



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:59 AM UTC

PDB ID : 7ZJQ / pdb_00007zjq
Title : Human TEAD3 in complex with 1-Cyclopentyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylic acid
Authors : Musil, D.; Sousa, C.M.
Deposited on : 2022-04-11
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

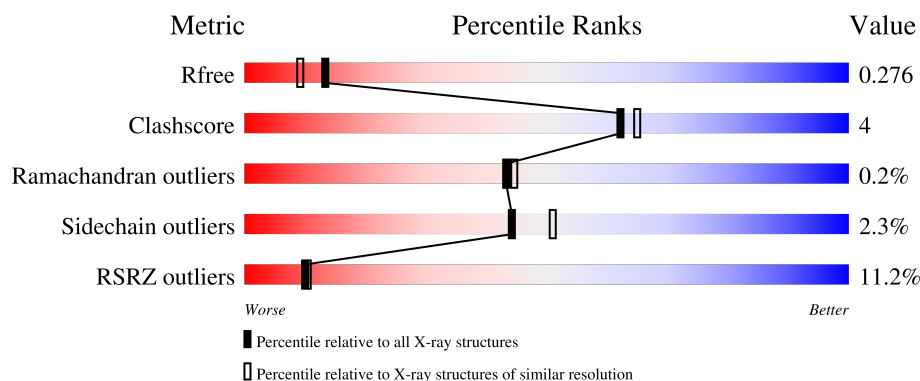
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	220	
2	B	220	
2	C	220	
2	D	220	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6986 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.

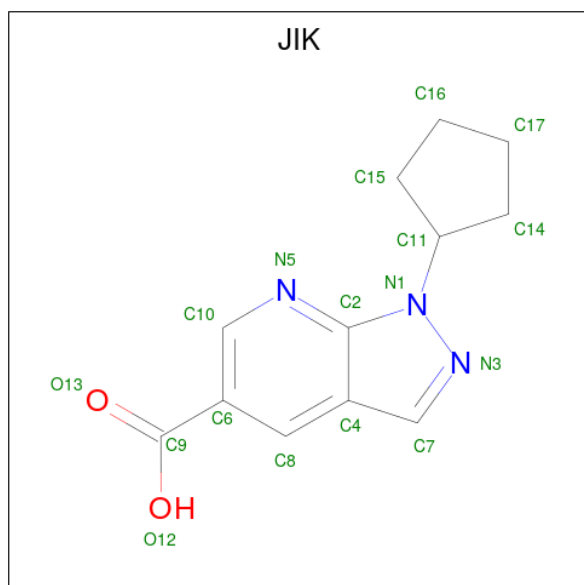
- Molecule 1 is a protein called Transcriptional enhancer factor TEF-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	26	2	0
			1719	1105	287	319	8			

- Molecule 2 is a protein called Transcriptional enhancer factor TEF-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	22	2	0
			1711	1101	288	314	8			
2	C	208	Total	C	N	O	S	18	2	0
			1707	1098	288	313	8			
2	D	208	Total	C	N	O	S	25	1	0
			1697	1092	285	312	8			

- Molecule 3 is 1-cyclopentylpyrazolo[3,4-b]pyridine-5-carboxylic acid (CCD ID: JIK) (formula: C₁₂H₁₃N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	12	3	2		
3	B	1	Total	C	N	O	0	0
			17	12	3	2		
3	C	1	Total	C	N	O	0	0
			17	12	3	2		
3	D	1	Total	C	N	O	0	0
			17	12	3	2		

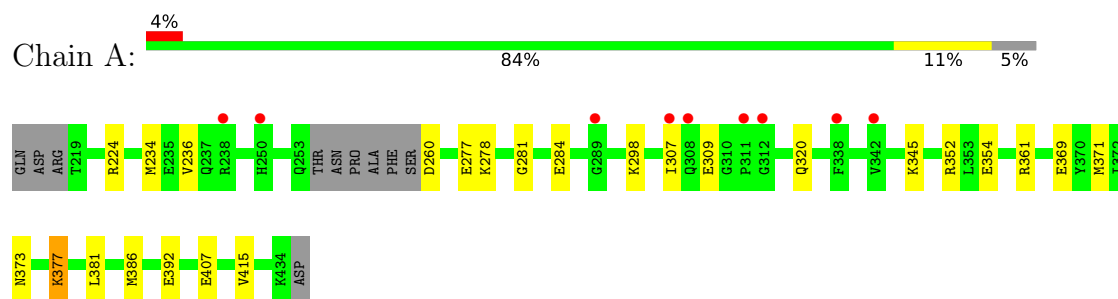
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	17	Total	O	0	0
			17	17		
4	C	29	Total	O	0	0
			29	29		
4	D	19	Total	O	0	0
			19	19		

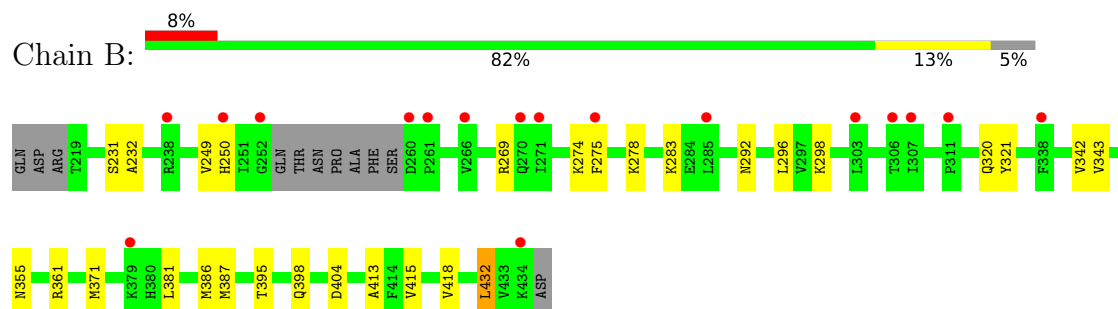
3 Residue-property plots [i](#)

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.

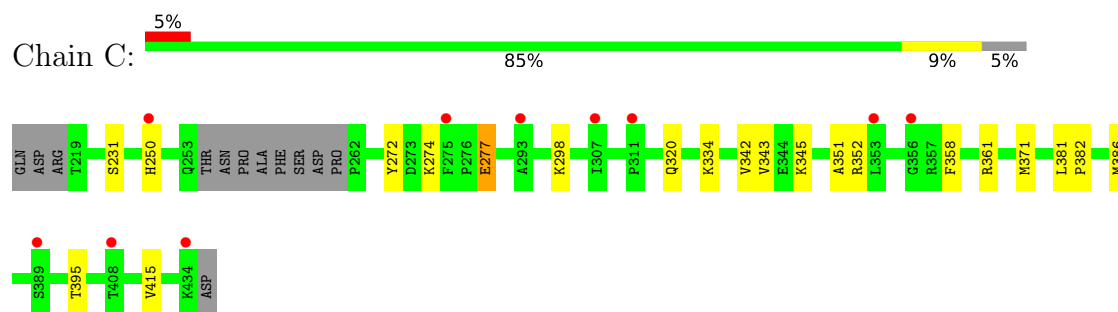
- Molecule 1: Transcriptional enhancer factor TEF-5



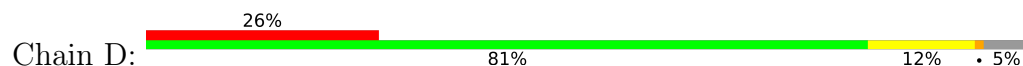
- Molecule 2: Transcriptional enhancer factor TEF-5

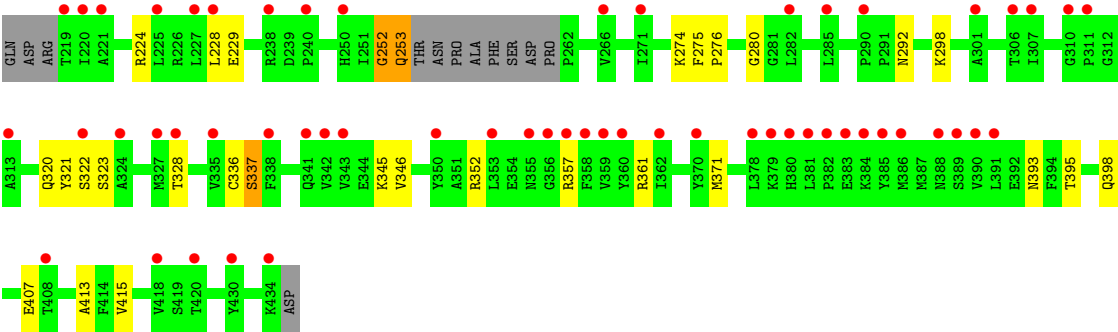


- Molecule 2: Transcriptional enhancer factor TEF-5



- Molecule 2: Transcriptional enhancer factor TEF-5





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.47Å 121.66Å 154.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.77 – 2.10 47.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.77-2.10) 98.2 (47.77-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.8 (3-FEB-2022)	Depositor
R, R_{free}	0.257 , 0.279 0.253 , 0.276	Depositor DCC
R_{free} test set	3597 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	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	0.96	EDS
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSX, JIK

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	0.69	0/1756	1.01	0/2369
2	B	0.66	0/1756	0.99	0/2370
2	C	0.69	0/1749	0.99	0/2359
2	D	0.68	1/1738 (0.1%)	1.02	2/2344 (0.1%)
All	All	0.68	1/6999 (0.0%)	1.00	2/9442 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	337	SER	N-CA	-5.20	1.40	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	252	GLY	CA-C-N	5.05	130.79	121.70
2	D	252	GLY	C-N-CA	5.05	130.79	121.70

There are no chirality outliers.

There are no planarity outliers.

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	1719	0	1694	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1711	0	1694	15	0
2	C	1707	0	1685	10	0
2	D	1697	0	1679	18	0
3	A	17	0	0	1	0
3	B	17	0	0	1	0
3	C	17	0	0	1	0
3	D	17	0	0	2	0
4	A	19	0	0	0	0
4	B	17	0	0	0	0
4	C	29	0	0	0	0
4	D	19	0	0	1	0
All	All	6986	0	6752	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASN:HB3	1:A:377:LYS:NZ	1.77	0.98
1:A:371:MET:HE2	3:A:501:JIK:N5	1.90	0.86
2:B:296:LEU:HB2	2:B:432:LEU:HD11	1.63	0.80
1:A:373:ASN:HB3	1:A:377:LYS:HZ1	1.45	0.78
1:A:373:ASN:HB3	1:A:377:LYS:HZ2	1.48	0.78
2:C:342:VAL:HG12	2:C:343:VAL:HG23	1.72	0.69
2:D:371:MET:HE2	3:D:501:JIK:N5	2.11	0.65
2:B:342:VAL:HG12	2:B:343:VAL:HG23	1.76	0.65
2:D:228:LEU:HD11	2:D:322:SER:HB3	1.79	0.65
1:A:236:VAL:HG12	1:A:307:ILE:HD12	1.82	0.61
2:B:355:ASN:ND2	2:D:328:THR:OG1	2.28	0.61
2:C:381:LEU:HD22	2:C:386:MET:HE2	1.83	0.60
2:B:387:MET:HB2	2:B:418:VAL:HG21	1.83	0.60
1:A:298:LYS:HD3	1:A:415:VAL:HG23	1.87	0.57
2:C:351:ALA:HB1	2:C:358:PHE:HB3	1.86	0.56
2:D:252:GLY:O	2:D:253:GLN:HB2	2.05	0.55
2:D:322:SER:CB	2:D:357:ARG:HE	2.20	0.55
2:C:298:LYS:HD3	2:C:415:VAL:HG23	1.89	0.54
2:D:298:LYS:HD3	2:D:415:VAL:HG23	1.89	0.53
1:A:354:GLU:OE1	1:A:361:ARG:NH2	2.42	0.53
2:B:296:LEU:CB	2:B:432:LEU:HD11	2.36	0.53
2:B:381:LEU:HD22	2:B:386:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:LYS:HD3	2:B:415:VAL:HG23	1.93	0.50
2:D:320:GLN:HG2	2:D:361:ARG:HG2	1.94	0.50
1:A:381:LEU:HD22	1:A:386:MET:HE2	1.93	0.50
2:D:371:MET:HE2	3:D:501:JIK:C10	2.41	0.50
1:A:320:GLN:HG2	1:A:361:ARG:HG2	1.93	0.49
2:C:320:GLN:HG2	2:C:361:ARG:HG2	1.92	0.49
2:B:320:GLN:HG2	2:B:361:ARG:HG2	1.94	0.49
2:C:371:MET:HE2	3:C:501:JIK:N5	2.28	0.48
2:D:321:TYR:OH	2:D:398:GLN:NE2	2.46	0.48
2:D:322:SER:HB2	2:D:357:ARG:HE	1.78	0.47
2:C:272:TYR:O	2:C:277:GLU:OE2	2.33	0.47
2:D:229:GLU:HG2	4:D:603:HOH:O	2.14	0.47
2:B:231:SER:HB3	2:B:250[B]:HIS:HD2	1.80	0.45
2:C:231:SER:HB3	2:C:250[B]:HIS:HD2	1.82	0.45
1:A:345:LYS:HG3	2:D:346:VAL:HB	1.98	0.45
2:D:224:ARG:NH2	2:D:407:GLU:OE2	2.49	0.45
1:A:234:MET:HE3	1:A:234:MET:HB2	1.93	0.44
2:B:274:LYS:HB3	2:B:395:THR:HG21	2.00	0.43
1:A:224:ARG:NH2	1:A:407:GLU:OE2	2.49	0.43
2:B:269:ARG:HH22	2:B:283:LYS:HE3	1.83	0.43
1:A:234:MET:HE1	1:A:309:GLU:HG3	2.01	0.43
2:D:276:PRO:HD3	2:D:336:CYS:SG	2.59	0.42
2:B:275:PHE:CZ	2:B:413:ALA:HB1	2.55	0.42
2:B:321:TYR:OH	2:B:398:GLN:NE2	2.53	0.42
1:A:369:GLU:HG3	2:D:280:GLY:HA3	2.01	0.42
2:C:274:LYS:HB3	2:C:395:THR:HG21	2.00	0.42
2:C:382:PRO:HD2	2:C:386:MET:HE1	2.01	0.41
1:A:277:GLU:O	1:A:281:GLY:HA3	2.21	0.41
2:B:232:ALA:HB3	2:B:249:VAL:HG22	2.03	0.41
2:D:275:PHE:CZ	2:D:413:ALA:HB1	2.56	0.40
2:D:274:LYS:HB3	2:D:395:THR:HG21	2.03	0.40
2:D:337:SER:HA	2:D:393:ASN:O	2.21	0.40
2:B:371:MET:HE2	3:B:501:JIK:N5	2.36	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	207/220 (94%)	204 (99%)	2 (1%)	1 (0%)	24	22
2	B	207/220 (94%)	203 (98%)	3 (1%)	1 (0%)	24	22
2	C	206/220 (94%)	203 (98%)	3 (2%)	0	100	100
2	D	205/220 (93%)	198 (97%)	7 (3%)	0	100	100
All	All	825/880 (94%)	808 (98%)	15 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
2	B	278	LYS

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	191/198 (96%)	186 (97%)	5 (3%)	40	46
2	B	191/199 (96%)	188 (98%)	3 (2%)	55	64
2	C	190/199 (96%)	186 (98%)	4 (2%)	47	54
2	D	189/199 (95%)	184 (97%)	5 (3%)	40	46
All	All	761/795 (96%)	744 (98%)	17 (2%)	44	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	ASP
1	A	284	GLU
1	A	352	ARG
1	A	377	LYS
1	A	392	GLU
2	B	292	ASN
2	B	404	ASP
2	B	432	LEU
2	C	277	GLU
2	C	334	LYS
2	C	345	LYS
2	C	352	ARG
2	D	253	GLN
2	D	292	ASN
2	D	323	SER
2	D	345	LYS
2	D	352	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	304	ASN
1	A	355	ASN
1	A	363	HIS
1	A	398	GLN
2	B	237	GLN
2	B	304	ASN
2	B	355	ASN
2	B	398	GLN
2	B	427	HIS
2	C	398	GLN
2	C	406	GLN
2	C	427	HIS
2	D	398	GLN
2	D	406	GLN
2	D	427	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSX	A	336	1	3,6,7	0.83	0	1,6,8	0.30	0

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
1	CSX	A	336	1	-	0/2/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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
3	JIK	B	501	-	19,19,19	1.62	4 (21%)	25,27,27	2.56	10 (40%)
3	JIK	D	501	-	19,19,19	1.58	4 (21%)	25,27,27	2.64	10 (40%)
3	JIK	C	501	-	19,19,19	1.75	4 (21%)	25,27,27	3.07	11 (44%)
3	JIK	A	501	-	19,19,19	1.55	3 (15%)	25,27,27	2.55	8 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JIK	B	501	-	-	0/8/15/15	0/3/3/3
3	JIK	D	501	-	-	3/8/15/15	0/3/3/3
3	JIK	C	501	-	-	2/8/15/15	0/3/3/3
3	JIK	A	501	-	-	0/8/15/15	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	JIK	O13-C9	4.33	1.35	1.22
3	B	501	JIK	O13-C9	4.17	1.34	1.22
3	A	501	JIK	O13-C9	4.07	1.34	1.22
3	D	501	JIK	O13-C9	3.95	1.34	1.22
3	C	501	JIK	C4-C7	3.68	1.46	1.42
3	B	501	JIK	C4-C7	3.49	1.46	1.42
3	A	501	JIK	C4-C7	3.43	1.46	1.42
3	D	501	JIK	C4-C7	3.23	1.46	1.42
3	B	501	JIK	O12-C9	-2.93	1.21	1.30
3	C	501	JIK	O12-C9	-2.76	1.22	1.30
3	D	501	JIK	O12-C9	-2.71	1.22	1.30
3	A	501	JIK	O12-C9	-2.68	1.22	1.30
3	D	501	JIK	N1-N3	2.51	1.40	1.37
3	C	501	JIK	C7-N3	-2.17	1.29	1.32
3	B	501	JIK	N1-N3	2.10	1.39	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	JIK	C7-N3-N1	7.61	111.15	105.95
3	C	501	JIK	N5-C2-N1	6.58	134.62	126.05
3	C	501	JIK	C4-C7-N3	-6.55	107.11	112.05
3	D	501	JIK	C7-N3-N1	6.35	110.29	105.95
3	A	501	JIK	C7-N3-N1	6.12	110.13	105.95
3	B	501	JIK	C7-N3-N1	5.84	109.94	105.95
3	D	501	JIK	C4-C7-N3	-5.75	107.71	112.05
3	B	501	JIK	C4-C7-N3	-5.63	107.80	112.05
3	A	501	JIK	C4-C7-N3	-5.50	107.90	112.05
3	C	501	JIK	C4-C2-N5	-5.37	119.66	126.88
3	B	501	JIK	N5-C2-N1	4.74	132.22	126.05
3	A	501	JIK	C4-C2-N5	-4.56	120.75	126.88
3	A	501	JIK	N5-C2-N1	4.49	131.89	126.05
3	B	501	JIK	C4-C2-N5	-4.36	121.02	126.88
3	D	501	JIK	N5-C2-N1	4.11	131.40	126.05
3	D	501	JIK	C4-C2-N5	-4.08	121.40	126.88
3	D	501	JIK	C11-N1-N3	3.78	127.84	119.79
3	D	501	JIK	C2-N1-N3	-3.38	108.91	110.94
3	A	501	JIK	C11-N1-N3	3.37	126.97	119.79
3	B	501	JIK	C11-N1-N3	3.25	126.72	119.79
3	A	501	JIK	C2-N1-N3	-3.18	109.03	110.94
3	C	501	JIK	C2-C4-C7	2.95	106.75	104.40
3	C	501	JIK	C16-C15-C11	-2.85	98.20	104.61
3	C	501	JIK	C2-N1-N3	-2.78	109.28	110.94
3	B	501	JIK	C2-N1-N3	-2.47	109.46	110.94
3	D	501	JIK	C4-C8-C6	-2.43	117.49	121.32
3	A	501	JIK	C4-C8-C6	-2.42	117.51	121.32
3	C	501	JIK	C8-C4-C2	2.39	120.36	117.93
3	C	501	JIK	C4-C2-N1	-2.39	105.72	107.16
3	D	501	JIK	C2-N1-C11	-2.32	123.20	128.97
3	D	501	JIK	C16-C15-C11	-2.29	99.45	104.61
3	B	501	JIK	C4-C8-C6	-2.27	117.75	121.32
3	C	501	JIK	O12-C9-C6	2.22	120.54	114.84
3	D	501	JIK	O12-C9-C6	2.22	120.53	114.84
3	B	501	JIK	O12-C9-O13	-2.21	118.61	123.35
3	C	501	JIK	C4-C8-C6	-2.20	117.85	121.32
3	B	501	JIK	C2-N1-C11	-2.10	123.75	128.97
3	B	501	JIK	C2-C4-C7	2.07	106.05	104.40
3	A	501	JIK	C2-N1-C11	-2.00	124.00	128.97

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	JIK	C15-C11-N1-N3
3	C	501	JIK	C14-C11-N1-C2
3	D	501	JIK	C14-C11-N1-C2
3	D	501	JIK	C14-C11-N1-N3
3	C	501	JIK	C14-C11-N1-N3

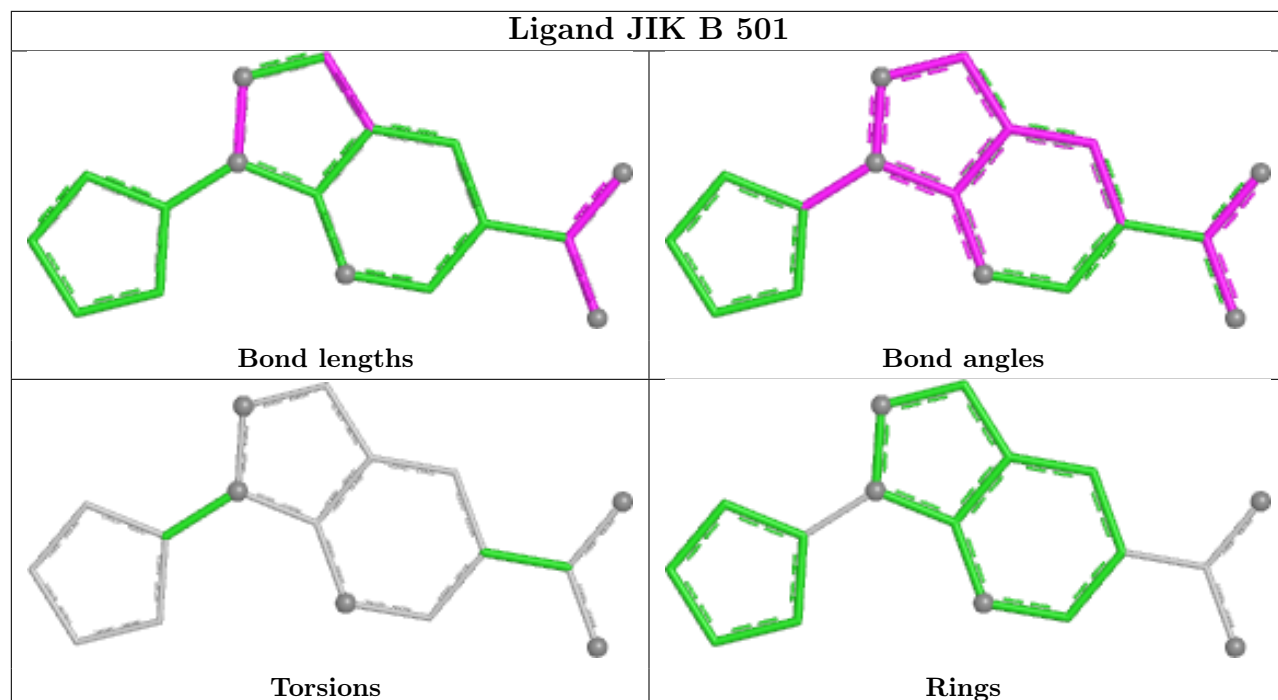
There are no ring outliers.

4 monomers are involved in 5 short contacts:

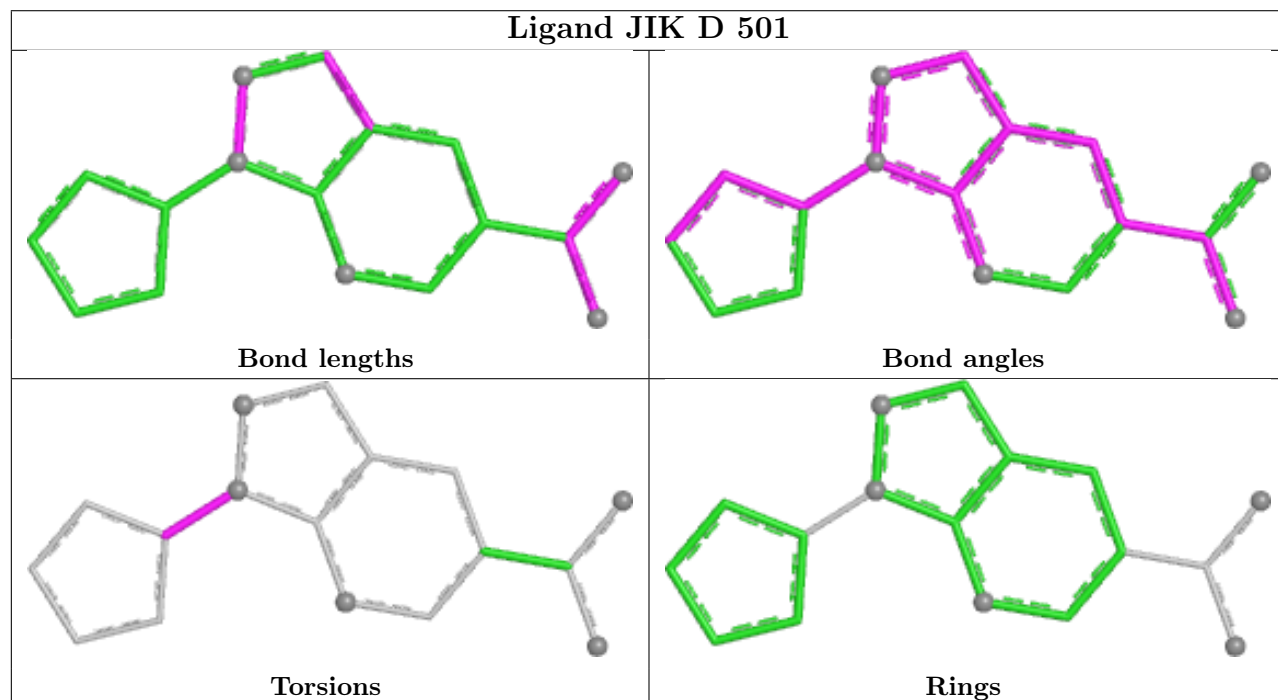
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	JIK	1	0
3	D	501	JIK	2	0
3	C	501	JIK	1	0
3	A	501	JIK	1	0

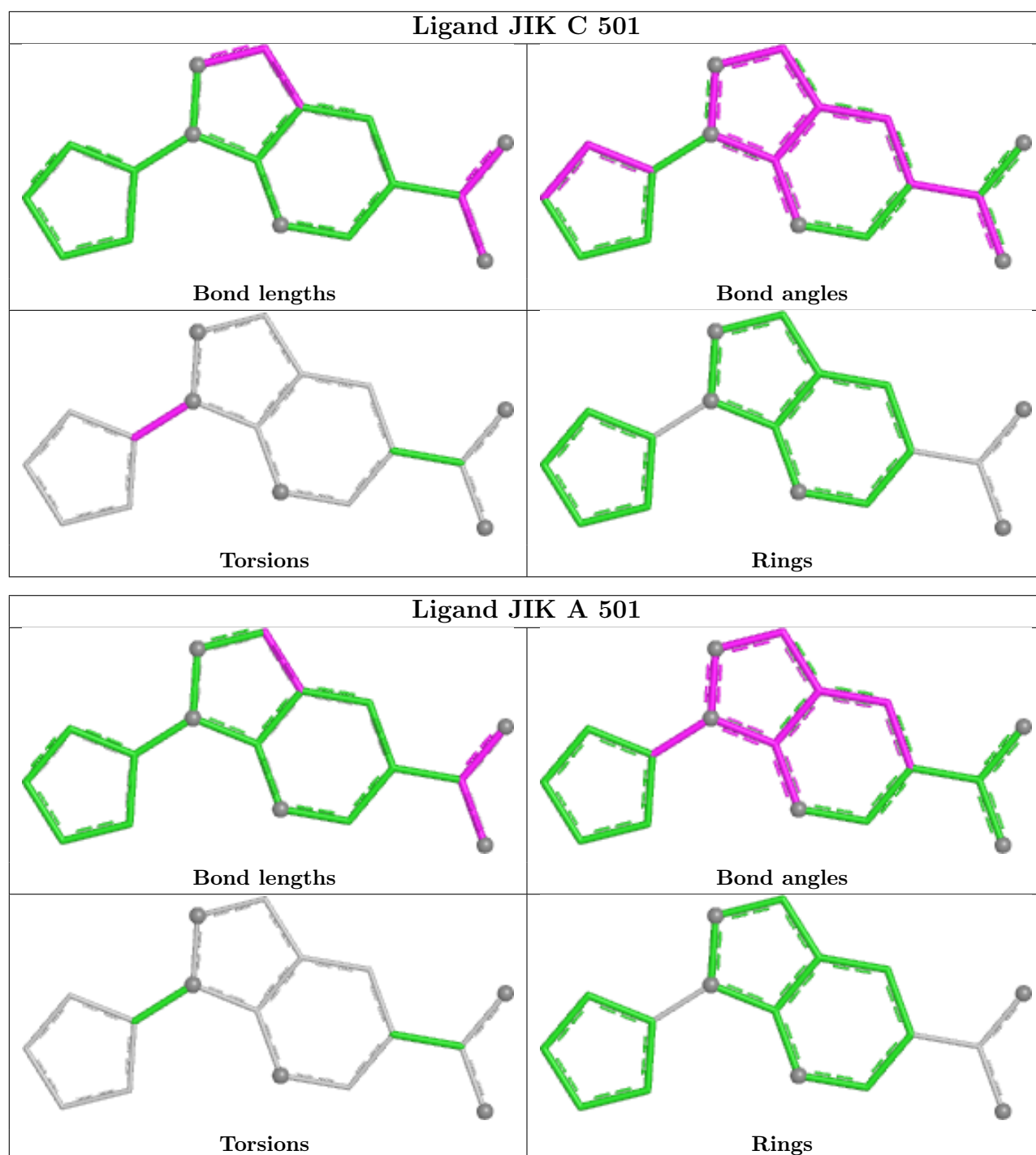
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 JIK B 501



Ligand JIK D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/220 (95%)	0.73	9 (4%) 40 41	38, 81, 116, 139	10 (4%)
2	B	209/220 (95%)	0.84	17 (8%) 18 19	40, 90, 129, 144	9 (4%)
2	C	208/220 (94%)	0.80	10 (4%) 35 38	39, 83, 109, 120	7 (3%)
2	D	208/220 (94%)	1.41	57 (27%) 1 1	38, 95, 152, 171	8 (3%)
All	All	834/880 (94%)	0.94	93 (11%) 10 10	38, 87, 129, 171	34 (4%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	385	TYR	4.9
2	D	358	PHE	4.5
1	A	250[A]	HIS	4.2
2	D	307	ILE	4.1
2	C	250[A]	HIS	3.7
2	D	353	LEU	3.6
2	D	389	SER	3.4
2	D	359	VAL	3.4
2	D	306	THR	3.3
2	B	250[A]	HIS	3.3
2	B	285	LEU	3.1
2	D	219	THR	3.1
2	D	408	THR	3.1
2	B	338	PHE	3.0
2	D	324	ALA	3.0
2	C	311	PRO	3.0
2	B	270	GLN	2.9
2	B	303	LEU	2.9
2	D	381	LEU	2.9
2	D	338	PHE	2.9
2	D	250[A]	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	266	VAL	2.9
2	C	434	LYS	2.9
2	D	388	ASN	2.8
2	B	252	GLY	2.8
2	D	228	LEU	2.8
2	D	342	VAL	2.8
2	D	311	PRO	2.8
2	D	380	HIS	2.7
2	B	311	PRO	2.7
2	D	418	VAL	2.7
2	C	356	GLY	2.7
2	D	420	THR	2.7
2	D	290	PRO	2.7
2	D	383	GLU	2.7
2	D	386	MET	2.7
2	D	384	LYS	2.7
2	D	238	ARG	2.7
2	D	391	LEU	2.7
2	D	390	VAL	2.7
1	A	342	VAL	2.6
2	D	434	LYS	2.6
1	A	238	ARG	2.6
2	D	430	TYR	2.6
2	D	313	ALA	2.6
2	C	353	LEU	2.6
2	D	341	GLN	2.5
1	A	307	ILE	2.5
2	D	343	VAL	2.5
2	B	434	LYS	2.5
2	D	355	ASN	2.5
2	D	378	LEU	2.5
2	D	328	THR	2.5
2	D	322	SER	2.4
2	D	282	LEU	2.4
2	B	271	ILE	2.4
2	D	271	ILE	2.4
2	B	261	PRO	2.4
2	D	227	LEU	2.4
2	C	307	ILE	2.4
2	B	379	LYS	2.4
2	D	301	ALA	2.4
2	D	356	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	338	PHE	2.4
2	D	350	TYR	2.3
2	D	382	PRO	2.3
1	A	308	GLN	2.3
1	A	312	GLY	2.3
2	C	389	SER	2.3
2	B	307	ILE	2.3
1	A	311	PRO	2.3
2	D	221	ALA	2.3
2	D	370	TYR	2.3
2	B	275	PHE	2.3
2	D	327	MET	2.3
2	C	275	PHE	2.2
2	D	220	ILE	2.2
2	D	362	ILE	2.2
2	D	335	VAL	2.2
2	D	379	LYS	2.1
2	D	360	TYR	2.1
2	C	408	THR	2.1
2	D	240	PRO	2.1
2	B	266	VAL	2.1
2	D	310	GLY	2.1
2	C	293	ALA	2.1
2	D	225	LEU	2.1
2	B	260	ASP	2.1
2	B	306	THR	2.1
2	D	285	LEU	2.0
2	B	238	ARG	2.0
1	A	289	GLY	2.0
2	D	357	ARG	2.0

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

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(Å ²)	Q<0.9
1	CSX	A	336	7/8	0.91	0.11	65,66,68,68	0

6.3 Carbohydrates [i](#)

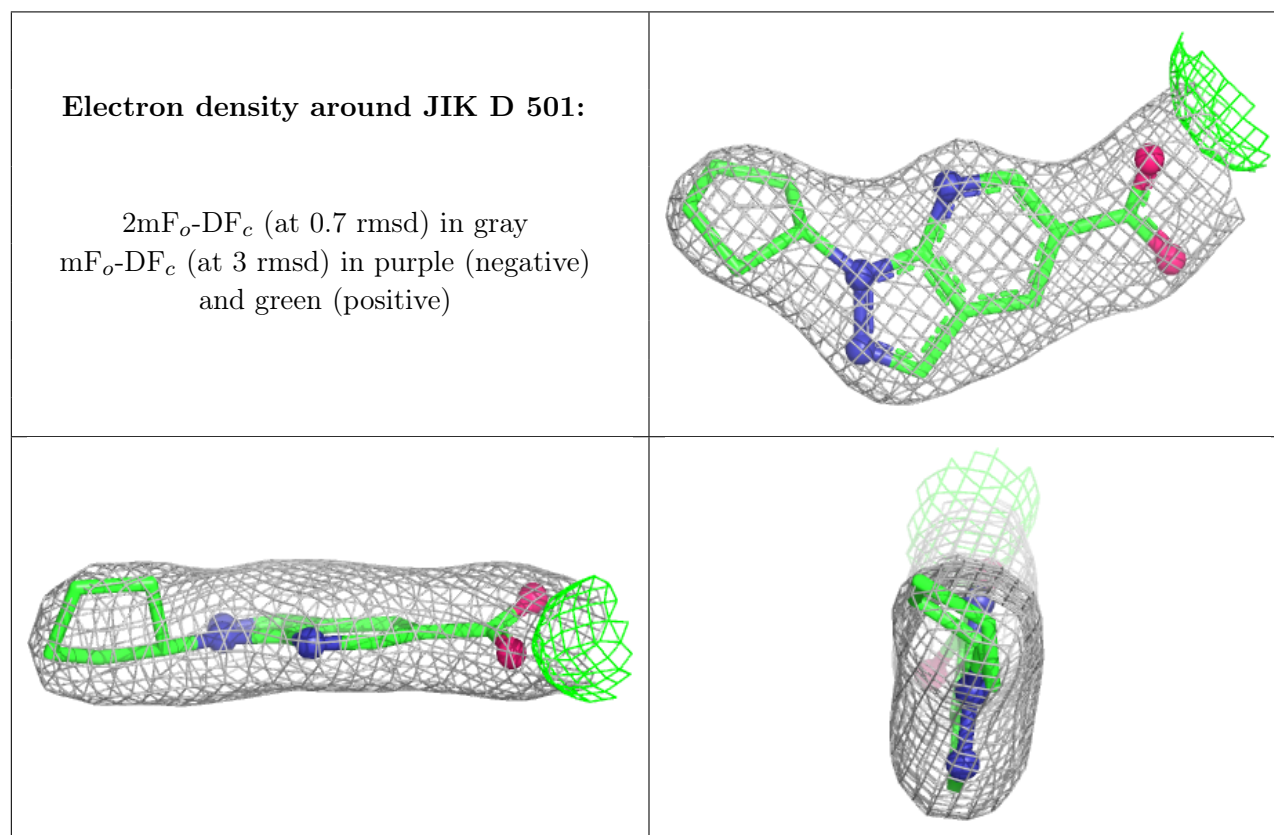
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

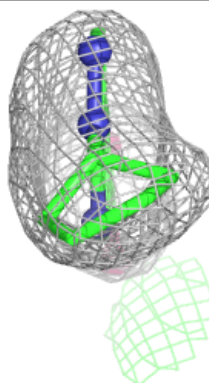
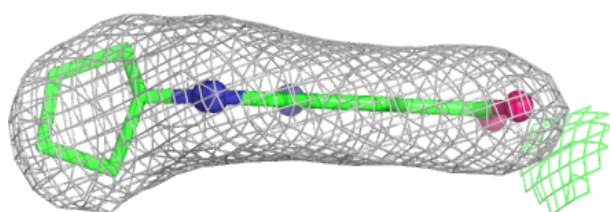
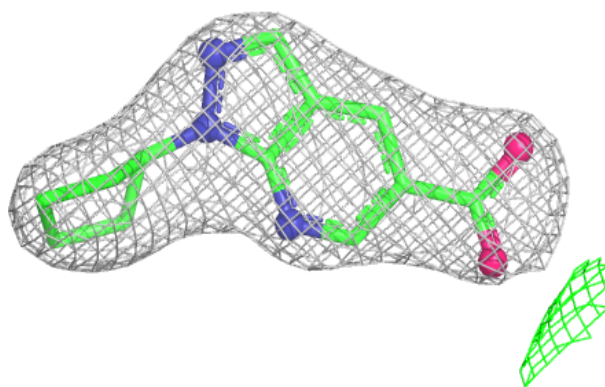
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JIK	D	501	17/17	0.94	0.11	74,76,78,78	0
3	JIK	C	501	17/17	0.95	0.12	75,77,78,78	0
3	JIK	B	501	17/17	0.95	0.10	78,79,80,80	0
3	JIK	A	501	17/17	0.96	0.09	73,74,76,76	0

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.

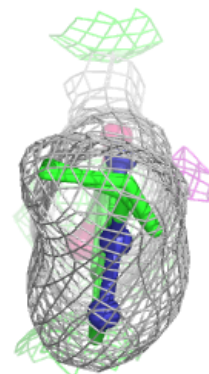
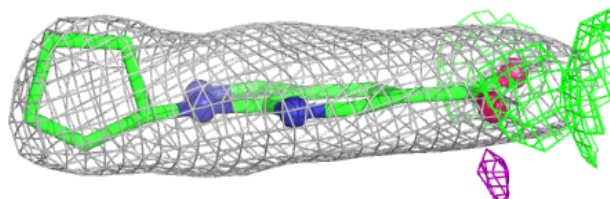
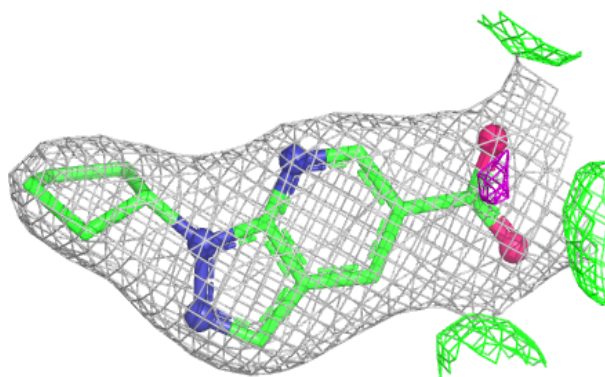


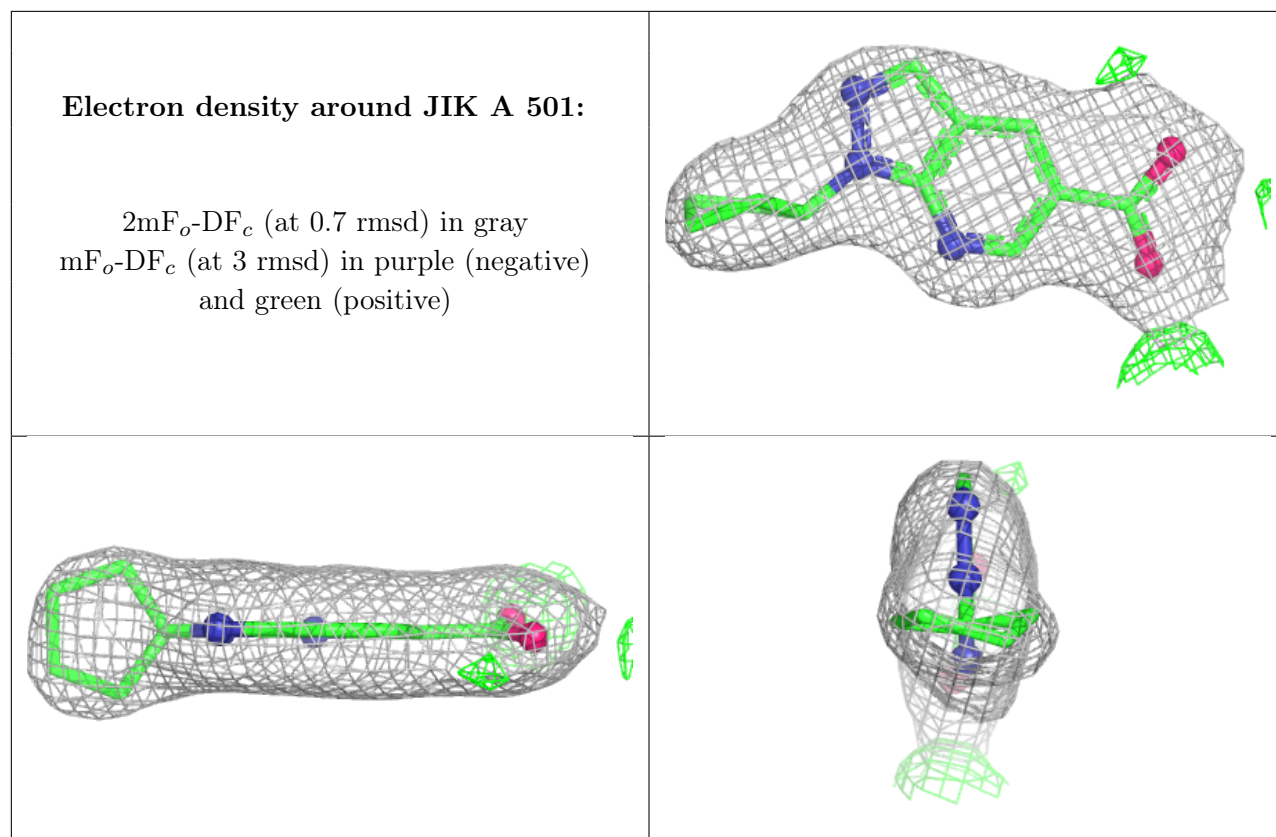
Electron density around JIK C 501:

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

**Electron density around JIK 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.