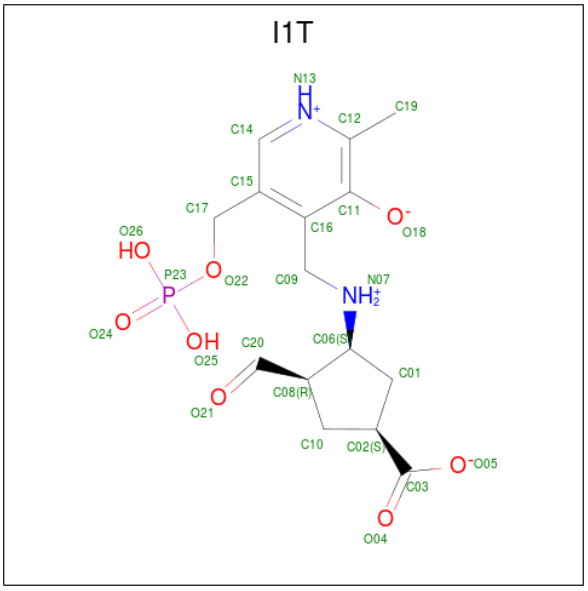
There are 3 unique types of molecules in this entry. The entry contains 10134 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3157	2028	532	585	12			
1	B	403	Total	C	N	O	S	0	0	0
			3157	2028	532	585	12			
1	C	402	Total	C	N	O	S	0	0	0
			3150	2023	531	584	12			

- Molecule 2 is (1S,3R,4S)-3-formyl-4-[({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)amino]cyclopentane-1-carboxylic acid (three-letter code: I1T) (formula: $C_{15}H_{21}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	15	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			26	15	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			26	15	2	8	1		

- Molecule 3 is water.

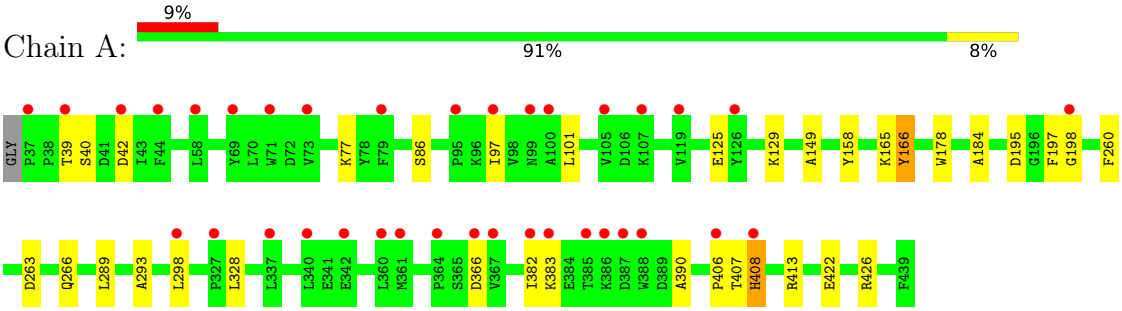
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		
3	B	166	Total	O	0	0
			166	166		
3	C	248	Total	O	0	0
			248	248		

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.

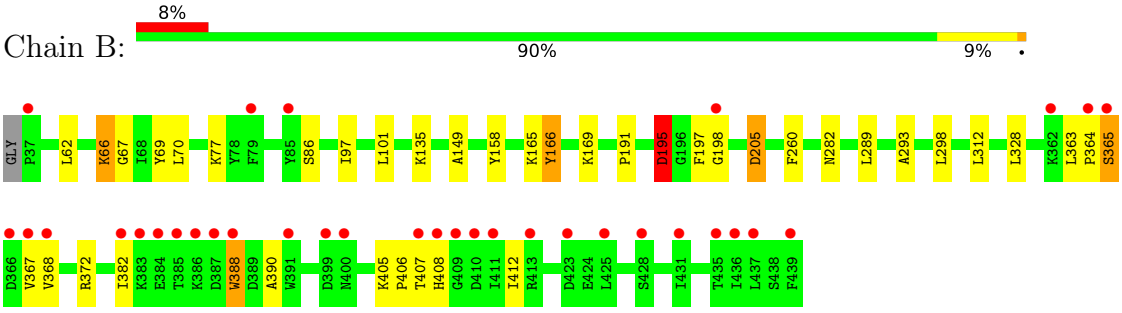
• Molecule 1: Ornithine aminotransferase, mitochondrial

Chain A:



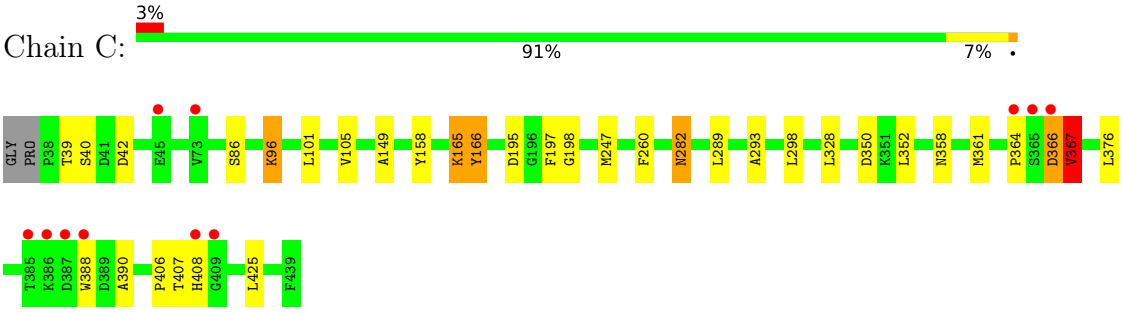
• Molecule 1: Ornithine aminotransferase, mitochondrial

Chain B:



• Molecule 1: Ornithine aminotransferase, mitochondrial

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.83Å 115.83Å 187.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.22 – 1.91 44.22 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.22-1.91) 99.4 (44.22-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.256 , 0.269 0.255 , 0.268	Depositor DCC
R_{free} test set	5651 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 20.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.068 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10134	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: I1T

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	0.59	1/3231 (0.0%)	0.78	4/4387 (0.1%)
1	B	0.56	1/3231 (0.0%)	0.78	8/4387 (0.2%)
1	C	0.62	1/3223 (0.0%)	0.81	5/4375 (0.1%)
All	All	0.59	3/9685 (0.0%)	0.79	17/13149 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	1
1	C	0	1
All	All	1	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLY	N-CA	9.08	1.59	1.46
1	C	198	GLY	N-CA	6.19	1.55	1.46
1	B	195	ASP	CB-CG	-5.19	1.40	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	GLY	N-CA-C	-10.34	87.26	113.10
1	C	198	GLY	N-CA-C	-9.69	88.87	113.10
1	B	198	GLY	N-CA-C	-9.18	90.15	113.10
1	A	195	ASP	CB-CG-OD1	7.07	124.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	TYR	CB-CA-C	6.54	123.49	110.40
1	A	166	TYR	CB-CA-C	6.41	123.21	110.40
1	C	166	TYR	CB-CA-C	6.24	122.88	110.40
1	B	195	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	365	SER	N-CA-CB	6.03	119.54	110.50
1	B	205	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	365	SER	CB-CA-C	5.67	120.86	110.10
1	B	165	LYS	C-N-CA	5.45	135.34	121.70
1	A	165	LYS	C-N-CA	5.43	135.27	121.70
1	C	195	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	165	LYS	C-N-CA	5.32	135.00	121.70
1	B	165	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	C	350	ASP	CB-CG-OD1	5.11	122.90	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	365	SER	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	PHE	Peptide
1	B	197	PHE	Peptide
1	C	197	PHE	Peptide

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	3157	0	3163	18	0
1	B	3157	0	3163	19	0
1	C	3150	0	3156	22	0
2	A	26	0	0	2	0
2	B	26	0	0	1	0
2	C	26	0	0	1	0
3	A	178	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	166	0	0	0	0
3	C	248	0	0	1	0
All	All	10134	0	9482	60	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 3.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:O	1:C:105:VAL:HG13	1.83	0.78
1:B:169:LYS:HE3	1:B:205:ASP:OD2	1.85	0.77
1:C:96:LYS:NZ	3:C:602:HOH:O	2.19	0.71
1:A:39:THR:HG23	1:A:42:ASP:H	1.56	0.70
1:C:39:THR:HG23	1:C:42:ASP:H	1.55	0.70
1:B:62:LEU:HD22	1:B:70:LEU:HB3	1.79	0.64
1:B:405:LYS:HG3	1:B:406:PRO:HD2	1.81	0.62
1:C:101:LEU:HD12	1:C:328:LEU:HD11	1.81	0.61
1:B:101:LEU:HD12	1:B:328:LEU:HD11	1.83	0.61
1:A:101:LEU:HD12	1:A:328:LEU:HD11	1.85	0.59
2:C:501:I1T:N07	2:C:501:I1T:O18	2.36	0.58
1:A:266:GLN:OE1	1:A:413:ARG:NH1	2.36	0.58
1:C:158:TYR:OH	1:C:166:TYR:HA	2.05	0.57
1:B:158:TYR:OH	1:B:166:TYR:HA	2.05	0.57
1:A:158:TYR:OH	1:A:166:TYR:HA	2.04	0.56
1:A:39:THR:HG22	1:A:42:ASP:CG	2.27	0.55
1:B:363:LEU:HB2	1:B:368:VAL:HG21	1.88	0.55
1:B:390:ALA:HB1	1:B:406:PRO:HB3	1.88	0.55
1:A:422:GLU:OE2	1:A:426:ARG:NH1	2.37	0.54
1:B:86:SER:O	1:B:293:ALA:HB2	2.08	0.54
1:C:390:ALA:HB1	1:C:406:PRO:HB3	1.89	0.53
1:B:282:ASN:HB3	1:C:282:ASN:HB3	1.91	0.53
1:C:39:THR:HG22	1:C:42:ASP:CG	2.29	0.52
1:B:191:PRO:O	1:B:195:ASP:HB2	2.10	0.52
1:B:382:ILE:HD11	1:B:412:ILE:HD12	1.91	0.52
1:A:86:SER:O	1:A:293:ALA:HB2	2.10	0.51
1:A:382:ILE:HD11	1:A:390:ALA:N	2.26	0.51
1:B:135:LYS:HE2	1:B:312:LEU:HD21	1.93	0.51
1:A:390:ALA:HB1	1:A:406:PRO:HB3	1.93	0.51
1:C:86:SER:O	1:C:293:ALA:HB2	2.11	0.50
1:A:407:THR:O	1:A:408:HIS:CG	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ASP:O	1:C:367:VAL:HG12	2.12	0.49
1:C:407:THR:O	1:C:408:HIS:CG	2.65	0.49
1:B:407:THR:O	1:B:408:HIS:CG	2.65	0.48
2:B:501:I1T:O18	2:B:501:I1T:N07	2.47	0.48
1:A:97:ILE:HG22	1:A:298:LEU:HD22	1.96	0.47
1:C:39:THR:HG22	1:C:42:ASP:OD2	2.16	0.46
1:B:97:ILE:HG22	1:B:298:LEU:HD22	1.98	0.46
1:C:364:PRO:O	1:C:367:VAL:HG12	2.15	0.46
1:A:125:GLU:CG	1:A:129:LYS:HE2	2.46	0.46
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.99	0.45
1:C:364:PRO:O	1:C:366:ASP:O	2.35	0.45
1:A:39:THR:HG22	1:A:42:ASP:OD2	2.17	0.44
1:B:66:LYS:HD3	1:B:67:GLY:N	2.32	0.44
1:C:358:ASN:HD22	1:C:361:MET:HE3	1.83	0.44
1:B:382:ILE:HG23	1:B:388:TRP:CZ2	2.54	0.43
1:C:101:LEU:HD12	1:C:328:LEU:CD1	2.48	0.42
1:C:366:ASP:OD1	1:C:366:ASP:N	2.52	0.42
1:A:178:TRP:HA	2:A:501:I1T:C14	2.50	0.42
1:B:149:ALA:HB2	1:B:289:LEU:HD21	2.01	0.41
1:C:149:ALA:HB2	1:C:289:LEU:HD21	2.02	0.41
1:C:39:THR:OG1	1:C:40:SER:N	2.53	0.41
1:B:364:PRO:O	1:B:367:VAL:HG12	2.20	0.41
1:B:69:TYR:CG	1:B:77:LYS:HE3	2.56	0.41
1:C:352:LEU:HB3	1:C:425:LEU:HD22	2.03	0.41
1:A:39:THR:OG1	1:A:40:SER:N	2.54	0.41
1:A:178:TRP:CZ2	1:A:184:ALA:HA	2.56	0.41
1:C:96:LYS:CD	1:C:96:LYS:O	2.69	0.41
1:A:263:ASP:OD2	2:A:501:I1T:N13	2.54	0.40
1:C:376:LEU:HD23	1:C:376:LEU:HA	1.98	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	401/404 (99%)	383 (96%)	17 (4%)	1 (0%)	47 38
1	B	401/404 (99%)	383 (96%)	18 (4%)	0	100 100
1	C	400/404 (99%)	380 (95%)	19 (5%)	1 (0%)	41 31
All	All	1202/1212 (99%)	1146 (95%)	54 (4%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	367	VAL
1	A	408	HIS

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	337/337 (100%)	333 (99%)	4 (1%)	71 69
1	B	337/337 (100%)	331 (98%)	6 (2%)	59 53
1	C	336/337 (100%)	327 (97%)	9 (3%)	44 36
All	All	1010/1011 (100%)	991 (98%)	19 (2%)	57 51

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	260	PHE
1	A	366	ASP
1	A	383	LYS
1	B	66	LYS
1	B	195	ASP
1	B	260	PHE
1	B	365	SER
1	B	372	ARG
1	B	388	TRP
1	C	96	LYS

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Mol	Chain	Res	Type
1	C	165	LYS
1	C	247	MET
1	C	260	PHE
1	C	282	ASN
1	C	298	LEU
1	C	366	ASP
1	C	367	VAL
1	C	388	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	358	ASN
1	C	266	GLN
1	C	282	ASN
1	C	358	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)

3 ligands are modelled in this entry.

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	I1T	B	501	-	27,27,27	3.66	10 (37%)	31,39,39	1.95	6 (19%)
2	I1T	A	501	-	27,27,27	3.82	10 (37%)	31,39,39	1.75	5 (16%)
2	I1T	C	501	-	27,27,27	3.69	10 (37%)	31,39,39	1.75	5 (16%)

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	I1T	B	501	-	1/1/5/6	4/16/29/29	0/2/2/2
2	I1T	A	501	-	-	3/16/29/29	0/2/2/2
2	I1T	C	501	-	2/2/5/6	4/16/29/29	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	I1T	C11-C12	13.44	1.54	1.40
2	A	501	I1T	C11-C12	13.21	1.54	1.40
2	B	501	I1T	C11-C12	12.10	1.53	1.40
2	A	501	I1T	C15-C16	10.21	1.54	1.40
2	B	501	I1T	C15-C16	10.06	1.54	1.40
2	C	501	I1T	C15-C16	8.67	1.52	1.40
2	A	501	I1T	C14-N13	6.58	1.48	1.34
2	B	501	I1T	C14-N13	6.16	1.47	1.34
2	C	501	I1T	C14-N13	5.33	1.45	1.34
2	C	501	I1T	C08-C20	4.99	1.58	1.50
2	B	501	I1T	C08-C20	4.49	1.57	1.50
2	A	501	I1T	C08-C20	3.70	1.56	1.50
2	B	501	I1T	O18-C11	3.04	1.44	1.37
2	C	501	I1T	C11-C16	-2.98	1.35	1.40
2	B	501	I1T	P23-O22	2.82	1.69	1.60
2	C	501	I1T	P23-O22	2.78	1.69	1.60
2	A	501	I1T	C06-N07	2.59	1.52	1.47
2	A	501	I1T	C17-C15	2.53	1.57	1.50
2	A	501	I1T	O18-C11	2.52	1.42	1.37
2	A	501	I1T	C01-C06	-2.49	1.49	1.54
2	B	501	I1T	C01-C06	-2.47	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	I1T	C01-C06	-2.45	1.49	1.54
2	B	501	I1T	C06-N07	2.37	1.52	1.47
2	A	501	I1T	P23-O22	2.33	1.67	1.60
2	C	501	I1T	C02-C03	2.30	1.55	1.51
2	C	501	I1T	C06-N07	2.29	1.52	1.47
2	C	501	I1T	O18-C11	2.28	1.42	1.37
2	A	501	I1T	C02-C03	2.14	1.55	1.51
2	B	501	I1T	C17-C15	2.11	1.56	1.50
2	B	501	I1T	C11-C16	-2.01	1.37	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	I1T	C08-C06-N07	6.83	123.64	112.81
2	A	501	I1T	C08-C06-N07	6.23	122.68	112.81
2	C	501	I1T	C08-C06-N07	5.79	121.99	112.81
2	A	501	I1T	C10-C08-C06	3.54	106.81	100.61
2	B	501	I1T	C10-C08-C06	3.31	106.40	100.61
2	C	501	I1T	C14-C15-C16	3.00	120.24	118.12
2	C	501	I1T	C10-C08-C06	2.83	105.56	100.61
2	B	501	I1T	C01-C06-C08	2.65	108.15	104.23
2	B	501	I1T	O25-P23-O22	-2.40	100.34	106.73
2	A	501	I1T	O05-C03-C02	2.36	120.39	114.21
2	C	501	I1T	C01-C06-C08	2.17	107.45	104.23
2	C	501	I1T	O05-C03-C02	2.15	119.83	114.21
2	A	501	I1T	O21-C20-C08	-2.12	120.21	125.16
2	A	501	I1T	C19-C12-N13	2.05	121.68	117.67
2	B	501	I1T	O05-C03-C02	2.05	119.57	114.21
2	B	501	I1T	C19-C12-N13	2.02	121.61	117.67

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	I1T	C02
2	C	501	I1T	C02
2	C	501	I1T	C08

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	I1T	C01-C06-N07-C09
2	B	501	I1T	N07-C09-C16-C11

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Mol	Chain	Res	Type	Atoms
2	B	501	I1T	N07-C09-C16-C15
2	C	501	I1T	C01-C06-N07-C09
2	A	501	I1T	N07-C09-C16-C15
2	C	501	I1T	N07-C09-C16-C15
2	C	501	I1T	N07-C09-C16-C11
2	A	501	I1T	N07-C09-C16-C11
2	A	501	I1T	C01-C06-N07-C09
2	C	501	I1T	C10-C02-C03-O05
2	B	501	I1T	C17-O22-P23-O24

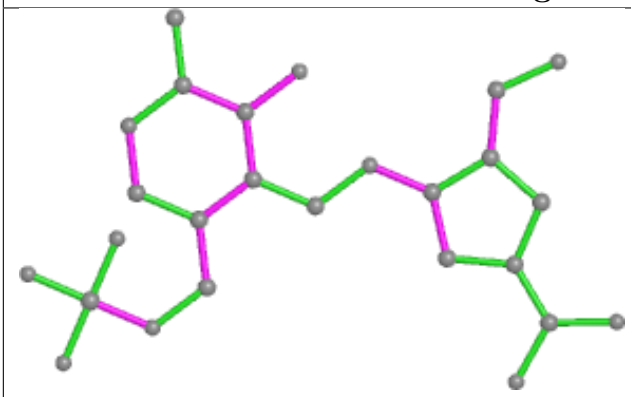
There are no ring outliers.

3 monomers are involved in 4 short contacts:

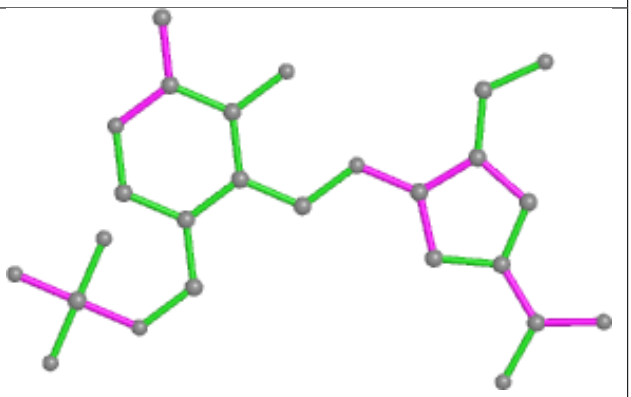
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	I1T	1	0
2	A	501	I1T	2	0
2	C	501	I1T	1	0

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.

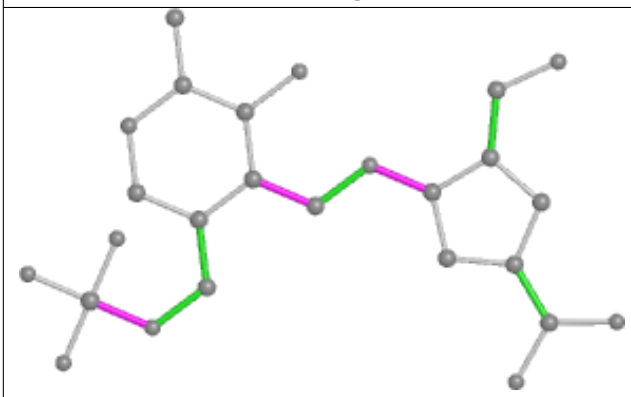
Ligand I1T B 501



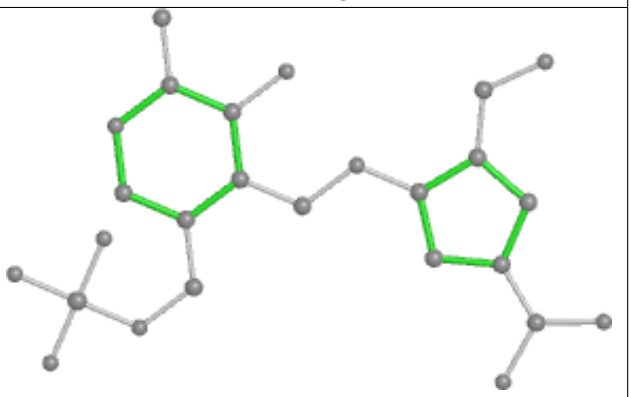
Bond lengths



Bond angles

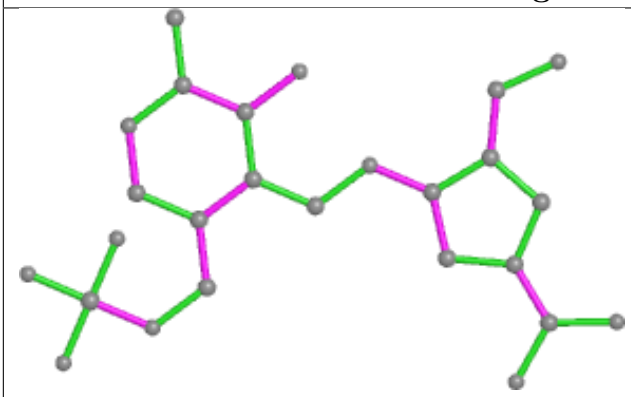


Torsions

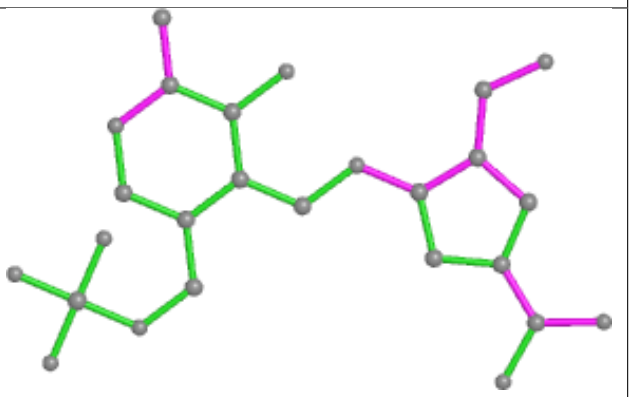


Rings

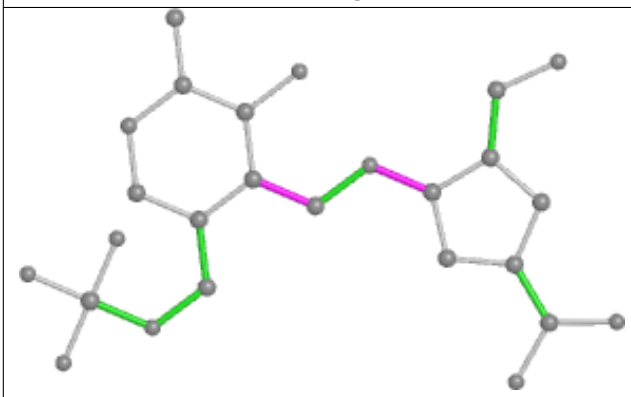
Ligand I1T A 501



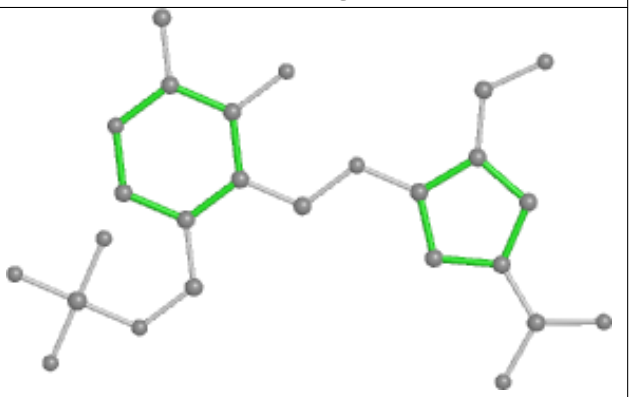
Bond lengths



Bond angles

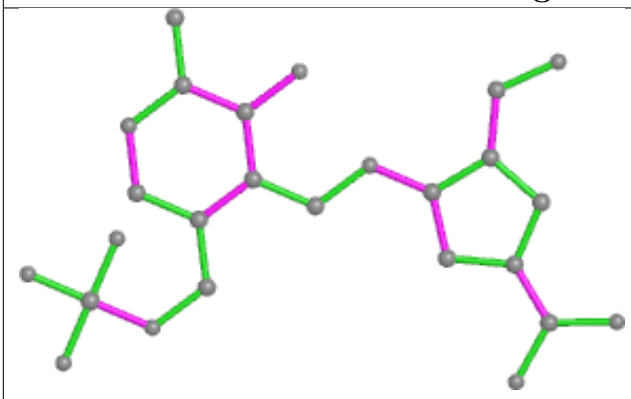


Torsions

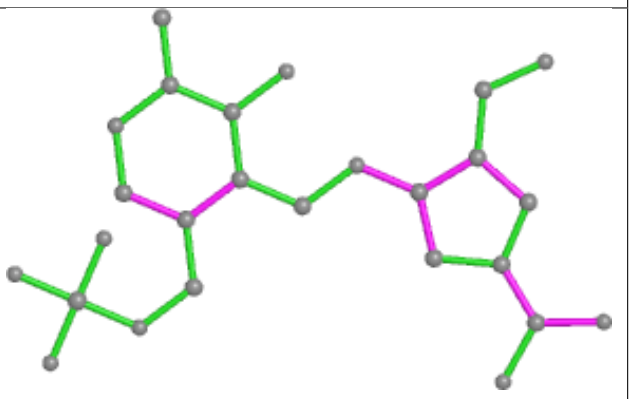


Rings

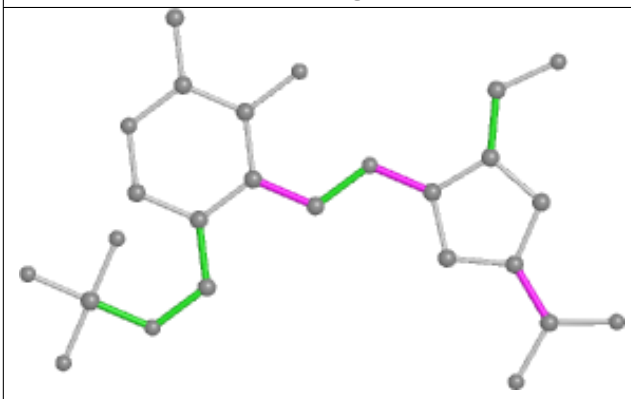
Ligand I1T C 501



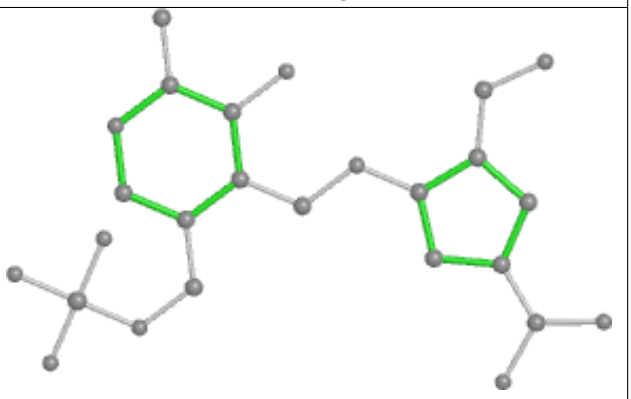
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	403/404 (99%)	0.79	36 (8%)	9	11	14, 22, 27, 35	0
1	B	403/404 (99%)	0.64	34 (8%)	11	13	14, 22, 27, 32	0
1	C	402/404 (99%)	0.44	11 (2%)	54	57	14, 20, 27, 37	0
All	All	1208/1212 (99%)	0.63	81 (6%)	17	20	14, 22, 27, 37	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	LEU	6.9
1	A	367	VAL	6.1
1	A	387	ASP	5.5
1	A	73	VAL	5.2
1	B	388	TRP	5.1
1	B	367	VAL	4.6
1	C	387	ASP	4.5
1	B	365	SER	4.5
1	B	436	ILE	4.4
1	A	382	ILE	4.2
1	A	385	THR	4.1
1	B	383	LYS	4.1
1	B	408	HIS	3.9
1	C	388	TRP	3.8
1	B	382	ILE	3.8
1	B	439	PHE	3.7
1	B	385	THR	3.7
1	B	386	LYS	3.7
1	B	366	ASP	3.7
1	A	408	HIS	3.5
1	B	411	ILE	3.5
1	A	100	ALA	3.4
1	A	383	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	71	TRP	3.3
1	A	342	GLU	3.3
1	A	198	GLY	3.3
1	A	97	ILE	3.3
1	B	409	GLY	3.1
1	C	386	LYS	3.1
1	A	386	LYS	3.0
1	B	362	LYS	3.0
1	A	37	PRO	3.0
1	B	400	ASN	2.9
1	B	410	ASP	2.8
1	C	73	VAL	2.8
1	A	327	PRO	2.8
1	A	361	MET	2.8
1	C	365	SER	2.8
1	A	406	PRO	2.7
1	B	391	TRP	2.7
1	B	364	PRO	2.7
1	C	408	HIS	2.7
1	B	387	ASP	2.7
1	B	37	PRO	2.6
1	A	119	VAL	2.6
1	B	368	VAL	2.6
1	A	99	ASN	2.5
1	A	79	PHE	2.5
1	B	425	LEU	2.5
1	A	298	LEU	2.5
1	C	385	THR	2.4
1	A	364	PRO	2.4
1	B	413	ARG	2.4
1	A	366	ASP	2.4
1	C	45	GLU	2.4
1	A	107	LYS	2.3
1	A	44	PHE	2.3
1	A	388	TRP	2.3
1	B	428	SER	2.3
1	A	42	ASP	2.3
1	A	39	THR	2.3
1	B	79	PHE	2.3
1	A	105	VAL	2.2
1	B	407	THR	2.2
1	A	69	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	384	GLU	2.2
1	A	95	PRO	2.2
1	B	85	TYR	2.2
1	A	58	LEU	2.2
1	A	126	TYR	2.2
1	A	360	LEU	2.1
1	B	423	ASP	2.1
1	C	366	ASP	2.1
1	C	409	GLY	2.1
1	A	337	LEU	2.1
1	B	435	THR	2.1
1	B	431	ILE	2.1
1	B	399	ASP	2.1
1	B	198	GLY	2.0
1	A	340	LEU	2.0
1	C	364	PRO	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)

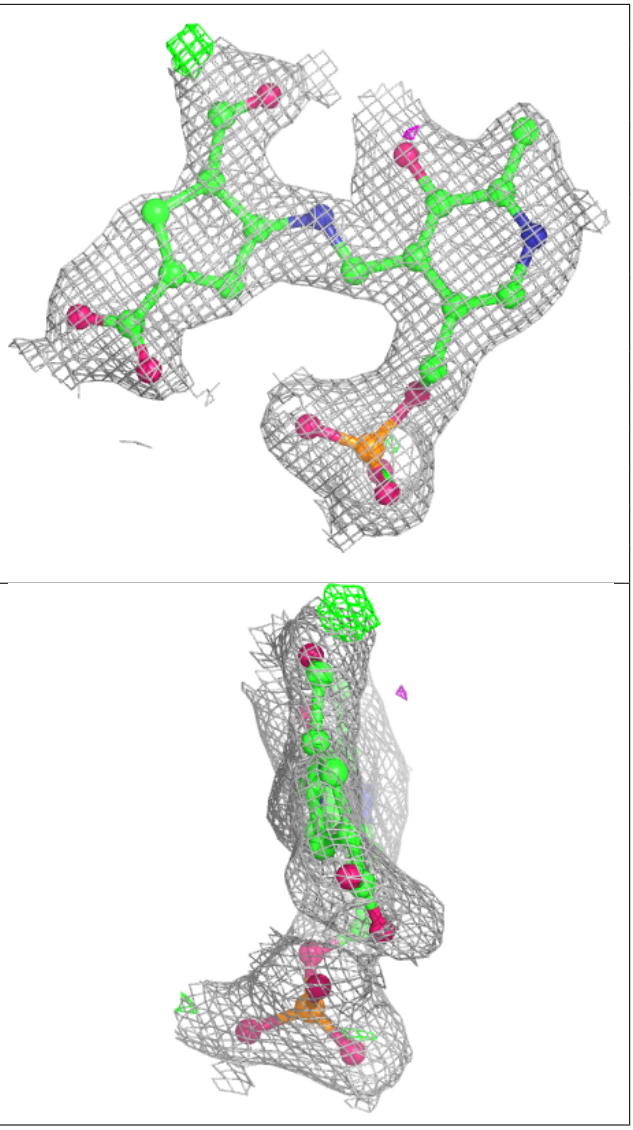
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

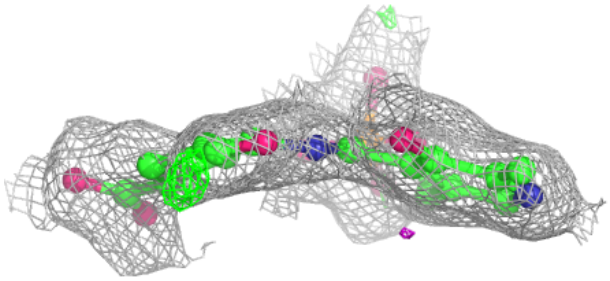
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	I1T	B	501	26/26	0.92	0.15	32,38,50,54	0
2	I1T	A	501	26/26	0.93	0.16	33,37,51,52	0
2	I1T	C	501	26/26	0.94	0.15	28,31,47,49	0

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 I1T B 501:

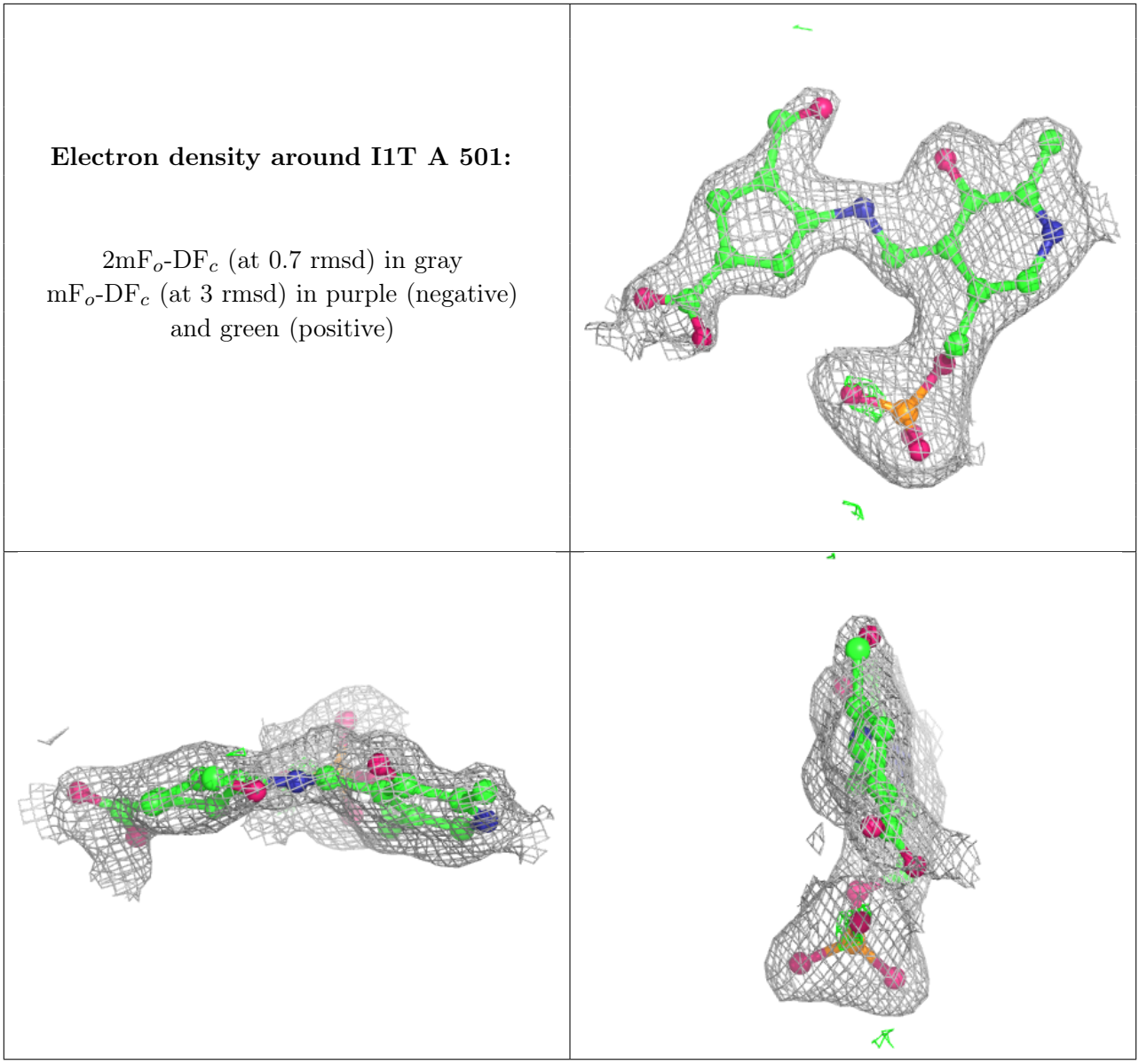
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





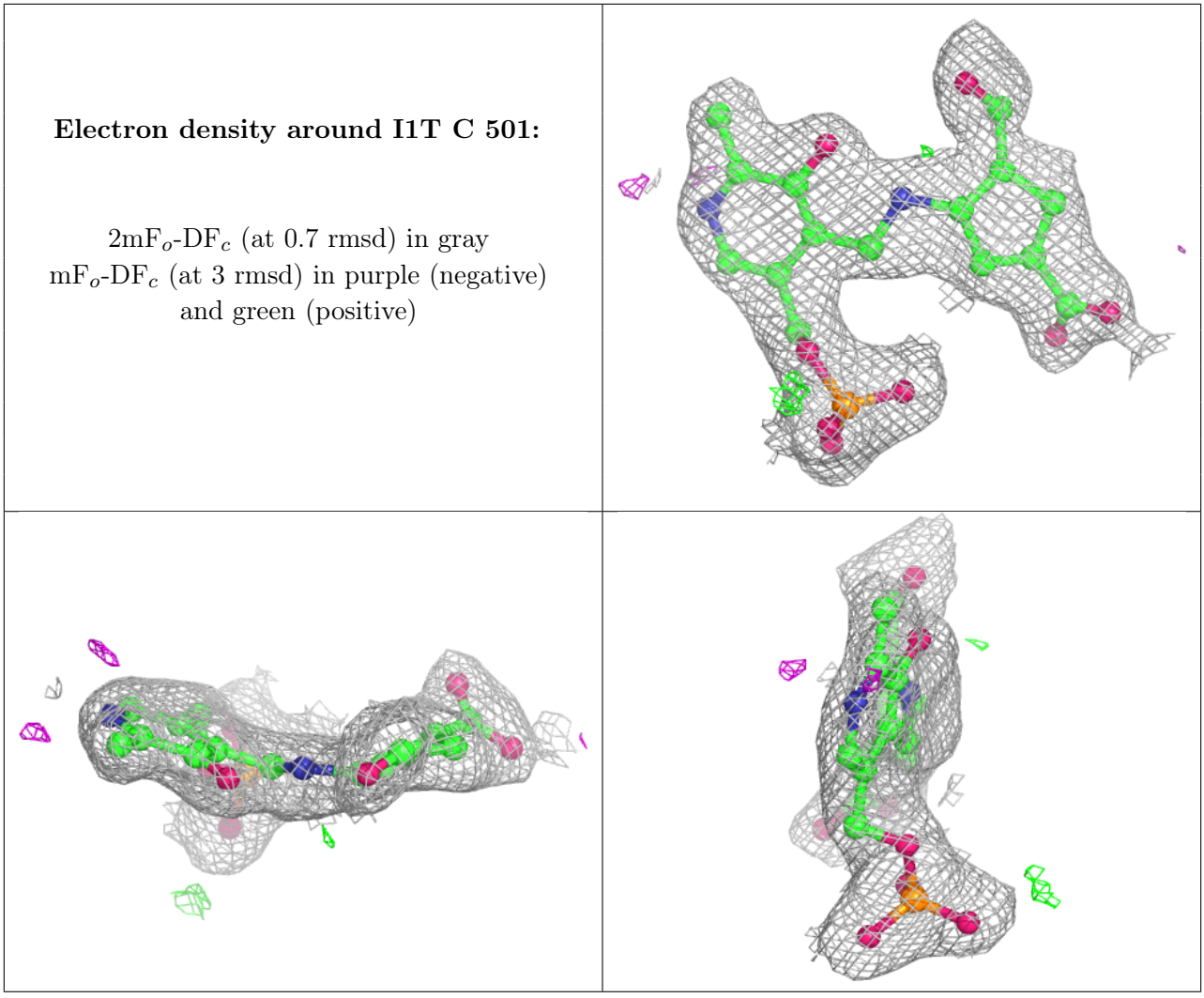
Electron density around I1T A 501:

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



Electron density around I1T C 501:

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



6.5 Other polymers

There are no such residues in this entry.