



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 28, 2020 – 02:34 PM EST

PDB ID : 7JX9
Title : The crystal structure of human ornithine aminotransferase with an intermediate bound during inactivation by (1S,3S)-3-amino-4-(hexafluoropropan-2-ylid enyl)-cyclopentane-1-carboxylic acid.
Authors : Butrin, A.; Beaupre, B.; Shen, S.; Silverman, R.B.; Moran, G.; Liu, D.
Deposited on : 2020-08-26
Resolution : 1.96 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 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 : 2.16
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) : 2.16

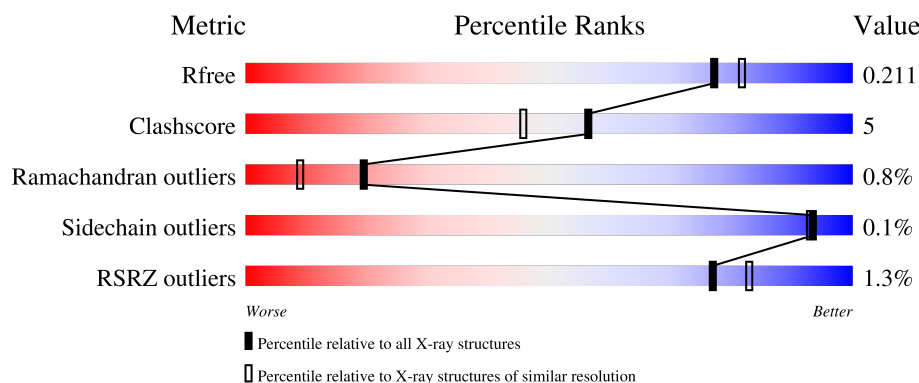
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	404	<div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	B	404	<div> <div> <div></div> <div>88%</div> <div>9%</div> </div> </div>
1	C	404	<div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>

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	IF1	A	501	X	-	-	-
2	IF1	B	501	X	-	-	-
2	IF1	C	501	X	-	-	-

2 Entry composition [i](#)

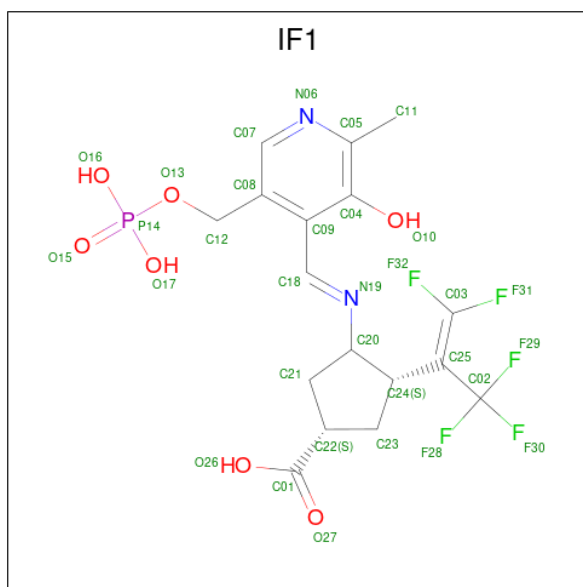
There are 4 unique types of molecules in this entry. The entry contains 10219 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	402	Total	C	N	O	S	0	2	0
			3167	2032	536	587	12			
1	B	402	Total	C	N	O	S	0	0	0
			3150	2023	531	584	12			
1	C	402	Total	C	N	O	S	0	2	0
			3167	2032	536	587	12			

- Molecule 2 is (1S,3S,4S)-3-[(E)-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methylidene)amino]-4-(1,1,3,3,3-pentafluoroprop-1-en-2-yl)cyclopentane-1-carboxylic acid (three-letter code: IF1) (formula: C₁₇H₁₈F₅N₂O₇P) (labeled as "Ligand of Interest" by depositor).



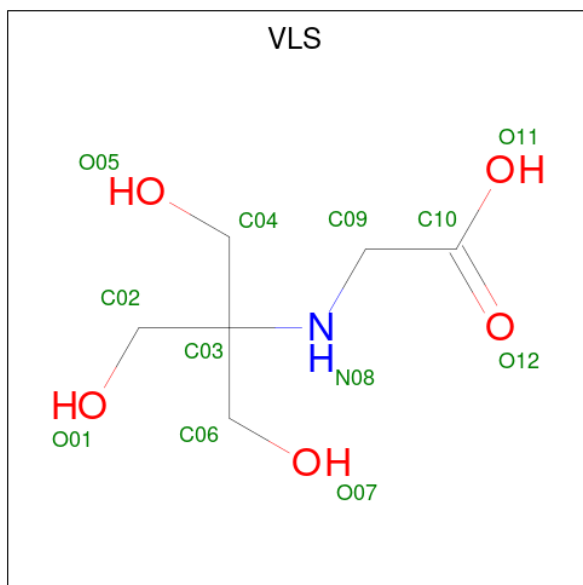
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0
			32	17	5	2	7	1	
2	B	1	Total	C	F	N	O	P	0
			32	17	5	2	7	1	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	P	0	0
			32	17	5	2	7	1		

- Molecule 3 is N-[1,3-dihydroxy-2-(hydroxymethyl)propan-2-yl]glycine (three-letter code: VLS) (formula: $C_6H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	1	5		
3	C	1	Total	C	N	O	0	0
			12	6	1	5		

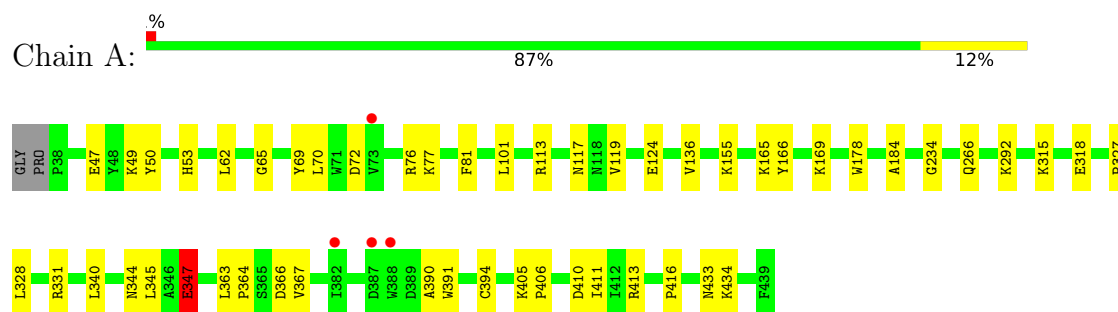
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	198	Total	O	0	0
			198	198		
4	C	222	Total	O	0	0
			222	222		

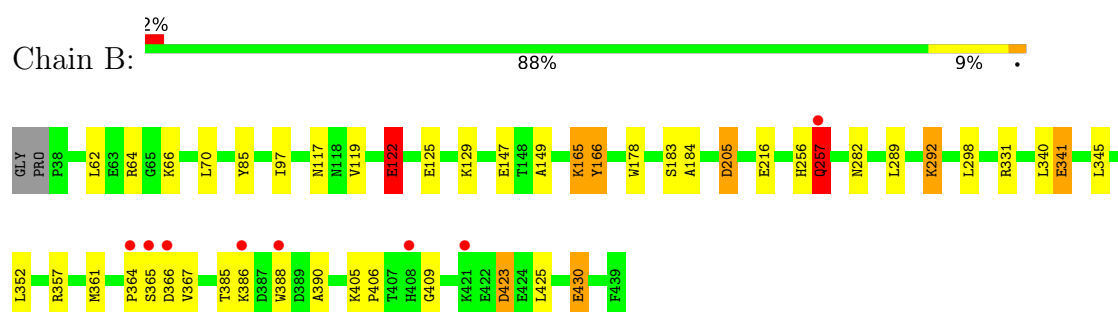
3 Residue-property plots

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.

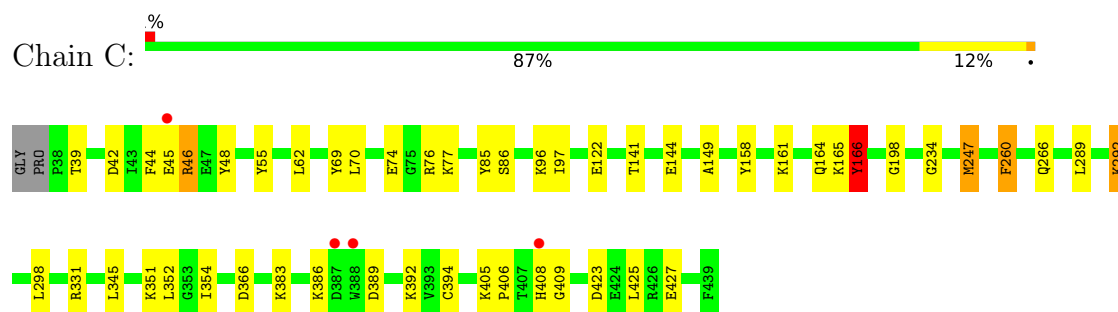
- Molecule 1: Ornithine aminotransferase, mitochondrial



- Molecule 1: Ornithine aminotransferase, mitochondrial



- Molecule 1: Ornithine aminotransferase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.30Å 115.30Å 185.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.21 – 1.96 87.92 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.21-1.96) 99.2 (87.92-1.96)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.186 , 0.213 0.184 , 0.211	Depositor DCC
R_{free} test set	5120 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10219	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: VLS, IF1

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	0.52	2/3240 (0.1%)	0.71	4/4397 (0.1%)
1	B	0.52	0/3223	0.97	20/4375 (0.5%)
1	C	0.52	0/3240	0.72	6/4397 (0.1%)
All	All	0.52	2/9703 (0.0%)	0.81	30/13169 (0.2%)

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	3
1	B	0	11
1	C	0	6
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	GLU	CB-CG	-5.72	1.41	1.52
1	A	347	GLU	CD-OE2	-5.60	1.19	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	ASP	CB-CG-OD1	19.51	135.86	118.30
1	B	423	ASP	CB-CG-OD2	-17.29	102.74	118.30
1	B	341	GLU	OE1-CD-OE2	-13.56	107.03	123.30
1	B	122	GLU	OE1-CD-OE2	-12.58	108.20	123.30
1	B	341	GLU	CG-CD-OE1	11.61	141.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	ASP	CB-CG-OD1	-11.37	108.06	118.30
1	C	260	PHE	CB-CG-CD2	-11.21	112.95	120.80
1	B	257	GLN	N-CA-C	-10.83	81.76	111.00
1	B	257	GLN	CB-CA-C	-10.32	89.76	110.40
1	B	423	ASP	OD1-CG-OD2	-9.49	105.28	123.30
1	B	257	GLN	CG-CD-NE2	-8.62	96.02	116.70
1	A	347	GLU	OE1-CD-OE2	-8.59	112.99	123.30
1	B	122	GLU	CG-CD-OE2	-8.26	101.79	118.30
1	B	122	GLU	CG-CD-OE1	8.23	134.76	118.30
1	B	341	GLU	CG-CD-OE2	-8.15	102.00	118.30
1	B	257	GLN	N-CA-CB	7.66	124.39	110.60
1	B	205	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	347	GLU	CG-CD-OE1	7.41	133.11	118.30
1	A	315	LYS	CD-CE-NZ	7.33	128.56	111.70
1	C	354	ILE	CG1-CB-CG2	-7.19	95.58	111.40
1	C	46	ARG	CG-CD-NE	6.74	125.94	111.80
1	B	166	TYR	N-CA-CB	6.25	121.85	110.60
1	C	260	PHE	CB-CG-CD1	6.15	125.10	120.80
1	C	166	TYR	N-CA-CB	5.96	121.33	110.60
1	A	347	GLU	CG-CD-OE2	-5.88	106.55	118.30
1	B	205	ASP	N-CA-C	-5.66	95.72	111.00
1	B	257	GLN	CB-CG-CD	5.58	126.11	111.60
1	B	165	LYS	C-N-CA	5.45	135.33	121.70
1	B	430	GLU	CA-CB-CG	5.42	125.33	113.40
1	C	247	MET	CG-SD-CE	-5.08	92.08	100.20

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LYS	Mainchain,Peptide
1	A	347	GLU	Sidechain
1	B	122	GLU	Sidechain
1	B	165	LYS	Mainchain,Peptide
1	B	205	ASP	Sidechain
1	B	256	HIS	Peptide
1	B	257	GLN	Sidechain,Mainchain
1	B	341	GLU	Sidechain
1	B	386	LYS	Peptide
1	B	423	ASP	Sidechain
1	B	430	GLU	Sidechain
1	C	165	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	C	198	GLY	Mainchain,Peptide
1	C	260	PHE	Sidechain
1	C	386	LYS	Peptide
1	C	44	PHE	Mainchain

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	3167	0	3172	34	0
1	B	3150	0	3156	27	0
1	C	3167	0	3172	33	0
2	A	32	0	0	1	0
2	B	32	0	0	1	0
2	C	32	0	0	2	0
3	A	12	0	0	0	0
3	C	12	0	0	0	0
4	A	195	0	0	6	0
4	B	198	0	0	5	0
4	C	222	0	0	7	0
All	All	10219	0	9500	95	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 5.

All (95) 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:B:216:GLU:OE2	4:B:601:HOH:O	1.98	0.82
1:C:351:LYS:NZ	4:C:603:HOH:O	2.23	0.72
1:B:340:LEU:HD23	1:B:345:LEU:HD12	1.71	0.71
1:C:405:LYS:HG3	1:C:406:PRO:HD2	1.75	0.69
1:C:164:GLN:OE1	4:C:601:HOH:O	2.09	0.68
1:C:122:GLU:OE2	1:C:331:ARG:NH1	2.27	0.68
1:C:39:THR:HG22	1:C:42:ASP:OD1	1.95	0.66
1:B:364:PRO:HG2	1:B:367:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:HD12	1:C:70:LEU:HB3	1.77	0.66
1:A:62:LEU:HD12	1:A:70:LEU:HB3	1.79	0.64
1:A:53:HIS:ND1	4:A:604:HOH:O	2.30	0.64
1:A:101:LEU:HD12	1:A:328:LEU:HD11	1.81	0.62
1:A:169:LYS:HE3	4:A:605:HOH:O	1.98	0.62
1:B:357:ARG:O	1:B:361:MET:HG3	2.00	0.62
1:B:292:LYS:NZ	2:B:501:IF1:F32	2.24	0.61
1:C:409:GLY:N	4:C:605:HOH:O	2.35	0.59
1:A:49:LYS:HD3	1:A:50:TYR:CZ	2.39	0.57
1:A:344:ASN:HB3	1:A:347:GLU:OE2	2.04	0.57
1:B:117:ASN:ND2	4:B:605:HOH:O	2.33	0.57
1:A:47:GLU:OE1	4:A:601:HOH:O	2.17	0.57
1:C:39:THR:HG23	1:C:42:ASP:H	1.70	0.57
1:A:364:PRO:O	1:A:367:VAL:HG12	2.05	0.56
1:C:234:GLY:HA3	1:C:266:GLN:HE22	1.70	0.56
1:A:405:LYS:HG3	1:A:406:PRO:HD2	1.89	0.55
1:B:122:GLU:OE1	1:B:331:ARG:NH1	2.31	0.54
1:C:141:THR:OG1	1:C:144:GLU:HG3	2.06	0.54
1:A:390:ALA:HB1	1:A:406:PRO:HB3	1.91	0.53
1:A:113[A]:ARG:NH2	4:A:609:HOH:O	2.40	0.53
2:A:501:IF1:F32	2:A:501:IF1:F30	2.05	0.53
1:A:434:LYS:NZ	4:A:610:HOH:O	2.42	0.53
1:B:125:GLU:OE2	1:B:129:LYS:NZ	2.38	0.52
1:C:408:HIS:C	4:C:605:HOH:O	2.48	0.52
1:B:64:ARG:HD2	4:B:607:HOH:O	2.10	0.52
1:A:363:LEU:HD21	1:A:433:ASN:ND2	2.25	0.52
1:A:119:VAL:HG11	1:A:331:ARG:HG2	1.91	0.52
1:A:69:TYR:CD1	1:A:77:LYS:HE3	2.45	0.52
1:C:86[B]:SER:O	1:C:86[B]:SER:OG	2.26	0.51
1:A:81:PHE:CD1	1:A:416:PRO:HB3	2.46	0.51
1:A:72:ASP:OD1	1:A:76:ARG:HD2	2.10	0.51
1:B:62:LEU:HD12	1:B:70:LEU:HB3	1.92	0.51
1:C:86[B]:SER:OG	4:C:602:HOH:O	2.20	0.51
1:C:408:HIS:N	4:C:605:HOH:O	2.36	0.50
1:A:81:PHE:CE1	1:A:416:PRO:HB3	2.47	0.50
1:A:266:GLN:HE22	1:A:413:ARG:NH2	2.09	0.49
1:A:65:GLY:HA3	1:A:70:LEU:HD23	1.94	0.49
1:B:85:TYR:O	1:B:292:LYS:HD3	2.11	0.49
1:C:389:ASP:OD2	1:C:392:LYS:HG3	2.13	0.49
1:A:366:ASP:OD1	4:A:602:HOH:O	2.19	0.48
1:B:352:LEU:HB3	1:B:425:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD21	1:A:433:ASN:HD22	1.78	0.48
1:A:234:GLY:O	1:A:413:ARG:NH1	2.46	0.47
1:B:64:ARG:NH2	4:B:603:HOH:O	2.26	0.47
1:B:97:ILE:HG22	1:B:298:LEU:HD22	1.97	0.47
1:A:394:CYS:SG	1:A:406:PRO:HD3	2.55	0.47
1:A:410:ASP:OD1	1:A:411:ILE:HG13	2.14	0.47
1:B:149:ALA:HB2	1:B:289:LEU:HD21	1.96	0.47
1:C:55:TYR:OH	2:C:501:IF1:O26	2.23	0.47
1:A:124:GLU:HG2	1:A:136:VAL:CG1	2.46	0.46
1:C:96:LYS:HG2	1:C:96:LYS:O	2.14	0.46
1:B:282:ASN:HB2	1:C:247:MET:CE	2.46	0.46
1:C:149:ALA:HB2	1:C:289:LEU:HD21	1.96	0.46
1:C:161:LYS:HE2	4:C:702:HOH:O	2.15	0.45
1:A:155:LYS:NZ	1:A:318:GLU:OE1	2.48	0.45
1:B:390:ALA:HB1	1:B:406:PRO:HB3	1.98	0.45
1:A:340:LEU:HD23	1:A:345:LEU:HD12	1.97	0.45
1:C:69:TYR:CD1	1:C:77:LYS:HE2	2.51	0.45
1:C:366:ASP:O	1:C:383:LYS:HE2	2.17	0.45
1:C:352:LEU:HB3	1:C:425:LEU:HD22	1.98	0.44
1:B:367:VAL:HB	1:B:388:TRP:CZ2	2.52	0.44
1:A:62:LEU:CD1	1:A:70:LEU:HB3	2.46	0.44
1:A:117:ASN:CG	1:A:327:PRO:HG3	2.38	0.44
1:B:178:TRP:CZ2	1:B:184:ALA:HA	2.53	0.44
1:B:64:ARG:NE	4:B:603:HOH:O	2.44	0.44
1:C:423:ASP:O	1:C:427:GLU:HG3	2.18	0.43
1:A:405:LYS:CG	1:A:406:PRO:HD2	2.48	0.43
1:B:66:LYS:HA	1:B:66:LYS:HD3	1.93	0.42
1:B:147:GLU:OE2	1:B:183:SER:HB2	2.19	0.42
1:C:45:GLU:O	1:C:48:TYR:HB3	2.19	0.42
1:C:394:CYS:SG	1:C:406:PRO:HD3	2.60	0.42
1:C:85:TYR:HB3	1:C:292:LYS:NZ	2.35	0.42
1:B:405:LYS:HG3	1:B:406:PRO:HD2	2.01	0.41
1:B:385:THR:HG1	1:B:388:TRP:HD1	1.68	0.41
1:A:178:TRP:CZ2	1:A:184:ALA:HA	2.55	0.41
1:B:119:VAL:HG11	1:B:331:ARG:HG2	2.01	0.41
1:C:158:TYR:OH	1:C:166:TYR:HA	2.20	0.41
1:C:62:LEU:CD1	1:C:70:LEU:HB3	2.48	0.41
1:A:391:TRP:HZ3	1:A:405:LYS:HE3	1.85	0.41
1:B:364:PRO:C	1:B:366:ASP:H	2.23	0.41
2:C:501:IF1:F30	2:C:501:IF1:F32	2.19	0.41
1:C:39:THR:HG22	1:C:42:ASP:CG	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLU:OE1	1:C:76:ARG:NH2	2.53	0.41
1:A:124:GLU:HG2	1:A:136:VAL:HG13	2.03	0.41
1:C:97:ILE:HG22	1:C:298:LEU:HD22	2.02	0.40
1:B:367:VAL:HB	1:B:388:TRP:CH2	2.56	0.40
1:C:345:LEU:HD23	1:C:345:LEU:HA	1.89	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	402/404 (100%)	382 (95%)	18 (4%)	2 (0%)	29	17
1	B	400/404 (99%)	377 (94%)	18 (4%)	5 (1%)	12	3
1	C	402/404 (100%)	383 (95%)	17 (4%)	2 (0%)	29	17
All	All	1204/1212 (99%)	1142 (95%)	53 (4%)	9 (1%)	19	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	TYR
1	B	257	GLN
1	C	166	TYR
1	A	166	TYR
1	B	292	LYS
1	A	292	LYS
1	C	292	LYS
1	B	365	SER
1	B	409	GLY

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	338/337 (100%)	338 (100%)	0	100	100
1	B	336/337 (100%)	336 (100%)	0	100	100
1	C	338/337 (100%)	337 (100%)	1 (0%)	92	92
All	All	1012/1011 (100%)	1011 (100%)	1 (0%)	93	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	46	ARG

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	164	GLN
1	A	266	GLN
1	A	358	ASN
1	A	400	ASN
1	A	433	ASN
1	C	56	HIS
1	C	266	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	IF1	C	501	-	29,33,33	3.27	11 (37%)	36,50,50	2.50	5 (13%)
3	VLS	A	502	-	8,11,11	0.83	0	10,14,14	1.00	1 (10%)
3	VLS	C	502	-	8,11,11	0.53	0	10,14,14	0.90	0
2	IF1	B	501	-	29,33,33	3.23	11 (37%)	36,50,50	2.56	5 (13%)
2	IF1	A	501	-	29,33,33	3.28	11 (37%)	36,50,50	2.53	6 (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	IF1	C	501	-	1/1/8/9	2/17/41/41	0/2/2/2
3	VLS	A	502	-	-	1/13/15/15	-
3	VLS	C	502	-	-	0/13/15/15	-
2	IF1	B	501	-	1/1/8/9	2/17/41/41	0/2/2/2
2	IF1	A	501	-	1/1/8/9	3/17/41/41	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IF1	C24-C20	-12.08	1.35	1.54
2	C	501	IF1	C24-C20	-11.96	1.36	1.54
2	B	501	IF1	C24-C20	-11.36	1.36	1.54
2	C	501	IF1	C23-C24	-7.67	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IF1	C23-C24	-7.54	1.38	1.54
2	B	501	IF1	C23-C24	-7.37	1.39	1.54
2	C	501	IF1	C09-C18	5.27	1.56	1.46
2	B	501	IF1	C09-C18	4.80	1.55	1.46
2	A	501	IF1	C09-C18	4.61	1.55	1.46
2	B	501	IF1	C21-C20	-4.43	1.44	1.52
2	C	501	IF1	C21-C20	-4.26	1.44	1.52
2	A	501	IF1	C21-C20	-4.19	1.44	1.52
2	A	501	IF1	C23-C22	3.99	1.69	1.54
2	B	501	IF1	C23-C22	3.83	1.68	1.54
2	C	501	IF1	C23-C22	3.73	1.68	1.54
2	B	501	IF1	P14-O17	3.15	1.67	1.54
2	B	501	IF1	O10-C04	2.90	1.43	1.37
2	B	501	IF1	C11-C05	2.62	1.54	1.50
2	A	501	IF1	C21-C22	2.59	1.64	1.54
2	B	501	IF1	C21-C22	2.59	1.64	1.54
2	C	501	IF1	C21-C22	2.56	1.64	1.54
2	A	501	IF1	O10-C04	2.54	1.42	1.37
2	C	501	IF1	O10-C04	2.43	1.42	1.37
2	A	501	IF1	F28-C02	2.37	1.42	1.32
2	C	501	IF1	F28-C02	2.36	1.42	1.32
2	B	501	IF1	C20-N19	2.34	1.50	1.46
2	B	501	IF1	F28-C02	2.29	1.42	1.32
2	A	501	IF1	C11-C05	2.28	1.54	1.50
2	A	501	IF1	P14-O15	-2.24	1.43	1.50
2	A	501	IF1	P14-O17	2.18	1.63	1.54
2	C	501	IF1	P14-O17	2.12	1.63	1.54
2	C	501	IF1	C11-C05	2.11	1.54	1.50
2	C	501	IF1	C20-N19	2.05	1.50	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	IF1	C23-C24-C20	10.40	116.95	102.74
2	B	501	IF1	C23-C24-C20	9.37	115.54	102.74
2	A	501	IF1	C23-C24-C20	8.63	114.53	102.74
2	B	501	IF1	C24-C20-N19	8.40	124.17	111.47
2	A	501	IF1	C24-C20-N19	6.86	121.85	111.47
2	C	501	IF1	C24-C20-N19	6.04	120.61	111.47
2	A	501	IF1	C21-C20-N19	5.71	122.17	112.71
2	A	501	IF1	F32-C03-C25	-5.60	117.67	125.30
2	B	501	IF1	C21-C20-N19	5.04	121.05	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	IF1	C21-C20-N19	4.88	120.79	112.71
2	C	501	IF1	F32-C03-C25	-4.34	119.39	125.30
2	B	501	IF1	F31-C03-C25	-3.97	119.89	125.30
2	A	501	IF1	F29-C02-C25	-3.06	103.75	112.82
2	C	501	IF1	F31-C03-C25	-3.03	121.17	125.30
2	B	501	IF1	F32-C03-C25	-2.62	121.72	125.30
2	A	501	IF1	F30-C02-C25	-2.08	106.66	112.82
3	A	502	VLS	C06-C03-N08	-2.00	103.00	109.03

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	501	IF1	C24
2	B	501	IF1	C20
2	A	501	IF1	C20

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	IF1	C21-C20-N19-C18
2	C	501	IF1	C24-C20-N19-C18
2	B	501	IF1	C21-C20-N19-C18
2	A	501	IF1	C21-C20-N19-C18
2	B	501	IF1	C24-C20-N19-C18
2	A	501	IF1	C24-C20-N19-C18
3	A	502	VLS	C02-C03-N08-C09
2	A	501	IF1	C12-O13-P14-O15

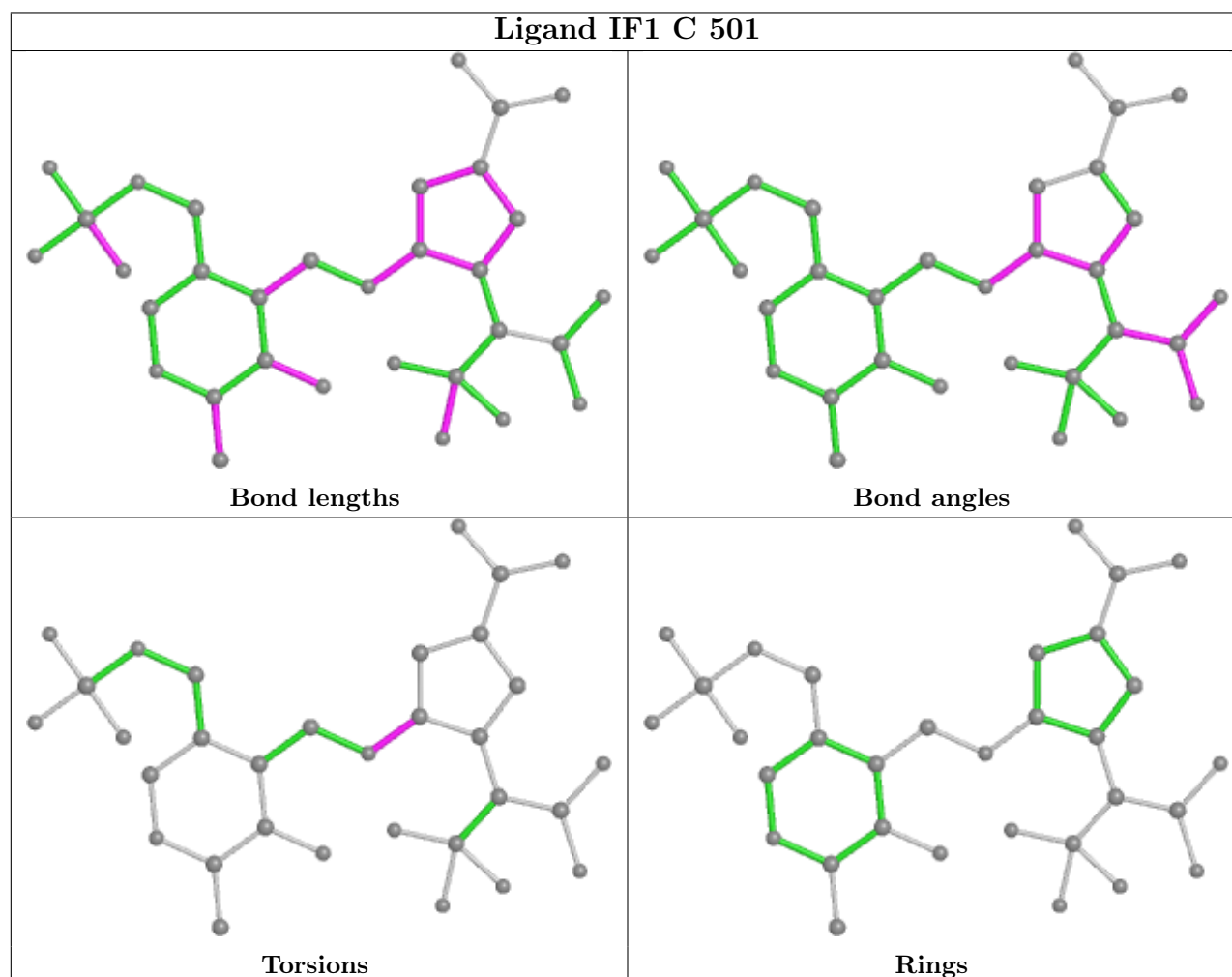
There are no ring outliers.

3 monomers are involved in 4 short contacts:

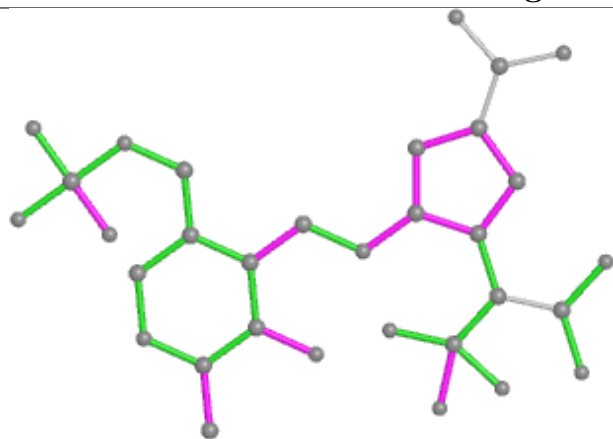
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	IF1	2	0
2	B	501	IF1	1	0
2	A	501	IF1	1	0

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

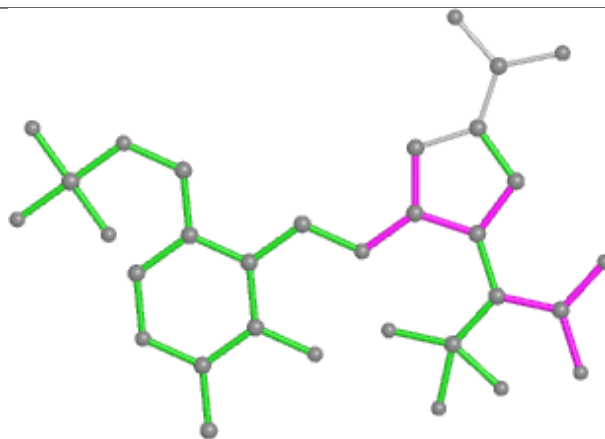
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



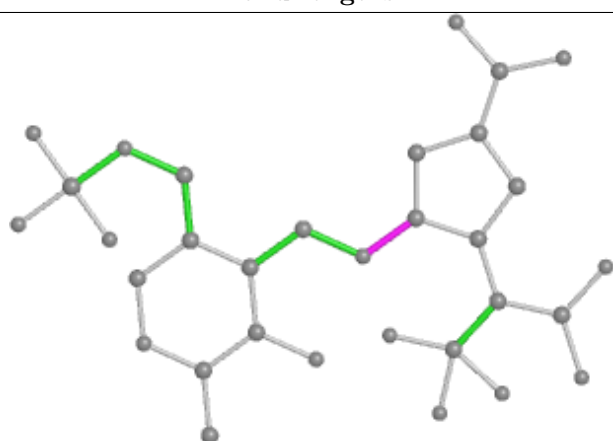
Ligand IF1 B 501



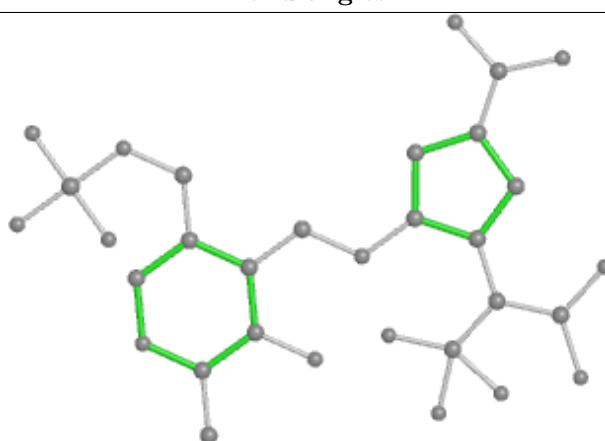
Bond lengths



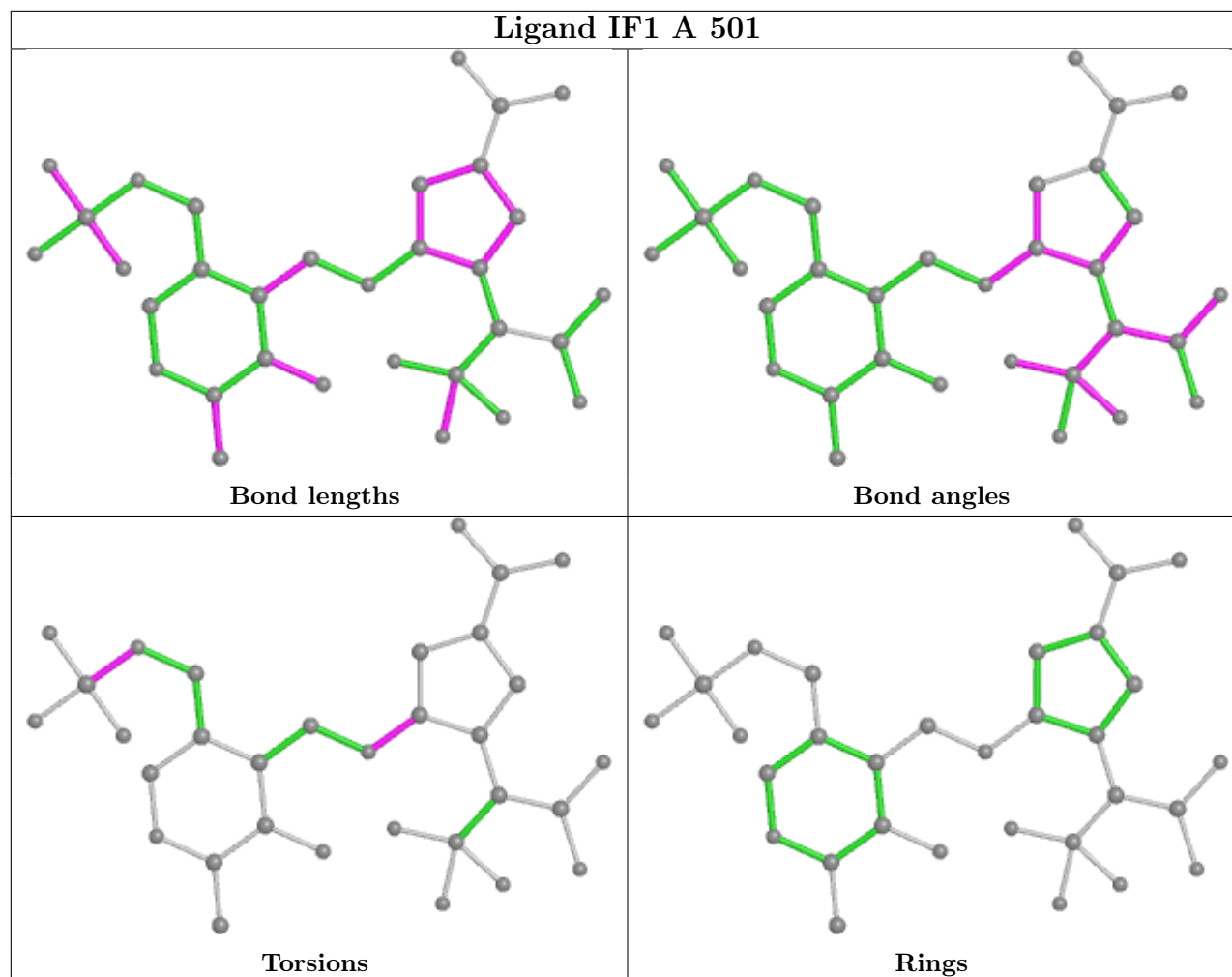
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	402/404 (99%)	-0.04	4 (0%) 82 87	18, 35, 56, 78	0
1	B	402/404 (99%)	-0.10	8 (1%) 65 73	19, 32, 58, 78	0
1	C	402/404 (99%)	-0.14	4 (0%) 82 87	18, 29, 51, 77	0
All	All	1206/1212 (99%)	-0.10	16 (1%) 77 83	18, 32, 56, 78	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	ASP	4.4
1	C	387	ASP	4.1
1	B	388	TRP	4.0
1	B	365	SER	3.5
1	A	388	TRP	3.4
1	C	388	TRP	3.1
1	B	364	PRO	2.7
1	B	408	HIS	2.5
1	A	73	VAL	2.4
1	B	257	GLN	2.4
1	A	382	ILE	2.4
1	B	366	ASP	2.2
1	B	421	LYS	2.2
1	B	386	LYS	2.2
1	C	45	GLU	2.0
1	C	408	HIS	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

There are no monosaccharides in this entry.

6.4 Ligands

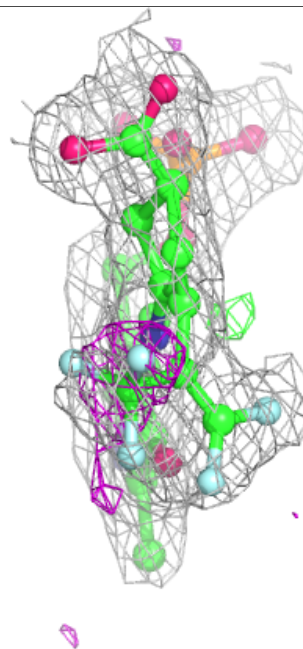
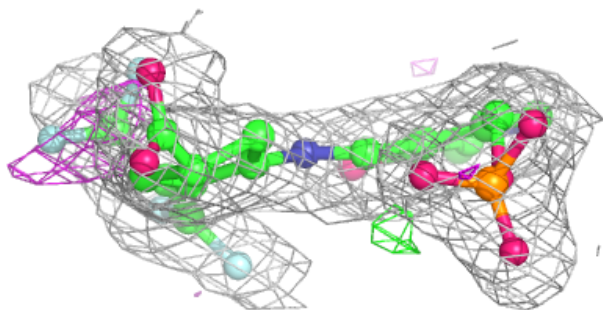
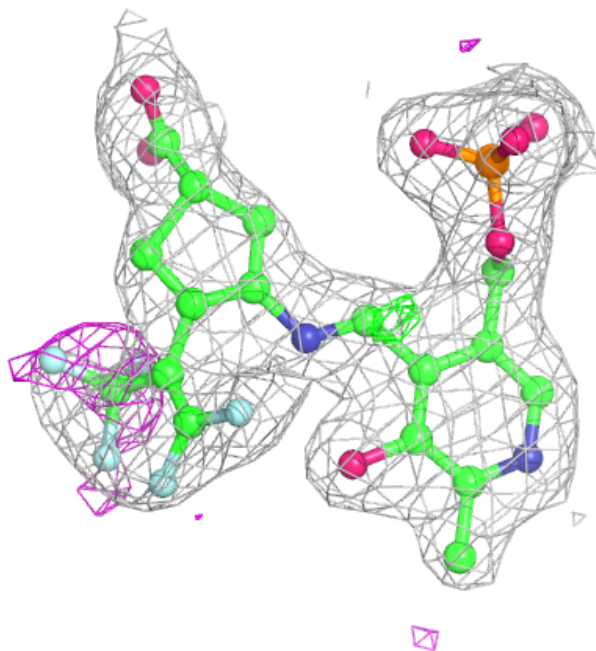
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	VLS	A	502	12/12	0.93	0.15	26,30,41,54	0
2	IF1	A	501	32/32	0.94	0.14	25,39,68,73	0
2	IF1	B	501	32/32	0.95	0.14	21,34,68,75	0
3	VLS	C	502	12/12	0.95	0.10	22,26,39,41	0
2	IF1	C	501	32/32	0.96	0.13	22,38,65,69	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.

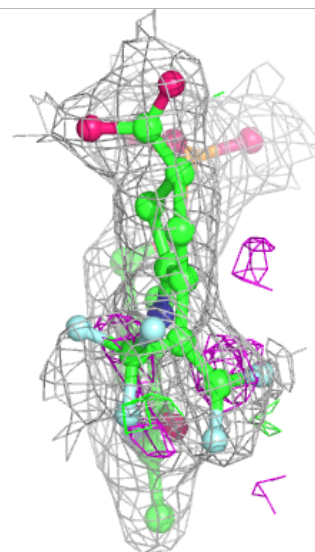
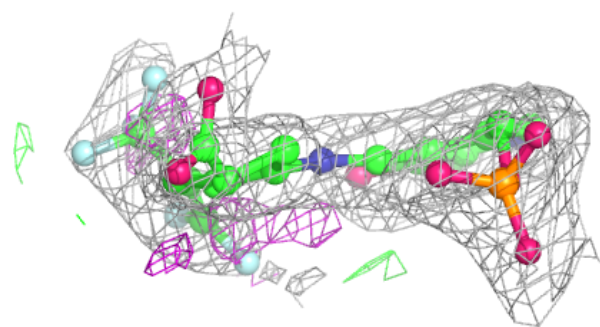
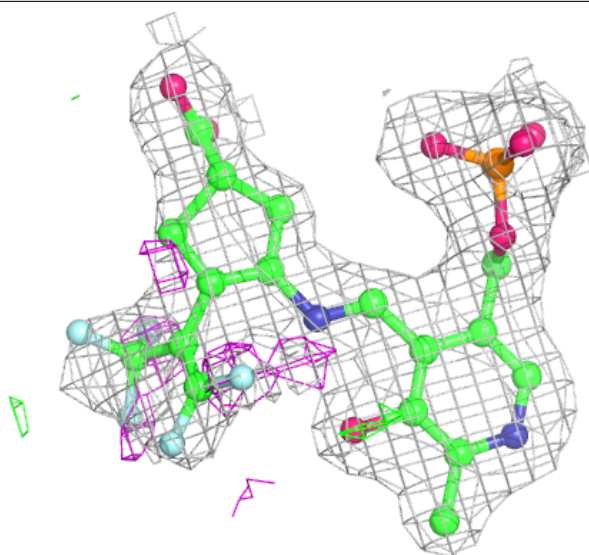
Electron density around IF1 A 501:

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



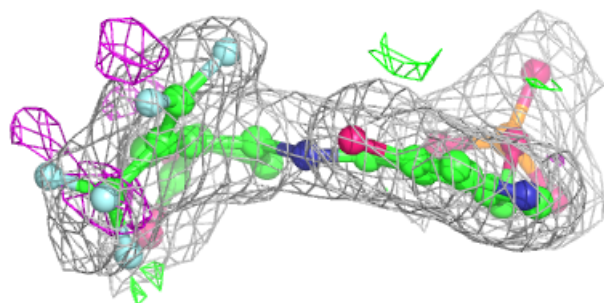
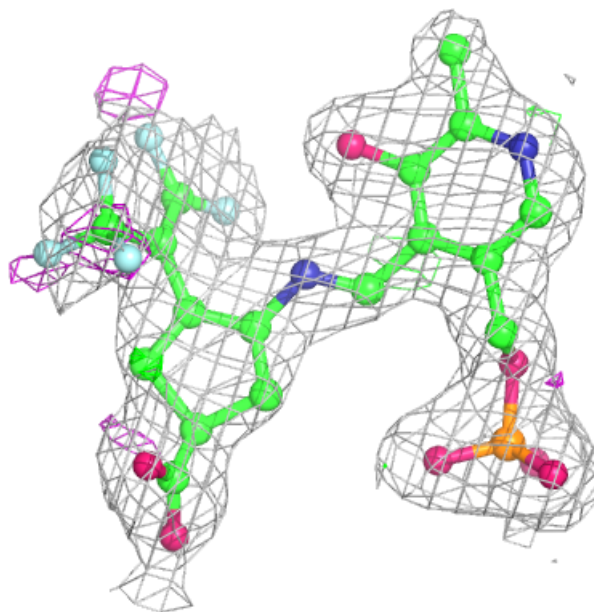
Electron density around IF1 B 501:

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



Electron density around IF1 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.