



Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2026 – 04:10 pm BST

PDB ID : 9GEM / pdb_00009gem
Title : Crystal structure of human NUDT14 in complex with MA-12
Authors : Koekemoer, L.; Dlamini, L.S.; Gurav, N.; Apostolidou, M.; Adcock, C.; McGown, A.; Spencer, J.; Huber, K.V.M.
Deposited on : 2024-08-07
Resolution : 2.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

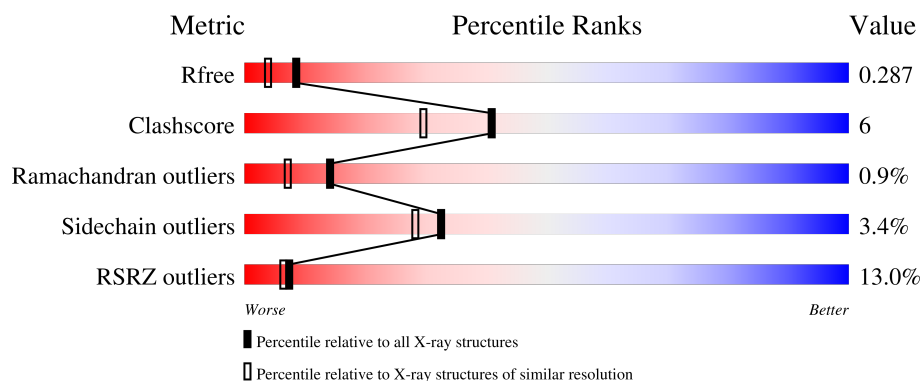
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	222	<div> <div>14%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>••</div> <div>9%</div> </div> </div>
1	B	222	<div> <div>10%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	222	<div> <div>12%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	222	<div> <div>11%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

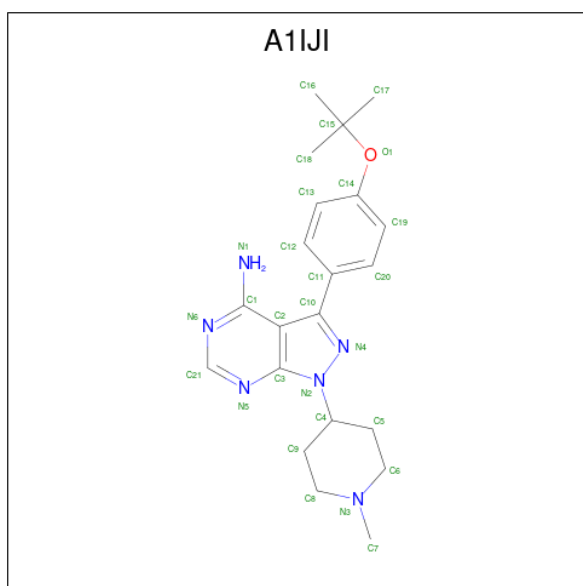
There are 3 unique types of molecules in this entry. The entry contains 12410 atoms, of which 6031 are hydrogens and 0 are deuteriums.

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 Uridine diphosphate glucose pyrophosphatase NUDT14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	202	Total	C	H	N	O	S	0	2	0
			3051	987	1495	274	289	6			
1	B	206	Total	C	H	N	O	S	0	0	0
			3116	1007	1529	277	296	7			
1	C	197	Total	C	H	N	O	S	0	2	0
			3014	976	1482	266	283	7			
1	D	194	Total	C	H	N	O	S	0	0	0
			2938	953	1441	261	277	6			

- Molecule 2 is 1-(1-methylpiperidin-4-yl)-3-[4-[(2-methylpropan-2-yl)oxy]phenyl]pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: A1IJI) (formula: C₂₁H₂₈N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			56	21	28	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			56	21	28	6	1		
2	D	1	Total	C	H	N	O	0	0
			56	21	28	6	1		

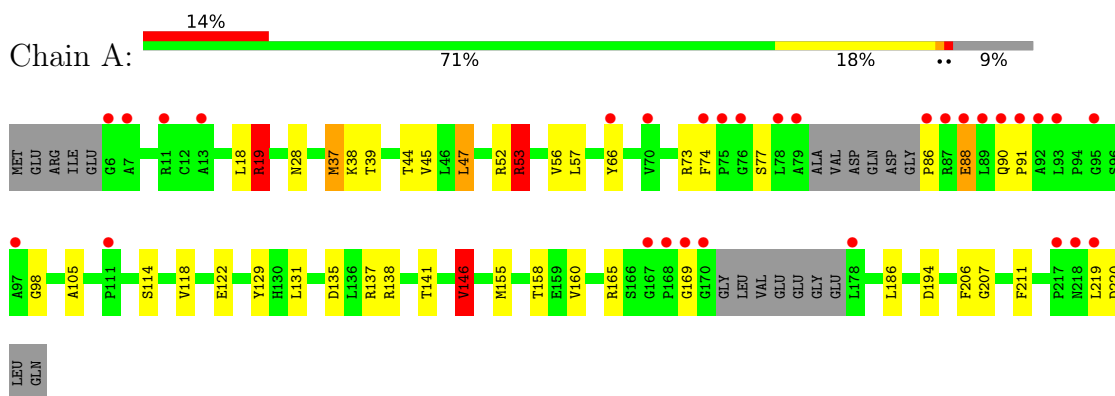
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	33	Total	O	0	0
			33	33		
3	C	15	Total	O	0	0
			15	15		
3	D	36	Total	O	0	0
			36	36		

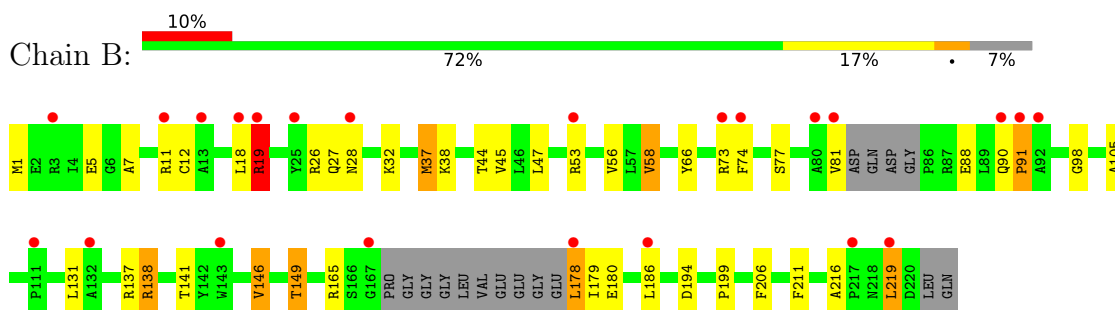
3 Residue-property plots [i](#)

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.

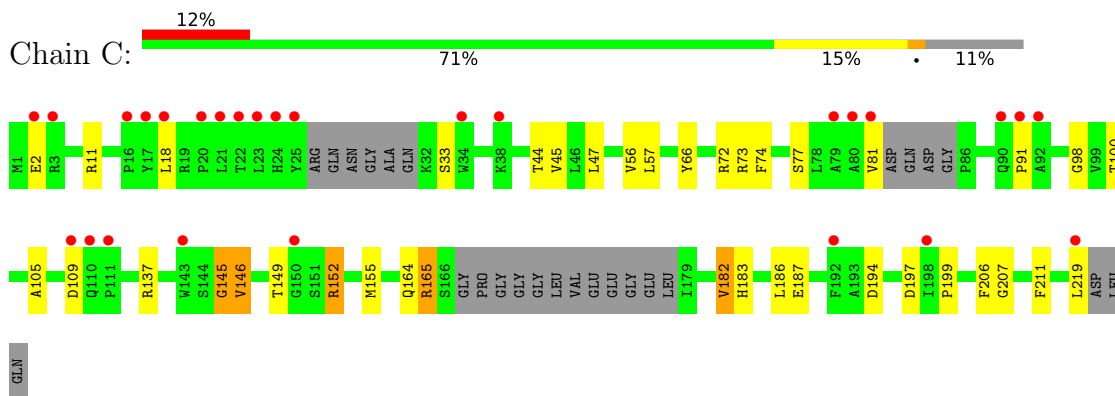
- Molecule 1: Uridine diphosphate glucose pyrophosphatase NUDT14



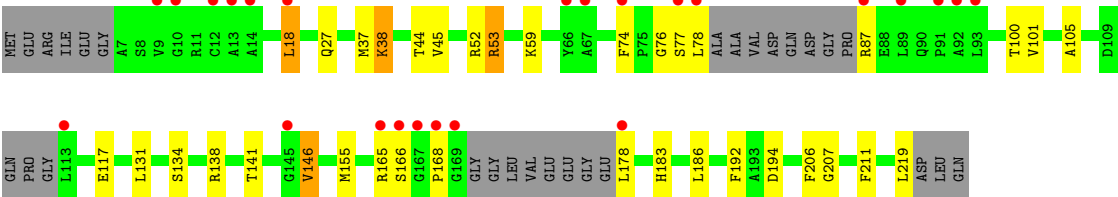
- Molecule 1: Uridine diphosphate glucose pyrophosphatase NUDT14



- Molecule 1: Uridine diphosphate glucose pyrophosphatase NUDT14



- Molecule 1: Uridine diphosphate glucose pyrophosphatase NUDT14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.92Å 107.19Å 78.11Å 90.00° 93.62° 90.00°	Depositor
Resolution (Å)	77.96 – 2.02 77.96 – 2.02	Depositor EDS
% Data completeness (in resolution range)	34.8 (77.96-2.02) 34.8 (77.96-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.77)	Depositor
R, R_{free}	0.215 , 0.287 0.215 , 0.287	Depositor DCC
R_{free} test set	1068 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12410	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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: A1IJI

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	0.89	1/1604 (0.1%)	1.47	18/2179 (0.8%)
1	B	0.87	1/1623 (0.1%)	1.46	12/2205 (0.5%)
1	C	0.83	0/1574	1.41	9/2138 (0.4%)
1	D	0.87	1/1531 (0.1%)	1.43	12/2080 (0.6%)
All	All	0.87	3/6332 (0.0%)	1.44	51/8602 (0.6%)

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	5
1	B	0	6
1	C	0	6
1	D	0	3
All	All	0	20

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ARG	NE-CZ	5.63	1.39	1.33
1	B	199	PRO	C-O	-5.10	1.20	1.24
1	D	138	ARG	NE-CZ	5.01	1.38	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	MET	CB-CA-C	-9.97	91.64	109.70
1	D	53	ARG	CB-CA-C	9.50	125.38	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	VAL	N-CA-CB	9.38	126.70	111.23
1	A	138	ARG	CD-NE-CZ	8.95	136.93	124.40
1	D	146	VAL	N-CA-CB	8.77	125.70	111.23
1	A	206	PHE	CA-CB-CG	-8.63	105.17	113.80
1	C	206	PHE	CA-CB-CG	-8.07	105.73	113.80
1	B	138	ARG	CD-NE-CZ	7.59	135.03	124.40
1	B	149	THR	CA-CB-OG1	-7.49	98.36	109.60
1	A	19	ARG	CG-CD-NE	7.12	127.66	112.00
1	D	138	ARG	CD-NE-CZ	7.06	134.28	124.40
1	D	53	ARG	N-CA-CB	-7.00	101.34	111.70
1	A	86	PRO	CA-N-CD	-6.76	102.54	112.00
1	D	206	PHE	CA-CB-CG	-6.66	107.14	113.80
1	B	206	PHE	CA-CB-CG	-6.66	107.14	113.80
1	A	90	GLN	N-CA-CB	-6.56	102.81	111.40
1	B	37	MET	CG-SD-CE	-6.41	86.80	100.90
1	A	53[A]	ARG	CB-CA-C	6.39	120.96	111.89
1	A	53[B]	ARG	CB-CA-C	6.39	120.96	111.89
1	D	168	PRO	CB-CA-C	6.35	118.48	111.56
1	D	59	LYS	N-CA-CB	-6.16	100.88	110.55
1	A	220	ASP	CA-CB-CG	6.15	118.75	112.60
1	B	141	THR	CA-CB-OG1	-6.11	100.43	109.60
1	C	194	ASP	CB-CA-C	-5.97	100.87	110.79
1	C	164	GLN	OE1-CD-NE2	5.91	128.51	122.60
1	C	199	PRO	N-CA-CB	5.88	106.21	102.92
1	B	19	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	D	117	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	135	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	141	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	158	THR	OG1-CB-CG2	5.75	120.79	109.30
1	A	194	ASP	CA-CB-CG	5.75	118.34	112.60
1	B	194	ASP	CB-CA-C	-5.68	101.35	110.79
1	B	28	ASN	CB-CA-C	5.65	121.66	110.42
1	C	109	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	53	ARG	CB-CA-C	5.52	119.73	111.89
1	A	37	MET	CB-CG-SD	-5.50	96.20	112.70
1	A	146	VAL	N-CA-CB	5.49	120.29	111.23
1	A	28	ASN	CB-CA-C	5.38	120.02	111.95
1	A	194	ASP	CB-CA-C	-5.37	101.87	110.79
1	D	194	ASP	CB-CA-C	-5.37	100.69	110.63
1	D	100	THR	CA-CB-OG1	-5.36	101.56	109.60
1	D	183	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	141	THR	CA-CB-OG1	-5.32	101.63	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	88	GLU	CB-CG-CD	5.22	121.47	112.60
1	B	28	ASN	CA-CB-CG	5.19	117.79	112.60
1	C	152	ARG	CB-CA-C	-5.18	99.93	109.46
1	C	100	THR	CA-CB-OG1	-5.13	101.91	109.60
1	C	197	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	2	GLU	CB-CA-C	-5.00	100.57	110.27

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	169	GLY	Peptide
1	A	19	ARG	Sidechain
1	A	53[A]	ARG	Sidechain
1	A	53[B]	ARG	Sidechain
1	B	138	ARG	Sidechain
1	B	165	ARG	Sidechain
1	B	19	ARG	Sidechain
1	B	26	ARG	Sidechain
1	B	73	ARG	Sidechain
1	B	91	PRO	Peptide
1	C	137	ARG	Sidechain
1	C	145	GLY	Peptide
1	C	152	ARG	Sidechain
1	C	165	ARG	Sidechain
1	C	72	ARG	Sidechain
1	C	73	ARG	Sidechain
1	D	165	ARG	Sidechain
1	D	52	ARG	Sidechain
1	D	53	ARG	Sidechain

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	1556	1495	1519	27	0
1	B	1587	1529	1568	28	0
1	C	1532	1482	1510	15	0
1	D	1497	1441	1477	14	0
2	A	28	28	0	0	0
2	B	28	28	0	0	0
2	D	28	28	0	0	0
3	A	39	0	0	7	0
3	B	33	0	0	8	0
3	C	15	0	0	1	0
3	D	36	0	0	4	0
All	All	6379	6031	6074	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ILE:HG22	3:B:411:HOH:O	1.51	1.08
1:D:131:LEU:HA	3:D:403:HOH:O	1.73	0.89
1:C:57:LEU:HB2	1:C:182:VAL:HG22	1.63	0.81
1:A:131:LEU:HB3	3:A:418:HOH:O	1.86	0.75
1:C:11:ARG:NH1	1:C:81:VAL:O	2.20	0.75
1:C:145:GLY:HA3	1:C:149:THR:HG23	1.68	0.74
1:A:37:MET:SD	1:B:37:MET:HE1	2.32	0.70
1:D:74:PHE:O	1:D:77:SER:OG	2.09	0.70
1:C:74:PHE:O	1:C:77:SER:OG	2.09	0.69
1:B:131:LEU:HA	3:B:407:HOH:O	1.92	0.69
1:A:74:PHE:O	1:A:77:SER:OG	2.12	0.66
1:B:18:LEU:O	1:B:38:LYS:O	2.15	0.65
1:B:74:PHE:O	1:B:77:SER:OG	2.14	0.65
1:A:88:GLU:HG2	3:A:435:HOH:O	1.96	0.64
1:D:27:GLN:N	3:D:401:HOH:O	2.31	0.63
1:A:73:ARG:NH1	1:D:76:GLY:HA2	2.14	0.63
1:D:18:LEU:O	1:D:38:LYS:O	2.17	0.62
1:D:155:MET:HE1	1:D:207:GLY:HA2	1.80	0.62
1:A:18:LEU:O	1:A:38:LYS:O	2.20	0.59
1:A:44:THR:HG22	1:A:105:ALA:HB2	1.85	0.58
1:B:7:ALA:HA	3:B:412:HOH:O	2.01	0.58
1:D:44:THR:HG22	1:D:105:ALA:HB2	1.85	0.58
1:B:7:ALA:CA	3:B:412:HOH:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:THR:HG22	1:C:105:ALA:HB2	1.86	0.57
1:C:187:GLU:HB3	3:C:314:HOH:O	2.05	0.57
1:A:37:MET:CE	1:A:37:MET:HA	2.33	0.57
1:C:74:PHE:CD2	1:C:91:PRO:HG2	2.40	0.56
1:A:122:GLU:HG2	3:A:406:HOH:O	2.06	0.56
1:A:37:MET:HA	1:A:37:MET:HE3	1.90	0.54
1:B:44:THR:HG22	1:B:105:ALA:HB2	1.88	0.54
1:B:149:THR:HG23	3:B:401:HOH:O	2.07	0.54
1:C:145:GLY:HA3	1:C:149:THR:CG2	2.35	0.54
1:C:57:LEU:HB2	1:C:182:VAL:CG2	2.36	0.53
1:A:52[A]:ARG:HD3	1:A:165:ARG:HH12	1.74	0.52
1:A:74:PHE:CD2	1:A:91:PRO:HG2	2.43	0.52
1:A:37:MET:HE3	1:A:37:MET:CA	2.39	0.51
1:B:137:ARG:CG	3:B:406:HOH:O	2.59	0.51
1:A:186:LEU:HD11	1:A:211:PHE:CE2	2.46	0.50
3:A:425:HOH:O	1:B:37:MET:CE	2.58	0.50
1:A:73:ARG:CZ	1:D:76:GLY:HA2	2.40	0.50
1:A:129:TYR:CE2	1:A:160:VAL:HG21	2.49	0.48
1:B:7:ALA:HB1	3:B:412:HOH:O	2.14	0.48
1:A:37:MET:HE1	3:A:425:HOH:O	2.13	0.48
1:C:165:ARG:HH12	1:C:183:HIS:CE1	2.32	0.47
1:B:137:ARG:HG2	3:B:406:HOH:O	2.15	0.47
1:C:155:MET:HE1	1:C:207:GLY:HA2	1.97	0.46
1:A:165:ARG:NE	3:A:409:HOH:O	2.48	0.46
1:C:186:LEU:HD11	1:C:211:PHE:CE2	2.51	0.46
1:D:78:LEU:O	1:D:87:ARG:NH2	2.48	0.46
1:B:186:LEU:HD11	1:B:211:PHE:CE2	2.51	0.46
1:B:216:ALA:HA	1:B:219:LEU:HD22	1.98	0.46
1:B:12:CYS:SG	1:B:18:LEU:HD12	2.56	0.45
1:B:1:MET:CE	1:B:180:GLU:HB3	2.46	0.45
1:B:66:TYR:HB2	1:B:98:GLY:HA3	1.99	0.44
1:A:37:MET:SD	1:B:37:MET:CE	3.03	0.44
1:A:37:MET:CE	1:B:37:MET:HE1	2.47	0.44
1:B:58:VAL:HG13	1:B:179:ILE:HG23	2.00	0.43
1:A:47:LEU:HB2	1:A:56:VAL:HB	2.00	0.43
1:D:18:LEU:C	1:D:37:MET:HE3	2.43	0.43
1:B:58:VAL:HG13	1:B:179:ILE:CG2	2.48	0.43
1:B:27:GLN:HB3	1:B:32:LYS:HE2	2.01	0.43
1:B:1:MET:HB2	1:B:178:LEU:HD12	2.00	0.43
1:A:155:MET:HE1	1:A:207:GLY:HA2	2.00	0.43
1:C:66:TYR:HB2	1:C:98:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:SER:N	3:D:402:HOH:O	2.33	0.42
1:D:192:PHE:HD1	3:D:405:HOH:O	2.02	0.42
1:B:88:GLU:OE1	1:B:90:GLN:NE2	2.49	0.42
1:C:47:LEU:HB2	1:C:56:VAL:HB	2.01	0.42
1:A:114:SER:O	1:A:118:VAL:HG23	2.20	0.42
1:B:74:PHE:CD2	1:B:91:PRO:HG2	2.54	0.42
1:B:47:LEU:HB2	1:B:56:VAL:HB	2.02	0.42
1:A:37:MET:HB3	1:A:39:THR:HG23	2.03	0.41
1:C:145:GLY:C	1:C:146:VAL:HG23	2.45	0.41
1:A:57:LEU:HG	3:A:411:HOH:O	2.20	0.41
1:B:186:LEU:HD12	1:B:186:LEU:HA	1.89	0.40
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.89	0.40
1:D:101:VAL:HG11	1:D:192:PHE:HZ	1.86	0.40
1:D:186:LEU:HD11	1:D:211:PHE:CE2	2.56	0.40
1:A:66:TYR:HB2	1:A:98:GLY:HA3	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	198/222 (89%)	186 (94%)	10 (5%)	2 (1%)	12	5
1	B	200/222 (90%)	188 (94%)	11 (6%)	1 (0%)	24	17
1	C	191/222 (86%)	180 (94%)	9 (5%)	2 (1%)	12	5
1	D	186/222 (84%)	176 (95%)	8 (4%)	2 (1%)	11	5
All	All	775/888 (87%)	730 (94%)	38 (5%)	7 (1%)	14	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	B	146	VAL
1	C	146	VAL
1	D	166	SER
1	C	33	SER
1	D	146	VAL
1	A	19	ARG

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	166/180 (92%)	160 (96%)	6 (4%)	31	26
1	B	169/180 (94%)	161 (95%)	8 (5%)	23	16
1	C	165/180 (92%)	161 (98%)	4 (2%)	43	41
1	D	160/180 (89%)	155 (97%)	5 (3%)	35	31
All	All	660/720 (92%)	637 (96%)	23 (4%)	32	27

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

Mol	Chain	Res	Type
1	A	45	VAL
1	A	47	LEU
1	A	53[A]	ARG
1	A	53[B]	ARG
1	A	146	VAL
1	A	219	LEU
1	B	5	GLU
1	B	11	ARG
1	B	19	ARG
1	B	45	VAL
1	B	58	VAL
1	B	81	VAL
1	B	178	LEU
1	B	219	LEU
1	C	18	LEU

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Mol	Chain	Res	Type
1	C	45	VAL
1	C	182	VAL
1	C	219	LEU
1	D	18	LEU
1	D	38	LYS
1	D	45	VAL
1	D	178	LEU
1	D	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	153	GLN
1	B	60	GLN
1	B	153	GLN
1	B	164	GLN
1	B	214	GLN
1	C	40	HIS
1	C	110	GLN
1	C	153	GLN
1	C	190	GLN
1	C	214	GLN
1	D	153	GLN
1	D	214	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A1IJI	A	301	-	31,31,31	0.80	0	46,46,46	1.62	10 (21%)
2	A1IJI	D	301	-	31,31,31	1.46	3 (9%)	46,46,46	1.69	9 (19%)
2	A1IJI	B	301	-	31,31,31	0.91	1 (3%)	46,46,46	1.90	12 (26%)

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	A1IJI	A	301	-	-	2/13/23/23	0/4/4/4
2	A1IJI	D	301	-	-	2/13/23/23	0/4/4/4
2	A1IJI	B	301	-	-	0/13/23/23	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	A1IJI	O1-C15	5.98	1.60	1.46
2	B	301	A1IJI	C2-C10	2.89	1.47	1.43
2	D	301	A1IJI	C4-N2	2.55	1.49	1.46
2	D	301	A1IJI	C2-C1	2.17	1.44	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	A1IJI	C10-N4-N2	5.92	109.56	106.88
2	B	301	A1IJI	C11-C10-N4	-4.86	112.44	118.92
2	B	301	A1IJI	C2-C10-C11	4.68	136.91	131.22
2	A	301	A1IJI	C10-N4-N2	4.32	108.83	106.88
2	A	301	A1IJI	C9-C4-N2	-4.11	108.27	111.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1IJI	C3-N2-N4	-4.07	108.73	110.95
2	B	301	A1IJI	C3-C2-C10	-4.05	102.19	104.71
2	B	301	A1IJI	C1-C2-C10	3.93	142.59	139.09
2	D	301	A1IJI	C3-N2-N4	-3.54	109.02	110.95
2	B	301	A1IJI	C10-N4-N2	3.19	108.32	106.88
2	D	301	A1IJI	C20-C11-C10	3.09	124.52	120.64
2	B	301	A1IJI	C12-C11-C10	-3.05	116.80	120.64
2	A	301	A1IJI	C12-C11-C10	3.00	124.40	120.64
2	B	301	A1IJI	C8-N3-C6	2.98	113.69	109.52
2	B	301	A1IJI	O1-C15-C17	2.95	120.63	107.82
2	B	301	A1IJI	C20-C11-C10	2.94	124.33	120.64
2	A	301	A1IJI	C20-C11-C10	-2.63	117.33	120.64
2	A	301	A1IJI	C3-C2-C10	2.58	106.31	104.71
2	B	301	A1IJI	C2-C1-N6	2.53	120.97	118.71
2	B	301	A1IJI	C2-C3-N5	-2.51	124.30	126.94
2	A	301	A1IJI	C2-C10-C11	2.49	134.24	131.22
2	B	301	A1IJI	O1-C15-C16	-2.48	97.04	107.82
2	D	301	A1IJI	C2-C10-C11	2.40	134.13	131.22
2	A	301	A1IJI	C15-O1-C14	2.37	130.39	121.52
2	A	301	A1IJI	C2-C10-N4	-2.33	108.89	110.27
2	D	301	A1IJI	C8-N3-C6	2.32	112.77	109.52
2	D	301	A1IJI	O1-C15-C17	2.29	117.75	107.82
2	D	301	A1IJI	C15-O1-C14	2.23	129.89	121.52
2	D	301	A1IJI	C2-C10-N4	-2.21	108.96	110.27
2	D	301	A1IJI	C18-C15-C17	-2.12	105.61	111.16
2	A	301	A1IJI	C11-C10-N4	-2.06	116.18	118.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

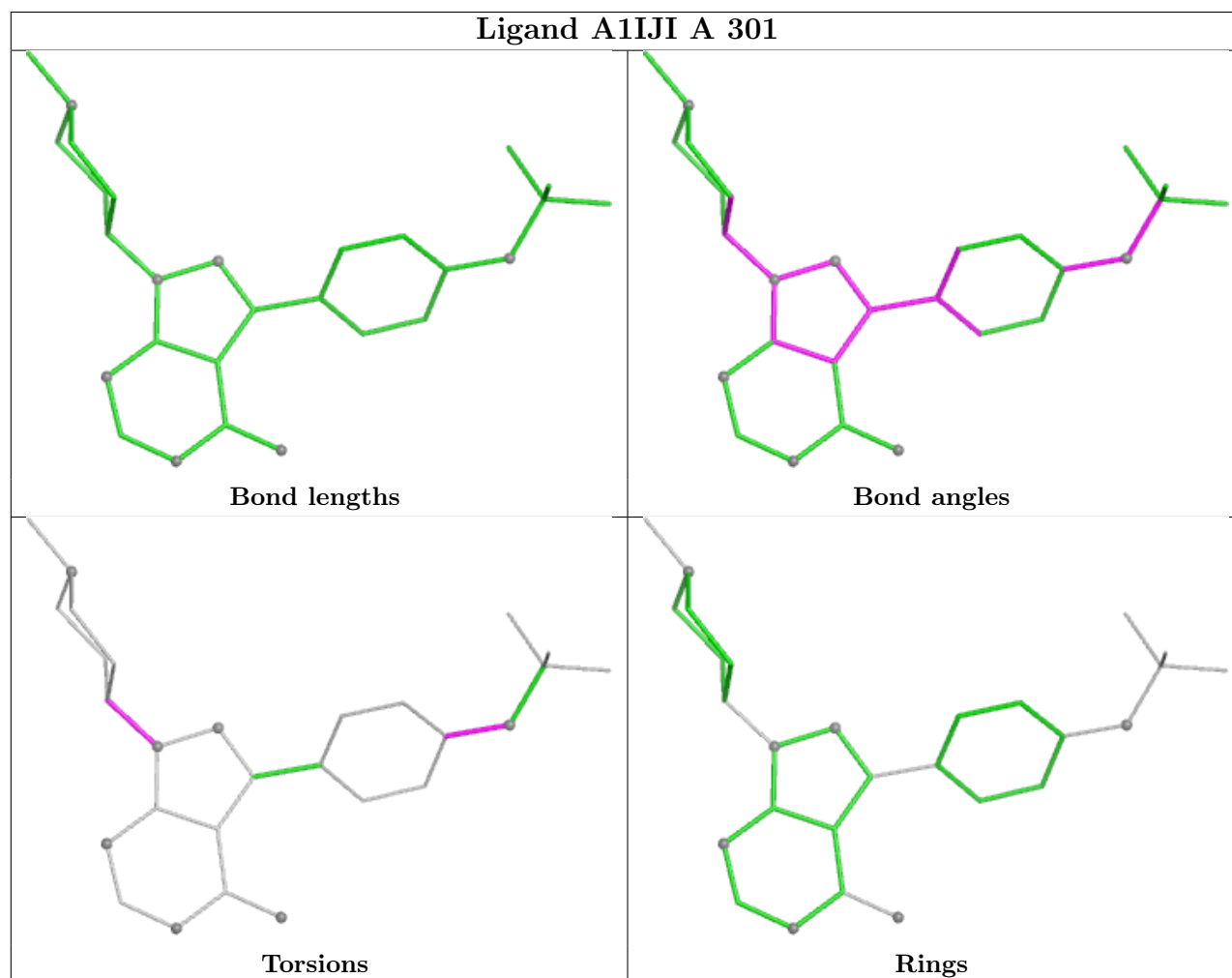
Mol	Chain	Res	Type	Atoms
2	D	301	A1IJI	C5-C4-N2-C3
2	D	301	A1IJI	C9-C4-N2-C3
2	A	301	A1IJI	C5-C4-N2-C3
2	A	301	A1IJI	C19-C14-O1-C15

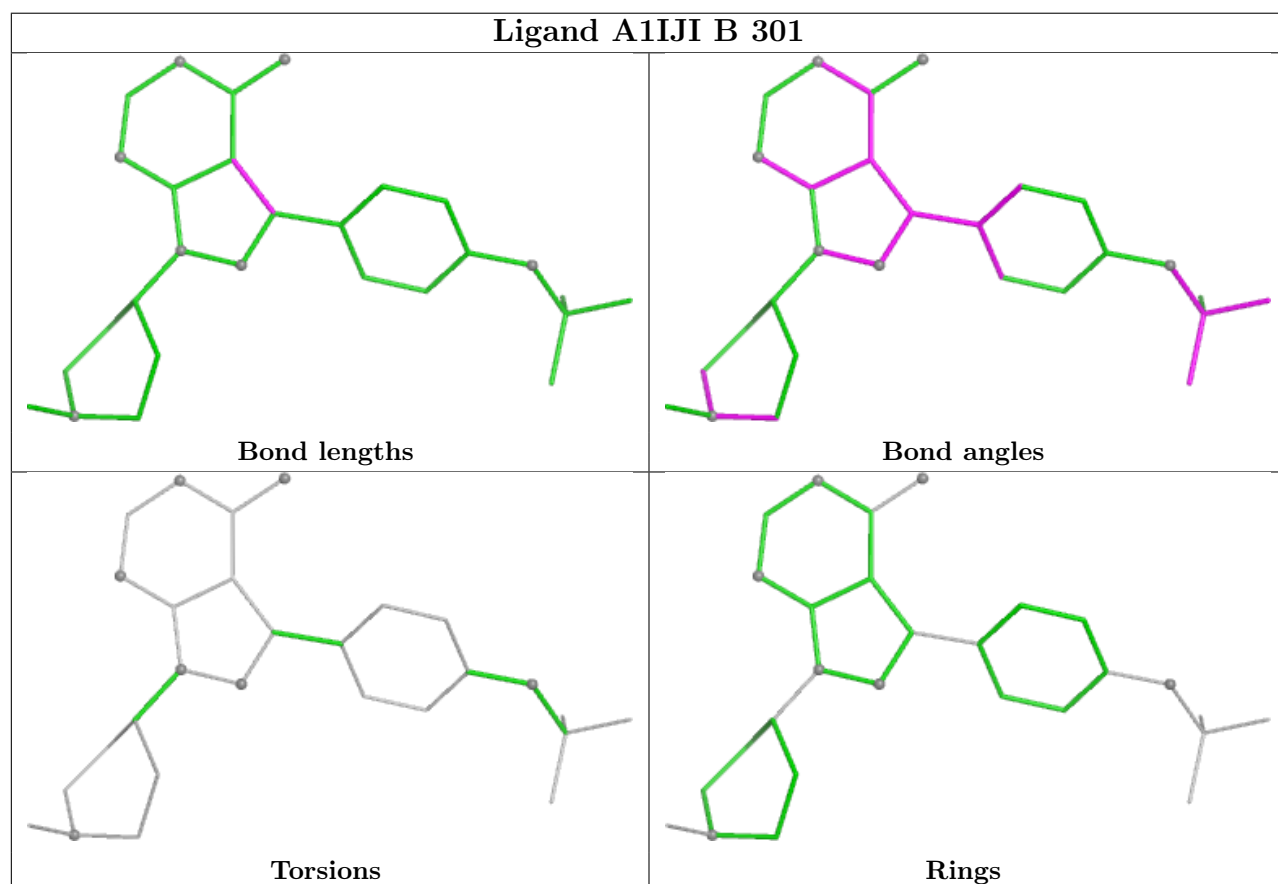
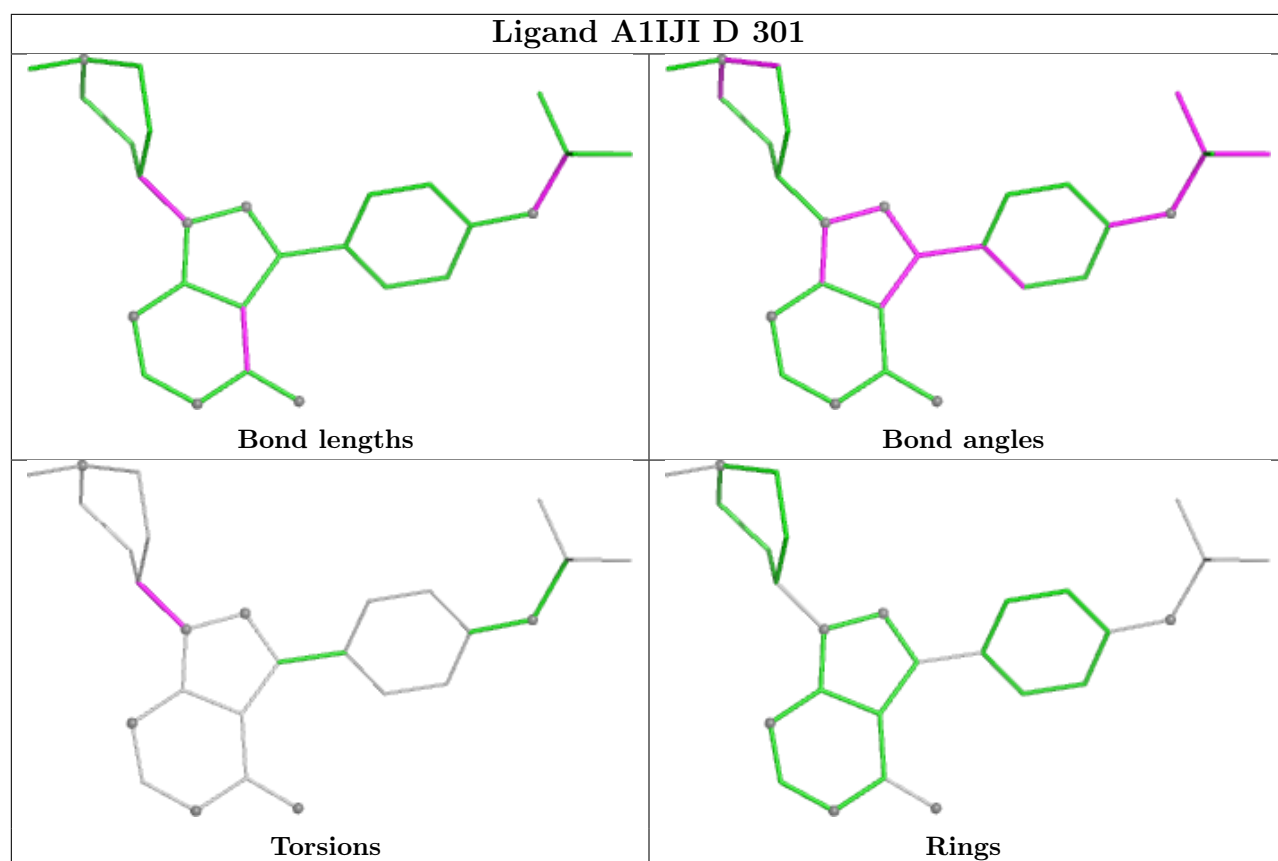
There are no ring outliers.

No monomer is involved in short contacts.

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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	202/222 (90%)	0.53	30 (14%) 5 5	5, 21, 75, 106	1 (0%)
1	B	206/222 (92%)	0.55	23 (11%) 10 9	5, 28, 67, 101	0
1	C	197/222 (88%)	0.69	27 (13%) 6 6	7, 31, 72, 107	1 (0%)
1	D	194/222 (87%)	0.60	24 (12%) 8 7	6, 23, 81, 110	0
All	All	799/888 (89%)	0.59	104 (13%) 7 6	5, 26, 73, 110	2 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	LEU	6.7
1	D	167	GLY	5.3
1	D	10	GLY	5.0
1	D	13	ALA	5.0
1	D	168	PRO	4.9
1	D	89	LEU	4.8
1	A	91	PRO	4.8
1	D	91	PRO	4.8
1	C	91	PRO	4.7
1	C	81	VAL	4.5
1	B	91	PRO	4.4
1	C	25	TYR	4.3
1	D	166	SER	4.3
1	A	74	PHE	4.2
1	C	92	ALA	4.1
1	A	78	LEU	4.0
1	C	22	THR	3.9
1	D	9	VAL	3.8
1	A	13	ALA	3.8
1	D	67	ALA	3.7
1	A	89	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	178	LEU	3.7
1	B	74	PHE	3.7
1	D	66	TYR	3.6
1	C	111	PRO	3.6
1	B	25	TYR	3.6
1	C	110	GLN	3.5
1	A	178	LEU	3.5
1	A	66	TYR	3.5
1	B	81	VAL	3.5
1	A	167	GLY	3.3
1	D	18	LEU	3.2
1	D	78	LEU	3.2
1	A	170	GLY	3.2
1	A	11	ARG	3.2
1	A	90	GLN	3.2
1	C	2	GLU	3.1
1	A	111	PRO	3.1
1	D	178	LEU	3.1
1	A	7	ALA	3.1
1	B	13	ALA	3.1
1	D	169	GLY	3.0
1	D	74	PHE	3.0
1	B	19	ARG	2.9
1	C	23	LEU	2.9
1	B	217	PRO	2.9
1	C	20	PRO	2.9
1	C	150	GLY	2.9
1	C	16	PRO	2.8
1	A	97	ALA	2.8
1	B	219	LEU	2.8
1	C	3	ARG	2.8
1	C	17	TYR	2.8
1	A	169	GLY	2.7
1	C	192	PHE	2.7
1	C	38	LYS	2.7
1	A	168	PRO	2.7
1	B	167	GLY	2.7
1	A	92	ALA	2.6
1	D	93	LEU	2.6
1	D	113	LEU	2.6
1	C	109	ASP	2.6
1	A	79	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	86	PRO	2.6
1	A	76	GLY	2.5
1	A	88	GLU	2.5
1	A	70	VAL	2.5
1	B	92	ALA	2.5
1	B	111	PRO	2.5
1	B	90	GLN	2.4
1	D	14	ALA	2.4
1	A	75	PRO	2.4
1	B	132	ALA	2.4
1	C	79	ALA	2.4
1	D	92	ALA	2.4
1	C	219	LEU	2.4
1	B	11	ARG	2.4
1	B	53	ARG	2.4
1	C	21	LEU	2.4
1	B	143	TRP	2.4
1	C	24	HIS	2.4
1	A	93	LEU	2.3
1	D	145	GLY	2.3
1	D	87	ARG	2.3
1	C	34	TRP	2.3
1	B	80	ALA	2.3
1	C	90	GLN	2.3
1	C	198	ILE	2.2
1	B	28	ASN	2.2
1	A	6	GLY	2.2
1	A	95	GLY	2.2
1	C	143	TRP	2.2
1	B	18	LEU	2.2
1	B	3	ARG	2.2
1	A	219	LEU	2.2
1	D	165	ARG	2.2
1	A	217	PRO	2.1
1	A	87	ARG	2.1
1	B	73	ARG	2.1
1	D	77	SER	2.1
1	C	80	ALA	2.1
1	B	186	LEU	2.1
1	A	218	ASN	2.1
1	D	12	CYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

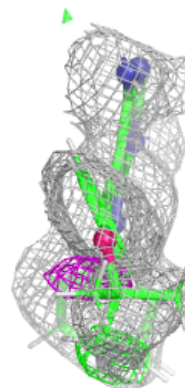
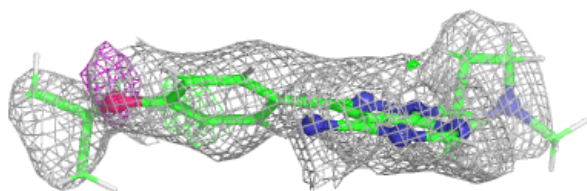
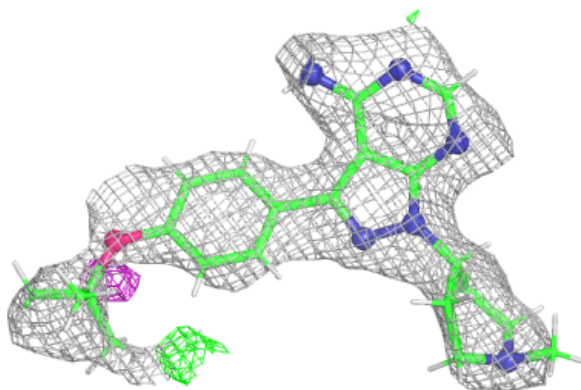
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1IJI	D	301	28/28	0.82	0.12	22,37,46,48	0
2	A1IJI	A	301	28/28	0.91	0.09	19,37,50,54	0
2	A1IJI	B	301	28/28	0.93	0.09	15,27,43,43	0

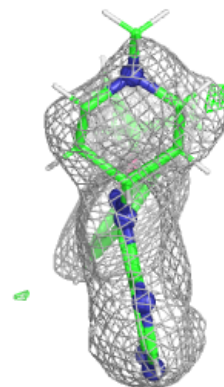
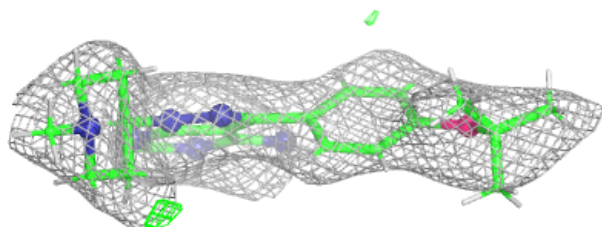
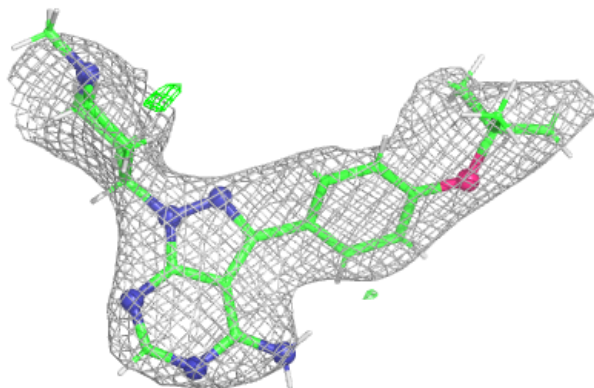
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

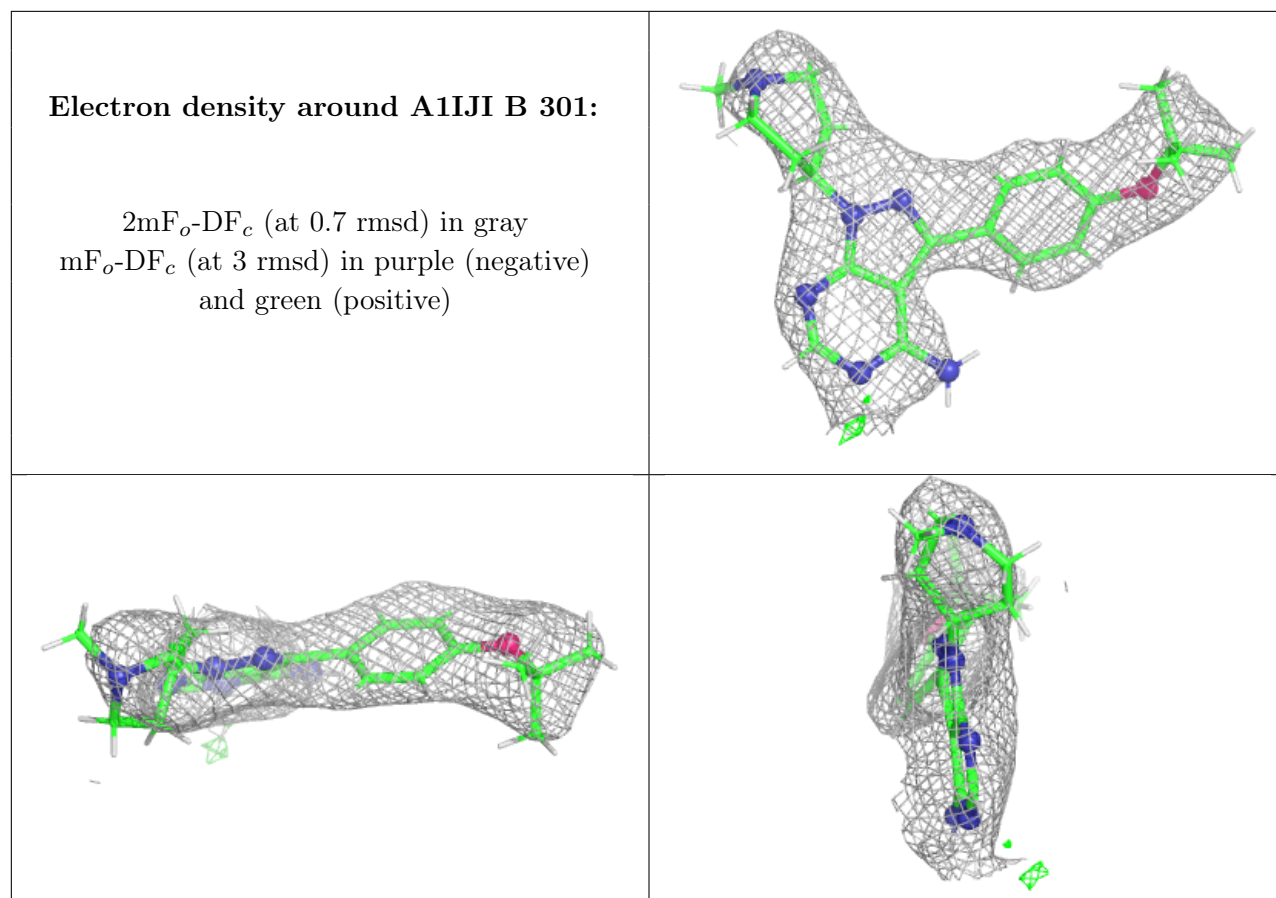
Electron density around A1IJI D 301:

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

**Electron density around A1IJI A 301:**

$2mF_o-DF_c$ (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.