



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 6QX2 / pdb_00006qx2
Title : 3.4A structure of benzoisoxazole 3 with S.aureus DNA gyrase and DNA
Authors : Bax, B.D.
Deposited on : 2019-03-06
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

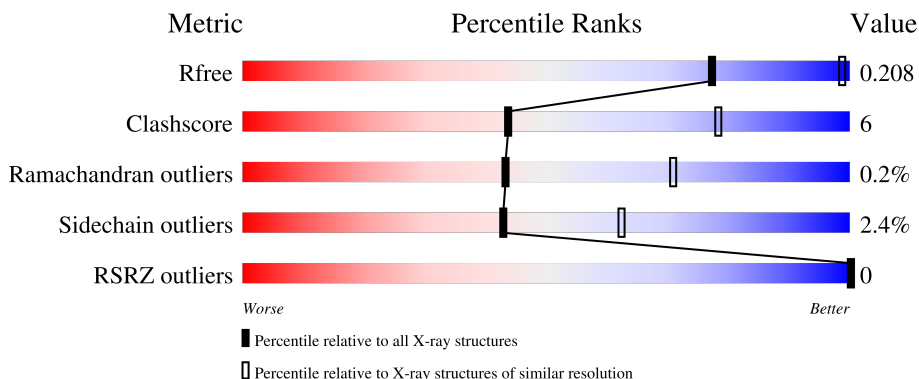
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	B	186	
1	S	186	
1	b	186	
1	s	186	
2	A	490	

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Mol	Chain	Length	Quality of chain
2	C	490	 88% 10% .
2	L	490	 88% 10% .
2	R	490	 87% 11% ..
2	T	490	 87% 10% ..
2	a	490	 87% 11% .
2	c	490	 87% 10% .
2	j	490	 87% 11% ..
2	l	490	 88% 10% .
2	r	490	 86% 12% ..
2	t	490	 87% 11% .
3	D	188	 86% 13% .
3	U	188	 87% 12% .
3	m	188	 87% 12% .
4	E	20	 45% 50% 5%
4	F	20	 60% 35% 5%
4	N	20	 55% 40% 5%
4	O	20	 70% 30%
4	W	20	 35% 60% 5%
4	e	20	 50% 45% 5%
4	n	20	 40% 45% 15%
4	v	20	 75% 20% 5%
4	w	20	 50% 40% 10%
5	K	187	 85% 14% ..
6	J	480	 87% 12% .
7	M	189	 87% 13%

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Mol	Chain	Length	Quality of chain
8	V	19	 58%37%5%
8	o	19	 58%32%5%5%
9	d	181	 86%13%.
10	f	17	 71%24%6%
11	k	188	 88%11%.
12	u	187	 87%13%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 68236 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 DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	185	Total	C	N	O	S	0	5	0
			1441	900	252	278	11			
1	S	185	Total	C	N	O	S	0	5	0
			1439	898	249	281	11			
1	b	185	Total	C	N	O	S	0	5	0
			1430	893	246	280	11			
1	s	186	Total	C	N	O	S	0	4	0
			1434	896	249	278	11			

- Molecule 2 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	479	Total	C	N	O	S	0	13	0
			3846	2387	693	748	18			
2	C	482	Total	C	N	O	S	0	8	0
			3784	2354	678	735	17			
2	L	481	Total	C	N	O	S	0	6	0
			3785	2354	681	733	17			
2	R	482	Total	C	N	O	S	0	11	0
			3830	2382	685	746	17			
2	T	481	Total	C	N	O	S	0	8	0
			3793	2362	680	734	17			
2	a	481	Total	C	N	O	S	0	12	0
			3802	2365	678	742	17			
2	c	482	Total	C	N	O	S	0	8	0
			3784	2357	677	733	17			
2	j	482	Total	C	N	O	S	0	13	0
			3848	2392	691	747	18			
2	l	481	Total	C	N	O	S	0	6	0
			3784	2357	681	729	17			
2	r	484	Total	C	N	O	S	0	15	0
			3870	2403	697	752	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	t	481	Total	C	N	O	S	0	10	0
			3809	2371	685	736	17			

- Molecule 3 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	188	Total	C	N	O	S	0	2	0
			1447	906	247	285	9			
3	U	188	Total	C	N	O	S	0	3	0
			1463	917	248	289	9			
3	m	188	Total	C	N	O	S	0	1	0
			1442	906	246	281	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	544	THR	-	linker	UNP P0A0K8
D	545	GLY	-	linker	UNP P0A0K8
U	544	THR	-	linker	UNP P0A0K8
U	545	GLY	-	linker	UNP P0A0K8
m	544	THR	-	linker	UNP P0A0K8
m	545	GLY	-	linker	UNP P0A0K8

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	20	Total	C	N	O	P	0	3	0
			455	215	89	130	21			
4	F	20	Total	C	N	O	P	0	0	0
			392	184	74	115	19			
4	N	20	Total	C	N	O	P	0	3	0
			455	215	89	130	21			
4	O	20	Total	C	N	O	P	0	0	0
			392	184	74	115	19			
4	W	20	Total	C	N	O	P	0	0	0
			408	194	76	119	19			
4	e	20	Total	C	N	O	P	0	0	0
			392	185	74	114	19			
4	n	20	Total	C	N	O	P	0	2	0
			418	196	76	125	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	v	19	Total	C	N	O	P	0	2	0
			399	186	71	121	21			
4	w	20	Total	C	N	O	P	0	0	0
			400	189	75	117	19			

- Molecule 5 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	187	Total	C	N	O	S	0	4	0
			1439	898	247	283	11			

- Molecule 6 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	480	Total	C	N	O	S	0	15	0
			3862	2399	694	751	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	?	-	ARG	deletion	UNP Q99XG5

- Molecule 7 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	189	Total	C	N	O	S	0	3	0
			1468	920	249	290	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	544	THR	-	linker	UNP P66937
M	545	GLY	-	linker	UNP P66937

- Molecule 8 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	V	19	Total	C	N	O	P	0	0	0
			388	184	74	112	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	o	18	Total	C	N	O	P	0	0	0
			369	174	69	108	18			

- Molecule 9 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	d	181	Total	C	N	O	S	0	2	0
			1395	875	240	272	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	544	THR	-	linker	UNP P66937
d	545	GLY	-	linker	UNP P66937

- Molecule 10 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	f	17	Total	C	N	O	P	0	0	0
			348	164	64	103	17			

- Molecule 11 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	k	188	Total	C	N	O	S	0	4	0
			1453	910	251	281	11			

- Molecule 12 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

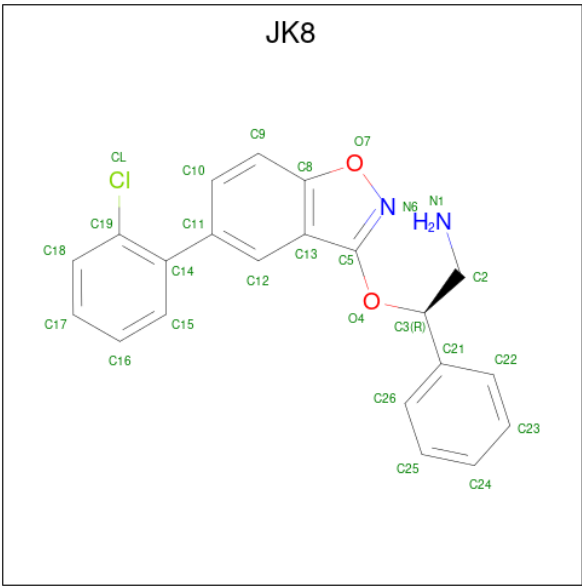
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	u	187	Total	C	N	O	S	0	3	0
			1460	915	248	288	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	544	THR	-	linker	UNP P66937
u	545	GLY	-	linker	UNP P66937

- Molecule 13 is (2 {R})-2-[[5-(2-chlorophenyl)-1,2-benzoxazol-3-yl]oxy]-2-phenyl-ethanamine

(CCD ID: JK8) (formula: C₂₁H₁₇ClN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total 26	C 21	Cl 1	N 2	O 2	0	0
13	C	1	Total 26	C 21	Cl 1	N 2	O 2	0	1
13	J	1	Total 26	C 21	Cl 1	N 2	O 2	0	0
13	L	1	Total 26	C 21	Cl 1	N 2	O 2	0	1
13	R	1	Total 26	C 21	Cl 1	N 2	O 2	0	0
13	U	1	Total 26	C 21	Cl 1	N 2	O 2	0	1
13	b	1	Total 26	C 21	Cl 1	N 2	O 2	0	0
13	d	1	Total 26	C 21	Cl 1	N 2	O 2	0	1
13	k	1	Total 26	C 21	Cl 1	N 2	O 2	0	0
13	l	1	Total 26	C 21	Cl 1	N 2	O 2	0	1
13	s	1	Total 26	C 21	Cl 1	N 2	O 2	0	0
13	t	1	Total 26	C 21	Cl 1	N 2	O 2	0	1

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: DNA gyrase subunit B,DNA gyrase subunit B

Chain B: 



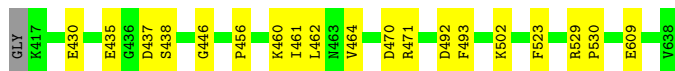
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

Chain S: 



- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

Chain b: 



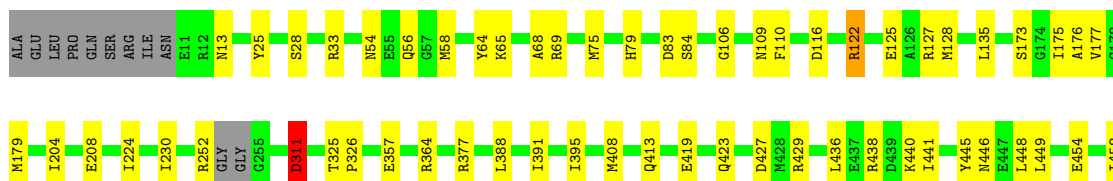
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

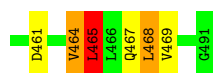
Chain s: 



- Molecule 2: DNA gyrase subunit A

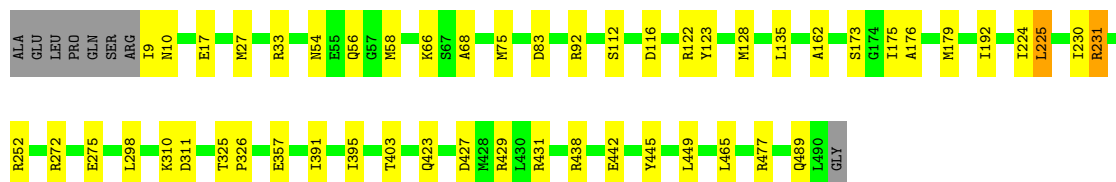
Chain A: 





• Molecule 2: DNA gyrase subunit A

Chain C: 88% 10% .



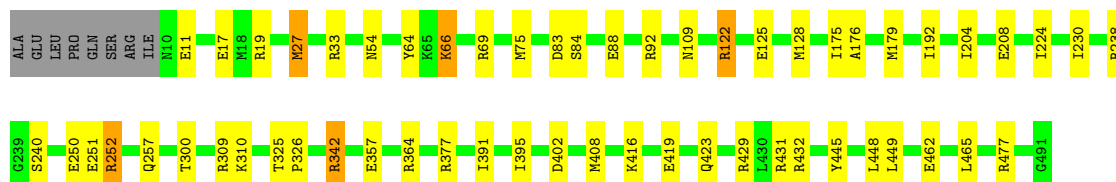
• Molecule 2: DNA gyrase subunit A

Chain L: 88% 10% .



• Molecule 2: DNA gyrase subunit A

Chain R: 87% 11% ..



• Molecule 2: DNA gyrase subunit A

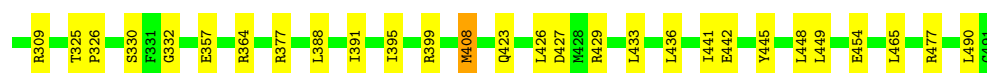
Chain T: 87% 10% ..



• Molecule 2: DNA gyrase subunit A

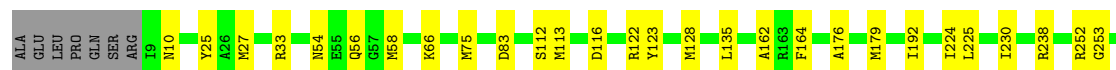
Chain a: 87% 11% .





- Molecule 2: DNA gyrase subunit A

Chain c: 87% 10%



- Molecule 2: DNA gyrase subunit A

Chain j: 87% 11%



- Molecule 2: DNA gyrase subunit A

Chain l: 88% 10%



- Molecule 2: DNA gyrase subunit A

Chain r: 86% 12%



- Molecule 2: DNA gyrase subunit A

Chain t: 87% 11%





- Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain D: 86% 13%



- Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain U: 87% 12%



- Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain m: 87% 12%



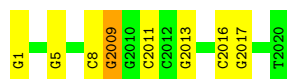
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain E: 45% 50% 5%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain F: 60% 35% 5%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain N: 55% 40% 5%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain O:  70% 30%



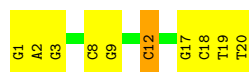
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain W:  35% 60% 5%

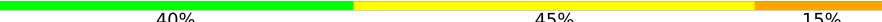


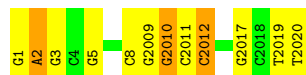
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain e:  50% 45% 5%



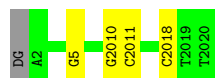
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain n:  40% 45% 15%



- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain v:  75% 20% 5%



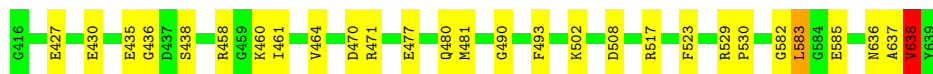
- Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain w:  50% 40% 10%



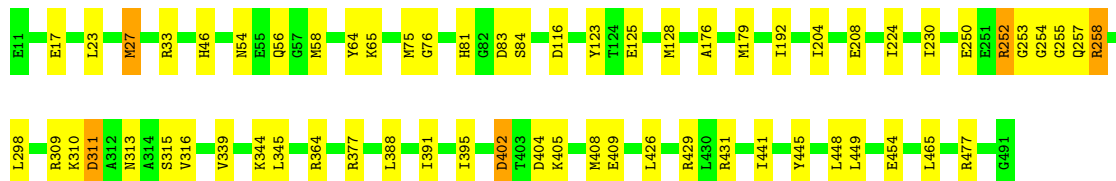
- Molecule 5: DNA gyrase subunit B,DNA gyrase subunit B

Chain K:  85% 14% ..



- Molecule 6: DNA gyrase subunit A

Chain J:  87% 12% .



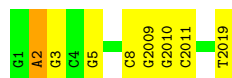
- Molecule 7: DNA gyrase subunit B,DNA gyrase subunit B

Chain M:  87% 13%



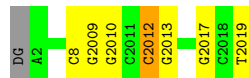
- Molecule 8: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain V:  58% 37% 5%



- Molecule 8: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain o:  58% 32% 5% 5%



- Molecule 9: DNA gyrase subunit B,DNA gyrase subunit B

Chain d:  86% 13% .



- Molecule 10: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain f:  71% 24% 6%



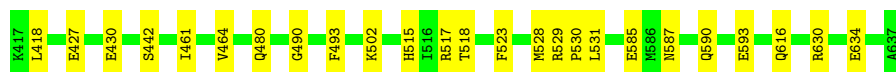
- Molecule 11: DNA gyrase subunit B,DNA gyrase subunit B

Chain k:  88% 11% .



- Molecule 12: DNA gyrase subunit B,DNA gyrase subunit B

Chain u:  87% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	187.64Å 410.12Å 93.94Å 90.00° 120.22° 90.00°	Depositor
Resolution (Å)	162.15 – 3.40 162.15 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.3 (162.15-3.40) 80.3 (162.15-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.208 0.179 , 0.208	Depositor DCC
R_{free} test set	6799 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 10.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.420 for -h-2*1,-k,l	Xtriage
Reported twinning fraction	0.525 for H, K, L 0.475 for -H-4/2L, -K, L	Depositor
Outliers	0 of 135780 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	68236	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.68% 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: JK8

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	B	1.08	1/1461 (0.1%)	1.54	1/1975 (0.1%)
1	S	1.09	0/1458	1.55	4/1971 (0.2%)
1	b	1.09	0/1450	1.54	2/1962 (0.1%)
1	s	1.08	0/1454	1.54	1/1966 (0.1%)
2	A	1.06	0/3896	1.49	4/5260 (0.1%)
2	C	1.03	0/3831	1.49	1/5179 (0.0%)
2	L	1.04	0/3833	1.50	2/5180 (0.0%)
2	R	1.06	0/3881	1.50	6/5241 (0.1%)
2	T	1.07	0/3844	1.51	3/5194 (0.1%)
2	a	1.04	0/3852	1.50	2/5206 (0.0%)
2	c	1.04	0/3835	1.49	1/5185 (0.0%)
2	j	1.06	1/3899 (0.0%)	1.51	5/5264 (0.1%)
2	l	1.03	0/3832	1.50	2/5177 (0.0%)
2	r	1.05	0/3921	1.50	7/5296 (0.1%)
2	t	1.05	1/3860 (0.0%)	1.48	0/5215
3	D	1.08	0/1469	1.53	0/1990
3	U	1.08	0/1486	1.54	3/2013 (0.1%)
3	m	1.07	0/1465	1.55	0/1985
4	E	0.50	0/511	0.86	2/789 (0.3%)
4	F	0.55	0/438	1.14	4/673 (0.6%)
4	N	0.52	0/510	0.95	4/785 (0.5%)
4	O	0.64	1/439 (0.2%)	0.96	2/677 (0.3%)
4	W	0.52	0/456	0.97	1/700 (0.1%)
4	e	0.57	0/439	1.06	3/677 (0.4%)
4	n	0.56	0/465	1.11	3/712 (0.4%)
4	v	0.46	0/443	0.95	2/677 (0.3%)
4	w	0.66	0/447	1.13	5/686 (0.7%)
5	K	1.10	0/1459	1.55	3/1974 (0.2%)
6	J	1.05	1/3912 (0.0%)	1.50	5/5278 (0.1%)
7	M	1.09	0/1491	1.54	1/2020 (0.0%)
8	V	0.54	0/434	1.10	2/666 (0.3%)
8	o	0.58	0/412	0.93	1/631 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	d	1.07	0/1416	1.55	1/1918 (0.1%)
10	f	0.57	1/389 (0.3%)	1.08	3/598 (0.5%)
11	k	1.09	0/1474	1.52	0/1994
12	u	1.09	0/1483	1.52	2/2007 (0.1%)
All	All	1.03	6/69345 (0.0%)	1.47	88/94721 (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
2	A	0	1
2	C	0	2
2	L	0	1
2	T	0	1
2	a	0	1
2	c	0	1
2	l	0	1
2	r	0	1
2	t	0	1
6	J	0	1
All	All	0	11

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	46	HIS	CE1-NE2	6.71	1.39	1.32
4	O	8	DC	O3'-P	6.48	1.70	1.61
1	B	471	ARG	CZ-NH2	6.15	1.41	1.33
2	t	46	HIS	CE1-NE2	5.75	1.38	1.32
2	j	11	GLU	C-O	5.57	1.31	1.24

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	2	DA	C4'-C3'-O3'	10.93	126.40	110.00
10	f	8	DC	C4'-C3'-O3'	10.57	125.85	110.00
4	F	2011	DC	O5'-P-OP2	-10.30	77.08	108.00
6	J	258	ARG	CG-CD-NE	9.52	132.95	112.00
4	F	2009	DG	O5'-C5'-C4'	9.40	124.90	110.80

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	311	ASP	Peptide
2	C	311	ASP	Peptide
2	C	9	ILE	Peptide
6	J	311	ASP	Mainchain
2	L	311	ASP	Peptide

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	B	1441	0	1381	26	0
1	S	1439	0	1374	18	0
1	b	1430	0	1354	13	0
1	s	1434	0	1372	14	0
2	A	3846	0	3780	88	0
2	C	3784	0	3713	47	1
2	L	3785	0	3731	38	0
2	R	3830	0	3769	47	1
2	T	3793	0	3740	53	0
2	a	3802	0	3718	52	0
2	c	3784	0	3717	46	1
2	j	3848	0	3786	52	0
2	l	3784	0	3744	43	0
2	r	3870	0	3787	47	1
2	t	3809	0	3753	41	0
3	D	1447	0	1376	23	0
3	U	1463	0	1388	16	0
3	m	1442	0	1376	18	0
4	E	455	0	247	34	0
4	F	392	0	214	7	0
4	N	455	0	248	20	0
4	O	392	0	213	5	0
4	W	408	0	227	21	0
4	e	392	0	210	20	0
4	n	418	0	226	18	0
4	v	399	0	214	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	w	400	0	222	6	0
5	K	1439	0	1367	16	0
6	J	3862	0	3802	60	0
7	M	1468	0	1390	16	0
8	V	388	0	215	17	0
8	o	369	0	203	9	0
9	d	1395	0	1326	27	0
10	f	348	0	191	9	0
11	k	1453	0	1393	19	0
12	u	1460	0	1390	19	0
13	A	26	0	0	0	0
13	C	26	0	0	2	0
13	J	26	0	0	4	0
13	L	26	0	0	2	0
13	R	26	0	0	3	0
13	U	26	0	0	3	0
13	b	26	0	0	1	0
13	d	26	0	0	2	0
13	k	26	0	0	2	0
13	l	26	0	0	2	0
13	s	26	0	0	1	0
13	t	26	0	0	5	0
All	All	68236	0	64157	809	2

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.

The worst 5 of 809 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)
7:M:581:LYS:CB	7:M:585:GLU:OE1	1.82	1.27
9:d:629:ARG:NH2	4:e:17:DG:OP1	1.65	1.26
4:E:1[A]:DG:O5'	4:E:1[A]:DG:C8	1.80	1.23
4:E:1[A]:DG:O5'	4:E:1[A]:DG:H8	1.12	1.22
2:A:58[B]:MET:HE2	2:A:58[B]:MET:HA	1.22	1.20

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:489:GLN:NE2	2:R:251:GLU:OE2[2_546]	1.63	0.57
2:c:315:SER:OG	2:r:257:GLN:NE2[2_444]	2.03	0.17

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	B	186/186 (100%)	176 (95%)	10 (5%)	0	100	100
1	S	185/186 (100%)	177 (96%)	8 (4%)	0	100	100
1	b	186/186 (100%)	177 (95%)	9 (5%)	0	100	100
1	s	186/186 (100%)	177 (95%)	9 (5%)	0	100	100
2	A	488/490 (100%)	471 (96%)	16 (3%)	1 (0%)	43	71
2	C	488/490 (100%)	470 (96%)	17 (4%)	1 (0%)	43	71
2	L	485/490 (99%)	467 (96%)	17 (4%)	1 (0%)	43	71
2	R	491/490 (100%)	473 (96%)	17 (4%)	1 (0%)	43	71
2	T	487/490 (99%)	470 (96%)	16 (3%)	1 (0%)	43	71
2	a	491/490 (100%)	472 (96%)	18 (4%)	1 (0%)	43	71
2	c	488/490 (100%)	470 (96%)	17 (4%)	1 (0%)	43	71
2	j	493/490 (101%)	475 (96%)	17 (3%)	1 (0%)	43	71
2	l	485/490 (99%)	467 (96%)	17 (4%)	1 (0%)	43	71
2	r	497/490 (101%)	476 (96%)	19 (4%)	2 (0%)	30	59
2	t	489/490 (100%)	472 (96%)	16 (3%)	1 (0%)	43	71
3	D	188/188 (100%)	180 (96%)	8 (4%)	0	100	100
3	U	189/188 (100%)	180 (95%)	9 (5%)	0	100	100
3	m	187/188 (100%)	178 (95%)	9 (5%)	0	100	100
5	K	187/187 (100%)	176 (94%)	10 (5%)	1 (0%)	24	54
6	J	491/480 (102%)	472 (96%)	17 (4%)	2 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	190/189 (100%)	182 (96%)	8 (4%)	0	100	100
9	d	179/181 (99%)	170 (95%)	9 (5%)	0	100	100
11	k	188/188 (100%)	177 (94%)	9 (5%)	2 (1%)	11	38
12	u	188/187 (100%)	180 (96%)	8 (4%)	0	100	100
All	All	8112/8110 (100%)	7785 (96%)	310 (4%)	17 (0%)	43	71

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	638	VAL
6	J	254	GLY
11	k	638	VAL
2	r	11	GLU
11	k	417	LYS

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	B	147/155 (95%)	145 (99%)	2 (1%)	59	70
1	S	148/155 (96%)	142 (96%)	6 (4%)	27	52
1	b	145/155 (94%)	143 (99%)	2 (1%)	59	70
1	s	146/155 (94%)	144 (99%)	2 (1%)	59	70
2	A	405/423 (96%)	394 (97%)	11 (3%)	39	60
2	C	394/423 (93%)	389 (99%)	5 (1%)	61	71
2	L	397/423 (94%)	391 (98%)	6 (2%)	57	69
2	R	402/423 (95%)	390 (97%)	12 (3%)	36	59
2	T	397/423 (94%)	384 (97%)	13 (3%)	33	57
2	a	395/423 (93%)	388 (98%)	7 (2%)	51	67
2	c	394/423 (93%)	388 (98%)	6 (2%)	57	69
2	j	403/423 (95%)	392 (97%)	11 (3%)	39	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	l	397/423 (94%)	388 (98%)	9 (2%)	44	63
2	r	403/423 (95%)	392 (97%)	11 (3%)	39	60
2	t	398/423 (94%)	392 (98%)	6 (2%)	57	69
3	D	147/157 (94%)	140 (95%)	7 (5%)	23	50
3	U	149/157 (95%)	143 (96%)	6 (4%)	28	53
3	m	146/157 (93%)	139 (95%)	7 (5%)	23	50
5	K	147/156 (94%)	141 (96%)	6 (4%)	27	52
6	J	406/414 (98%)	399 (98%)	7 (2%)	53	67
7	M	149/158 (94%)	143 (96%)	6 (4%)	28	53
9	d	141/152 (93%)	134 (95%)	7 (5%)	22	49
11	k	148/156 (95%)	146 (99%)	2 (1%)	59	70
12	u	149/156 (96%)	145 (97%)	4 (3%)	39	60
All	All	6553/6936 (94%)	6392 (98%)	161 (2%)	43	62

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	j	252	ARG
2	r	232[B]	ARG
2	j	364	ARG
2	l	238	ARG
2	r	440	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	l	390	HIS
2	l	467	GLN
2	t	10	ASN
2	L	257	GLN
2	L	10	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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$
13	JK8	b	701	-	29,29,29	1.36	5 (17%)	38,40,40	3.27	18 (47%)
13	JK8	J	501	-	29,29,29	1.39	4 (13%)	38,40,40	2.78	17 (44%)
13	JK8	L	501[A]	-	29,29,29	1.28	4 (13%)	38,40,40	2.42	12 (31%)
13	JK8	A	501	-	29,29,29	1.21	4 (13%)	38,40,40	1.70	6 (15%)
13	JK8	d	701[A]	-	29,29,29	1.23	4 (13%)	38,40,40	2.05	8 (21%)
13	JK8	s	701	-	29,29,29	1.53	4 (13%)	38,40,40	3.09	18 (47%)
13	JK8	k	701	-	29,29,29	1.42	5 (17%)	38,40,40	1.62	8 (21%)
13	JK8	t	501[A]	-	29,29,29	1.48	3 (10%)	38,40,40	2.28	13 (34%)
13	JK8	C	501[A]	-	29,29,29	1.26	4 (13%)	38,40,40	2.14	13 (34%)
13	JK8	U	701[A]	-	29,29,29	1.23	4 (13%)	38,40,40	2.18	8 (21%)
13	JK8	l	501[A]	-	29,29,29	1.51	5 (17%)	38,40,40	1.66	12 (31%)
13	JK8	R	501	-	29,29,29	1.21	3 (10%)	38,40,40	2.01	11 (28%)

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
13	JK8	b	701	-	-	1/14/14/14	0/4/4/4
13	JK8	J	501	-	-	5/14/14/14	0/4/4/4
13	JK8	L	501[A]	-	-	4/14/14/14	0/4/4/4
13	JK8	A	501	-	-	3/14/14/14	0/4/4/4
13	JK8	d	701[A]	-	-	5/14/14/14	0/4/4/4
13	JK8	s	701	-	-	3/14/14/14	0/4/4/4
13	JK8	k	701	-	-	2/14/14/14	0/4/4/4
13	JK8	t	501[A]	-	-	3/14/14/14	0/4/4/4
13	JK8	C	501[A]	-	-	5/14/14/14	0/4/4/4
13	JK8	U	701[A]	-	-	3/14/14/14	0/4/4/4
13	JK8	l	501[A]	-	-	3/14/14/14	0/4/4/4
13	JK8	R	501	-	-	4/14/14/14	0/4/4/4

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	s	701	JK8	C14-C11	-4.31	1.41	1.49
13	t	501[A]	JK8	C14-C11	-4.24	1.41	1.49
13	b	701	JK8	O7-N6	-4.09	1.39	1.43
13	C	501[A]	JK8	O7-N6	-3.86	1.39	1.43
13	t	501[A]	JK8	O7-N6	-3.82	1.39	1.43

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	s	701	JK8	O4-C3-C2	9.48	118.11	106.02
13	b	701	JK8	O4-C5-C13	8.23	133.41	118.20
13	b	701	JK8	C3-O4-C5	-7.47	105.45	116.64
13	J	501	JK8	O4-C5-C13	7.29	131.67	118.20
13	b	701	JK8	C10-C11-C14	-7.00	109.31	120.91

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

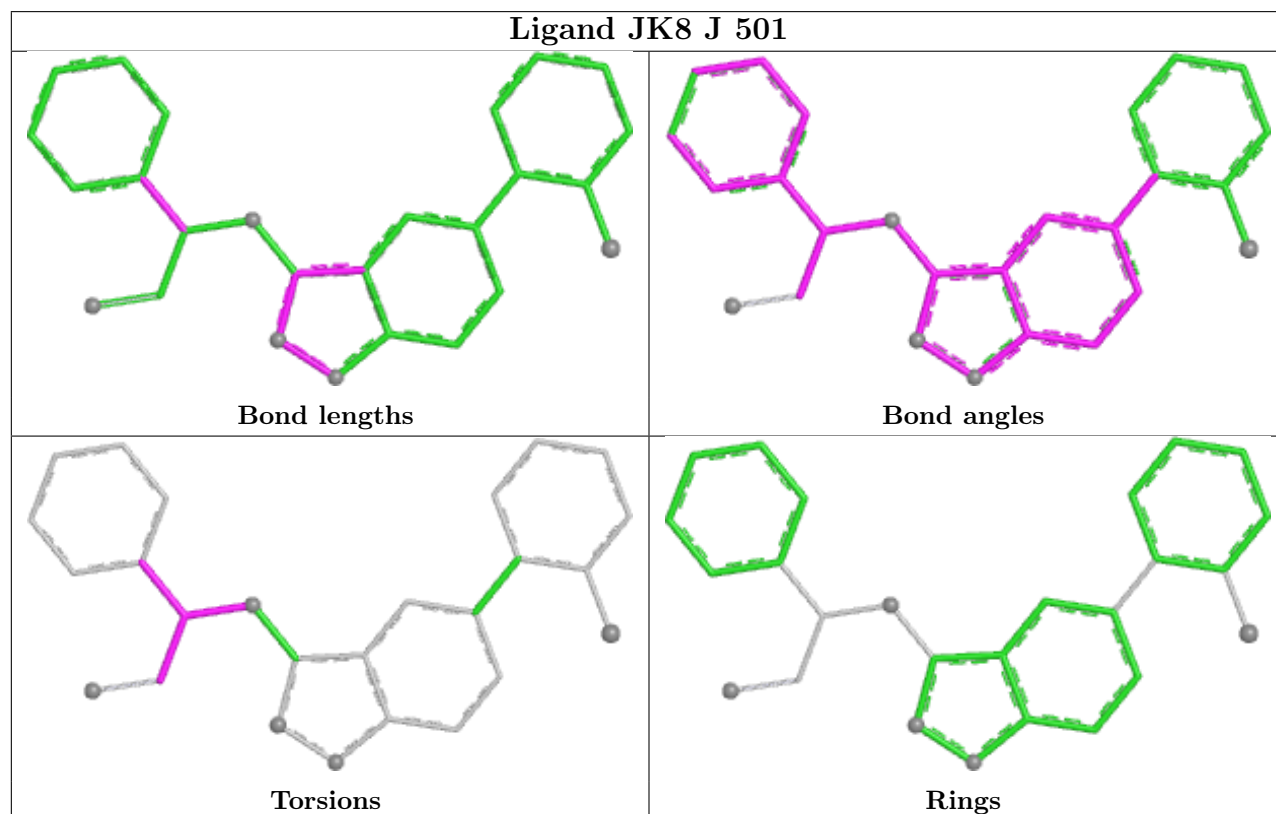
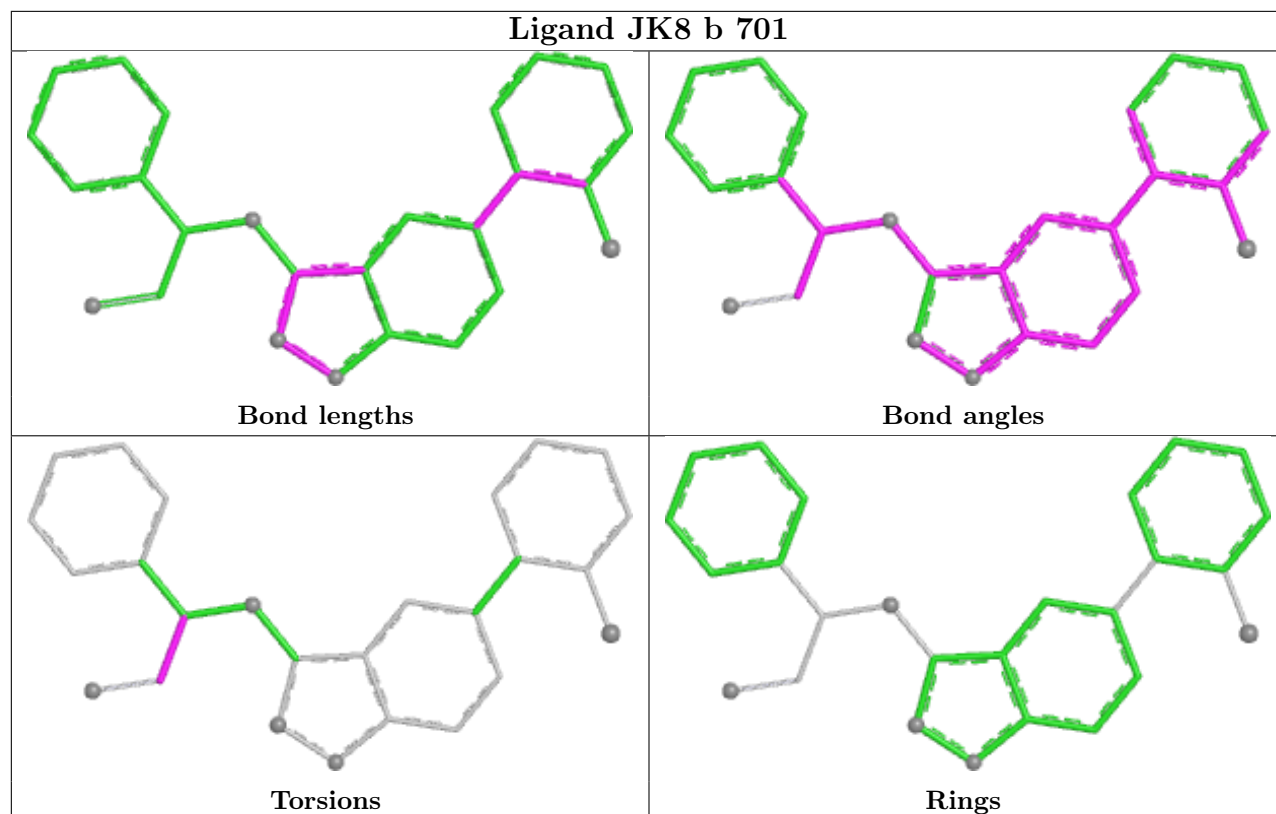
Mol	Chain	Res	Type	Atoms
13	A	501	JK8	N1-C2-C3-C21
13	A	501	JK8	N1-C2-C3-O4
13	A	501	JK8	C21-C3-O4-C5
13	C	501[A]	JK8	C22-C21-C3-C2
13	C	501[A]	JK8	C26-C21-C3-C2

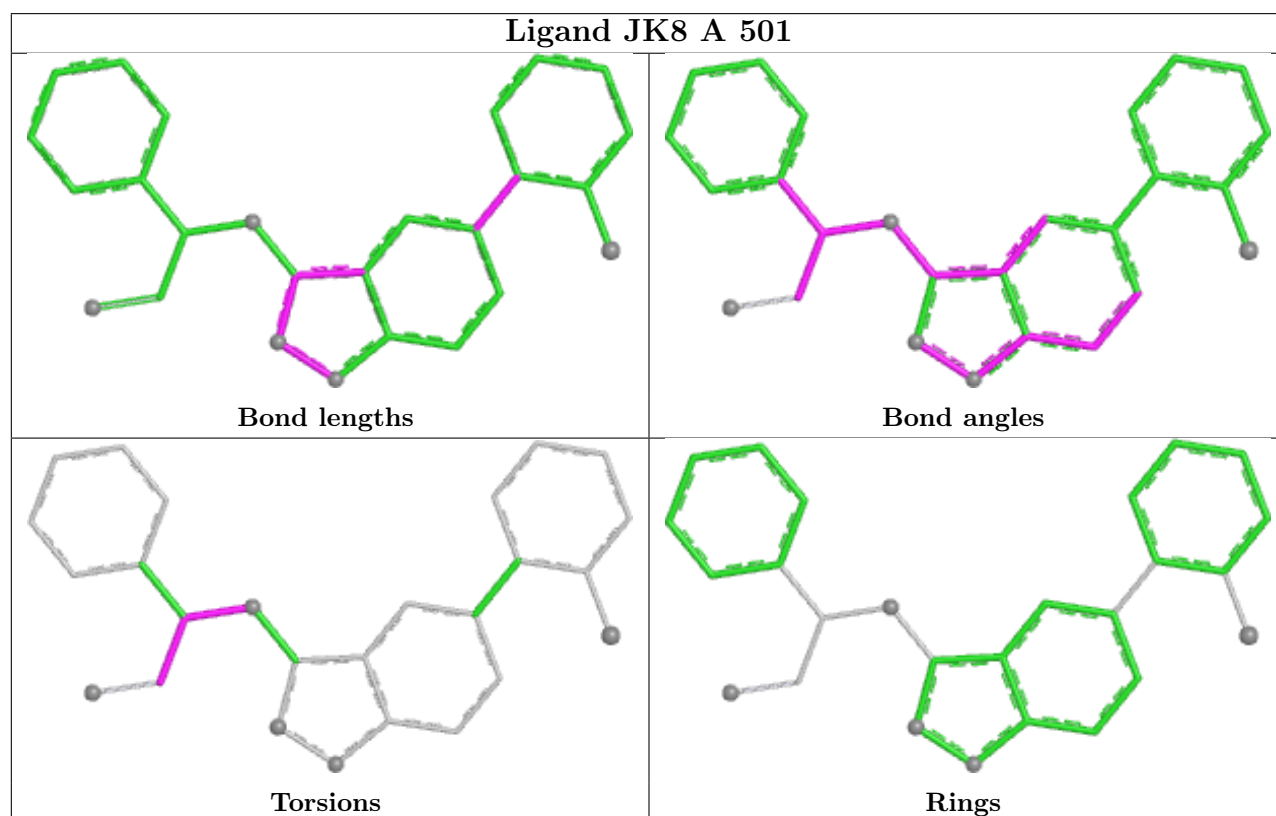
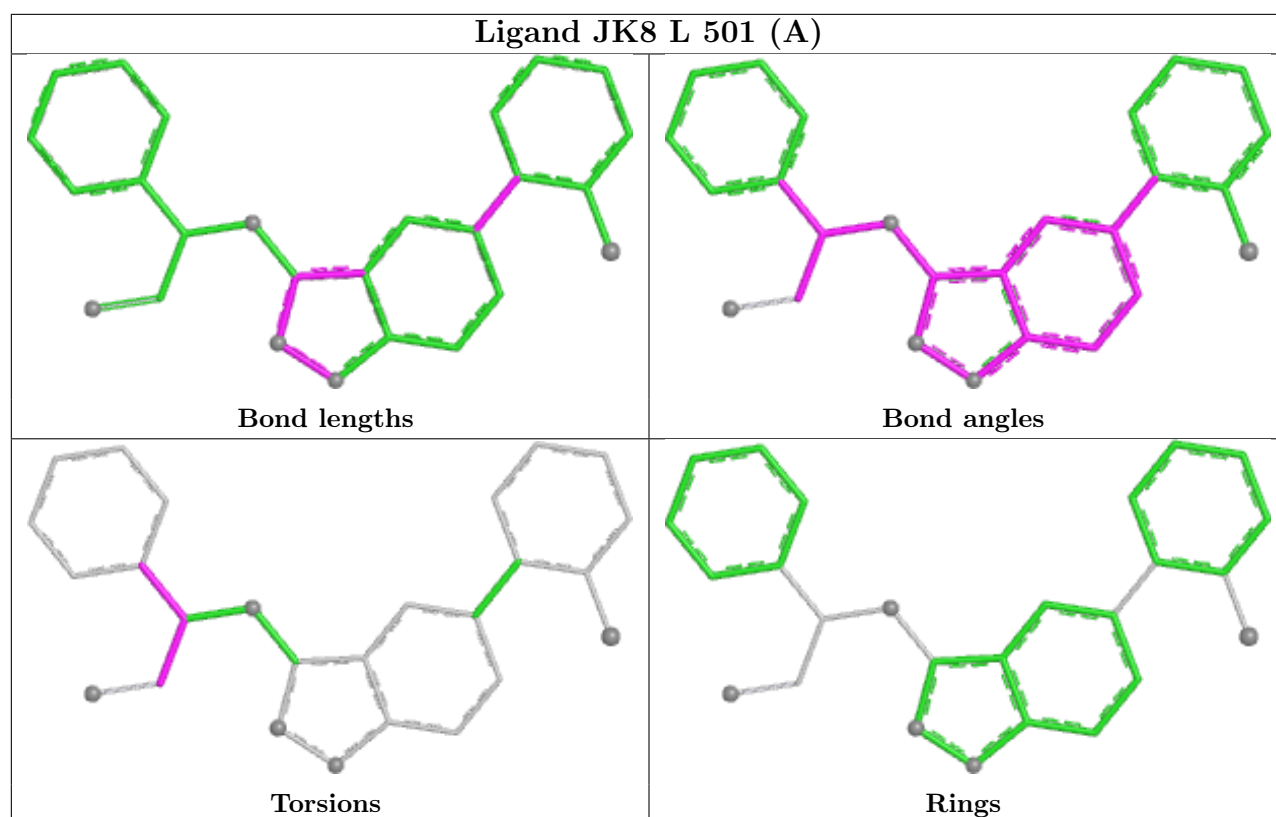
There are no ring outliers.

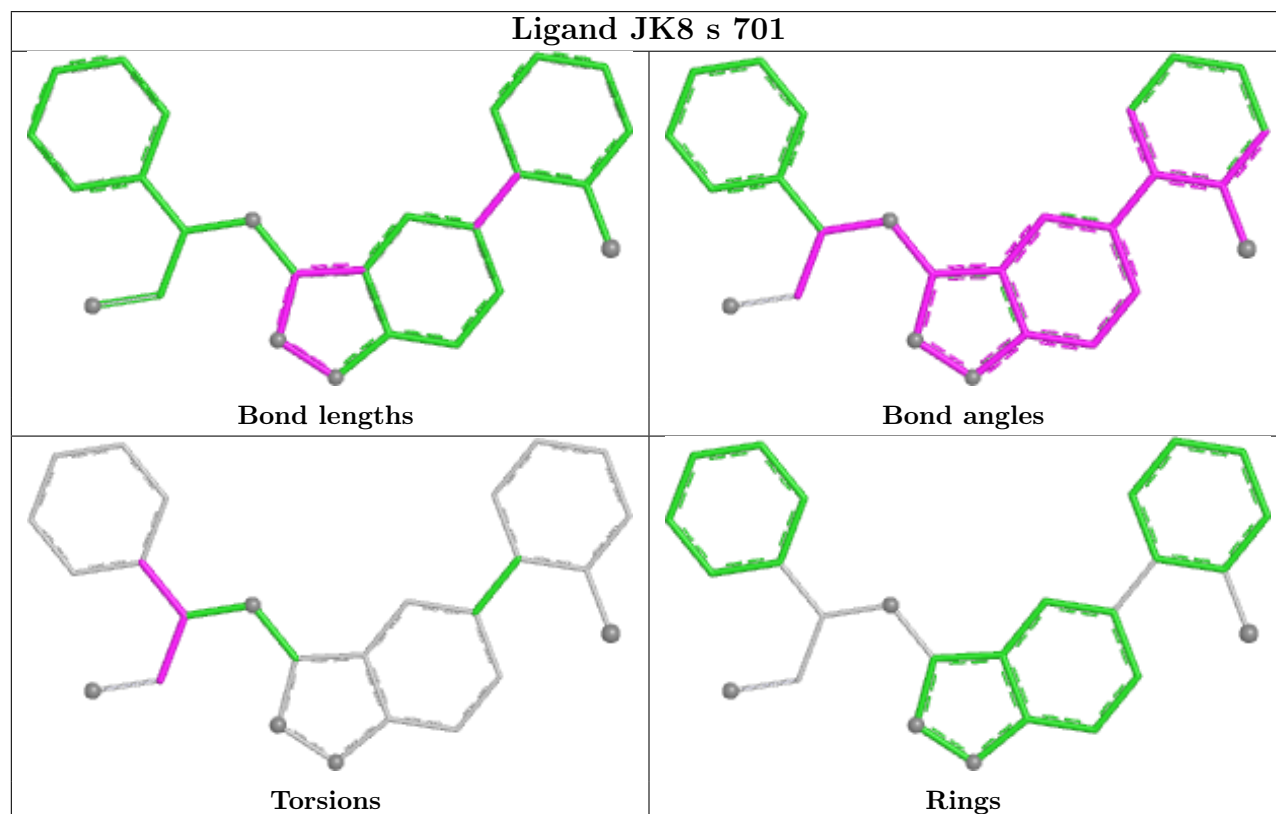
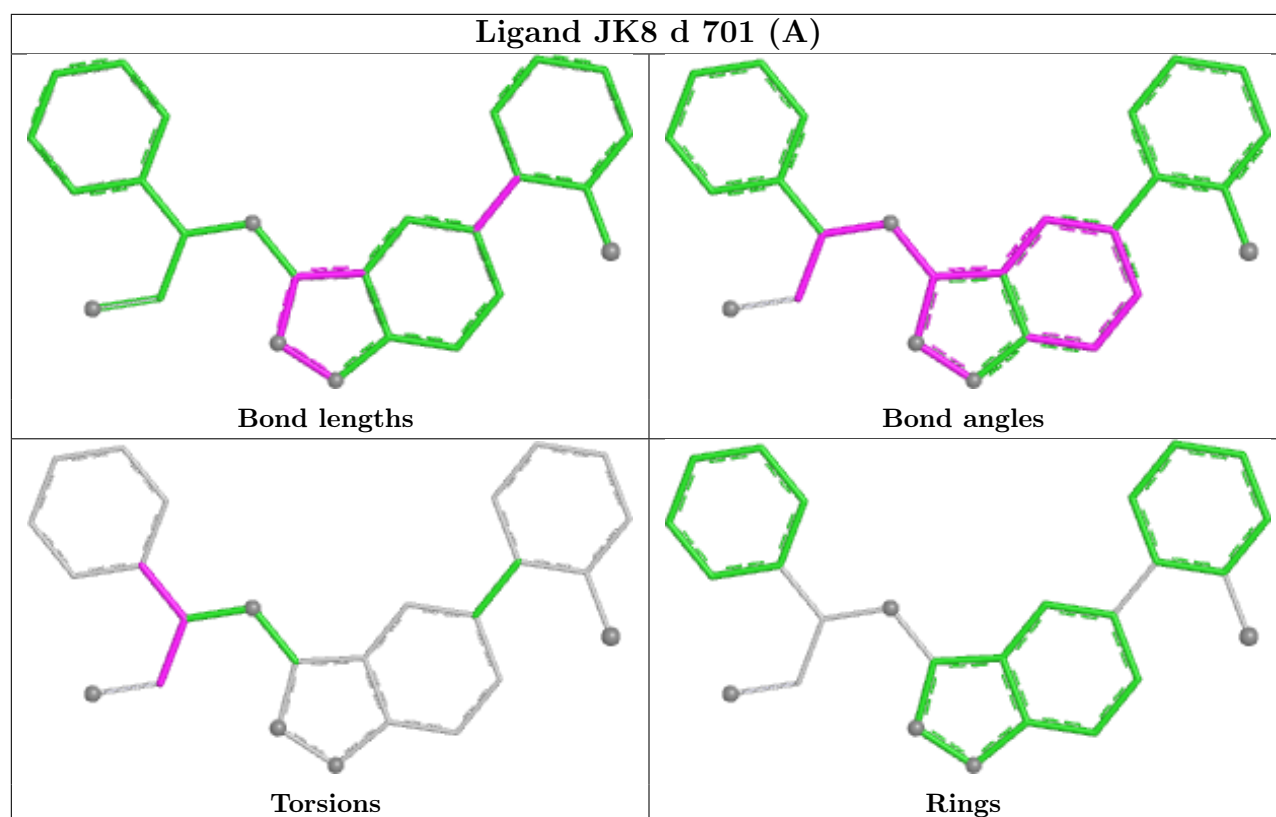
11 monomers are involved in 27 short contacts:

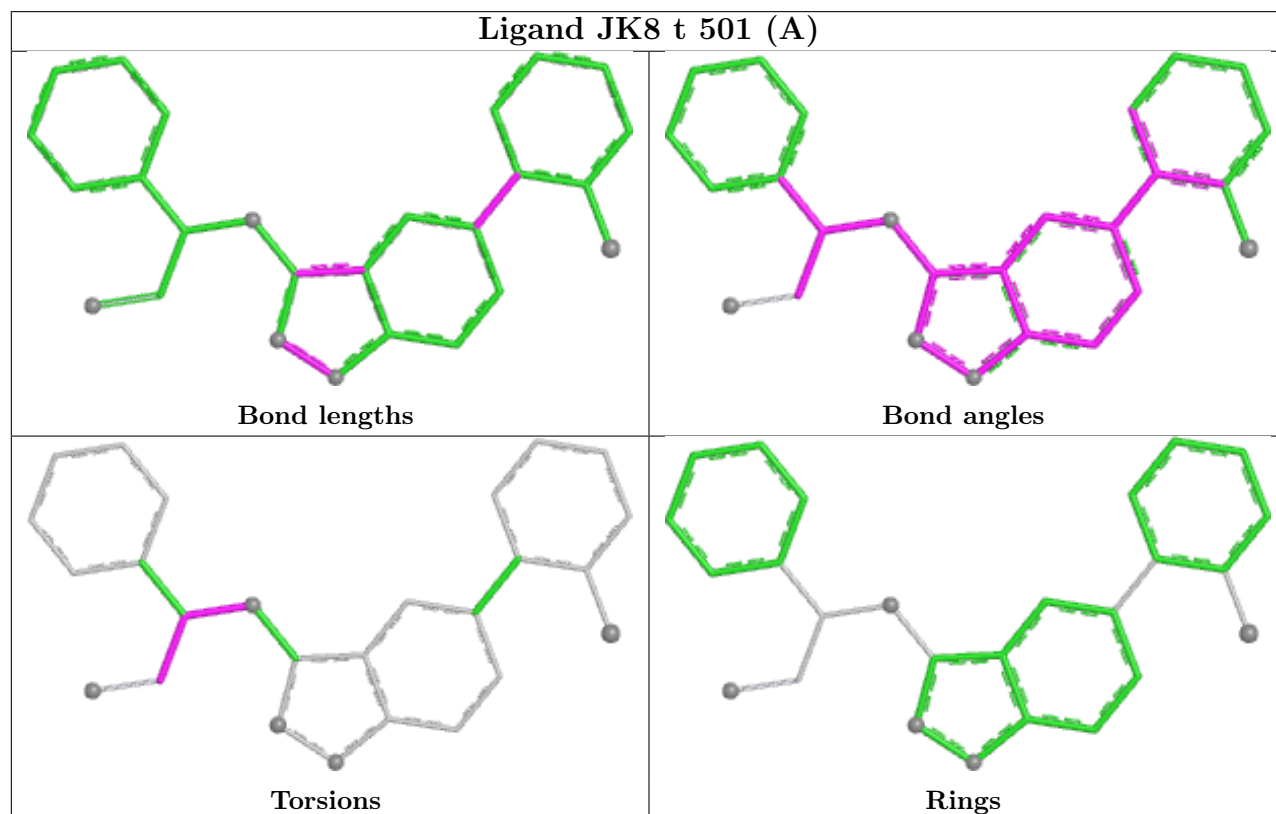
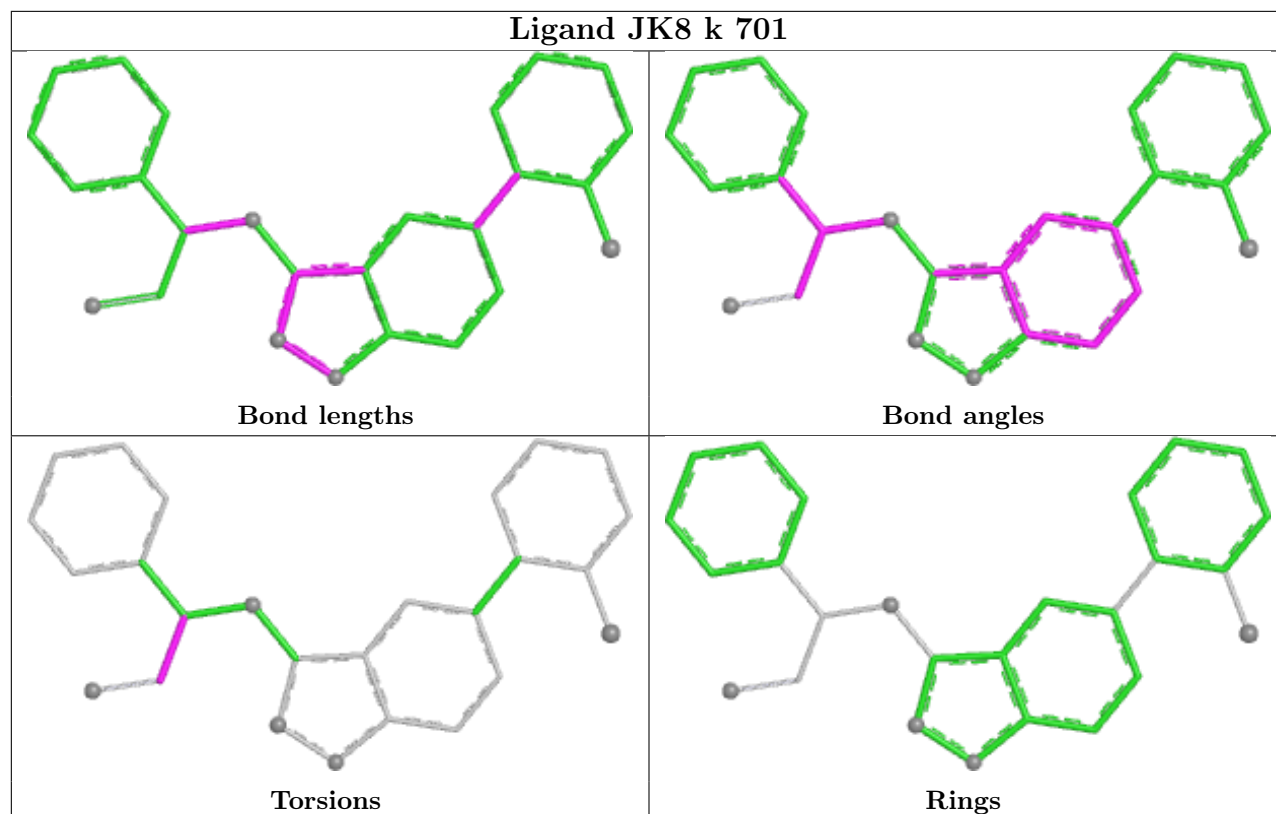
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	b	701	JK8	1	0
13	J	501	JK8	4	0
13	L	501[A]	JK8	2	0
13	d	701[A]	JK8	2	0
13	s	701	JK8	1	0
13	k	701	JK8	2	0
13	t	501[A]	JK8	5	0
13	C	501[A]	JK8	2	0
13	U	701[A]	JK8	3	0
13	l	501[A]	JK8	2	0
13	R	501	JK8	3	0

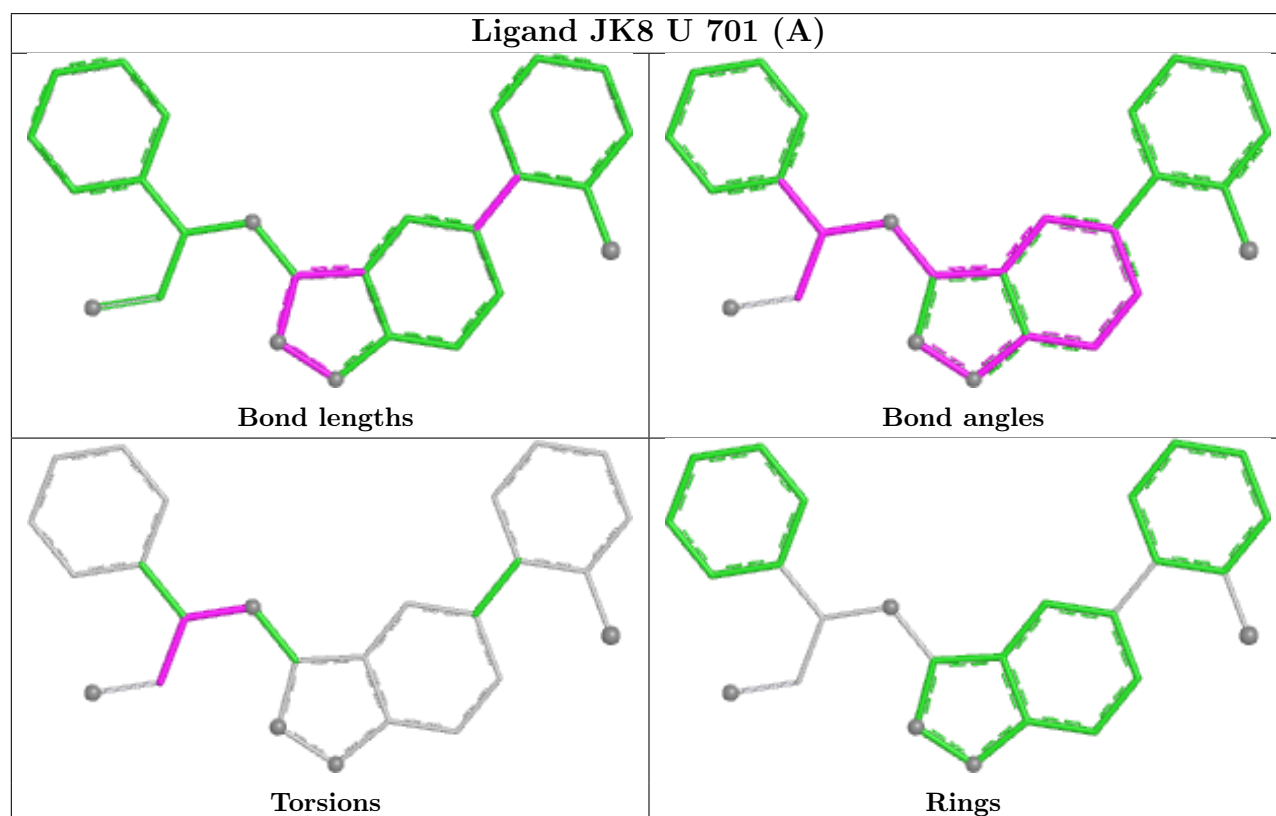
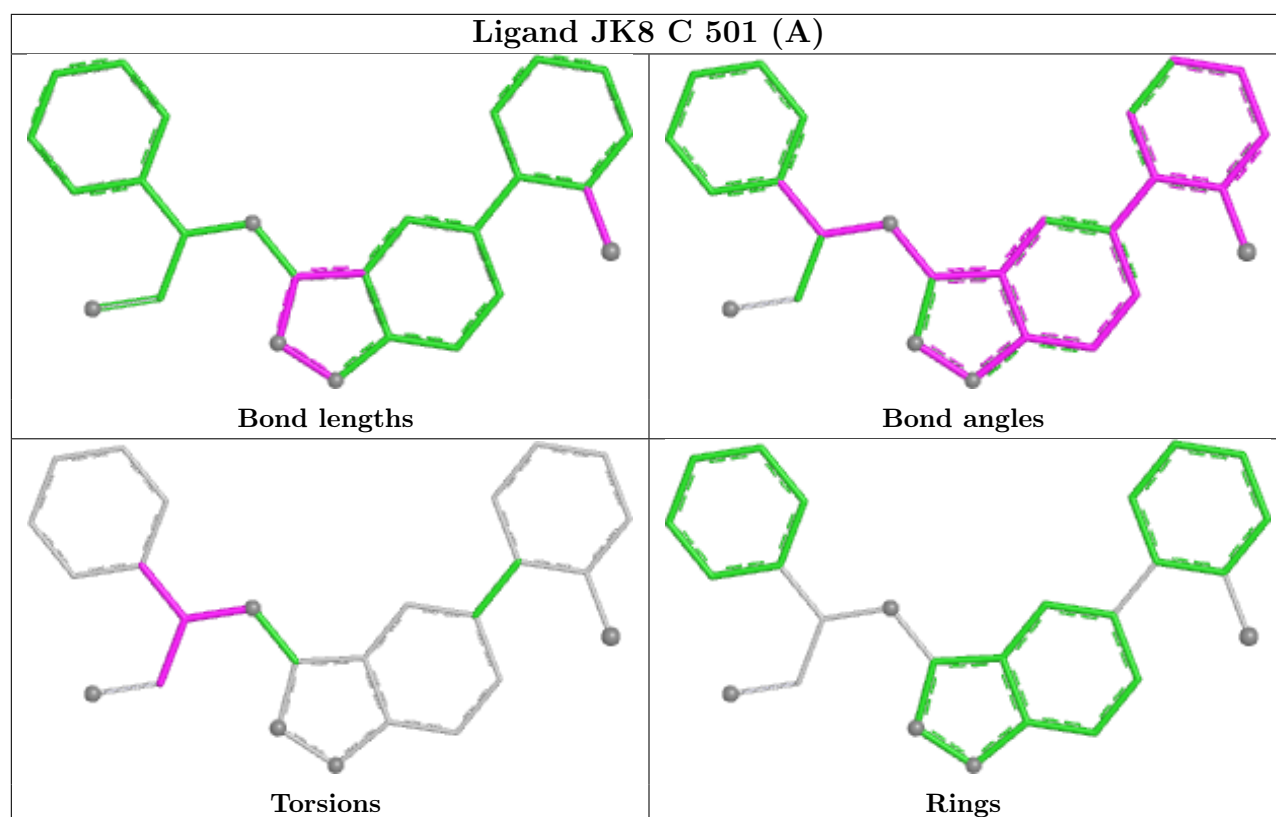
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

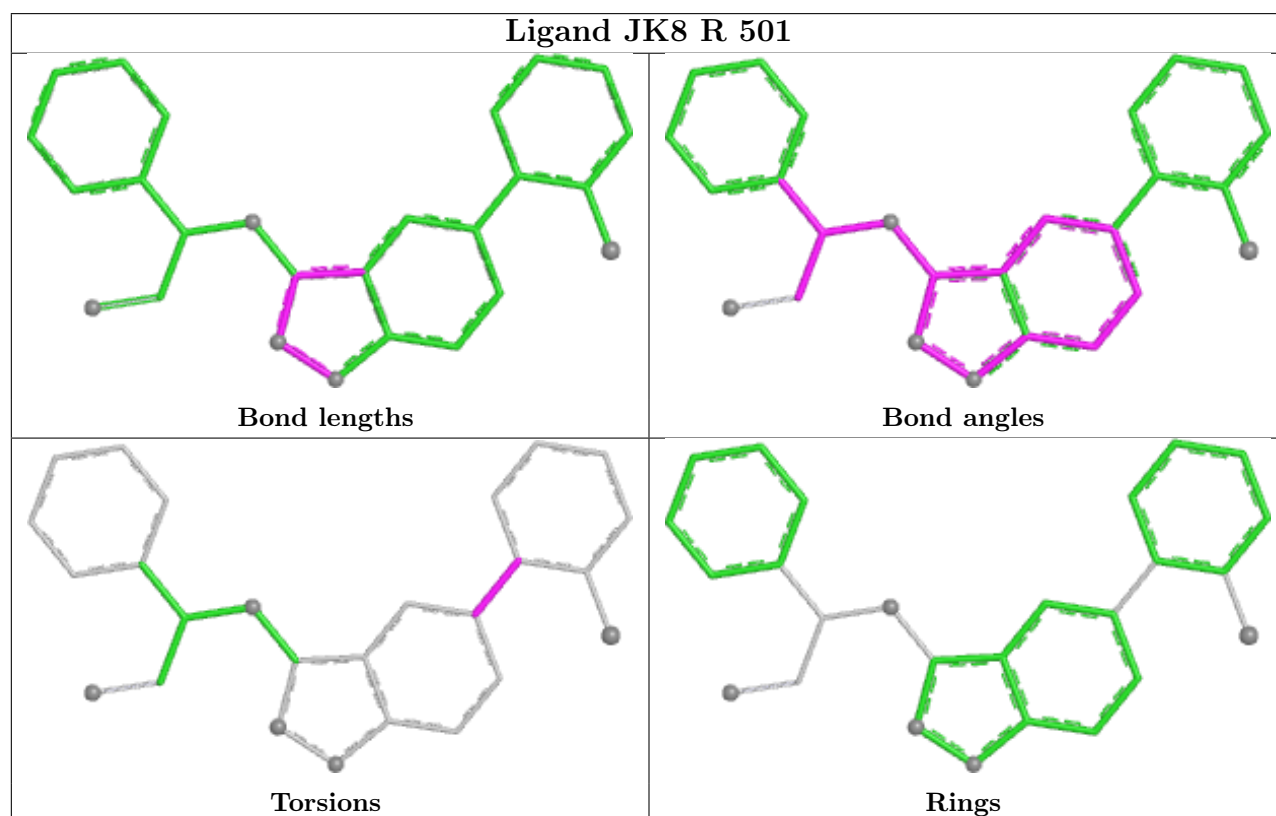
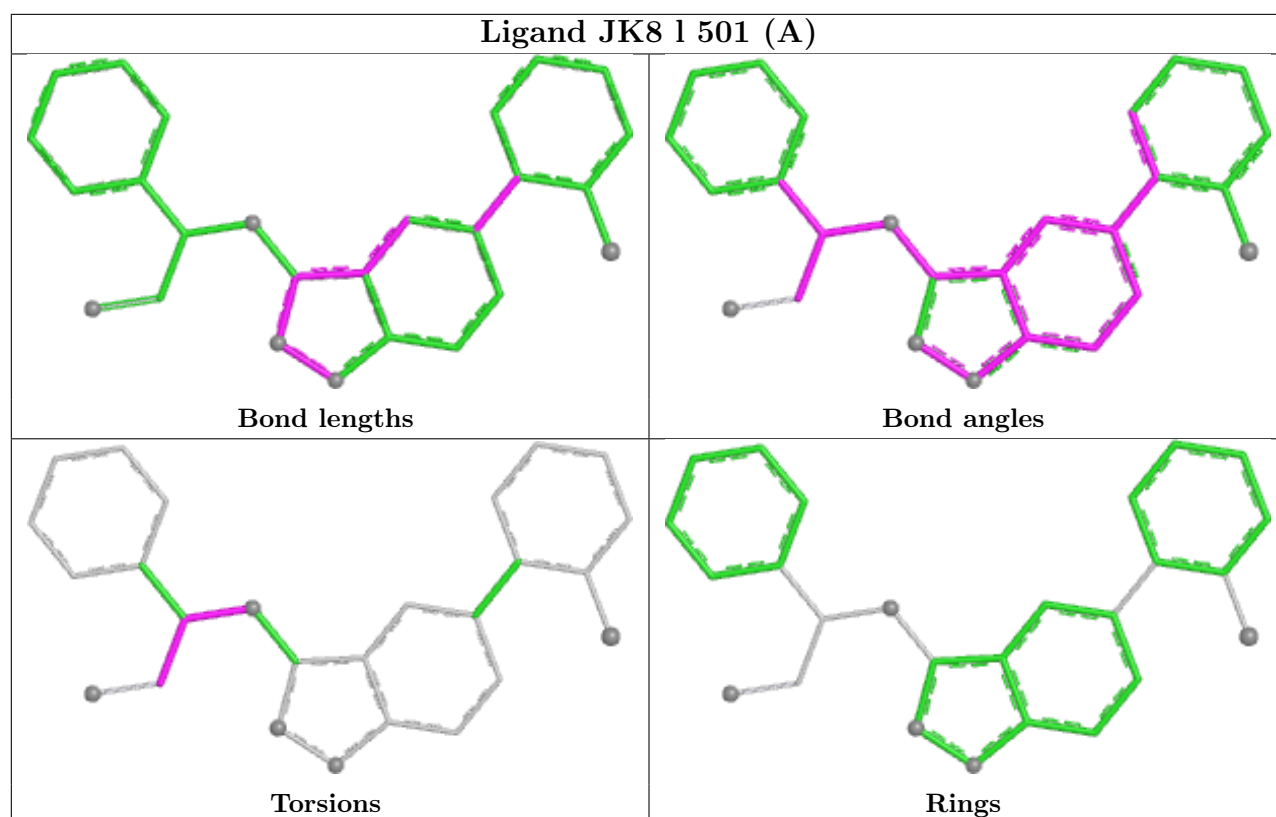












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
9	d	1
1	S	1
1	s	1
1	b	1
11	k	1
5	K	1
6	J	1
8	V	1
4	W	1
4	N	1
4	n	1
4	v	1
4	F	1
4	w	1
8	o	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	543:PRO	C	581:LYS	N	8.39
1	d	545:GLY	C	586:MET	N	8.19
1	S	543:PRO	C	581:LYS	N	7.73
1	s	543:PRO	C	581:LYS	N	7.36
1	b	543:PRO	C	581:LYS	N	7.01

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	B	185/186 (99%)	-1.23	0 100 100	39, 91, 124, 173	5 (2%)
1	S	185/186 (99%)	-1.45	0 100 100	26, 60, 84, 112	5 (2%)
1	b	185/186 (99%)	-1.34	0 100 100	36, 79, 114, 134	5 (2%)
1	s	186/186 (100%)	-1.41	0 100 100	30, 62, 95, 112	4 (2%)
2	A	479/490 (97%)	-1.36	0 100 100	25, 74, 105, 175	13 (2%)
2	C	482/490 (98%)	-1.44	0 100 100	24, 61, 90, 123	8 (1%)
2	L	481/490 (98%)	-1.53	0 100 100	16, 45, 73, 110	6 (1%)
2	R	482/490 (98%)	-1.56	0 100 100	16, 45, 70, 92	11 (2%)
2	T	481/490 (98%)	-1.54	0 100 100	13, 43, 67, 97	8 (1%)
2	a	481/490 (98%)	-1.42	0 100 100	25, 62, 89, 113	12 (2%)
2	c	482/490 (98%)	-1.43	0 100 100	24, 63, 100, 143	8 (1%)
2	j	482/490 (98%)	-1.51	0 100 100	16, 46, 73, 122	13 (2%)
2	l	481/490 (98%)	-1.52	0 100 100	21, 46, 78, 132	6 (1%)
2	r	484/490 (98%)	-1.52	0 100 100	14, 44, 74, 105	15 (3%)
2	t	481/490 (98%)	-1.53	0 100 100	14, 44, 77, 125	10 (2%)
3	D	188/188 (100%)	-1.35	0 100 100	33, 83, 117, 148	2 (1%)
3	U	188/188 (100%)	-1.35	0 100 100	34, 67, 94, 138	3 (1%)
3	m	188/188 (100%)	-1.32	0 100 100	34, 68, 109, 154	1 (0%)
4	E	20/20 (100%)	-1.44	0 100 100	34, 59, 112, 130	3 (15%)
4	F	20/20 (100%)	-1.56	0 100 100	32, 70, 103, 148	0
4	N	20/20 (100%)	-1.70	0 100 100	25, 39, 59, 61	3 (15%)
4	O	20/20 (100%)	-1.73	0 100 100	31, 49, 78, 88	0
4	W	20/20 (100%)	-1.73	0 100 100	29, 48, 88, 116	0
4	e	20/20 (100%)	-1.51	0 100 100	47, 81, 112, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9		
4	n	20/20 (100%)	-1.52	0	100	100	24, 48, 96, 143	2 (10%)
4	v	19/20 (95%)	-1.63	0	100	100	21, 38, 77, 95	2 (10%)
4	w	20/20 (100%)	-1.77	0	100	100	36, 42, 67, 81	0
5	K	187/187 (100%)	-1.45	0	100	100	22, 53, 88, 113	4 (2%)
6	J	480/480 (100%)	-1.49	0	100	100	17, 47, 76, 105	15 (3%)
7	M	189/189 (100%)	-1.42	0	100	100	30, 68, 96, 112	3 (1%)
8	V	19/19 (100%)	-1.53	0	100	100	27, 50, 95, 123	0
8	o	18/19 (94%)	-1.61	0	100	100	31, 43, 91, 98	0
9	d	181/181 (100%)	-1.22	0	100	100	38, 95, 125, 150	2 (1%)
10	f	17/17 (100%)	-1.53	0	100	100	63, 79, 110, 113	0
11	k	188/188 (100%)	-1.36	0	100	100	27, 60, 98, 136	4 (2%)
12	u	187/187 (100%)	-1.43	0	100	100	27, 60, 88, 151	3 (1%)
All	All	8246/8345 (98%)	-1.46	0	100	100	13, 56, 99, 175	176 (2%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
13	JK8	A	501	26/26	0.99	0.05	26,33,47,52	26
13	JK8	C	501[A]	26/26	0.99	0.03	42,63,68,68	0
13	JK8	J	501	26/26	0.99	0.04	33,46,54,57	0

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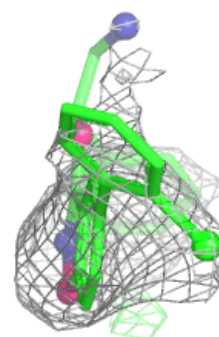
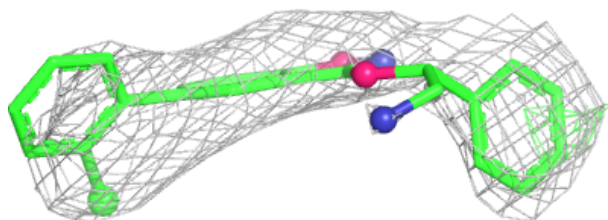
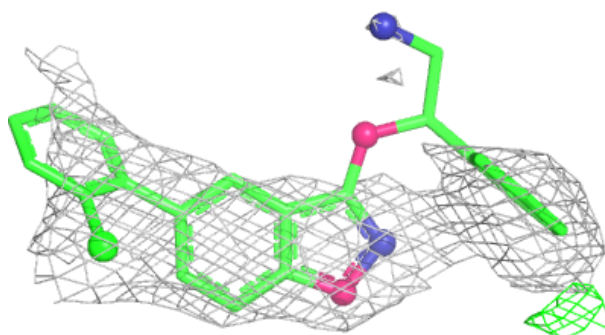
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	JK8	L	501[A]	26/26	0.99	0.04	20,21,29,30	26
13	JK8	R	501	26/26	0.99	0.05	16,17,18,22	26
13	JK8	U	701[A]	26/26	0.99	0.08	7,9,11,11	26
13	JK8	b	701	26/26	0.99	0.10	7,9,9,10	26
13	JK8	d	701[A]	26/26	0.99	0.05	34,42,60,61	26
13	JK8	k	701	26/26	0.99	0.04	36,47,69,71	0
13	JK8	l	501[A]	26/26	0.99	0.03	45,58,69,72	0
13	JK8	s	701	26/26	0.99	0.05	11,13,18,19	26
13	JK8	t	501[A]	26/26	1.00	0.04	26,31,33,43	26

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.

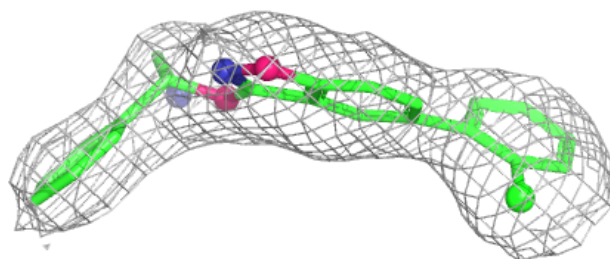
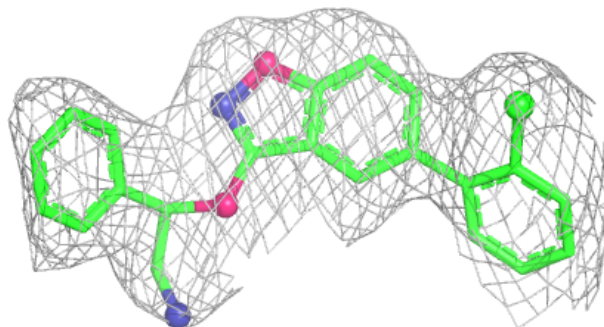
Electron density around JK8 A 501:

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

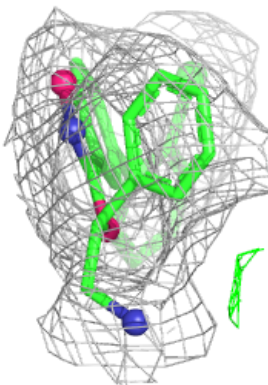
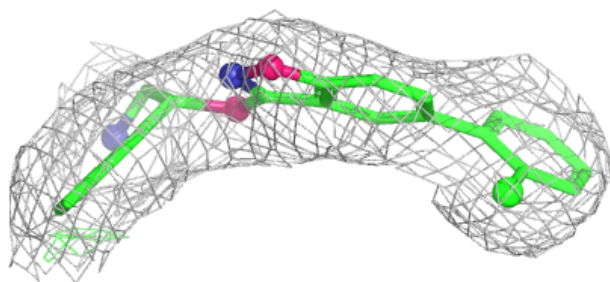
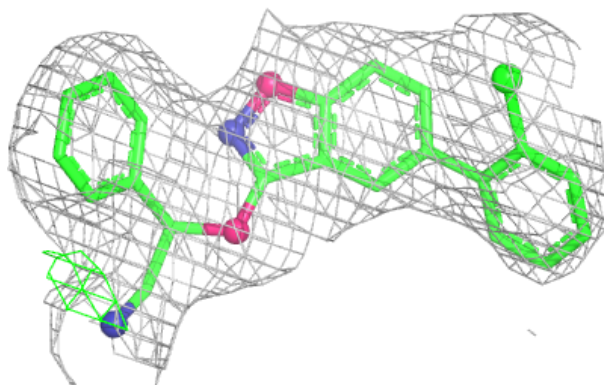


Electron density around JK8 C 501 (A):

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

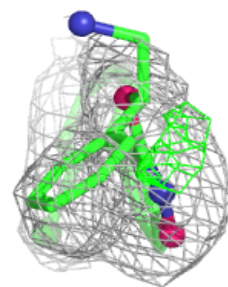
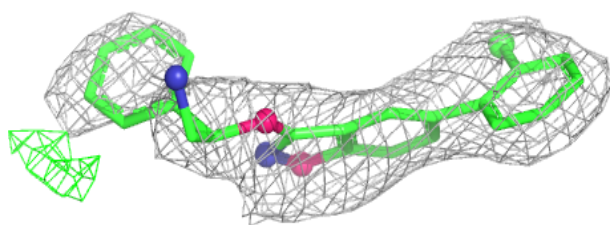
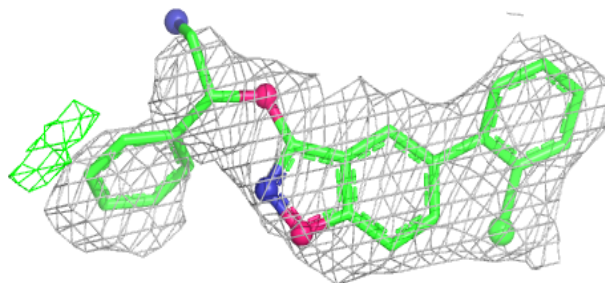
**Electron density around JK8 J 501:**

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and green (positive)

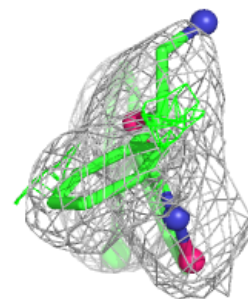
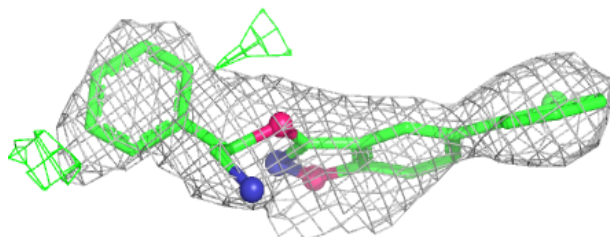
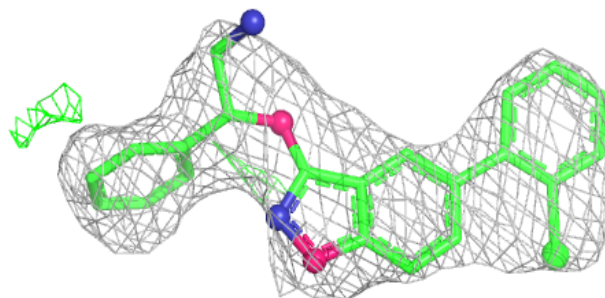


Electron density around JK8 L 501 (A):

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and green (positive)

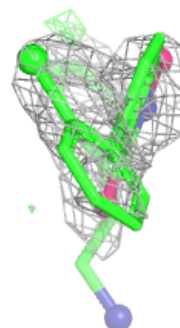
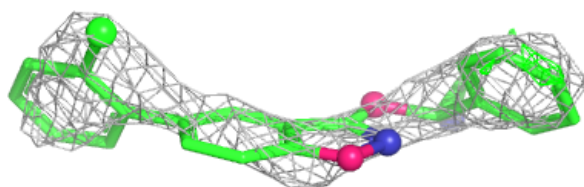
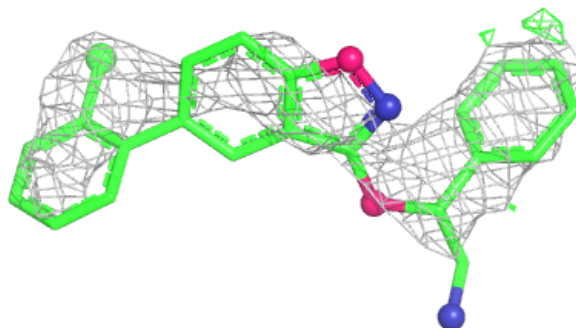
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and green (positive)

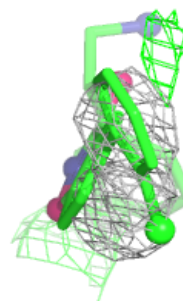
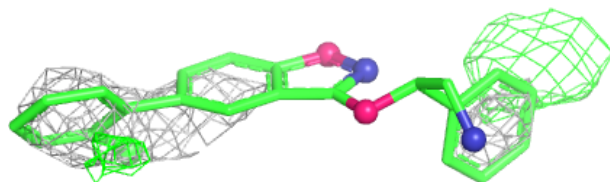


Electron density around JK8 U 701 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

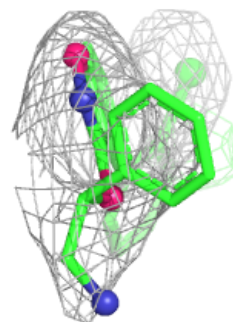
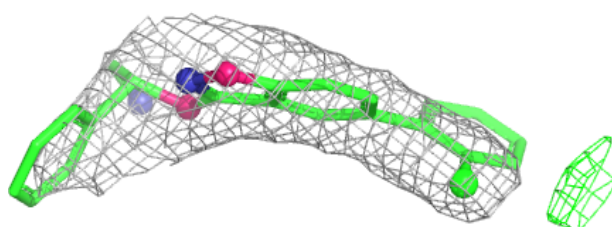
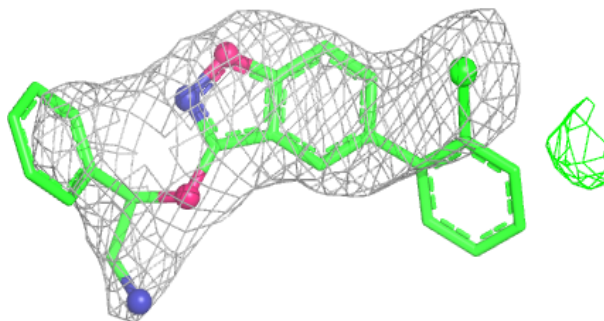
**Electron density around JK8 b 701:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

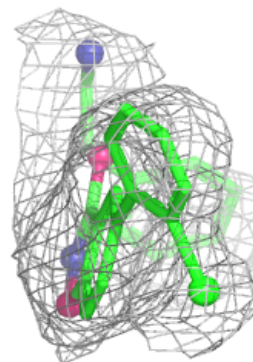
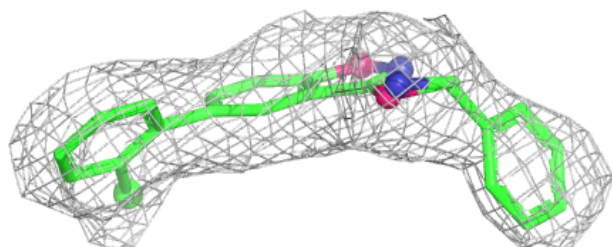
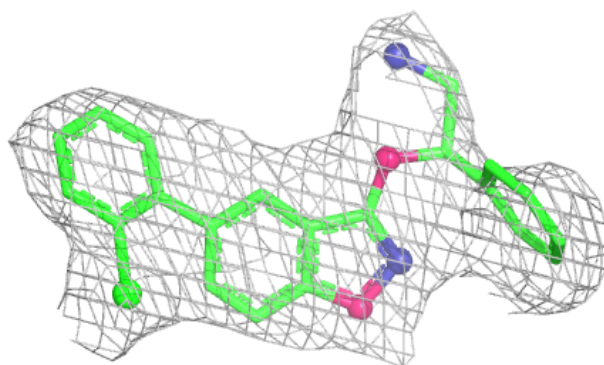


Electron density around JK8 d 701 (A):

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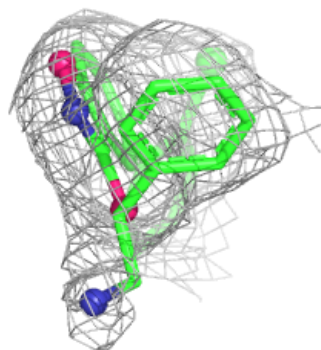
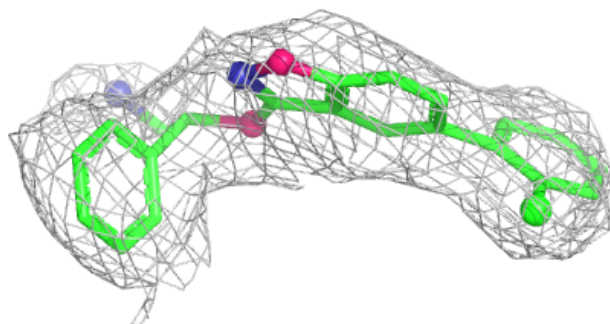
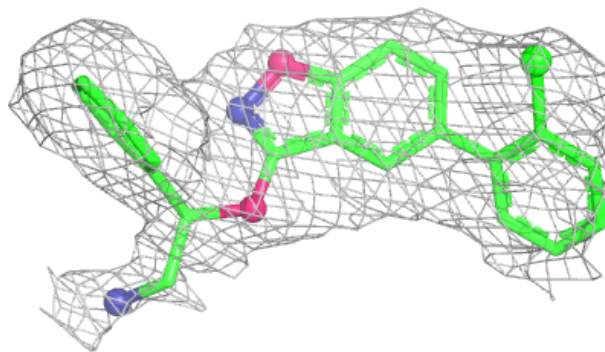
**Electron density around JK8 k 701:**

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and green (positive)

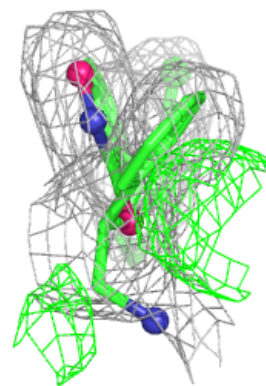
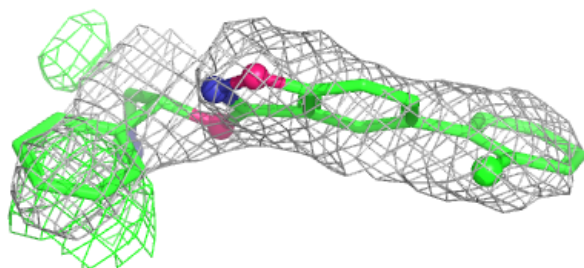
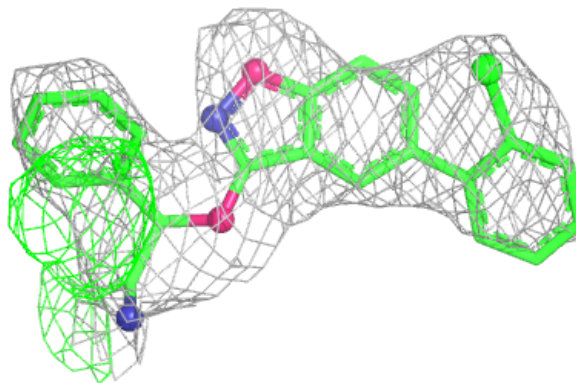


Electron density around JK8 I 501 (A):

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and green (positive)

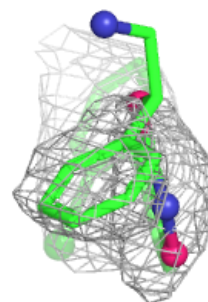
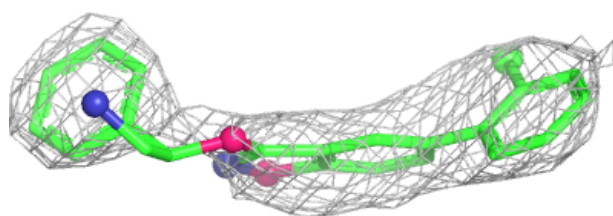
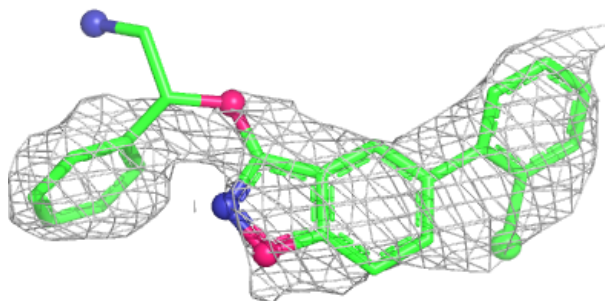
**Electron density around JK8 s 701:**

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and green (positive)



Electron density around JK8 t 501 (A):

$2mF_o-DF_c$ (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.