wwPDB X-ray Structure Validation Summary Report (i)

Jan 16, 2024 – 01:01 am GMT

PDB ID	:	6QX1
Title	:	2.7A structure of benzoisoxazole 3 with S.aureus DNA gyrase and DNA.
Authors	:	Bax, B.D.
Deposited on	:	2019-03-06
Resolution	:	2.65 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 (i) 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 (i)) were used in the production of this report:

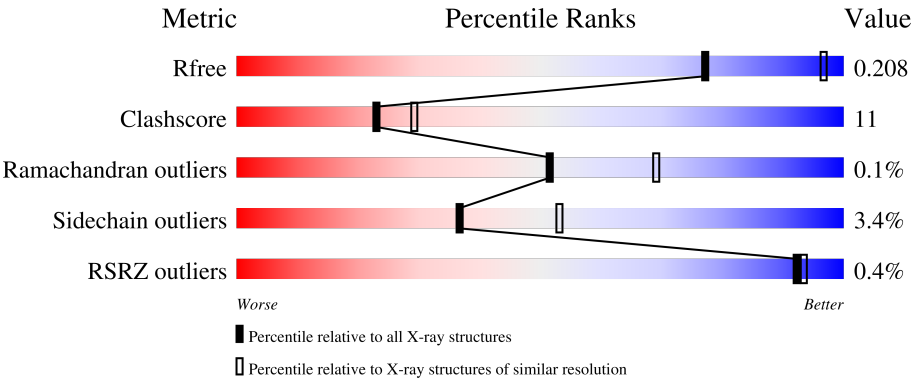
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	202	76% 16% 6%
1	D	202	78% 14% 6%
2	A	490	81% 15%
2	C	490	83% 13%
3	E	20	60% 30% 10%

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Mol	Chain	Length	Quality of chain
3	F	20	45% 50% 5%

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
5	JK8	B	702	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12028 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	189	Total	C	N	O	S	0	1	0
			1486	931	258	288	9			
1	D	189	Total	C	N	O	S	0	4	0
			1493	942	255	287	9			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	initiating methionine	UNP P66937
B	544	THR	-	expression tag	UNP P66937
B	545	GLY	-	expression tag	UNP P66937
B	580	TYR	-	expression tag	UNP P66937
B	581	LYS	-	expression tag	UNP P66937
B	582	GLY	-	expression tag	UNP P66937
B	583	LEU	-	expression tag	UNP P66937
B	584	GLY	-	expression tag	UNP P66937
B	585	GLU	-	expression tag	UNP P66937
B	586	MET	-	expression tag	UNP P66937
B	587	ASN	-	expression tag	UNP P66937
B	588	ALA	-	expression tag	UNP P66937
B	589	ASP	-	expression tag	UNP P66937
B	590	GLN	-	expression tag	UNP P66937
B	591	LEU	-	expression tag	UNP P66937
B	592	TRP	-	expression tag	UNP P66937
B	593	GLU	-	expression tag	UNP P66937
B	594	THR	-	expression tag	UNP P66937
B	595	THR	-	expression tag	UNP P66937
B	596	MET	-	expression tag	UNP P66937
B	597	ASN	-	expression tag	UNP P66937
B	598	PRO	-	expression tag	UNP P66937
B	599	GLU	-	expression tag	UNP P66937
B	600	HIS	-	expression tag	UNP P66937
B	601	ARG	-	expression tag	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	602	ALA	-	expression tag	UNP P66937
B	603	LEU	-	expression tag	UNP P66937
B	604	LEU	-	expression tag	UNP P66937
B	605	GLN	-	expression tag	UNP P66937
B	606	VAL	-	expression tag	UNP P66937
B	607	LYS	-	expression tag	UNP P66937
B	608	LEU	-	expression tag	UNP P66937
B	609	GLU	-	expression tag	UNP P66937
B	610	ASP	-	expression tag	UNP P66937
B	611	ALA	-	expression tag	UNP P66937
B	612	ILE	-	expression tag	UNP P66937
B	613	GLU	-	expression tag	UNP P66937
B	614	ALA	-	expression tag	UNP P66937
B	615	ASP	-	expression tag	UNP P66937
B	616	GLN	-	expression tag	UNP P66937
B	617	THR	-	expression tag	UNP P66937
B	618	PHE	-	expression tag	UNP P66937
B	619	GLU	-	expression tag	UNP P66937
B	620	MET	-	expression tag	UNP P66937
B	621	LEU	-	expression tag	UNP P66937
B	622	MET	-	expression tag	UNP P66937
B	623	GLY	-	expression tag	UNP P66937
B	624	ASP	-	expression tag	UNP P66937
B	625	VAL	-	expression tag	UNP P66937
B	626	VAL	-	expression tag	UNP P66937
B	627	GLU	-	expression tag	UNP P66937
B	628	ASN	-	expression tag	UNP P66937
B	629	ARG	-	expression tag	UNP P66937
B	630	ARG	-	expression tag	UNP P66937
B	631	GLN	-	expression tag	UNP P66937
B	632	PHE	-	expression tag	UNP P66937
B	633	ILE	-	expression tag	UNP P66937
B	634	GLU	-	expression tag	UNP P66937
B	635	ASP	-	expression tag	UNP P66937
B	636	ASN	-	expression tag	UNP P66937
B	637	ALA	-	expression tag	UNP P66937
B	638	VAL	-	expression tag	UNP P66937
B	639	TYR	-	expression tag	UNP P66937
B	640	ALA	-	expression tag	UNP P66937
B	641	ASN	-	expression tag	UNP P66937
B	642	LEU	-	expression tag	UNP P66937
B	643	ASP	-	expression tag	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	644	PHE	-	expression tag	UNP P66937
D	409	MET	-	initiating methionine	UNP P66937
D	544	THR	-	expression tag	UNP P66937
D	545	GLY	-	expression tag	UNP P66937
D	580	TYR	-	expression tag	UNP P66937
D	581	LYS	-	expression tag	UNP P66937
D	582	GLY	-	expression tag	UNP P66937
D	583	LEU	-	expression tag	UNP P66937
D	584	GLY	-	expression tag	UNP P66937
D	585	GLU	-	expression tag	UNP P66937
D	586	MET	-	expression tag	UNP P66937
D	587	ASN	-	expression tag	UNP P66937
D	588	ALA	-	expression tag	UNP P66937
D	589	ASP	-	expression tag	UNP P66937
D	590	GLN	-	expression tag	UNP P66937
D	591	LEU	-	expression tag	UNP P66937
D	592	TRP	-	expression tag	UNP P66937
D	593	GLU	-	expression tag	UNP P66937
D	594	THR	-	expression tag	UNP P66937
D	595	THR	-	expression tag	UNP P66937
D	596	MET	-	expression tag	UNP P66937
D	597	ASN	-	expression tag	UNP P66937
D	598	PRO	-	expression tag	UNP P66937
D	599	GLU	-	expression tag	UNP P66937
D	600	HIS	-	expression tag	UNP P66937
D	601	ARG	-	expression tag	UNP P66937
D	602	ALA	-	expression tag	UNP P66937
D	603	LEU	-	expression tag	UNP P66937
D	604	LEU	-	expression tag	UNP P66937
D	605	GLN	-	expression tag	UNP P66937
D	606	VAL	-	expression tag	UNP P66937
D	607	LYS	-	expression tag	UNP P66937
D	608	LEU	-	expression tag	UNP P66937
D	609	GLU	-	expression tag	UNP P66937
D	610	ASP	-	expression tag	UNP P66937
D	611	ALA	-	expression tag	UNP P66937
D	612	ILE	-	expression tag	UNP P66937
D	613	GLU	-	expression tag	UNP P66937
D	614	ALA	-	expression tag	UNP P66937
D	615	ASP	-	expression tag	UNP P66937
D	616	GLN	-	expression tag	UNP P66937
D	617	THR	-	expression tag	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
D	618	PHE	-	expression tag	UNP P66937
D	619	GLU	-	expression tag	UNP P66937
D	620	MET	-	expression tag	UNP P66937
D	621	LEU	-	expression tag	UNP P66937
D	622	MET	-	expression tag	UNP P66937
D	623	GLY	-	expression tag	UNP P66937
D	624	ASP	-	expression tag	UNP P66937
D	625	VAL	-	expression tag	UNP P66937
D	626	VAL	-	expression tag	UNP P66937
D	627	GLU	-	expression tag	UNP P66937
D	628	ASN	-	expression tag	UNP P66937
D	629	ARG	-	expression tag	UNP P66937
D	630	ARG	-	expression tag	UNP P66937
D	631	GLN	-	expression tag	UNP P66937
D	632	PHE	-	expression tag	UNP P66937
D	633	ILE	-	expression tag	UNP P66937
D	634	GLU	-	expression tag	UNP P66937
D	635	ASP	-	expression tag	UNP P66937
D	636	ASN	-	expression tag	UNP P66937
D	637	ALA	-	expression tag	UNP P66937
D	638	VAL	-	expression tag	UNP P66937
D	639	TYR	-	expression tag	UNP P66937
D	640	ALA	-	expression tag	UNP P66937
D	641	ASN	-	expression tag	UNP P66937
D	642	LEU	-	expression tag	UNP P66937
D	643	ASP	-	expression tag	UNP P66937
D	644	PHE	-	expression tag	UNP P66937

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	483	Total	C	N	O	S	0	4	0
			3868	2404	710	738	16			
2	C	481	Total	C	N	O	S	0	3	0
			3843	2389	702	736	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	P	0	1	0
			426	203	79	124	20			

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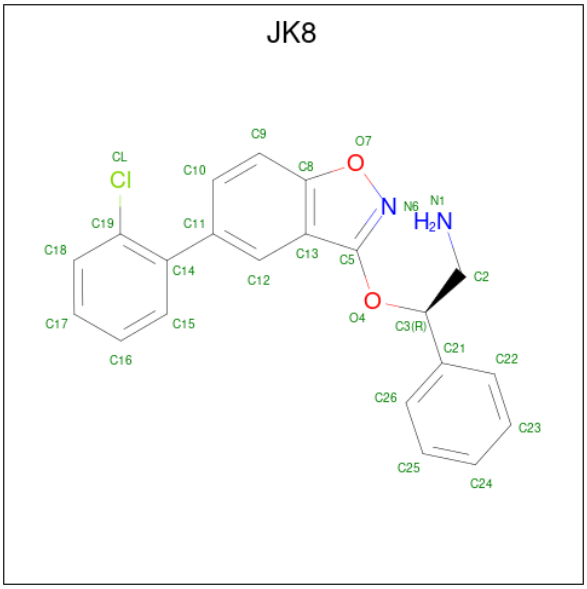
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	20	Total	C	N	O	P	0	5	0
			491	233	89	145	24			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

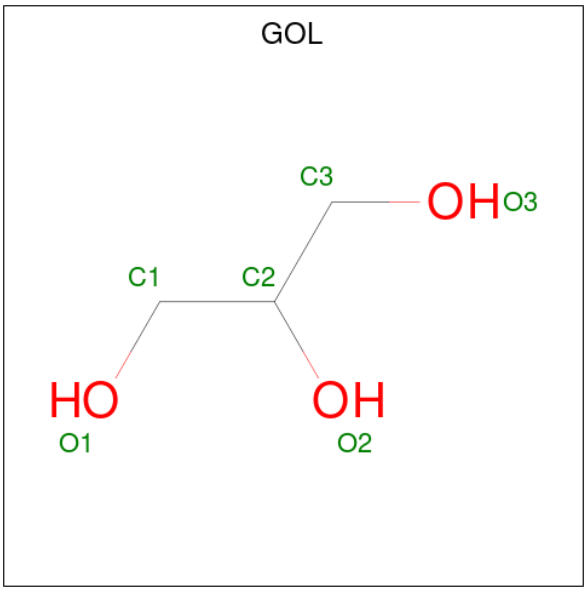
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		

- Molecule 5 is (2 {R})-2-[[5-(2-chlorophenyl)-1,2-benzoxazol-3-yl]oxy]-2-phenyl-ethanamine (three-letter code: JK8) (formula: $C_{21}H_{17}ClN_2O_2$) (labeled as "Ligand of Interest" by depositor).



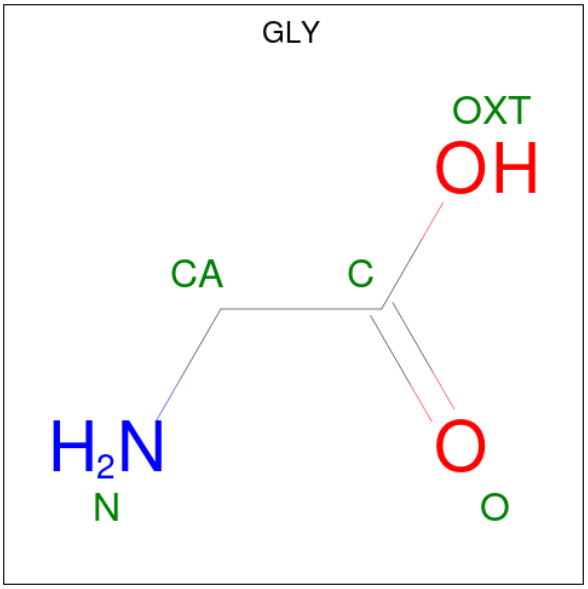
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	0	0
			26	21	1	2	2		
5	D	1	Total	C	Cl	N	O	0	1
			26	21	1	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0

- Molecule 7 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O 4 2 1 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Cl 1 1	0	0

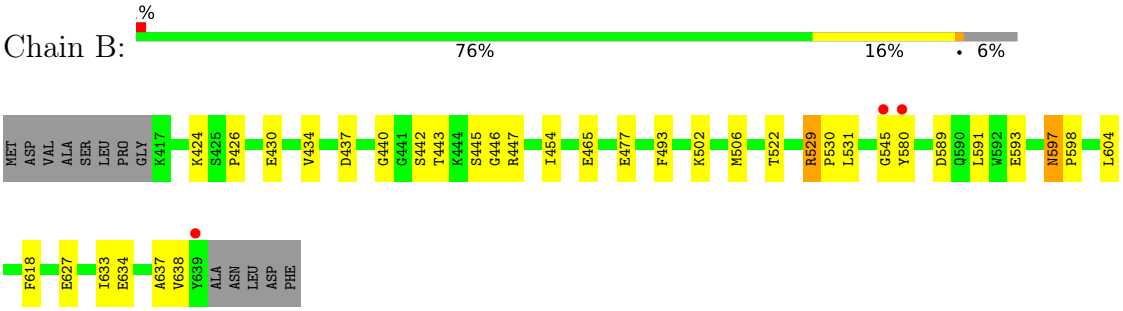
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	25	Total O 25 25	0	0
9	A	117	Total O 117 117	0	0
9	D	19	Total O 19 19	0	0
9	C	128	Total O 128 128	0	0
9	E	24	Total O 24 24	0	0
9	F	18	Total O 19 19	0	1

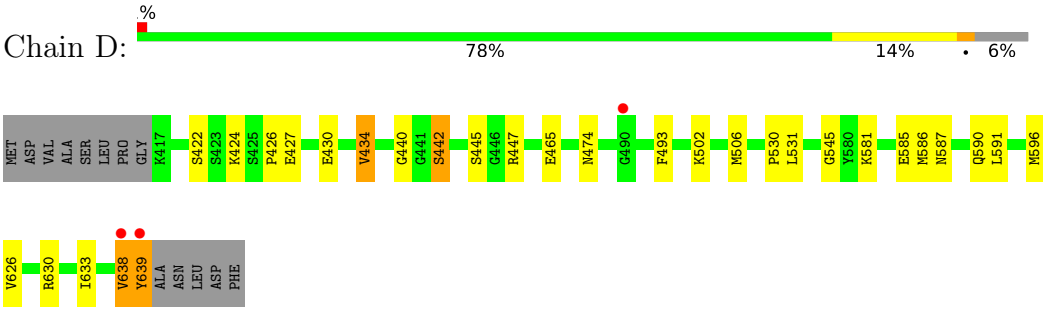
3 Residue-property plots (i)

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.

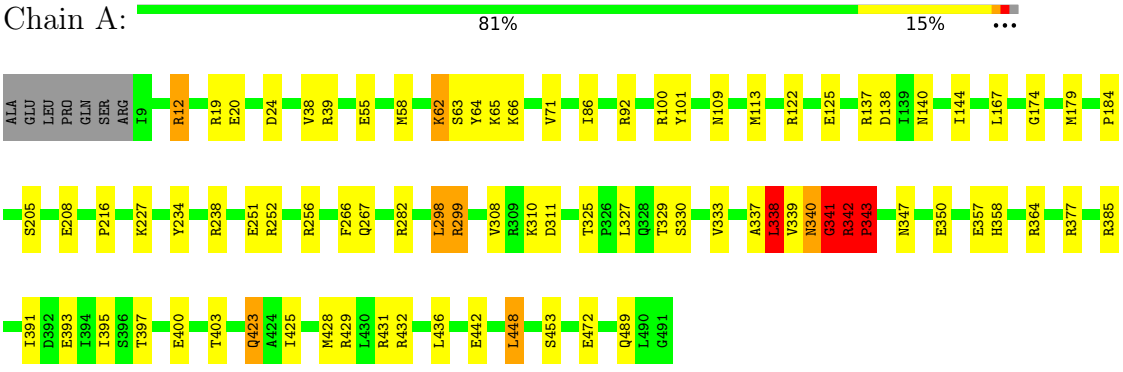
• Molecule 1: DNA gyrase subunit B



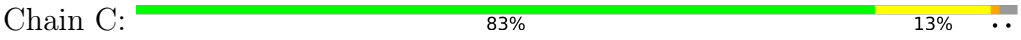
• Molecule 1: DNA gyrase subunit B

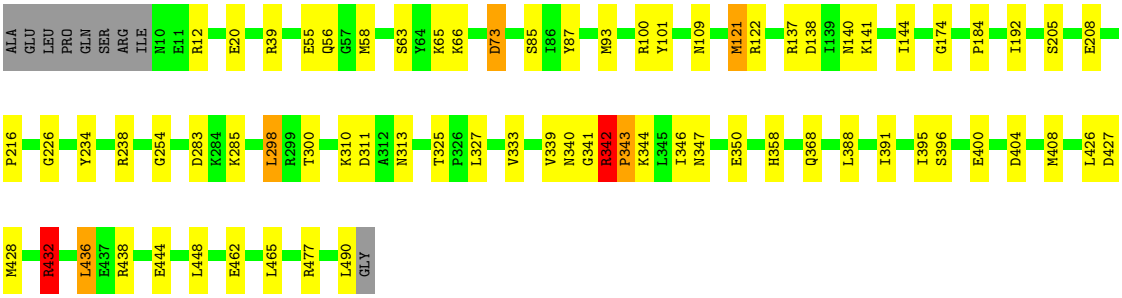


• Molecule 2: DNA gyrase subunit A



• Molecule 2: DNA gyrase subunit A



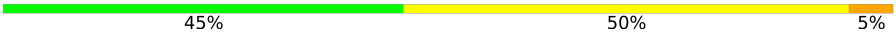


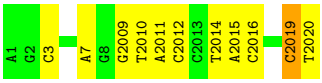
• Molecule 3: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain E:

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

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	93.19Å 93.19Å 408.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.52 – 2.65 57.45 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (57.52-2.65) 98.4 (57.45-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.162 , 0.206 0.164 , 0.208	Depositor DCC
R_{free} test set	2904 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.129 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12028	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: MN, CL, GOL, 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	0.58	2/1509 (0.1%)	0.93	1/2036 (0.0%)
1	D	0.48	0/1517	0.83	0/2050
2	A	0.99	18/3916 (0.5%)	1.28	27/5271 (0.5%)
2	C	0.99	14/3894 (0.4%)	1.15	15/5245 (0.3%)
3	E	0.90	2/476 (0.4%)	1.05	1/730 (0.1%)
3	F	0.77	1/548 (0.2%)	1.03	2/838 (0.2%)
All	All	0.88	37/11860 (0.3%)	1.12	46/16170 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	A	1	5
2	C	0	1
All	All	1	7

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	341	GLY	CA-C	24.40	1.90	1.51
2	C	342	ARG	NE-CZ	-23.05	1.03	1.33
2	C	342	ARG	CZ-NH1	19.83	1.58	1.33
2	C	342	ARG	CB-CG	18.76	2.03	1.52
2	A	341	GLY	C-O	16.18	1.49	1.23

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	342	ARG	NE-CZ-NH2	-26.07	107.26	120.30
2	A	342	ARG	NE-CZ-NH1	-23.14	108.73	120.30
2	C	342	ARG	CD-NE-CZ	19.01	150.21	123.60
2	C	342	ARG	CB-CA-C	-17.87	74.67	110.40
2	C	342	ARG	N-CA-CB	17.30	141.74	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	338	LEU	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	337	ALA	Peptide
2	A	338	LEU	Peptide
2	A	341	GLY	Mainchain
2	A	342	ARG	Sidechain
2	A	343	PRO	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1486	0	1457	38	0
1	D	1493	0	1449	32	0
2	A	3868	0	3931	54	0
2	C	3843	0	3899	72	0
3	E	426	0	238	54	0
3	F	491	0	273	58	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	26	0	0	11	0
5	D	26	0	0	8	0
6	A	12	0	16	0	0
6	C	6	0	8	0	0
6	E	12	0	16	3	0
7	C	4	0	2	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
9	A	117	0	0	8	0
9	B	25	0	0	2	0
9	C	128	0	0	8	0
9	D	19	0	0	0	0
9	E	24	0	0	1	0
9	F	19	0	0	1	0
All	All	12028	0	11289	262	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 262 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)
2:A:342:ARG:CD	2:A:342:ARG:CG	1.76	1.62
2:A:341:GLY:C	2:A:341:GLY:CA	1.90	1.40
2:C:342:ARG:C	2:C:342:ARG:CA	1.93	1.36
2:C:342:ARG:CG	2:C:342:ARG:CB	2.03	1.35
2:C:490:LEU:C	7:C:501:GLY:N	1.85	1.29

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	188/202 (93%)	179 (95%)	8 (4%)	1 (0%)	29 43
1	D	190/202 (94%)	184 (97%)	6 (3%)	0	100 100
2	A	485/490 (99%)	472 (97%)	12 (2%)	1 (0%)	47 64
2	C	482/490 (98%)	473 (98%)	9 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1345/1384 (97%)	1308 (97%)	35 (3%)	2 (0%)	51 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	580	TYR
2	A	338	LEU

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	156/168 (93%)	150 (96%)	6 (4%)	33 49
1	D	154/168 (92%)	144 (94%)	10 (6%)	17 26
2	A	419/423 (99%)	405 (97%)	14 (3%)	38 54
2	C	417/423 (99%)	407 (98%)	10 (2%)	49 67
All	All	1146/1182 (97%)	1106 (96%)	40 (4%)	37 52

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	639[A]	TYR
2	C	342	ARG
1	D	639[B]	TYR
2	C	121	MET
2	C	432	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	56	GLN
2	C	107	GLN
2	C	368	GLN

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Mol	Chain	Res	Type
2	A	10	ASN
1	B	597	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
6	GOL	E	2102	-	5,5,5	0.12	0	5,5,5	0.45	0
5	JK8	B	702	-	24,29,29	3.57	5 (20%)	29,40,40	3.23	18 (62%)
6	GOL	A	501	-	5,5,5	0.15	0	5,5,5	0.42	0
7	GLY	C	501	-	3,3,4	0.95	0	0,2,4	-	-
6	GOL	E	2101	-	5,5,5	0.17	0	5,5,5	0.45	0
6	GOL	C	503	-	5,5,5	0.10	0	5,5,5	0.36	0
6	GOL	A	502	-	5,5,5	0.14	0	5,5,5	0.66	0
5	JK8	D	702[A]	-	24,29,29	1.77	6 (25%)	29,40,40	2.48	10 (34%)

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
6	GOL	E	2102	-	-	2/4/4/4	-
5	JK8	B	702	-	-	1/12/14/14	0/4/4/4
6	GOL	A	501	-	-	2/4/4/4	-
7	GLY	C	501	-	-	0/0/1/2	-
6	GOL	E	2101	-	-	0/4/4/4	-
6	GOL	C	503	-	-	4/4/4/4	-
6	GOL	A	502	-	-	2/4/4/4	-
5	JK8	D	702[A]	-	-	1/12/14/14	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	702	JK8	C15-C14	-11.95	1.21	1.40
5	B	702	JK8	C18-C19	9.37	1.58	1.38
5	B	702	JK8	O4-C3	-5.97	1.39	1.44
5	D	702[A]	JK8	C14-C11	-4.74	1.40	1.49
5	D	702[A]	JK8	C5-C13	-4.38	1.41	1.45

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	702[A]	JK8	C5-O4-C3	-8.22	104.96	116.79
5	B	702	JK8	C11-C14-C19	-7.10	111.57	123.53
5	B	702	JK8	C10-C11-C14	-6.42	110.50	120.91
5	B	702	JK8	C17-C16-C15	5.62	128.75	120.19
5	B	702	JK8	C5-C13-C8	-4.65	100.24	106.59

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	702[A]	JK8	N1-C2-C3-C21
6	C	503	GOL	O1-C1-C2-O2
6	A	501	GOL	C1-C2-C3-O3
6	A	502	GOL	C1-C2-C3-O3
6	C	503	GOL	O1-C1-C2-C3

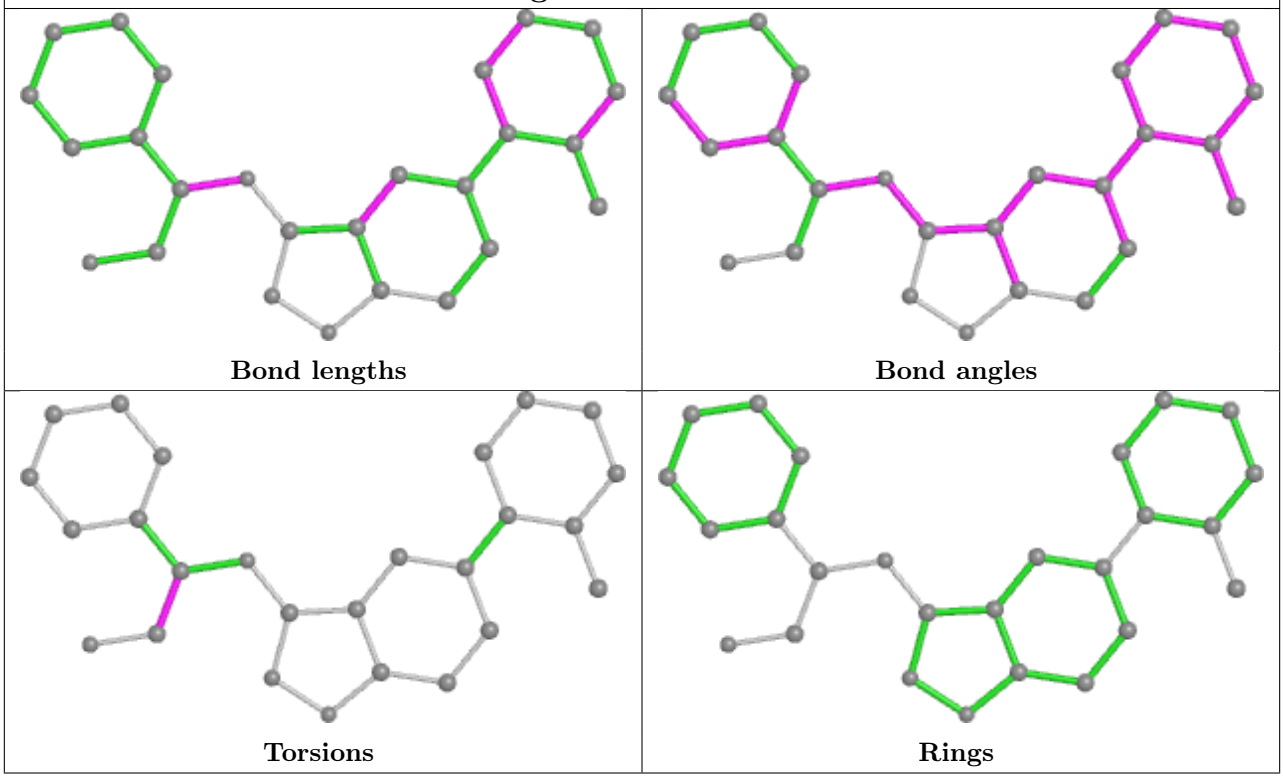
There are no ring outliers.

4 monomers are involved in 24 short contacts:

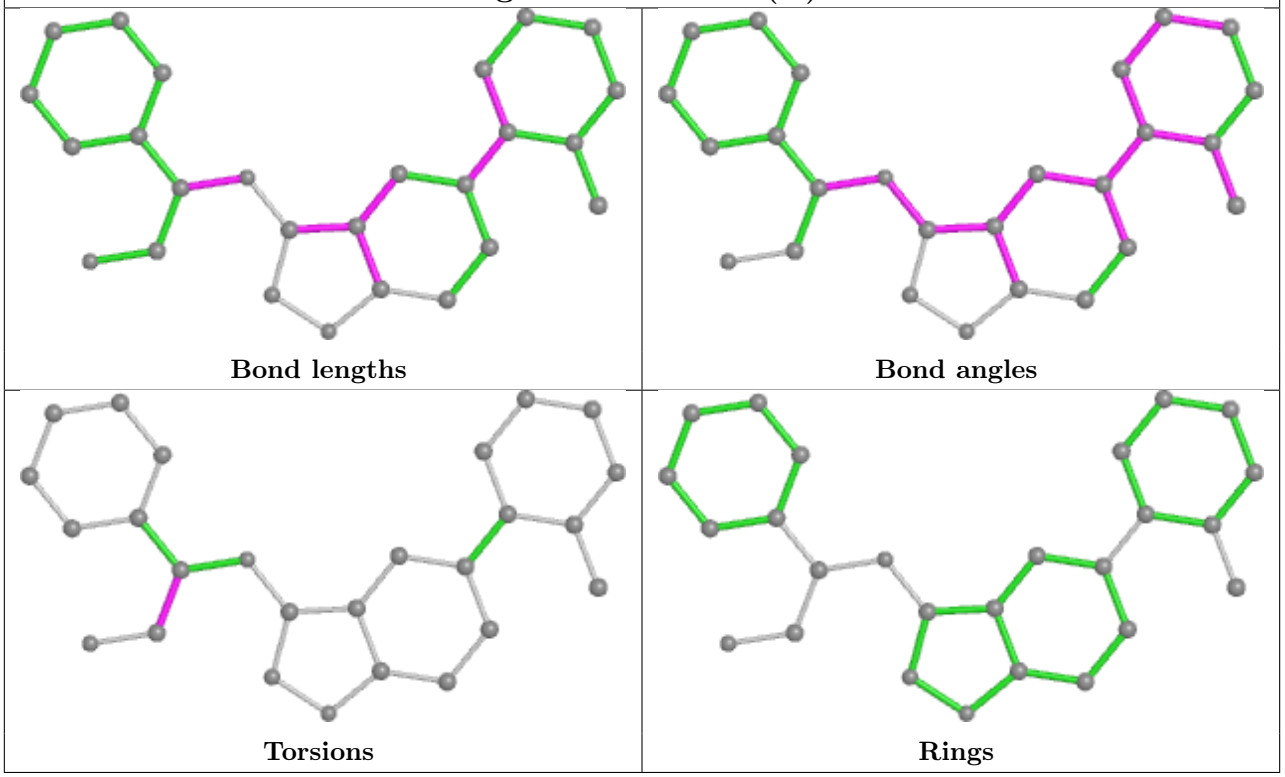
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	702	JK8	11	0
7	C	501	GLY	2	0
6	E	2101	GOL	3	0
5	D	702[A]	JK8	8	0

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 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 702



Ligand JK8 D 702 (A)



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
3	F	2
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	8:DG	O3'	2009[B]:DG	P	9.98
1	E	8:DG	O3'	2009:DG	P	7.42
1	F	8:DG	O3'	2009[A]:DG	P	6.96

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	189/202 (93%)	-0.36	3 (1%) 72 69	40, 63, 89, 114	0
1	D	189/202 (93%)	-0.24	3 (1%) 72 69	50, 78, 104, 124	0
2	A	483/490 (98%)	-0.48	0 100 100	33, 51, 77, 110	0
2	C	481/490 (98%)	-0.47	0 100 100	36, 52, 77, 108	0
3	E	20/20 (100%)	-0.75	0 100 100	47, 57, 148, 150	0
3	F	20/20 (100%)	-0.57	0 100 100	43, 67, 140, 153	0
All	All	1382/1424 (97%)	-0.43	6 (0%) 92 93	33, 56, 92, 153	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	639	TYR	3.7
1	D	639[A]	TYR	3.6
1	D	490	GLY	3.3
1	B	545	GLY	2.4
1	D	638[A]	VAL	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

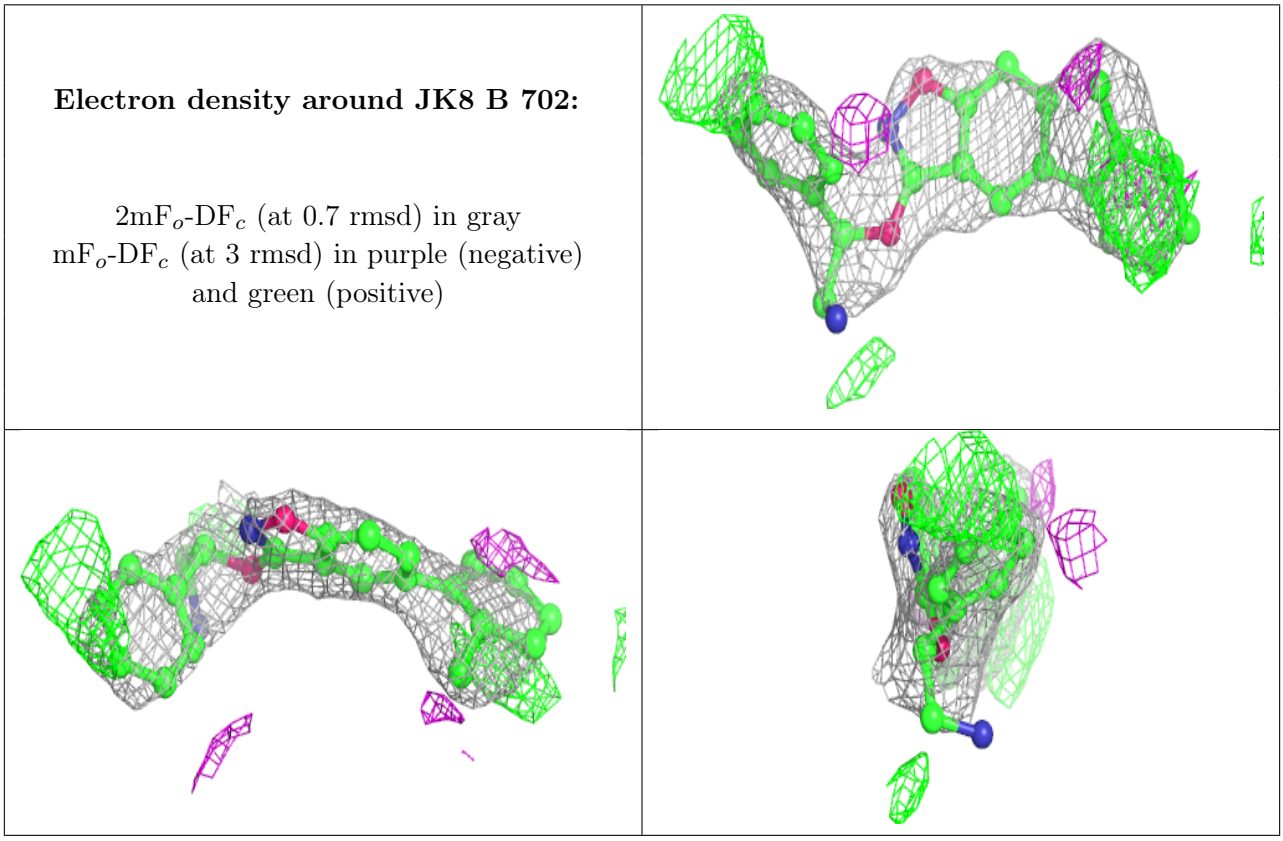
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	GOL	E	2102	6/6	0.80	0.16	84,91,96,98	0
7	GLY	C	501	4/5	0.84	0.50	78,96,96,106	0
5	JK8	B	702	26/26	0.85	0.34	49,55,59,63	26
6	GOL	C	503	6/6	0.85	0.23	98,102,104,105	0
6	GOL	A	501	6/6	0.88	0.33	88,100,102,113	0
5	JK8	D	702[A]	26/26	0.91	0.32	34,38,44,46	26
6	GOL	A	502	6/6	0.92	0.28	46,64,70,72	0
6	GOL	E	2101	6/6	0.95	0.11	61,69,74,77	0
8	CL	C	502	1/1	0.98	0.10	68,68,68,68	0
4	MN	D	701	1/1	0.99	0.13	63,63,63,63	0
4	MN	B	701	1/1	1.00	0.14	50,50,50,50	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.

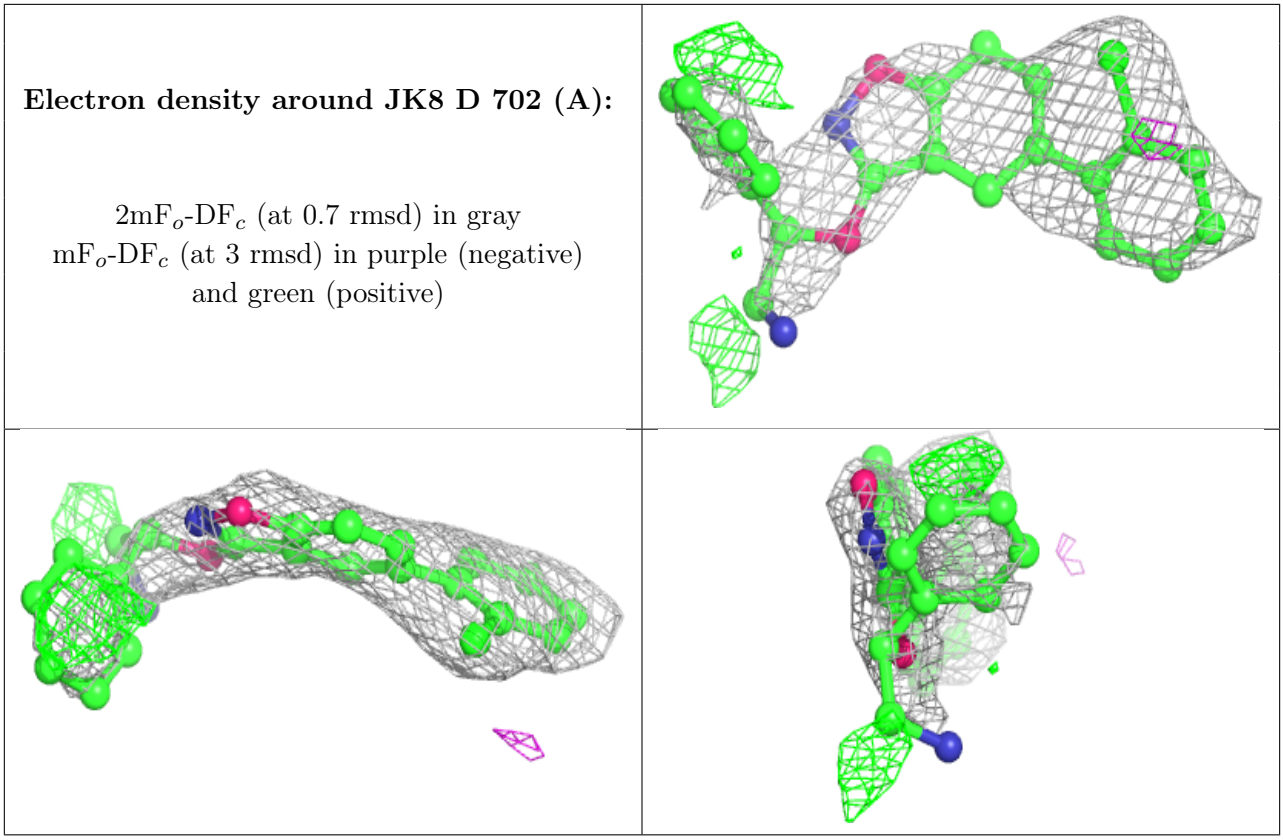
Electron density around JK8 B 702:

$2mF_o$-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 702 (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.