Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:51 PM BST

PDB ID	:	6QX2
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

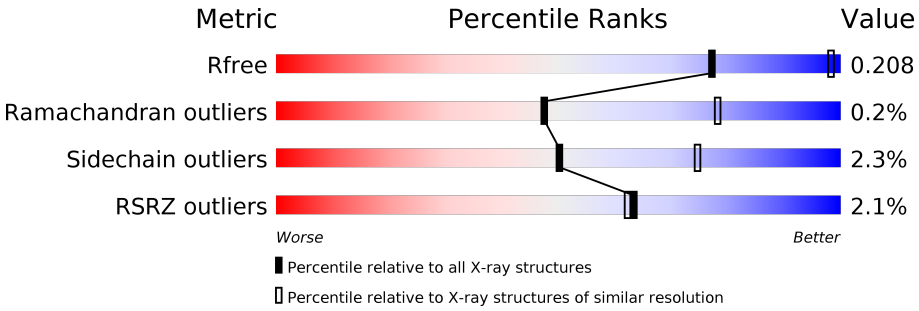
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1026 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	186	10% 97%
1	S	186	2% 96%
1	b	186	5% 98%
1	s	186	% 98%
2	A	490	4% 96%
2	C	490	% 97%
2	L	490	96%

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Mol	Chain	Length	Quality of chain
2	R	490	95%
2	T	490	96%
2	a	490	97%
2	c	490	97%
2	j	490	95%
2	l	490	97%
2	r	490	96%
2	t	490	97%
3	D	188	12% 96%
3	U	188	4% 96%
3	m	188	5% 96%
4	E	20	5% 85% 15%
4	F	20	90% 10%
4	N	20	90% 10%
4	O	20	90% 10%
4	W	20	85% 15%
4	e	20	90% 10%
4	n	20	80% 20%
4	v	20	90% 5% 5%
4	w	20	85% 15%
5	K	187	97%
6	J	480	98%
7	M	189	3% 96%
8	V	19	89% 11%
8	o	19	84% 11% 5%

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Mol	Chain	Length	Quality of chain
9	d	181	12% 96%
10	f	17	82% 18%
11	k	188	4% 98%
12	u	187	3% 97%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	JK8	b	701	-	-	-	X

2 Entry composition

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.

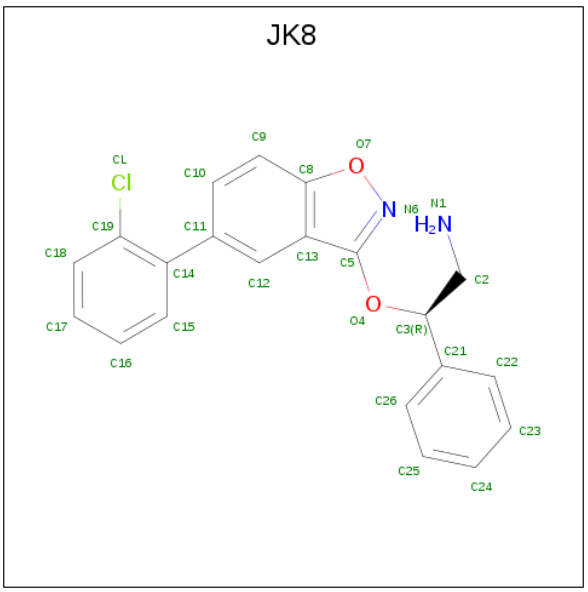
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	u	187	Total	C	N	O	S	0	3	0
			1460	915	248	288	9			

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

(three-letter code: JK8) (formula: $C_{21}H_{17}ClN_2O_2$).

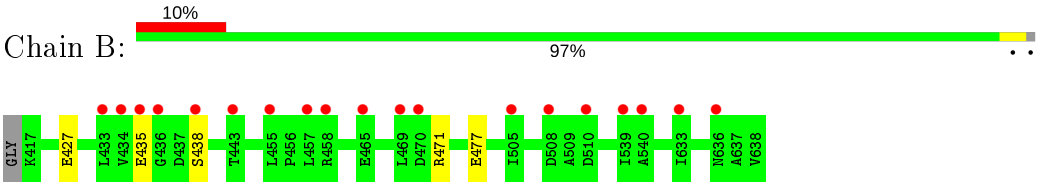


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	C	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		
13	J	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	L	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		
13	R	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
13	U	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2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

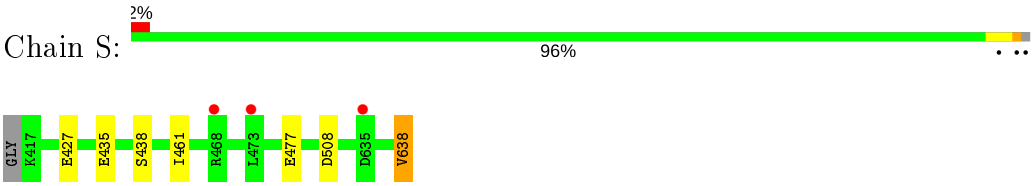
3 Residue-property plots (i)

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.

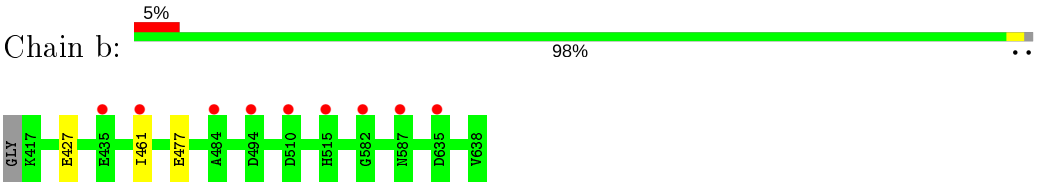
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



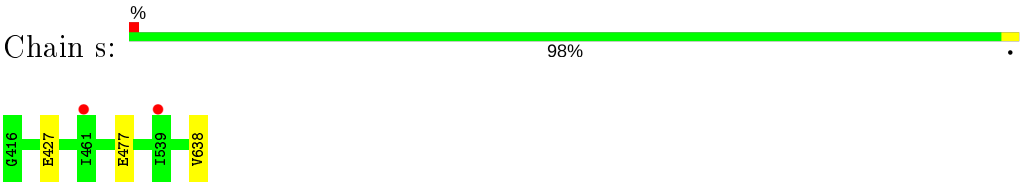
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



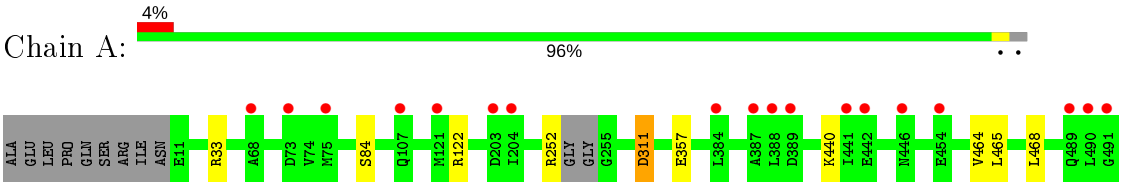
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B



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

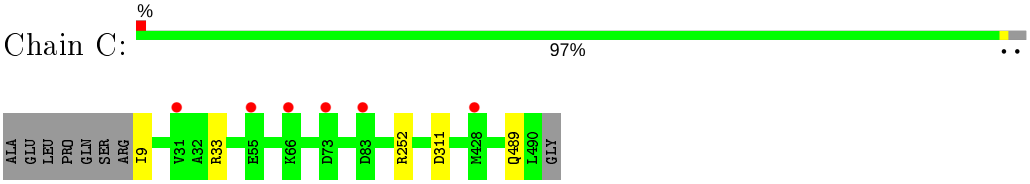


- Molecule 2: DNA gyrase subunit A



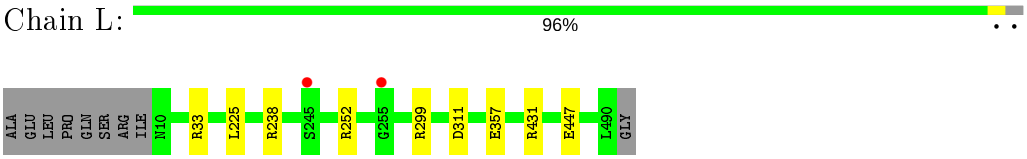
- Molecule 2: DNA gyrase subunit A

Chain C:



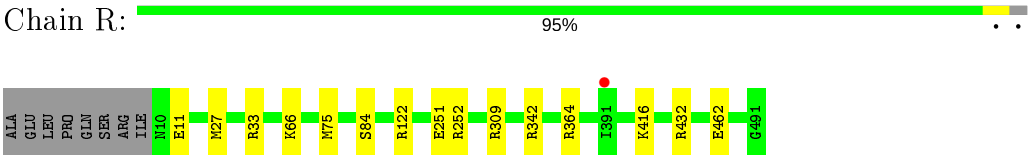
• Molecule 2: DNA gyrase subunit A

Chain L:



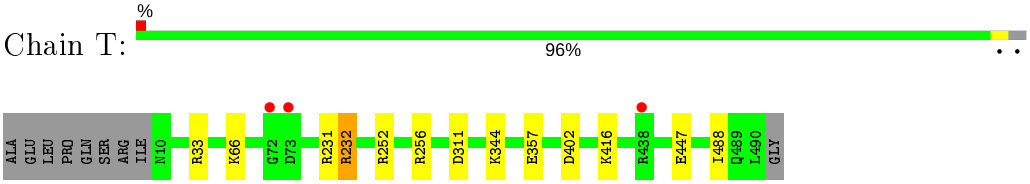
• Molecule 2: DNA gyrase subunit A

Chain R:



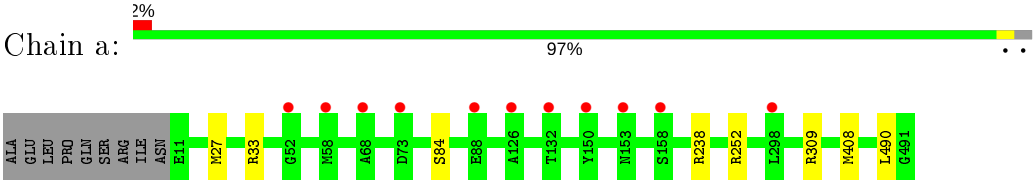
• Molecule 2: DNA gyrase subunit A

Chain T:



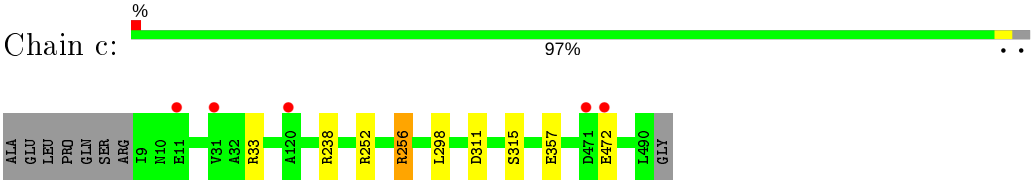
• Molecule 2: DNA gyrase subunit A

Chain a:



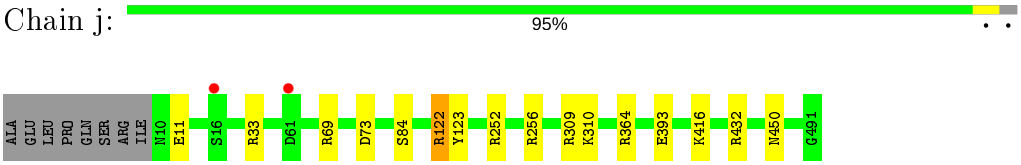
• Molecule 2: DNA gyrase subunit A

Chain c:



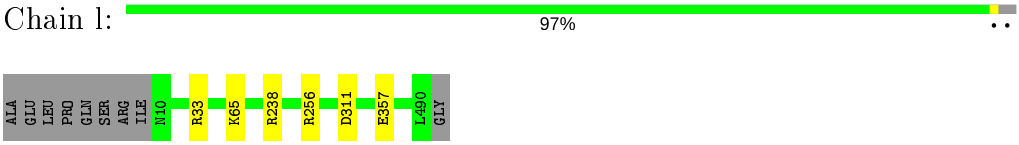
• Molecule 2: DNA gyrase subunit A

Chain j:



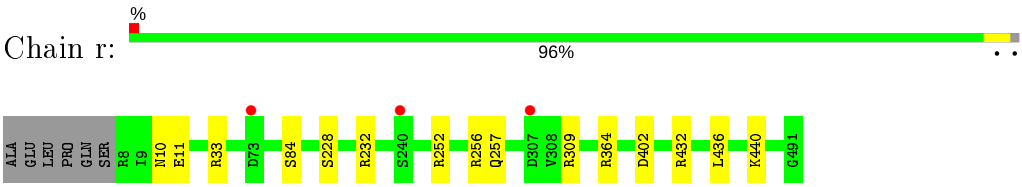
• Molecule 2: DNA gyrase subunit A

Chain l:



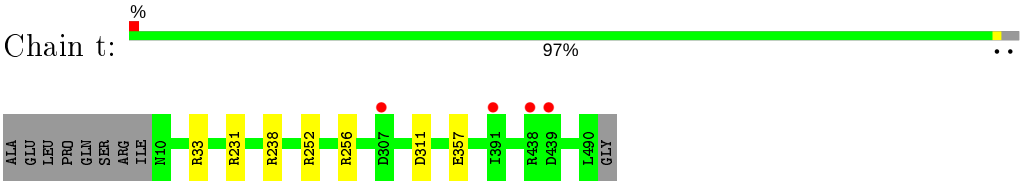
• Molecule 2: DNA gyrase subunit A

Chain r:



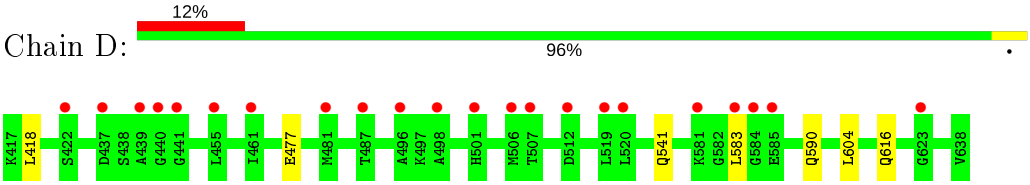
• Molecule 2: DNA gyrase subunit A

Chain t:



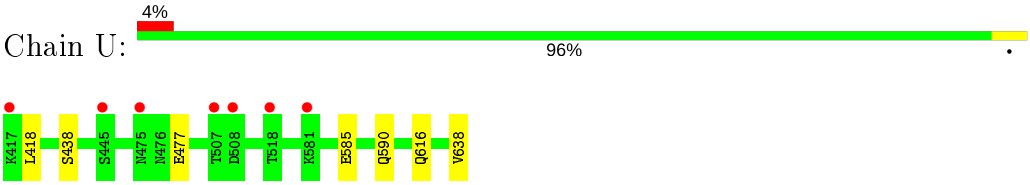
• Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain D:



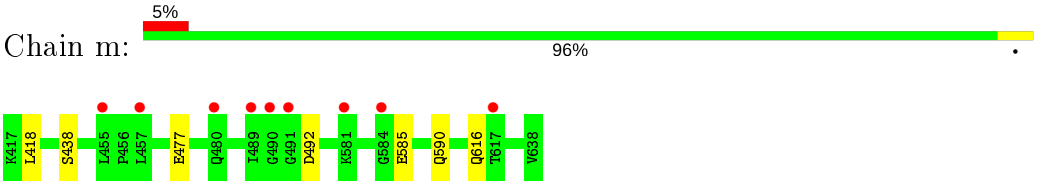
• Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain U:



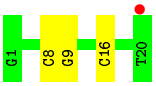
• Molecule 3: DNA gyrase subunit B,DNA gyrase subunit B

Chain m:



• 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:

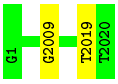


• Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain F:

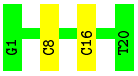
• Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain N:



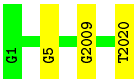
• Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain O:



• 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:

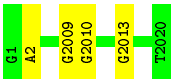


• Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain e:

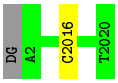
• Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain n:



• 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:

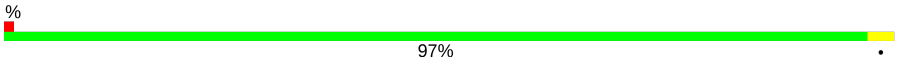


• Molecule 4: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain w:

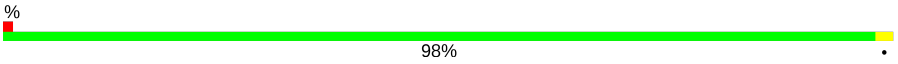
• Molecule 5: DNA gyrase subunit B,DNA gyrase subunit B

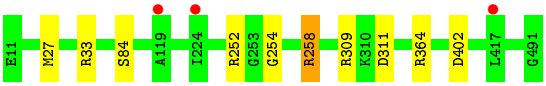
Chain K:



• Molecule 6: DNA gyrase subunit A

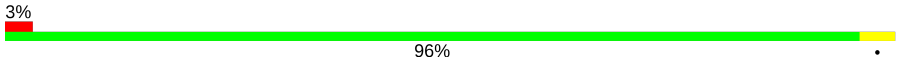
Chain J:

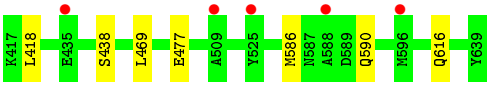




• Molecule 7: DNA gyrase subunit B,DNA gyrase subunit B

Chain M:



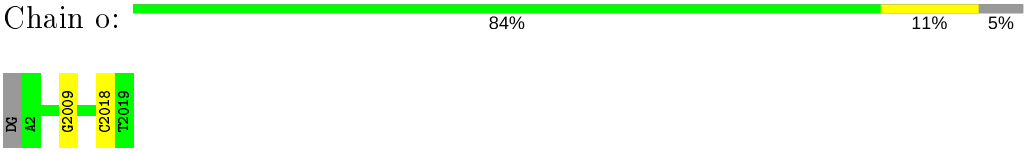


• Molecule 8: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain V:

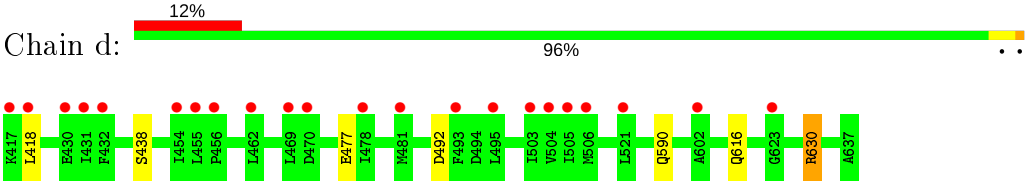
• Molecule 8: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain o:



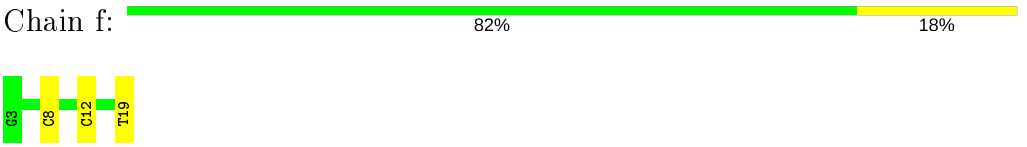
• Molecule 9: DNA gyrase subunit B,DNA gyrase subunit B

Chain d:



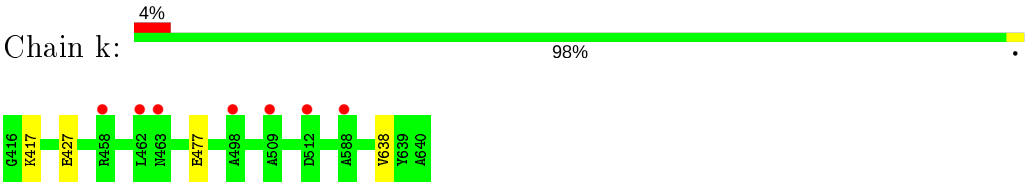
• Molecule 10: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain f:



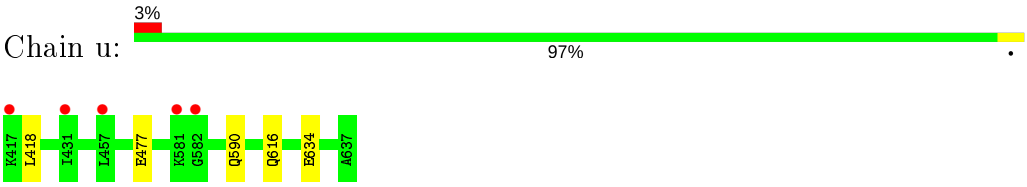
• Molecule 11: DNA gyrase subunit B,DNA gyrase subunit B

Chain k:



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

Chain u:



4 Data and refinement statistics (i)

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 – 3.40 162.14 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.3 (162.15-3.40) 80.3 (162.14-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.01%)	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)	0.30 , 4.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.420 for -h-2*l,-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	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.73	1/1461 (0.1%)	0.83	1/1975 (0.1%)
1	S	0.74	0/1458	0.83	1/1971 (0.1%)
1	b	0.73	0/1450	0.81	0/1962
1	s	0.72	0/1454	0.82	1/1966 (0.1%)
2	A	0.72	0/3896	0.83	2/5260 (0.0%)
2	C	0.70	0/3831	0.80	0/5179
2	L	0.72	0/3833	0.82	0/5180
2	R	0.73	0/3881	0.83	1/5241 (0.0%)
2	T	0.73	0/3844	0.83	2/5194 (0.0%)
2	a	0.72	0/3852	0.80	0/5206
2	c	0.71	1/3835 (0.0%)	0.81	1/5185 (0.0%)
2	j	0.73	0/3899	0.85	6/5264 (0.1%)
2	l	0.70	0/3832	0.82	0/5177
2	r	0.73	0/3921	0.82	0/5296
2	t	0.72	0/3860	0.80	0/5215
3	D	0.72	0/1469	0.80	0/1990
3	U	0.72	0/1486	0.81	1/2013 (0.0%)
3	m	0.72	0/1465	0.82	0/1985
4	E	0.63	1/511 (0.2%)	0.88	2/789 (0.3%)
4	F	0.67	0/438	1.53	4/673 (0.6%)
4	N	0.64	1/510 (0.2%)	0.92	1/785 (0.1%)
4	O	0.82	1/439 (0.2%)	0.89	1/677 (0.1%)
4	W	0.69	1/456 (0.2%)	1.01	3/700 (0.4%)
4	e	0.75	1/439 (0.2%)	1.04	1/677 (0.1%)
4	n	0.74	0/465	1.09	4/712 (0.6%)
4	v	0.64	0/443	0.93	1/677 (0.1%)
4	w	0.83	1/447 (0.2%)	1.03	2/686 (0.3%)
5	K	0.74	0/1459	0.82	0/1974
6	J	0.72	0/3912	0.83	1/5278 (0.0%)
7	M	0.74	0/1491	0.82	1/2020 (0.0%)
8	V	0.73	0/434	1.10	3/666 (0.5%)
8	o	0.74	1/412 (0.2%)	0.97	1/631 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	d	0.72	0/1416	0.84	1/1918 (0.1%)
10	f	0.74	2/389 (0.5%)	0.97	2/598 (0.3%)
11	k	0.73	0/1474	0.80	0/1994
12	u	0.73	1/1483 (0.1%)	0.80	0/2007
All	All	0.72	12/69345 (0.0%)	0.84	44/94721 (0.0%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	8	DC	O3'-P	8.10	1.70	1.61
10	f	8	DC	O3'-P	6.56	1.69	1.61
1	B	471	ARG	CZ-NH2	6.46	1.41	1.33
4	e	8	DC	O3'-P	6.05	1.68	1.61
8	o	2018	DC	O3'-P	-5.98	1.53	1.61
4	N	2019	DT	O3'-P	-5.88	1.54	1.61
4	w	2019	DT	O3'-P	-5.72	1.54	1.61
4	E	8	DC	O3'-P	5.68	1.68	1.61
4	W	5	DG	O3'-P	-5.63	1.54	1.61
2	c	472	GLU	CD-OE1	-5.53	1.19	1.25
10	f	12	DC	O3'-P	-5.45	1.54	1.61
12	u	634	GLU	CD-OE1	5.20	1.31	1.25

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2011	DC	O5'-P-OP2	-28.01	77.08	110.70
4	F	2011	DC	O5'-P-OP1	13.31	126.67	110.70
6	J	258	ARG	CG-CD-NE	10.07	132.95	111.80
8	o	2009	DG	O5'-P-OP1	-9.72	96.95	105.70
8	V	2019	DT	O5'-P-OP1	-9.35	97.29	105.70
1	B	471	ARG	NE-CZ-NH2	9.25	124.92	120.30
4	F	2009	DG	P-O5'-C5'	-8.71	106.96	120.90
4	e	20	DT	O5'-P-OP2	-8.14	98.37	105.70
9	d	630	ARG	CG-CD-NE	-7.75	95.52	111.80
8	V	2019	DT	O5'-P-OP2	7.60	119.82	110.70
4	N	2009	DG	P-O5'-C5'	-7.59	108.75	120.90
4	W	2009	DG	O5'-P-OP2	-7.31	99.12	105.70
2	T	256	ARG	CG-CD-NE	-7.28	96.51	111.80
4	w	2009	DG	O5'-P-OP2	-7.05	99.36	105.70
2	A	311	ASP	CB-CG-OD1	6.75	124.38	118.30
2	R	252	ARG	N-CA-CB	-6.72	98.50	110.60
8	V	2	DA	C4'-C3'-O3'	6.68	126.40	109.70
4	W	2009	DG	P-O5'-C5'	-6.59	110.35	120.90
2	j	69	ARG	CB-CG-CD	6.59	128.73	111.60
10	f	8	DC	C4'-C3'-O3'	6.46	125.85	109.70
2	A	311	ASP	CB-CG-OD2	-6.32	112.61	118.30
4	n	2009	DG	O5'-P-OP1	-6.25	100.08	105.70
3	U	638	VAL	CA-C-O	6.12	132.96	120.10
4	E	9	DG	O5'-P-OP2	-5.99	100.31	105.70
4	W	2020	DT	O5'-P-OP1	5.95	117.83	110.70
1	s	638	VAL	CA-C-O	5.94	132.58	120.10
2	j	122	ARG	NE-CZ-NH2	5.93	123.27	120.30
2	T	232	ARG	CG-CD-NE	-5.66	99.91	111.80
4	n	2	DA	P-O5'-C5'	5.65	129.95	120.90
4	F	2009	DG	O5'-C5'-C4'	5.56	124.90	111.00
2	j	416	LYS	CA-CB-CG	5.50	125.49	113.40
1	S	638	VAL	CA-C-O	5.48	131.60	120.10
2	c	256	ARG	CG-CD-NE	-5.42	100.43	111.80
4	E	16	DC	C1'-O4'-C4'	-5.38	104.72	110.10
4	w	2016	DC	C1'-O4'-C4'	-5.35	104.75	110.10
4	O	16	DC	C1'-O4'-C4'	-5.33	104.77	110.10
2	j	11	GLU	CB-CA-C	5.14	120.68	110.40
4	n	2013	DG	O5'-P-OP2	-5.13	101.08	105.70
2	j	69	ARG	CG-CD-NE	-5.11	101.07	111.80
4	v	2016	DC	C1'-O4'-C4'	-5.10	105.00	110.10
7	M	586	MET	CG-SD-CE	5.07	108.31	100.20
10	f	19	DT	N1-C1'-C2'	5.07	122.23	112.60
2	j	123	TYR	CB-CG-CD2	5.07	124.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	n	2010	DG	P-O5'-C5'	-5.00	112.90	120.90

There are no chirality outliers.

All (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
2	T	311	ASP	Peptide
2	a	490	LEU	Peptide
2	c	311	ASP	Peptide
2	l	311	ASP	Peptide
2	r	10	ASN	Peptide
2	t	311	ASP	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	488/490 (100%)	470 (96%)	17 (4%)	1 (0%)	47	78
2	L	485/490 (99%)	467 (96%)	17 (4%)	1 (0%)	47	78
2	R	491/490 (100%)	473 (96%)	17 (4%)	1 (0%)	47	78
2	T	487/490 (99%)	470 (96%)	16 (3%)	1 (0%)	47	78
2	a	491/490 (100%)	472 (96%)	18 (4%)	1 (0%)	47	78
2	c	488/490 (100%)	470 (96%)	17 (4%)	1 (0%)	47	78
2	j	493/490 (101%)	475 (96%)	17 (3%)	1 (0%)	47	78
2	l	485/490 (99%)	467 (96%)	17 (4%)	1 (0%)	47	78
2	r	497/490 (101%)	476 (96%)	19 (4%)	2 (0%)	34	67
2	t	489/490 (100%)	472 (96%)	16 (3%)	1 (0%)	47	78
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%)	29	61
6	J	491/480 (102%)	472 (96%)	17 (4%)	2 (0%)	34	67
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%)	14	44
12	u	188/187 (100%)	180 (96%)	8 (4%)	0	100	100
All	All	8112/8110 (100%)	7785 (96%)	310 (4%)	17 (0%)	47	78

All (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
2	A	33	ARG
2	C	33	ARG
6	J	33	ARG
2	L	33	ARG
2	R	33	ARG
2	T	33	ARG

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Mol	Chain	Res	Type
2	a	33	ARG
2	c	33	ARG
2	j	33	ARG
2	l	33	ARG
2	r	33	ARG
2	t	33	ARG

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	B	147/155 (95%)	143 (97%)	4 (3%)	44	70
1	S	148/155 (96%)	141 (95%)	7 (5%)	26	57
1	b	145/155 (94%)	142 (98%)	3 (2%)	53	76
1	s	146/155 (94%)	144 (99%)	2 (1%)	67	83
2	A	405/423 (96%)	396 (98%)	9 (2%)	52	75
2	C	394/423 (93%)	393 (100%)	1 (0%)	92	97
2	L	397/423 (94%)	389 (98%)	8 (2%)	55	77
2	R	402/423 (95%)	390 (97%)	12 (3%)	41	68
2	T	397/423 (94%)	386 (97%)	11 (3%)	43	70
2	a	395/423 (93%)	389 (98%)	6 (2%)	65	82
2	c	394/423 (93%)	388 (98%)	6 (2%)	65	82
2	j	403/423 (95%)	392 (97%)	11 (3%)	44	70
2	l	397/423 (94%)	393 (99%)	4 (1%)	76	88
2	r	403/423 (95%)	391 (97%)	12 (3%)	41	68
2	t	398/423 (94%)	392 (98%)	6 (2%)	65	82
3	D	147/157 (94%)	140 (95%)	7 (5%)	25	56
3	U	149/157 (95%)	143 (96%)	6 (4%)	31	60
3	m	146/157 (93%)	139 (95%)	7 (5%)	25	56
5	K	147/156 (94%)	142 (97%)	5 (3%)	37	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	J	406/414 (98%)	399 (98%)	7 (2%)	60 80
7	M	149/158 (94%)	143 (96%)	6 (4%)	31 60
9	d	141/152 (93%)	134 (95%)	7 (5%)	24 54
11	k	148/156 (95%)	146 (99%)	2 (1%)	67 83
12	u	149/156 (96%)	145 (97%)	4 (3%)	44 70
All	All	6553/6936 (94%)	6400 (98%)	153 (2%)	50 74

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	427	GLU
1	B	435	GLU
1	B	438	SER
1	B	477	GLU
2	A	84	SER
2	A	122	ARG
2	A	252	ARG
2	A	357[A]	GLU
2	A	357[B]	GLU
2	A	440	LYS
2	A	464	VAL
2	A	465	LEU
2	A	468	LEU
3	D	418	LEU
3	D	477	GLU
3	D	541	GLN
3	D	583	LEU
3	D	590	GLN
3	D	604	LEU
3	D	616	GLN
2	C	252	ARG
5	K	427	GLU
5	K	438	SER
5	K	477	GLU
5	K	583	LEU
5	K	585	GLU
6	J	27	MET
6	J	84	SER
6	J	252	ARG
6	J	258	ARG

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Mol	Chain	Res	Type
6	J	309	ARG
6	J	364	ARG
6	J	402	ASP
7	M	418	LEU
7	M	438	SER
7	M	469	LEU
7	M	477	GLU
7	M	590	GLN
7	M	616	GLN
2	L	225	LEU
2	L	238	ARG
2	L	252	ARG
2	L	299	ARG
2	L	357	GLU
2	L	431	ARG
2	L	447[A]	GLU
2	L	447[B]	GLU
1	S	427	GLU
1	S	435	GLU
1	S	438	SER
1	S	461	ILE
1	S	477	GLU
1	S	508	ASP
1	S	638	VAL
2	R	11	GLU
2	R	27	MET
2	R	66	LYS
2	R	75	MET
2	R	84	SER
2	R	122	ARG
2	R	309	ARG
2	R	342	ARG
2	R	364	ARG
2	R	416	LYS
2	R	432	ARG
2	R	462	GLU
3	U	418	LEU
3	U	438	SER
3	U	477	GLU
3	U	585	GLU
3	U	590	GLN
3	U	616	GLN

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Mol	Chain	Res	Type
2	T	66	LYS
2	T	231	ARG
2	T	232	ARG
2	T	252	ARG
2	T	344	LYS
2	T	357	GLU
2	T	402	ASP
2	T	416	LYS
2	T	447[A]	GLU
2	T	447[B]	GLU
2	T	488	ILE
1	b	427	GLU
1	b	461	ILE
1	b	477	GLU
2	a	27	MET
2	a	84	SER
2	a	238	ARG
2	a	252	ARG
2	a	309	ARG
2	a	408	MET
9	d	418	LEU
9	d	438	SER
9	d	477	GLU
9	d	492	ASP
9	d	590	GLN
9	d	616	GLN
9	d	630	ARG
2	c	238	ARG
2	c	252	ARG
2	c	256	ARG
2	c	298[A]	LEU
2	c	298[B]	LEU
2	c	357	GLU
11	k	427	GLU
11	k	477	GLU
2	j	73	ASP
2	j	84	SER
2	j	122	ARG
2	j	252	ARG
2	j	256	ARG
2	j	309	ARG
2	j	310	LYS

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Mol	Chain	Res	Type
2	j	364	ARG
2	j	393	GLU
2	j	432	ARG
2	j	450	ASN
3	m	418	LEU
3	m	438	SER
3	m	477	GLU
3	m	492	ASP
3	m	585	GLU
3	m	590	GLN
3	m	616	GLN
2	l	65	LYS
2	l	238	ARG
2	l	256	ARG
2	l	357	GLU
1	s	427	GLU
1	s	477	GLU
2	r	84	SER
2	r	228	SER
2	r	232[A]	ARG
2	r	232[B]	ARG
2	r	252	ARG
2	r	256	ARG
2	r	309	ARG
2	r	364	ARG
2	r	402	ASP
2	r	432	ARG
2	r	436	LEU
2	r	440	LYS
12	u	418	LEU
12	u	477	GLU
12	u	590	GLN
12	u	616	GLN
2	t	231[A]	ARG
2	t	231[B]	ARG
2	t	238	ARG
2	t	252	ARG
2	t	256	ARG
2	t	357	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	46	HIS
2	A	467	GLN
3	D	541	GLN
2	C	10	ASN
2	C	390	HIS
5	K	476	ASN
5	K	480	GLN
5	K	636	ASN
6	J	107	GLN
6	J	257	GLN
6	J	313	ASN
2	L	10	ASN
2	L	257	GLN
2	L	390	HIS
2	T	10	ASN
2	T	257	GLN
2	T	390	HIS
2	T	423	GLN
2	a	257	GLN
2	c	390	HIS
2	j	313	ASN
2	j	450	ASN
2	l	10	ASN
2	l	257	GLN
2	l	390	HIS
2	r	107	GLN
2	t	10	ASN
2	t	257	GLN
2	t	390	HIS

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 monosaccharides 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	-	24,29,29	1.19	3 (12%)	29,40,40	3.07	12 (41%)
13	JK8	U	701[A]	-	24,29,29	1.24	4 (16%)	29,40,40	1.58	5 (17%)
13	JK8	d	701[A]	-	24,29,29	1.15	3 (12%)	29,40,40	1.74	5 (17%)
13	JK8	L	501[A]	-	24,29,29	1.32	4 (16%)	29,40,40	1.65	7 (24%)
13	JK8	s	701	-	24,29,29	1.66	4 (16%)	29,40,40	2.92	10 (34%)
13	JK8	l	501[A]	-	24,29,29	1.68	4 (16%)	29,40,40	1.49	6 (20%)
13	JK8	R	501	-	24,29,29	1.27	2 (8%)	29,40,40	1.41	5 (17%)
13	JK8	k	701	-	24,29,29	1.52	5 (20%)	29,40,40	1.45	4 (13%)
13	JK8	t	501[A]	-	24,29,29	1.51	5 (20%)	29,40,40	1.76	7 (24%)
13	JK8	J	501	-	24,29,29	1.41	5 (20%)	29,40,40	2.14	9 (31%)
13	JK8	C	501[A]	-	24,29,29	1.08	3 (12%)	29,40,40	2.05	9 (31%)
13	JK8	A	501	-	24,29,29	1.15	3 (12%)	29,40,40	1.41	5 (17%)

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	-	-	1/12/14/14	0/4/4/4
13	JK8	U	701[A]	-	-	3/12/14/14	0/4/4/4
13	JK8	d	701[A]	-	-	5/12/14/14	0/4/4/4
13	JK8	L	501[A]	-	-	4/12/14/14	0/4/4/4
13	JK8	s	701	-	-	3/12/14/14	0/4/4/4
13	JK8	l	501[A]	-	-	2/12/14/14	0/4/4/4
13	JK8	R	501	-	-	4/12/14/14	0/4/4/4
13	JK8	k	701	-	-	2/12/14/14	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	JK8	t	501[A]	-	-	2/12/14/14	0/4/4/4
13	JK8	J	501	-	-	4/12/14/14	0/4/4/4
13	JK8	C	501[A]	-	-	6/12/14/14	0/4/4/4
13	JK8	A	501	-	-	5/12/14/14	0/4/4/4

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	l	501[A]	JK8	C5-C13	-5.44	1.40	1.45
13	s	701	JK8	C5-C13	-5.08	1.40	1.45
13	k	701	JK8	C5-C13	-4.59	1.41	1.45
13	R	501	JK8	C5-C13	-4.31	1.41	1.45
13	s	701	JK8	C14-C11	-4.27	1.41	1.49
13	t	501[A]	JK8	C14-C11	-4.20	1.41	1.49
13	J	501	JK8	C21-C3	3.49	1.57	1.51
13	L	501[A]	JK8	C5-C13	-3.47	1.42	1.45
13	l	501[A]	JK8	C14-C11	-3.47	1.43	1.49
13	d	701[A]	JK8	C5-C13	-3.34	1.42	1.45
13	C	501[A]	JK8	C5-C13	-3.20	1.42	1.45
13	A	501	JK8	C5-C13	-3.20	1.42	1.45
13	b	701	JK8	C14-C11	-3.18	1.43	1.49
13	t	501[A]	JK8	C5-C13	-3.01	1.42	1.45
13	U	701[A]	JK8	C14-C11	-2.97	1.44	1.49
13	J	501	JK8	C5-C13	-2.95	1.42	1.45
13	U	701[A]	JK8	C5-C13	-2.91	1.42	1.45
13	l	501[A]	JK8	C12-C13	-2.90	1.36	1.42
13	k	701	JK8	C14-C11	-2.90	1.44	1.49
13	L	501[A]	JK8	C14-C11	-2.85	1.44	1.49
13	l	501[A]	JK8	C13-C8	-2.80	1.37	1.43
13	t	501[A]	JK8	C13-C8	-2.72	1.37	1.43
13	L	501[A]	JK8	O4-C3	2.72	1.47	1.44
13	d	701[A]	JK8	C14-C11	-2.71	1.44	1.49
13	U	701[A]	JK8	C13-C8	-2.67	1.37	1.43
13	J	501	JK8	C12-C13	-2.66	1.36	1.42
13	A	501	JK8	C13-C8	-2.64	1.37	1.43
13	t	501[A]	JK8	O4-C3	2.61	1.47	1.44
13	A	501	JK8	C14-C11	-2.60	1.44	1.49
13	s	701	JK8	C12-C13	-2.58	1.37	1.42
13	k	701	JK8	O4-C3	-2.52	1.42	1.44
13	J	501	JK8	O4-C3	2.48	1.47	1.44
13	k	701	JK8	C13-C8	-2.46	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	701[A]	JK8	C13-C8	-2.44	1.38	1.43
13	C	501[A]	JK8	C13-C8	-2.33	1.38	1.43
13	b	701	JK8	C5-C13	-2.30	1.43	1.45
13	s	701	JK8	C13-C8	-2.25	1.38	1.43
13	J	501	JK8	C13-C8	-2.23	1.38	1.43
13	t	501[A]	JK8	C12-C13	-2.21	1.37	1.42
13	b	701	JK8	C13-C8	-2.21	1.38	1.43
13	k	701	JK8	C12-C13	-2.17	1.37	1.42
13	C	501[A]	JK8	C19-CL	-2.14	1.68	1.73
13	U	701[A]	JK8	C12-C13	-2.13	1.37	1.42
13	R	501	JK8	C12-C13	-2.06	1.38	1.42
13	L	501[A]	JK8	C13-C8	-2.05	1.39	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	s	701	JK8	O4-C3-C2	9.48	118.11	106.02
13	b	701	JK8	C5-O4-C3	-7.88	105.45	116.79
13	b	701	JK8	C10-C11-C14	-7.16	109.31	120.91
13	d	701[A]	JK8	O4-C3-C2	6.64	114.50	106.02
13	s	701	JK8	C5-O4-C3	-6.32	107.70	116.79
13	J	501	JK8	C2-C3-C21	5.60	120.21	111.36
13	b	701	JK8	C14-C19-CL	-5.45	112.93	120.75
13	b	701	JK8	C11-C14-C19	-5.04	115.04	123.53
13	s	701	JK8	C14-C19-CL	-5.02	113.55	120.75
13	C	501[A]	JK8	C15-C14-C19	-4.62	112.52	117.63
13	t	501[A]	JK8	O4-C3-C2	4.62	111.91	106.02
13	s	701	JK8	C11-C14-C19	-4.39	116.13	123.53
13	b	701	JK8	C12-C11-C14	4.15	127.11	120.72
13	J	501	JK8	O4-C3-C21	4.02	119.55	111.92
13	A	501	JK8	O4-C3-C21	3.89	119.31	111.92
13	C	501[A]	JK8	C11-C14-C19	3.88	130.07	123.53
13	C	501[A]	JK8	C5-C13-C8	-3.85	101.35	106.59
13	b	701	JK8	C12-C13-C5	3.74	139.63	132.74
13	s	701	JK8	C11-C12-C13	-3.71	114.17	122.30
13	J	501	JK8	C5-O4-C3	-3.64	111.55	116.79
13	C	501[A]	JK8	C18-C19-CL	-3.61	111.16	118.41
13	C	501[A]	JK8	C18-C19-C14	3.61	125.65	121.29
13	U	701[A]	JK8	O4-C3-C2	3.58	110.59	106.02
13	s	701	JK8	C10-C11-C12	3.51	123.60	118.09
13	k	701	JK8	C5-C13-C8	-3.47	101.86	106.59
13	b	701	JK8	C10-C11-C12	3.46	123.51	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	L	501[A]	JK8	O4-C3-C21	3.45	118.47	111.92
13	t	501[A]	JK8	C12-C11-C14	-3.36	115.54	120.72
13	b	701	JK8	C15-C14-C11	3.35	125.29	118.68
13	k	701	JK8	C11-C12-C13	-3.31	115.04	122.30
13	J	501	JK8	C12-C11-C14	-3.31	115.61	120.72
13	l	501[A]	JK8	C11-C12-C13	-3.30	115.08	122.30
13	s	701	JK8	C18-C19-CL	3.30	125.03	118.41
13	J	501	JK8	C26-C21-C22	-3.29	114.19	118.29
13	b	701	JK8	C5-C13-C8	-3.28	102.12	106.59
13	L	501[A]	JK8	C10-C11-C12	3.26	123.21	118.09
13	l	501[A]	JK8	C10-C11-C12	3.26	123.21	118.09
13	t	501[A]	JK8	C15-C14-C19	3.20	121.18	117.63
13	b	701	JK8	O4-C3-C2	3.20	110.11	106.02
13	s	701	JK8	C15-C14-C19	3.16	121.13	117.63
13	U	701[A]	JK8	O4-C3-C21	3.13	117.87	111.92
13	L	501[A]	JK8	C10-C11-C14	-3.12	115.86	120.91
13	L	501[A]	JK8	C11-C12-C13	-3.09	115.54	122.30
13	A	501	JK8	C5-O4-C3	3.08	121.22	116.79
13	J	501	JK8	C25-C26-C21	3.04	124.41	120.65
13	t	501[A]	JK8	C11-C14-C19	-3.04	118.41	123.53
13	l	501[A]	JK8	O4-C3-C2	3.03	109.89	106.02
13	t	501[A]	JK8	C10-C11-C12	3.00	122.80	118.09
13	b	701	JK8	C11-C12-C13	-3.00	115.73	122.30
13	s	701	JK8	C10-C11-C14	-2.98	116.09	120.91
13	R	501	JK8	C5-O4-C3	-2.97	112.52	116.79
13	J	501	JK8	C10-C11-C12	2.94	122.71	118.09
13	b	701	JK8	C18-C19-CL	2.93	124.29	118.41
13	d	701[A]	JK8	C5-O4-C3	-2.91	112.60	116.79
13	k	701	JK8	O4-C3-C2	-2.83	102.41	106.02
13	U	701[A]	JK8	C10-C11-C12	2.82	122.51	118.09
13	A	501	JK8	O4-C3-C2	2.79	109.58	106.02
13	U	701[A]	JK8	C2-C3-C21	-2.78	106.96	111.36
13	U	701[A]	JK8	C12-C13-C5	2.75	137.80	132.74
13	R	501	JK8	C11-C12-C13	-2.74	116.31	122.30
13	L	501[A]	JK8	C12-C13-C5	2.72	137.74	132.74
13	J	501	JK8	C11-C12-C13	-2.70	116.39	122.30
13	t	501[A]	JK8	C12-C13-C5	2.48	137.30	132.74
13	d	701[A]	JK8	C11-C12-C13	-2.41	117.03	122.30
13	C	501[A]	JK8	O4-C3-C21	2.38	116.44	111.92
13	A	501	JK8	C5-C13-C8	-2.37	103.37	106.59
13	l	501[A]	JK8	C12-C11-C14	-2.36	117.07	120.72
13	C	501[A]	JK8	C9-C10-C11	2.36	124.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	501[A]	JK8	C12-C13-C5	2.29	136.95	132.74
13	A	501	JK8	C11-C12-C13	-2.28	117.31	122.30
13	d	701[A]	JK8	C12-C13-C5	2.27	136.92	132.74
13	k	701	JK8	C10-C11-C12	2.27	121.65	118.09
13	L	501[A]	JK8	C5-C13-C8	-2.26	103.50	106.59
13	l	501[A]	JK8	C5-O4-C3	-2.26	113.54	116.79
13	R	501	JK8	O4-C3-C2	2.25	108.90	106.02
13	J	501	JK8	O4-C3-C2	2.20	108.83	106.02
13	t	501[A]	JK8	C11-C12-C13	-2.18	117.53	122.30
13	l	501[A]	JK8	C15-C14-C11	-2.11	114.50	118.68
13	L	501[A]	JK8	O4-C3-C2	2.11	108.72	106.02
13	R	501	JK8	O4-C3-C21	2.09	115.89	111.92
13	d	701[A]	JK8	C5-C13-C8	-2.09	103.75	106.59
13	C	501[A]	JK8	C11-C12-C13	-2.07	117.77	122.30
13	R	501	JK8	C5-C13-C8	-2.05	103.79	106.59
13	s	701	JK8	C15-C14-C11	2.04	122.72	118.68

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	U	701[A]	JK8	C21-C3-O4-C5
13	d	701[A]	JK8	N1-C2-C3-C21
13	d	701[A]	JK8	N1-C2-C3-O4
13	l	501[A]	JK8	N1-C2-C3-C21
13	l	501[A]	JK8	N1-C2-C3-O4
13	s	701	JK8	N1-C2-C3-C21
13	R	501	JK8	C10-C11-C14-C19
13	R	501	JK8	C12-C11-C14-C19
13	k	701	JK8	N1-C2-C3-C21
13	k	701	JK8	N1-C2-C3-O4
13	t	501[A]	JK8	N1-C2-C3-C21
13	t	501[A]	JK8	N1-C2-C3-O4
13	J	501	JK8	C22-C21-C3-C2
13	J	501	JK8	C26-C21-C3-C2
13	J	501	JK8	N1-C2-C3-C21
13	J	501	JK8	N1-C2-C3-O4
13	C	501[A]	JK8	C22-C21-C3-C2
13	C	501[A]	JK8	C26-C21-C3-C2
13	C	501[A]	JK8	N1-C2-C3-C21
13	A	501	JK8	N1-C2-C3-C21
13	A	501	JK8	N1-C2-C3-O4

Continued on next page...

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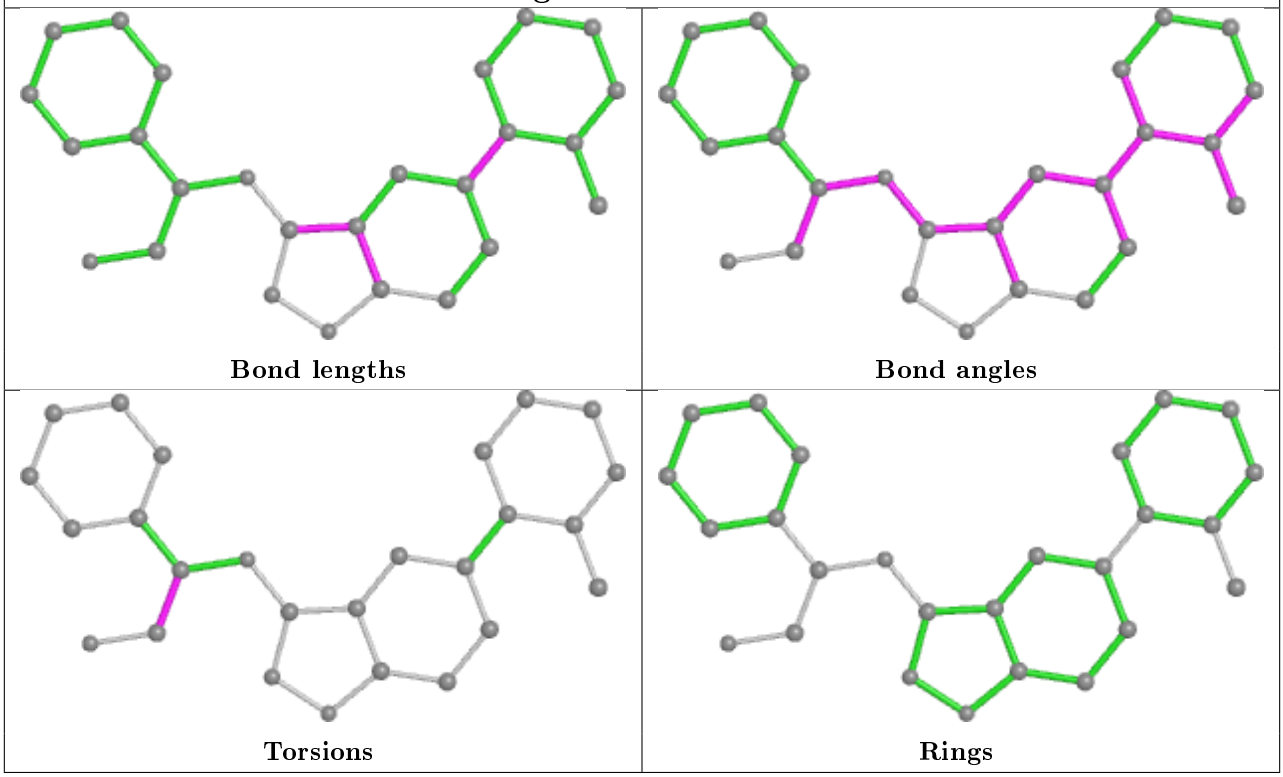
Mol	Chain	Res	Type	Atoms
13	A	501	JK8	C21-C3-O4-C5
13	U	701[A]	JK8	N1-C2-C3-C21
13	s	701	JK8	C22-C21-C3-C2
13	s	701	JK8	C26-C21-C3-C2
13	d	701[A]	JK8	C22-C21-C3-O4
13	d	701[A]	JK8	C26-C21-C3-O4
13	L	501[A]	JK8	C22-C21-C3-O4
13	b	701	JK8	N1-C2-C3-C21
13	L	501[A]	JK8	N1-C2-C3-C21
13	R	501	JK8	C12-C11-C14-C15
13	R	501	JK8	C10-C11-C14-C15
13	L	501[A]	JK8	C26-C21-C3-O4
13	L	501[A]	JK8	N1-C2-C3-O4
13	d	701[A]	JK8	C22-C21-C3-C2
13	U	701[A]	JK8	N1-C2-C3-O4
13	C	501[A]	JK8	C22-C21-C3-O4
13	C	501[A]	JK8	C26-C21-C3-O4
13	A	501	JK8	C26-C21-C3-O4
13	A	501	JK8	C22-C21-C3-O4
13	C	501[A]	JK8	C2-C3-O4-C5

There are no ring outliers.

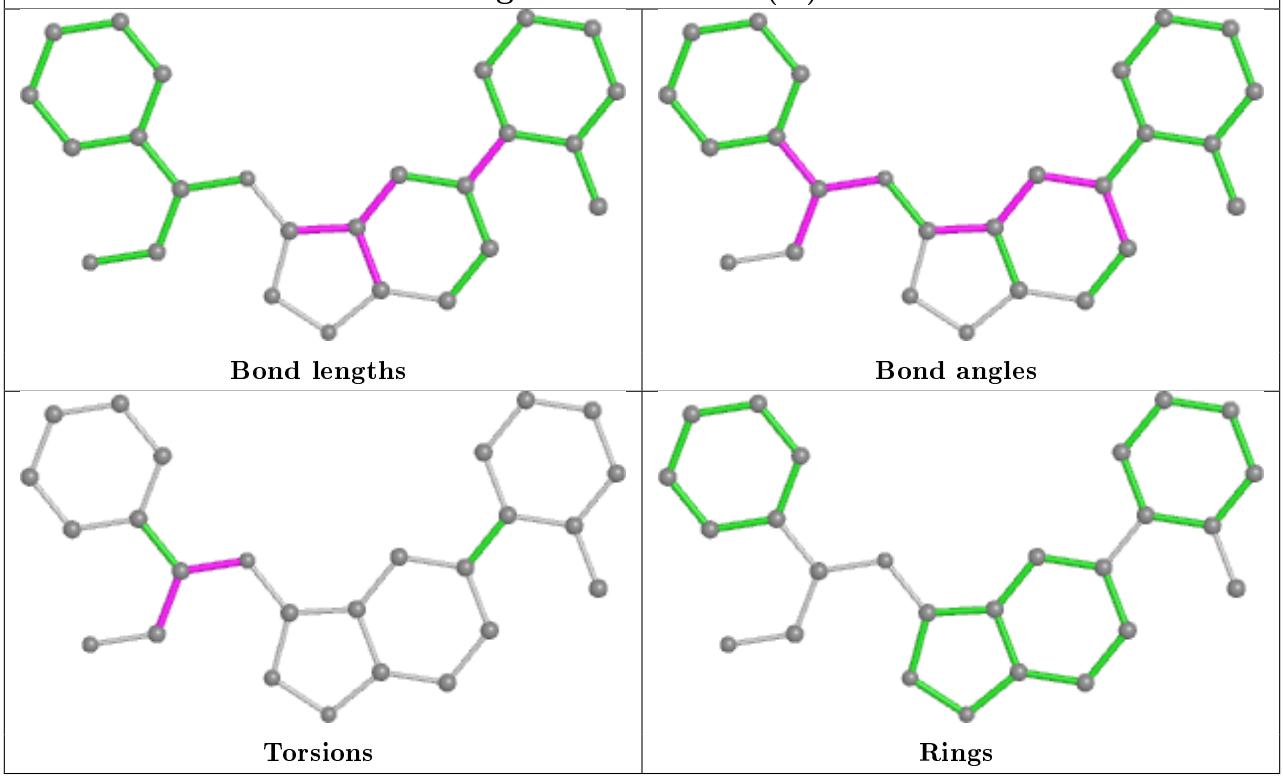
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

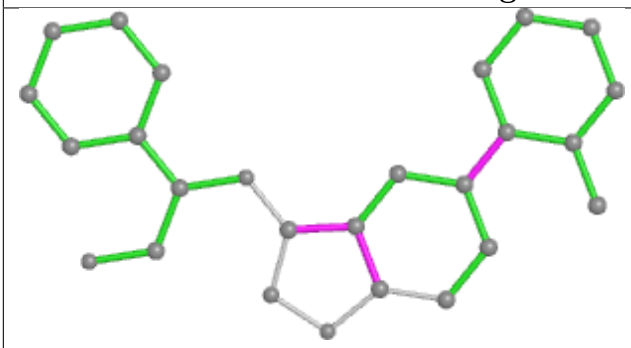
Ligand JK8 b 701



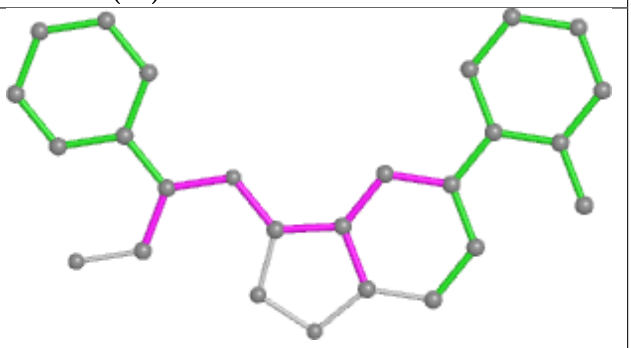
Ligand JK8 U 701 (A)



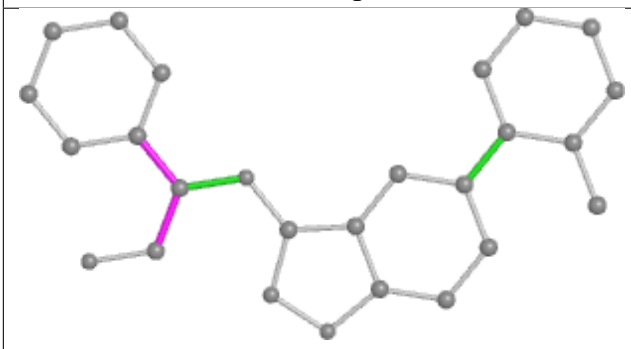
Ligand JK8 d 701 (A)



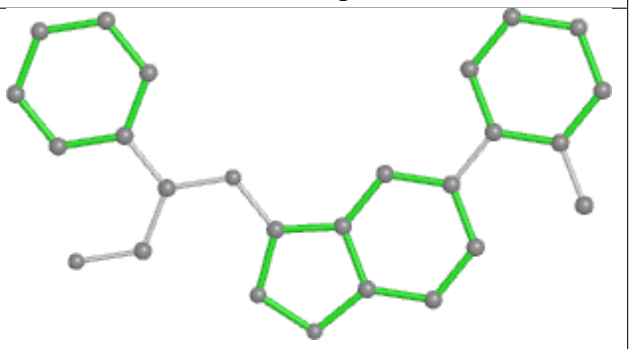
Bond lengths



Bond angles

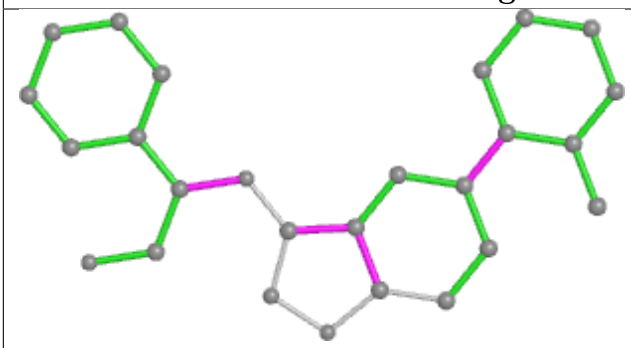


Torsions

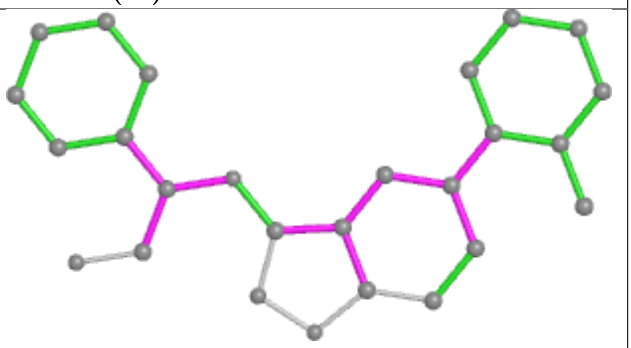


Rings

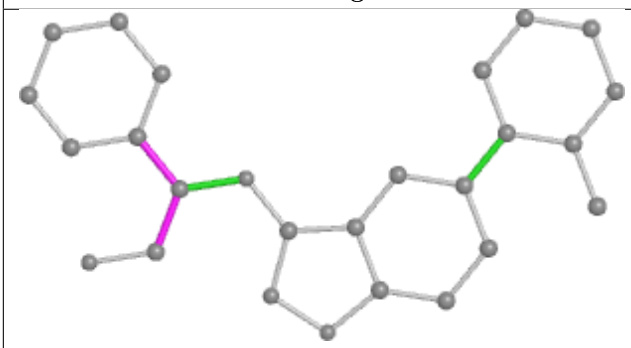
Ligand JK8 L 501 (A)



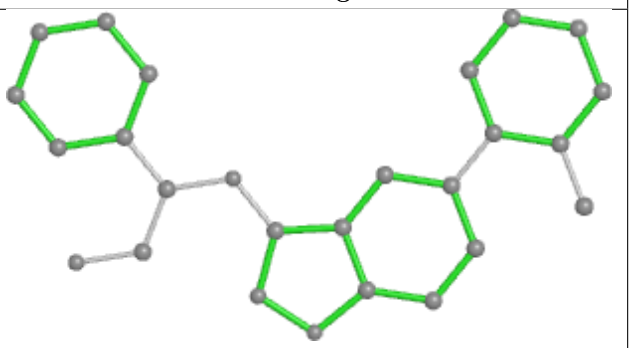
Bond lengths



Bond angles

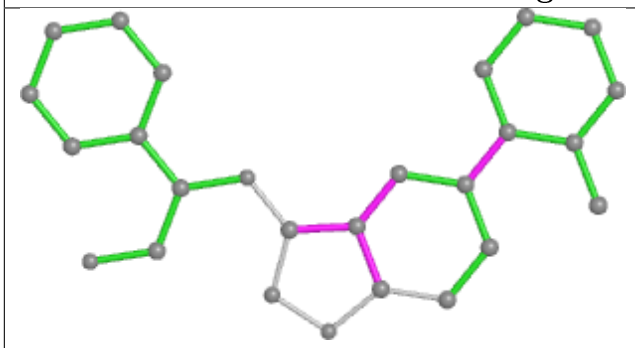


Torsions

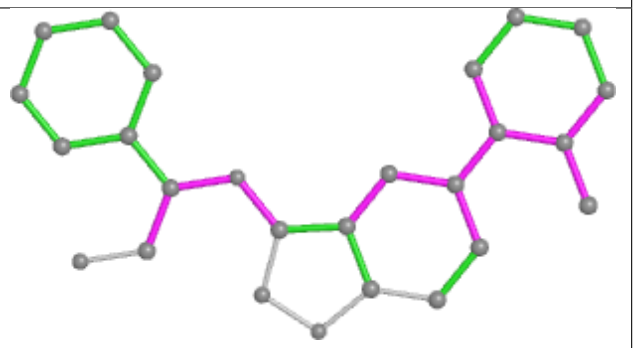


Rings

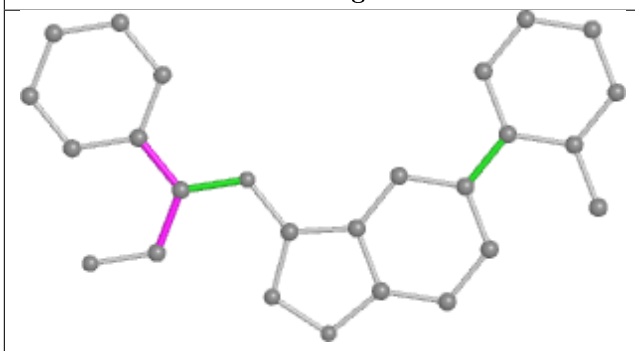
Ligand JK8 s 701



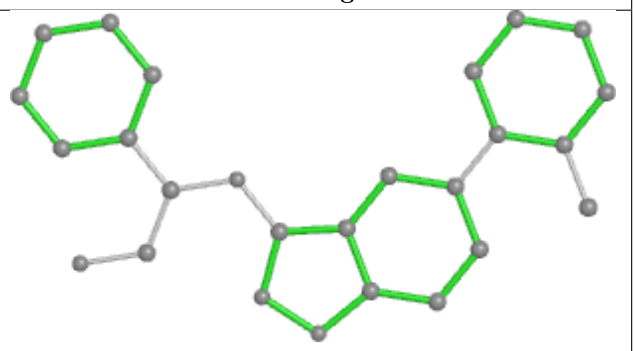
Bond lengths



Bond angles

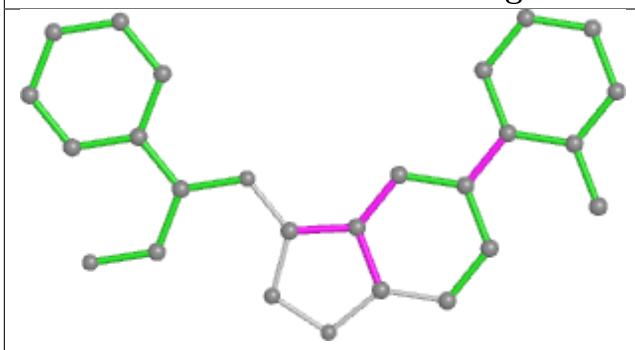


Torsions

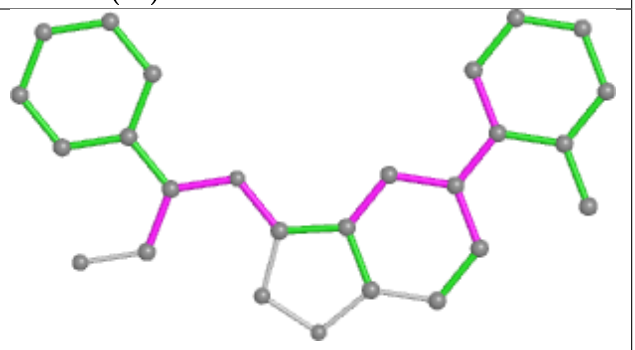


Rings

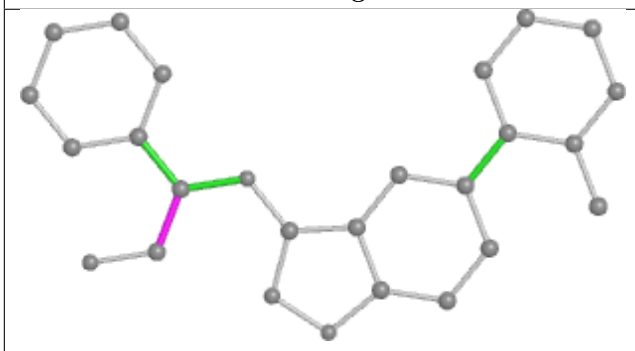
Ligand JK8 l 501 (A)



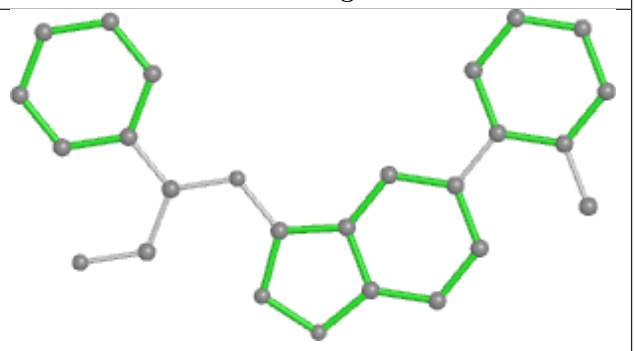
Bond lengths



Bond angles

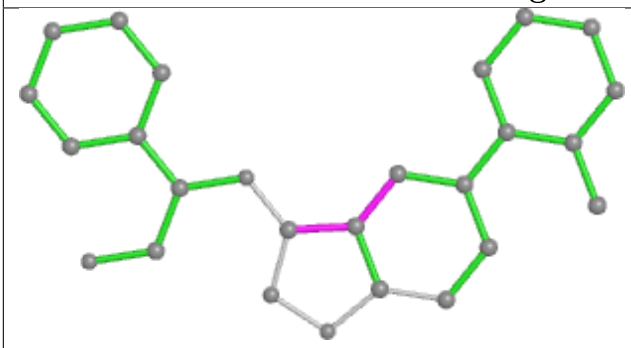


Torsions

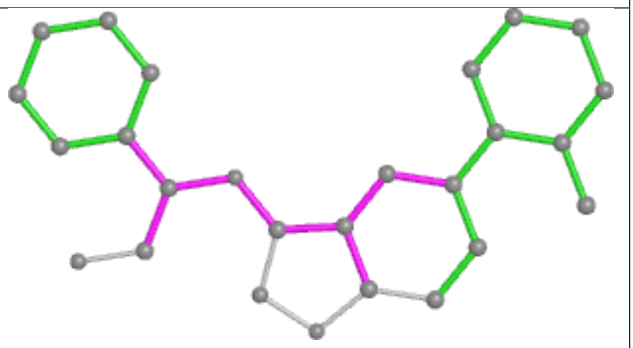


Rings

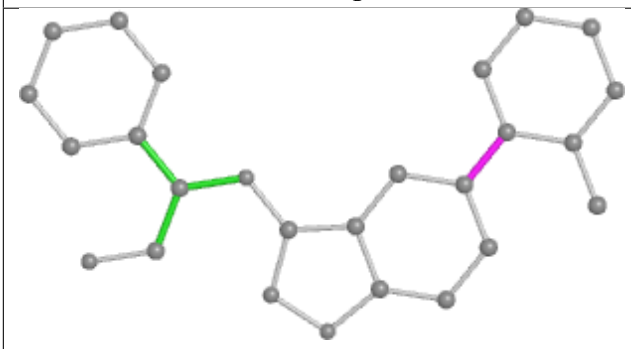
Ligand JK8 R 501



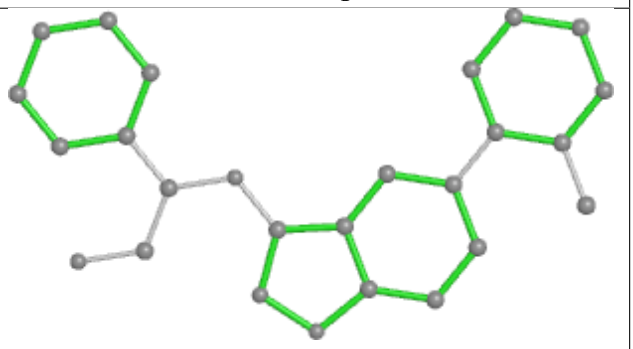
Bond lengths



Bond angles

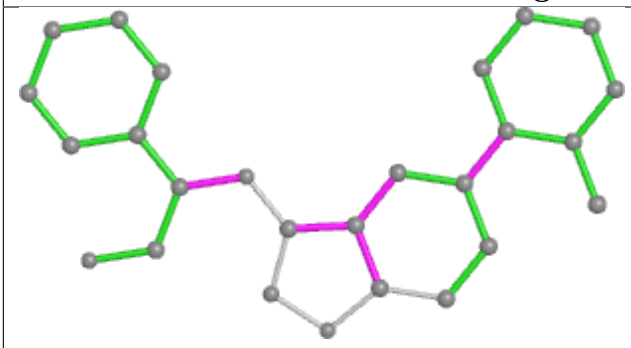


Torsions

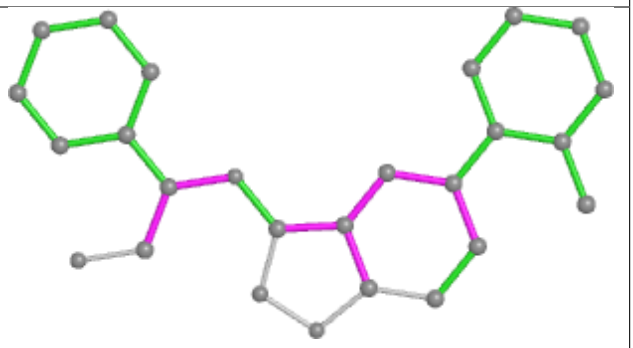


Rings

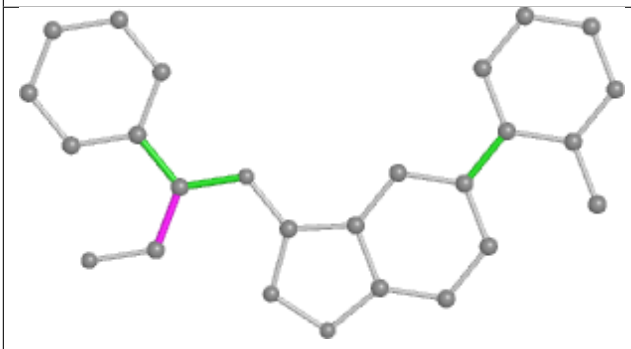
Ligand JK8 k 701



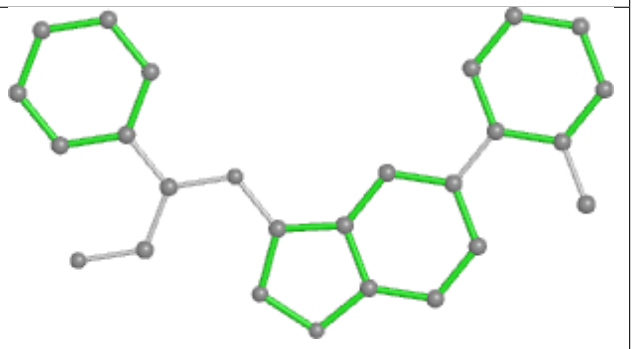
Bond lengths



Bond angles

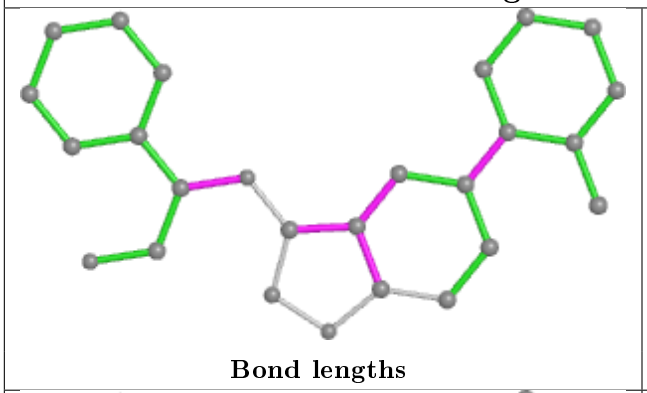


Torsions

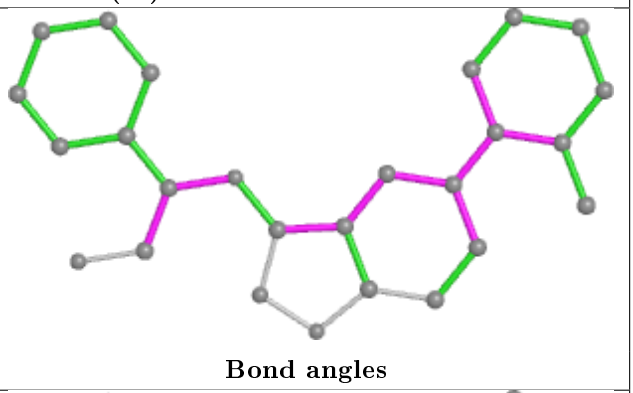


Rings

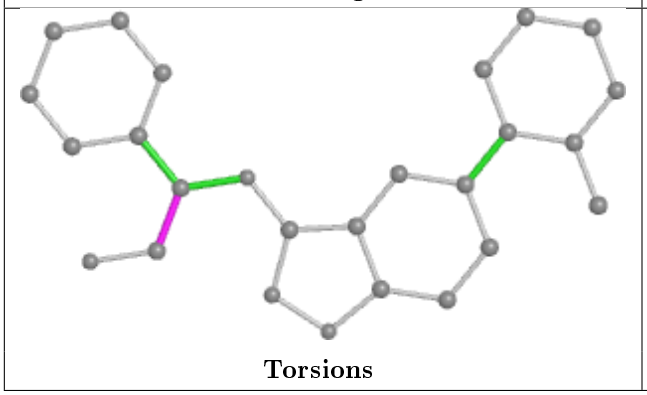
Ligand JK8 t 501 (A)



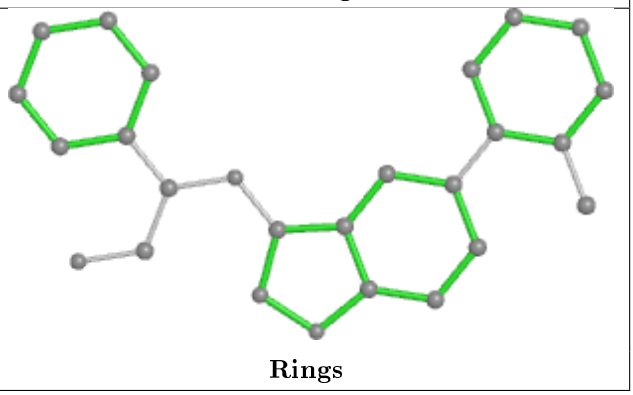
Bond lengths



Bond angles

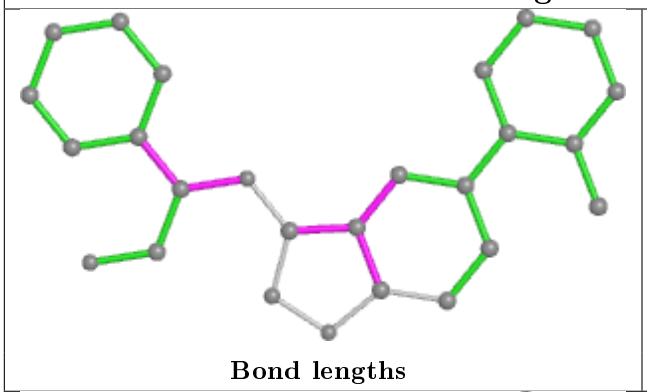


Torsions

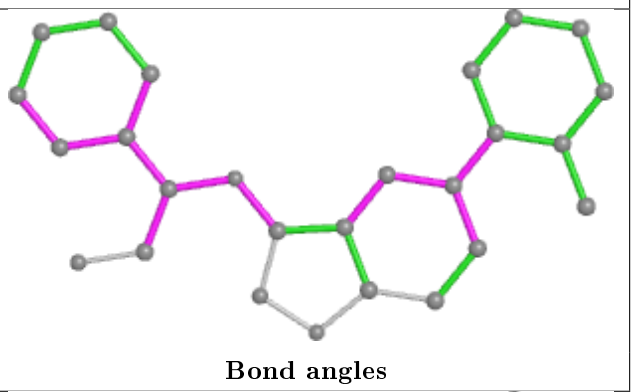


Rings

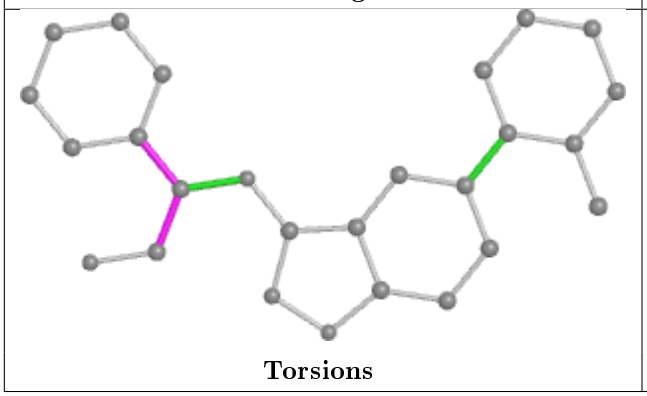
Ligand JK8 J 501



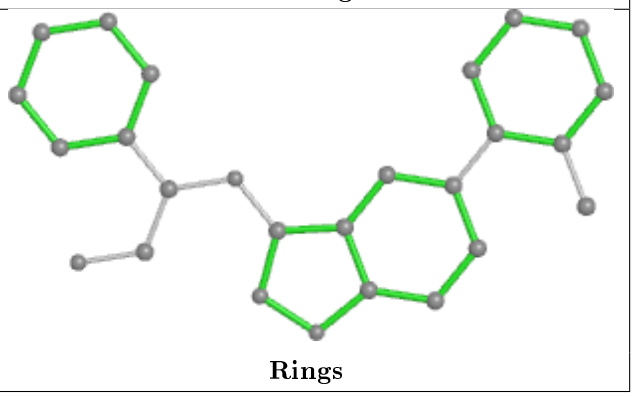
Bond lengths



Bond angles

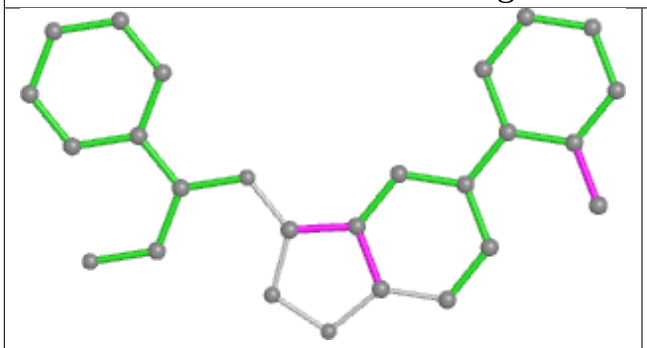


Torsions

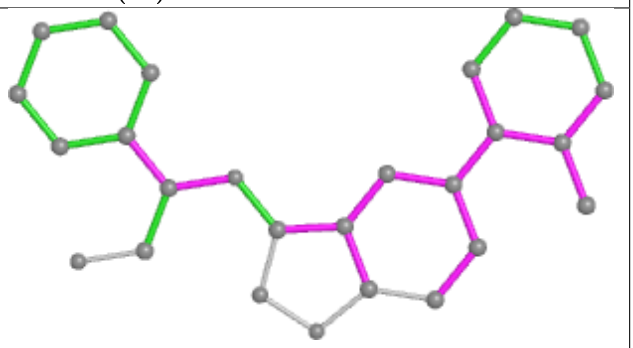


Rings

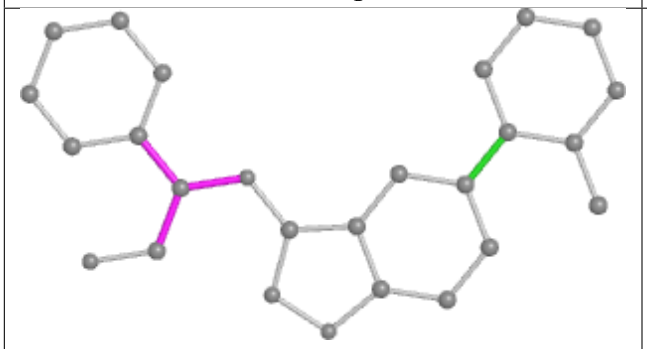
Ligand JK8 C 501 (A)



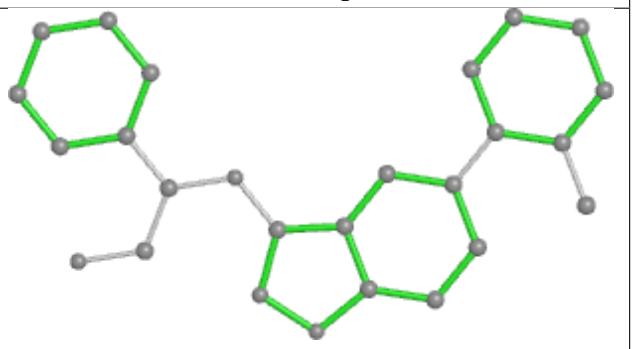
Bond lengths



Bond angles

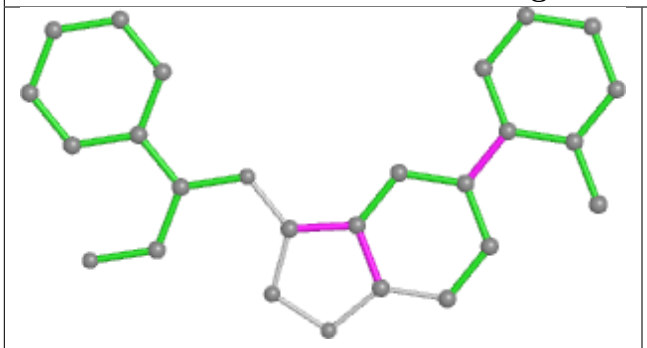


Torsions

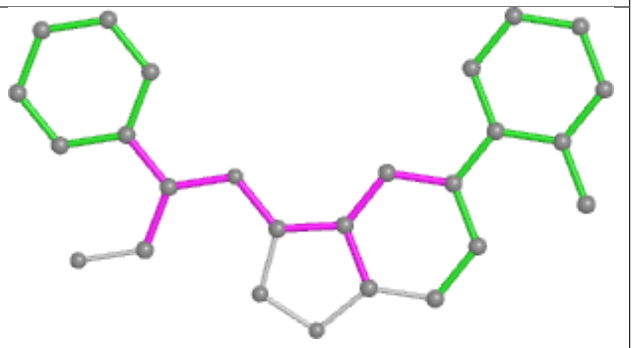


Rings

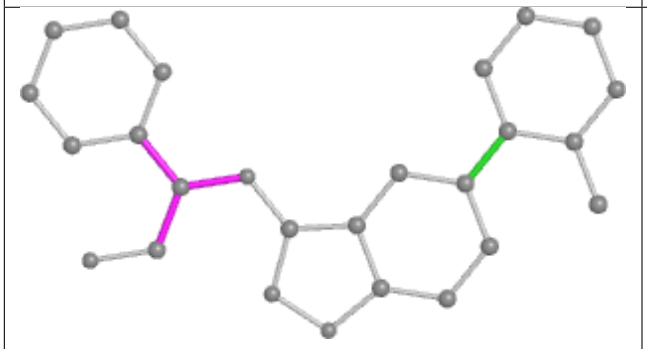
Ligand JK8 A 501



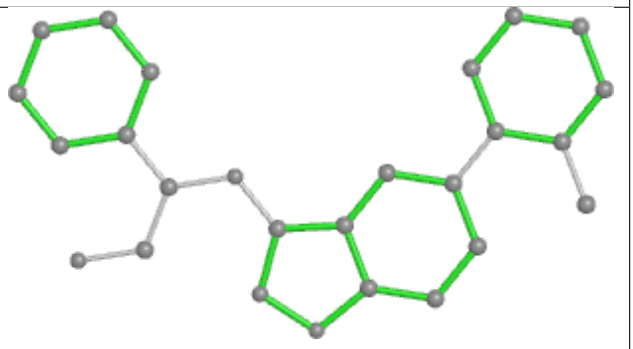
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

All 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
1	k	543:PRO	C	581:LYS	N	6.78
1	K	543:PRO	C	581:LYS	N	6.66
1	J	255:GLY	C	257:GLN	N	4.17
1	V	8:DC	O3'	2009:DG	P	3.75
1	W	8:DC	O3'	2009:DG	P	3.18
1	N	8:DC	O3'	2009:DG	P	3.10
1	n	8:DC	O3'	2009:DG	P	3.10
1	v	8:DC	O3'	2009:DG	P	3.10
1	F	8:DC	O3'	2009:DG	P	3.08
1	w	8:DC	O3'	2009:DG	P	3.02

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	8:DC	O3'	2009:DG	P	2.66

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	185/186 (99%)	0.71	19 (10%) 6 8	55, 92, 124, 173	0
1	S	185/186 (99%)	0.17	3 (1%) 72 70	26, 61, 84, 112	0
1	b	185/186 (99%)	0.42	9 (4%) 29 29	45, 79, 114, 134	0
1	s	186/186 (100%)	0.24	2 (1%) 80 79	36, 62, 95, 112	0
2	A	479/490 (97%)	0.28	18 (3%) 40 39	31, 74, 105, 175	0
2	C	482/490 (98%)	0.11	6 (1%) 79 77	24, 61, 90, 123	0
2	L	481/490 (98%)	-0.01	2 (0%) 92 92	16, 46, 73, 110	0
2	R	482/490 (98%)	-0.05	1 (0%) 95 95	17, 45, 70, 92	0
2	T	481/490 (98%)	-0.12	3 (0%) 89 89	20, 43, 67, 110	0
2	a	481/490 (98%)	0.20	11 (2%) 60 59	28, 63, 89, 113	0
2	c	482/490 (98%)	0.06	5 (1%) 82 81	31, 64, 100, 143	0
2	j	482/490 (98%)	-0.06	2 (0%) 92 92	20, 46, 73, 122	0
2	l	481/490 (98%)	-0.01	0 100 100	21, 47, 78, 132	0
2	r	484/490 (98%)	-0.01	3 (0%) 89 89	20, 45, 74, 105	0
2	t	481/490 (98%)	0.04	4 (0%) 86 85	14, 45, 77, 125	0
3	D	188/188 (100%)	0.58	22 (11%) 4 5	44, 83, 117, 148	0
3	U	188/188 (100%)	0.45	7 (3%) 41 40	36, 68, 99, 138	0
3	m	188/188 (100%)	0.33	9 (4%) 30 31	34, 68, 109, 154	0
4	E	20/20 (100%)	0.15	1 (5%) 28 29	34, 68, 112, 130	0
4	F	20/20 (100%)	-0.13	0 100 100	32, 70, 103, 148	0
4	N	20/20 (100%)	0.01	0 100 100	28, 45, 62, 68	0
4	O	20/20 (100%)	0.06	0 100 100	31, 49, 78, 88	0
4	W	20/20 (100%)	-0.10	0 100 100	29, 48, 88, 116	0
4	e	20/20 (100%)	-0.20	0 100 100	47, 81, 112, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
4	n	20/20 (100%)	0.17	0 100 100	34, 49, 96, 143	0
4	v	19/20 (95%)	0.02	0 100 100	21, 43, 77, 95	0
4	w	20/20 (100%)	-0.12	0 100 100	36, 42, 67, 81	0
5	K	187/187 (100%)	0.07	2 (1%) 80 79	22, 53, 88, 113	0
6	J	480/480 (100%)	0.05	3 (0%) 89 89	19, 48, 76, 105	0
7	M	189/189 (100%)	0.21	5 (2%) 56 54	33, 68, 96, 112	0
8	V	19/19 (100%)	0.05	0 100 100	27, 50, 95, 123	0
8	o	18/19 (94%)	-0.10	0 100 100	31, 43, 91, 98	0
9	d	181/181 (100%)	0.88	22 (12%) 4 5	45, 95, 125, 150	0
10	f	17/17 (100%)	0.02	0 100 100	63, 79, 110, 113	0
11	k	188/188 (100%)	0.32	7 (3%) 41 40	34, 61, 98, 136	0
12	u	187/187 (100%)	0.25	5 (2%) 54 53	27, 60, 88, 151	0
All	All	8246/8345 (98%)	0.13	171 (2%) 63 62	14, 56, 99, 175	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	d	418	LEU	6.9
1	B	435	GLU	5.7
2	A	442	GLU	5.7
1	B	510	ASP	5.1
9	d	455	LEU	5.1
7	M	588	ALA	5.0
2	A	387	ALA	4.9
7	M	509	ALA	4.7
9	d	417	LYS	4.5
1	B	434	VAL	4.4
3	m	490	GLY	4.3
3	D	506	MET	4.0
1	B	436	GLY	4.0
3	m	489	ILE	3.9
12	u	582	GLY	3.9
1	s	461	ILE	3.9
2	A	203	ASP	3.8
9	d	481	MET	3.8
9	d	623	GLY	3.7
11	k	458	ARG	3.7
1	B	540	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	A	68	ALA	3.6
12	u	581	LYS	3.5
2	A	490	LEU	3.5
2	t	438[A]	ARG	3.5
1	B	455	LEU	3.5
9	d	456	PRO	3.4
9	d	478	ILE	3.4
2	A	491	GLY	3.4
9	d	506	MET	3.4
1	B	470	ASP	3.3
3	D	507	THR	3.3
1	B	457	LEU	3.3
3	D	481	MET	3.2
3	D	512	ASP	3.2
9	d	454	ILE	3.2
12	u	417	LYS	3.2
2	T	438[A]	ARG	3.1
3	U	417	LYS	3.1
1	B	508	ASP	3.1
2	A	121	MET	3.1
2	a	68	ALA	3.1
2	a	58[A]	MET	3.1
3	U	507	THR	3.1
2	a	88[A]	GLU	3.1
2	a	158	SER	3.0
3	U	508	ASP	3.0
9	d	505	ILE	3.0
1	b	582	GLY	3.0
4	E	20	DT	3.0
11	k	463	ASN	3.0
1	b	510	ASP	3.0
2	A	107	GLN	3.0
2	a	73[A]	ASP	2.9
3	D	583	LEU	2.9
2	c	120	ALA	2.9
2	c	472	GLU	2.8
3	m	617	THR	2.8
1	b	515	HIS	2.8
3	D	422	SER	2.8
2	C	83	ASP	2.8
1	B	438	SER	2.8
3	m	584	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	U	518	THR	2.7
9	d	469	LEU	2.7
1	B	636	ASN	2.7
3	D	439	ALA	2.7
3	D	585	GLU	2.7
1	B	633	ILE	2.7
2	A	388	LEU	2.6
2	r	73[A]	ASP	2.6
2	C	31	VAL	2.6
2	t	307	ASP	2.6
11	k	588	ALA	2.6
1	b	435[A]	GLU	2.6
3	m	457	LEU	2.6
1	B	458[A]	ARG	2.6
3	U	475	ASN	2.6
1	b	461	ILE	2.6
12	u	431	ILE	2.5
2	t	439	ASP	2.5
9	d	470	ASP	2.5
3	U	581	LYS	2.5
9	d	432	PHE	2.5
3	D	501	HIS	2.5
2	c	11	GLU	2.5
2	C	55	GLU	2.5
1	b	484	ALA	2.5
3	D	584	GLY	2.5
2	a	153	ASN	2.5
3	m	480[A]	GLN	2.5
1	S	468	ARG	2.5
2	R	391	ILE	2.5
9	d	431	ILE	2.4
2	c	471	ASP	2.4
11	k	509	ALA	2.4
2	A	441	ILE	2.4
2	r	307	ASP	2.4
3	D	496	ALA	2.4
9	d	504	VAL	2.4
12	u	457	LEU	2.4
11	k	462	LEU	2.4
2	a	132	THR	2.4
3	m	581	LYS	2.4
2	A	489	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	r	240	SER	2.4
1	B	469	LEU	2.4
3	D	520	LEU	2.4
3	D	581	LYS	2.3
2	A	446	ASN	2.3
2	a	298	LEU	2.3
2	A	384	LEU	2.3
3	m	491	GLY	2.3
1	B	465	GLU	2.3
2	a	126	ALA	2.3
3	D	440	GLY	2.3
1	b	587	ASN	2.3
5	K	510	ASP	2.3
7	M	435[A]	GLU	2.3
9	d	521	LEU	2.3
11	k	498	ALA	2.3
2	C	66[A]	LYS	2.2
9	d	430	GLU	2.2
2	A	75	MET	2.2
7	M	525	TYR	2.2
9	d	495	LEU	2.2
3	D	461	ILE	2.2
2	A	454[A]	GLU	2.2
1	b	494	ASP	2.2
9	d	602	ALA	2.2
1	B	539	ILE	2.2
3	D	519	LEU	2.2
5	K	583	LEU	2.2
2	A	73[A]	ASP	2.2
1	s	539	ILE	2.2
3	D	623	GLY	2.2
2	C	73	ASP	2.2
2	L	255	GLY	2.2
2	T	72	GLY	2.2
9	d	462	LEU	2.2
9	d	493	PHE	2.2
2	A	389	ASP	2.2
1	B	433	LEU	2.1
2	c	31	VAL	2.1
3	D	441	GLY	2.1
1	S	473	LEU	2.1
3	m	455	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
9	d	503	ILE	2.1
1	S	635	ASP	2.1
3	D	498	ALA	2.1
2	C	428	MET	2.1
2	j	61	ASP	2.1
2	a	52	GLY	2.1
7	M	596	MET	2.1
6	J	119	ALA	2.1
11	k	512	ASP	2.1
6	J	224	ILE	2.1
1	B	443	THR	2.1
2	L	245	SER	2.1
3	U	445	SER	2.1
1	b	635	ASP	2.1
2	T	73	ASP	2.1
6	J	417	LEU	2.0
3	D	437	ASP	2.0
2	A	204	ILE	2.0
2	t	391	ILE	2.0
3	D	487	THR	2.0
2	j	16	SER	2.0
1	B	505	ILE	2.0
2	a	150	TYR	2.0
3	D	455	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

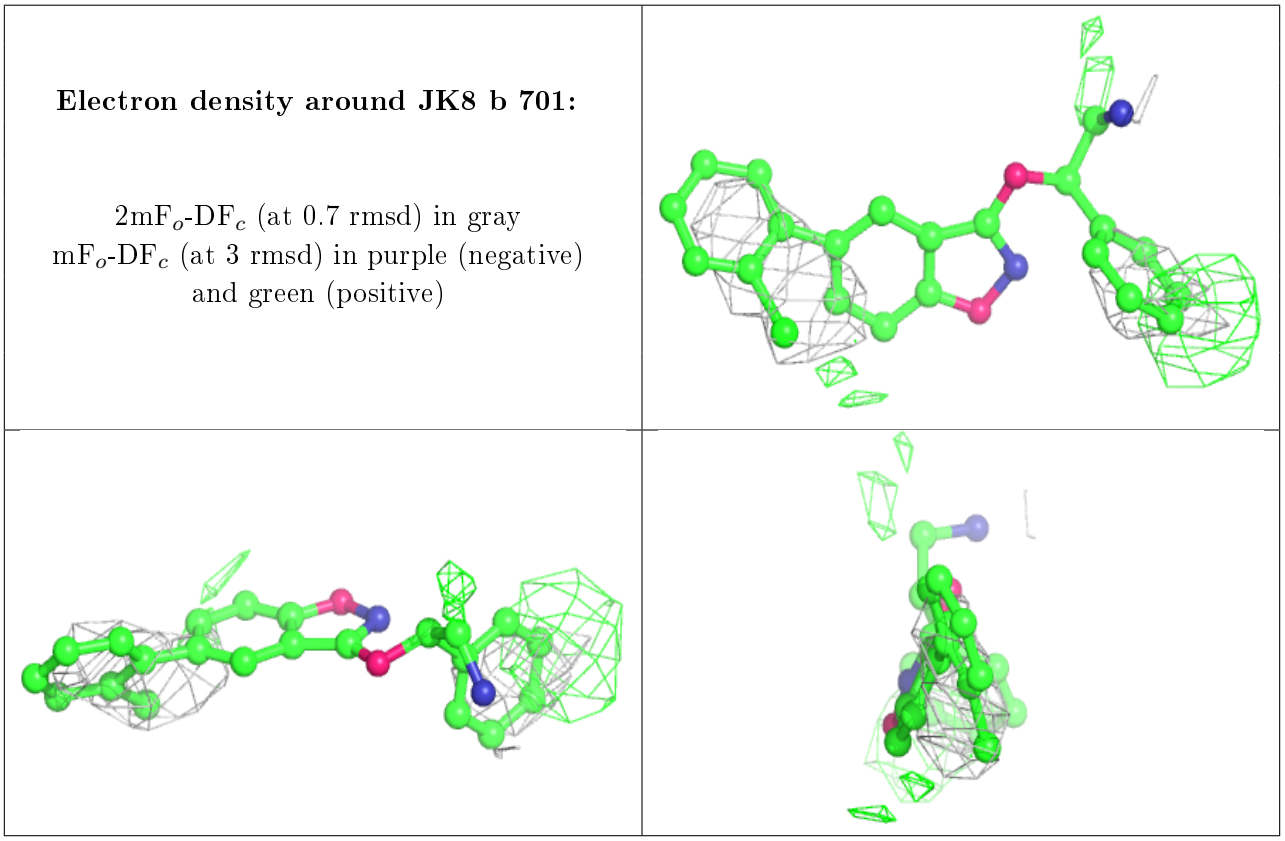
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	JK8	b	701	26/26	0.72	0.66	7,9,9,10	26
13	JK8	U	701[A]	26/26	0.84	0.56	7,9,11,11	26
13	JK8	d	701[A]	26/26	0.90	0.31	34,42,60,61	26
13	JK8	A	501	26/26	0.90	0.36	26,33,47,52	26
13	JK8	R	501	26/26	0.92	0.30	16,17,18,22	26
13	JK8	t	501[A]	26/26	0.92	0.40	26,31,33,43	26
13	JK8	s	701	26/26	0.92	0.30	11,13,18,19	26
13	JK8	L	501[A]	26/26	0.94	0.25	20,21,29,30	26
13	JK8	C	501[A]	26/26	0.94	0.22	42,63,68,68	0
13	JK8	l	501[A]	26/26	0.94	0.27	45,58,69,72	0
13	JK8	k	701	26/26	0.95	0.25	36,47,69,71	0
13	JK8	J	501	26/26	0.95	0.18	33,46,54,57	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.

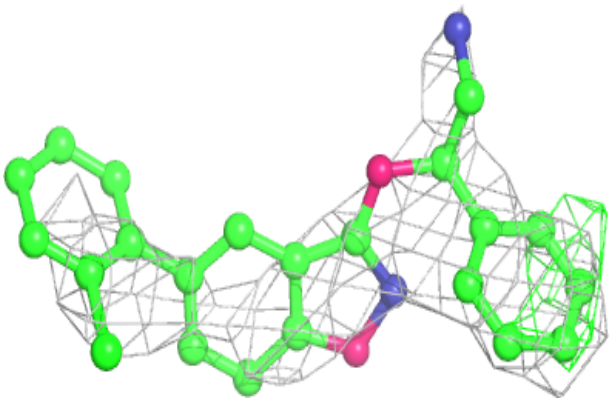
Electron density around JK8 b 701:

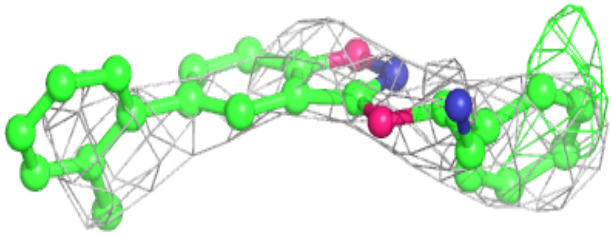
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

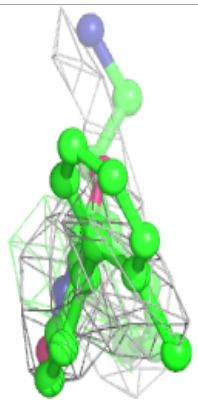


Electron density around JK8 U 701 (A):

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

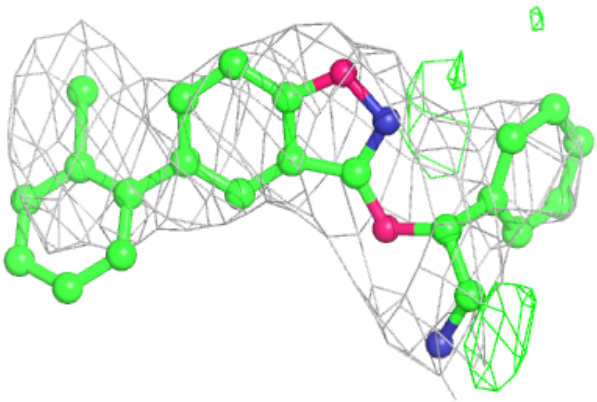


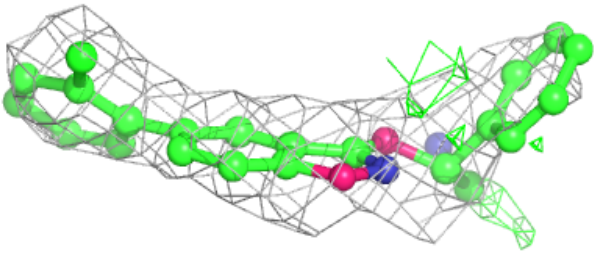


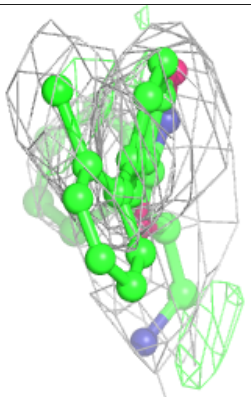


Electron density around JK8 d 701 (A):

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

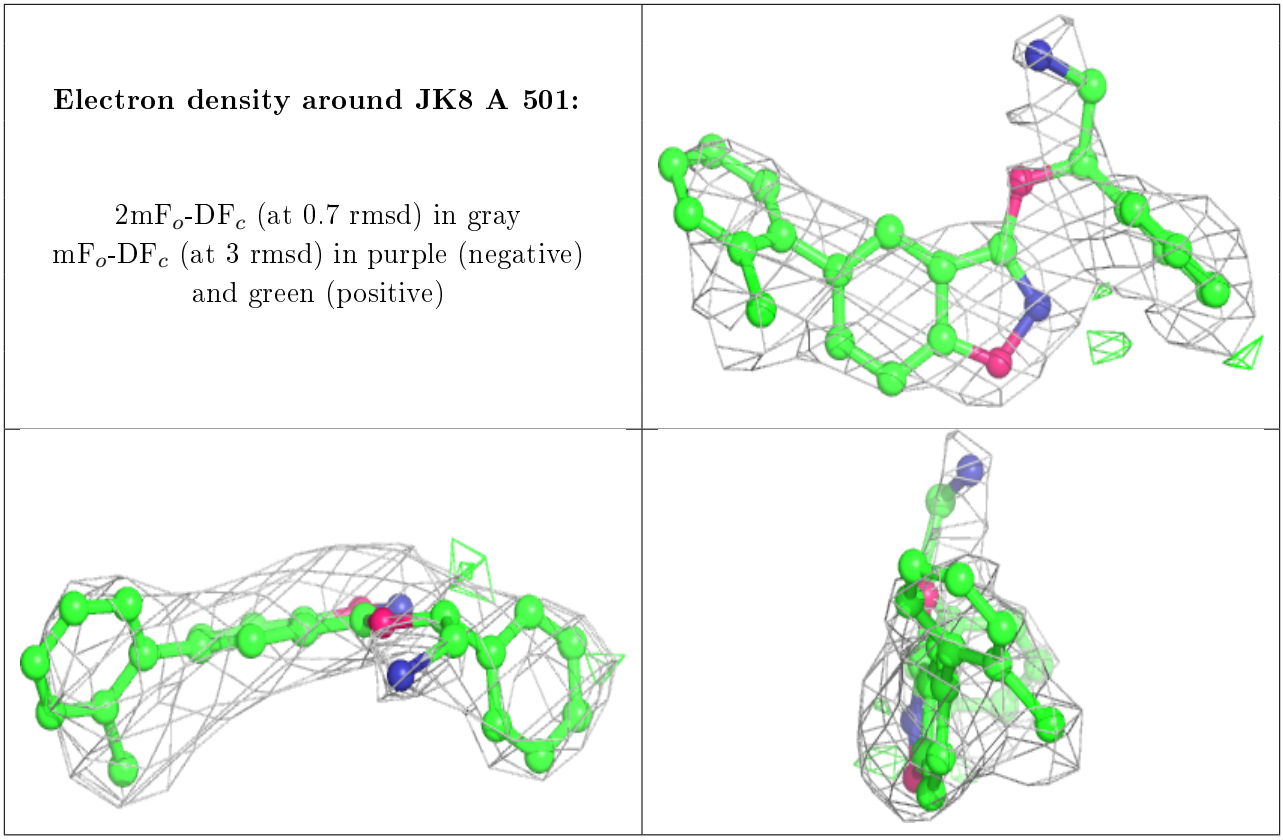






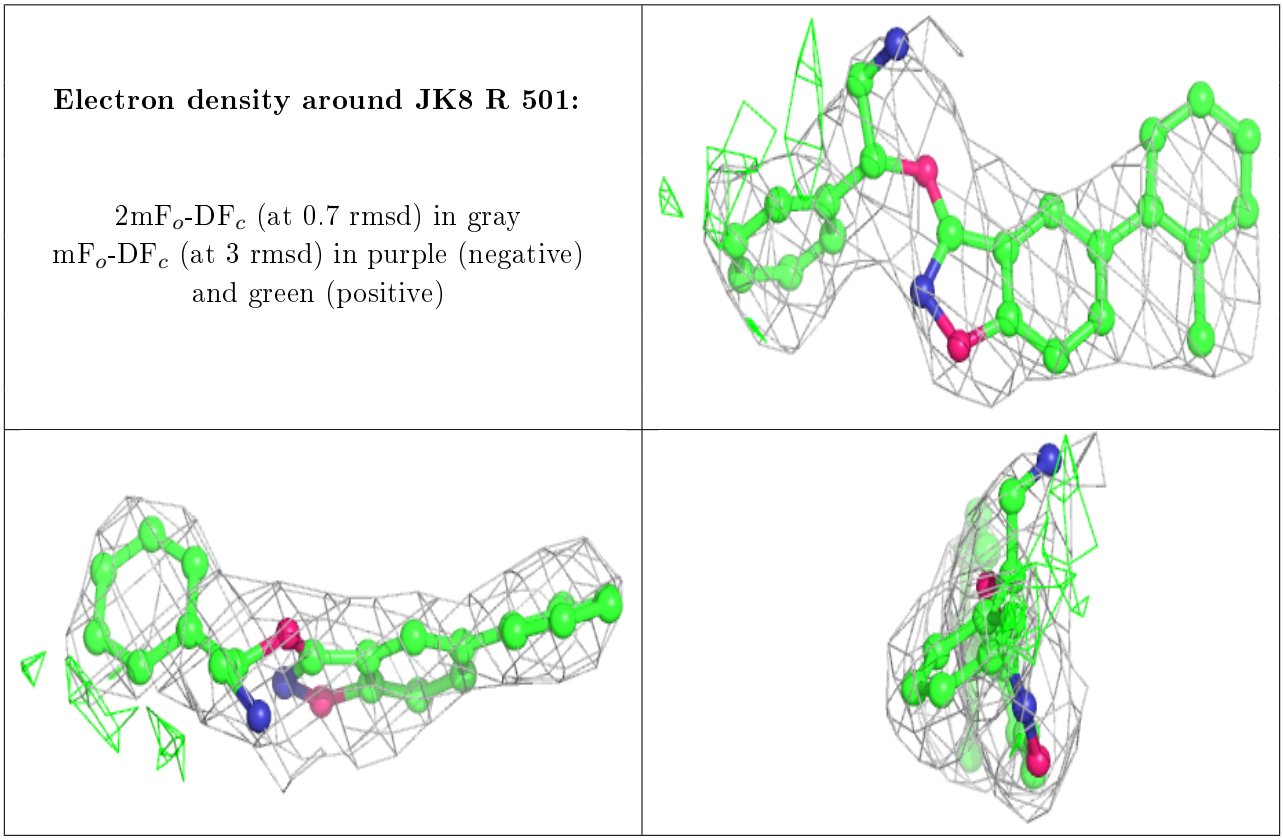
Electron density around JK8 A 501:

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



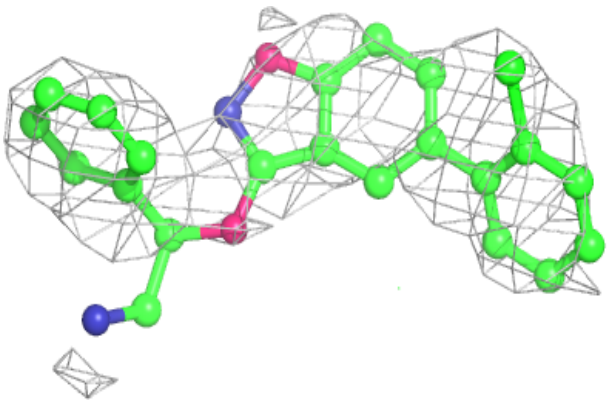
Electron density around JK8 R 501:

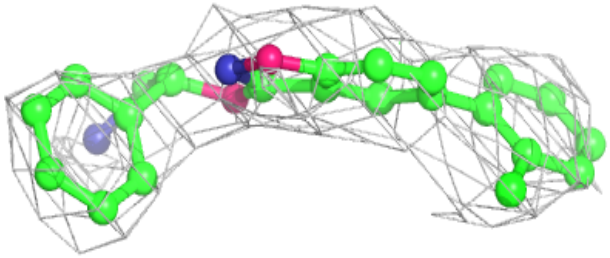
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

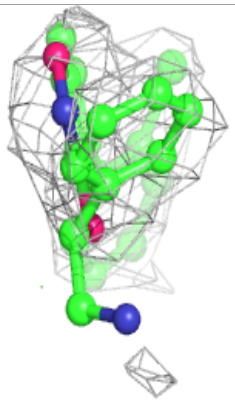


Electron density around JK8 t 501 (A):

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

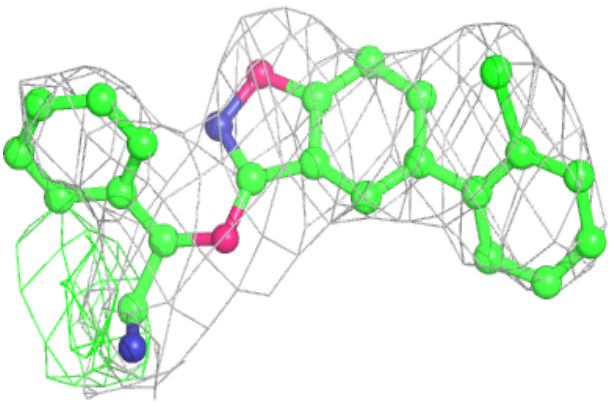


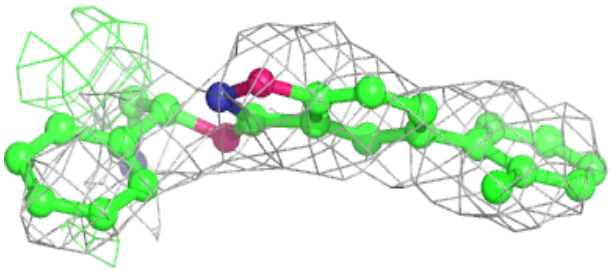


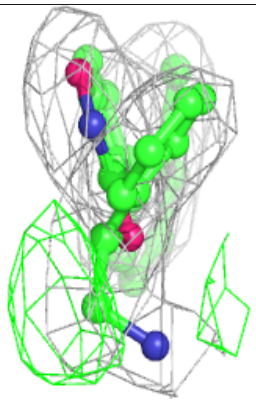


Electron density around JK8 s 701:

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

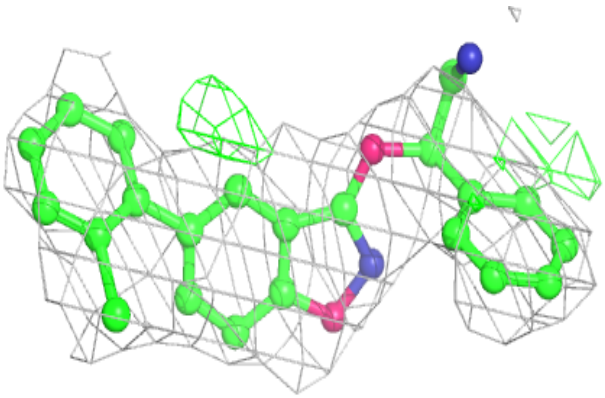


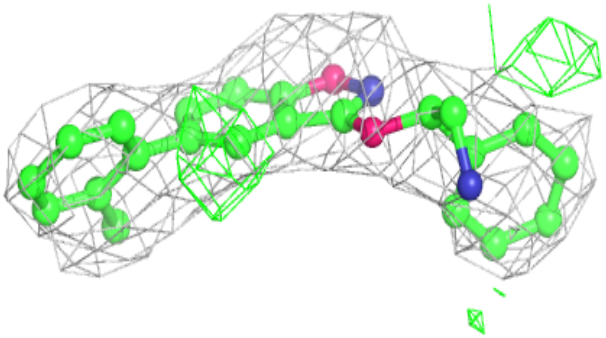


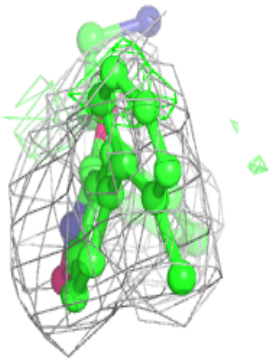


Electron density around JK8 L 501 (A):

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

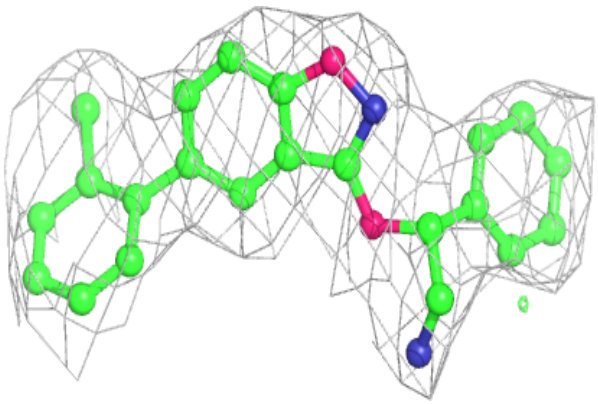


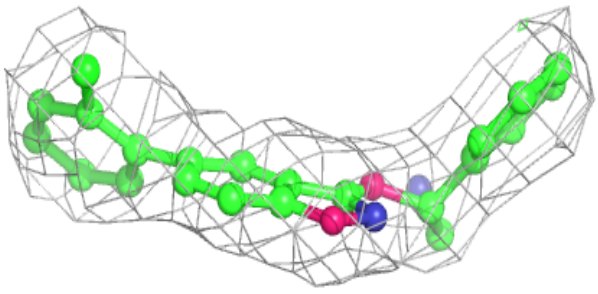


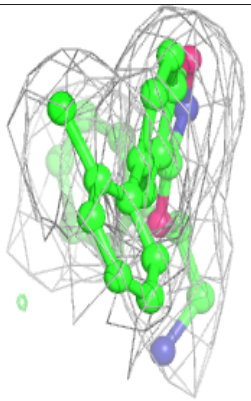


Electron density around JK8 C 501 (A):

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

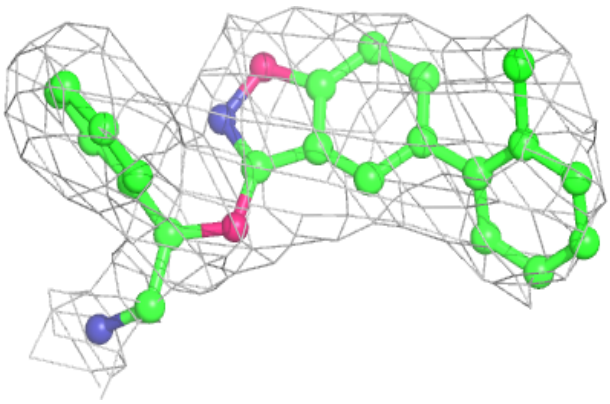


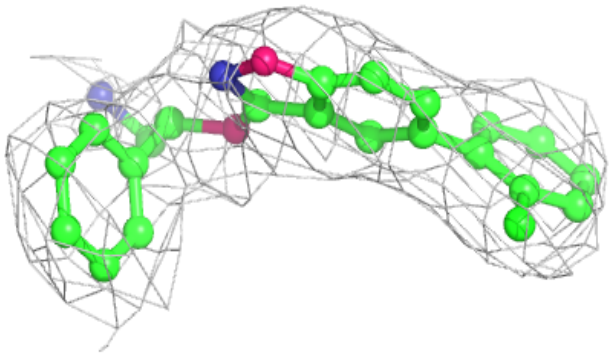


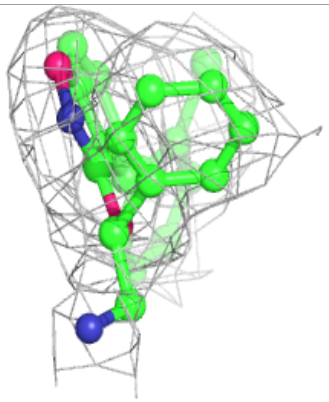


Electron density around JK8 l 501 (A):

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

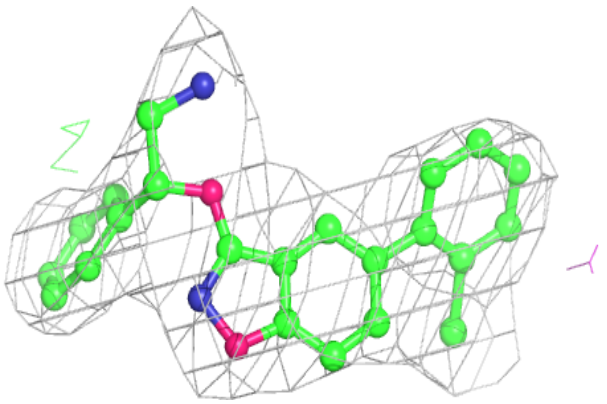


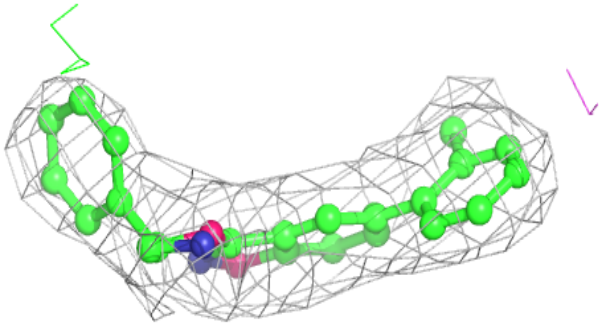


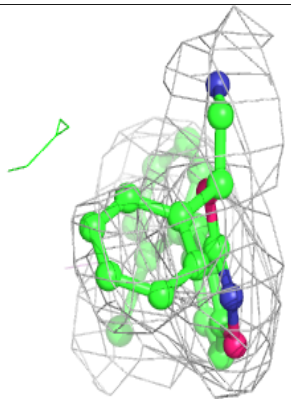


Electron density around JK8 k 701:

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

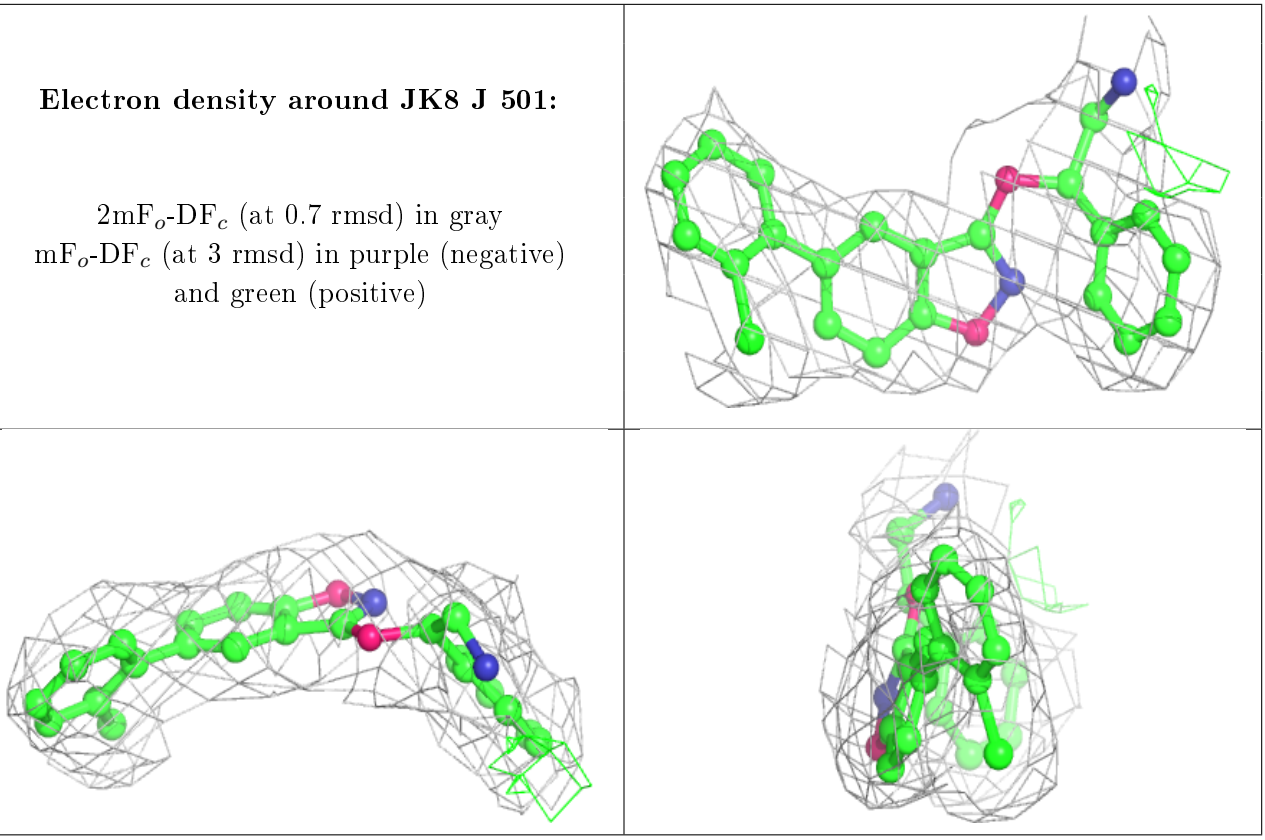






Electron density around JK8 J 501:

$2mF_o$-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.