



# Full wwPDB X-ray Structure Validation Report i

Jun 19, 2024 – 02:12 PM JST

PDB ID : 8K9V  
Title : Crystal structure of plasmodium LysRS complexing with ASP3026 derived LysRS inhibitor 3 (ADKI3)  
Authors : Zhou, J.; Xia, M.; Yang, G.; Li, P.; Fang, P.  
Deposited on : 2023-08-01  
Resolution : 1.92 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

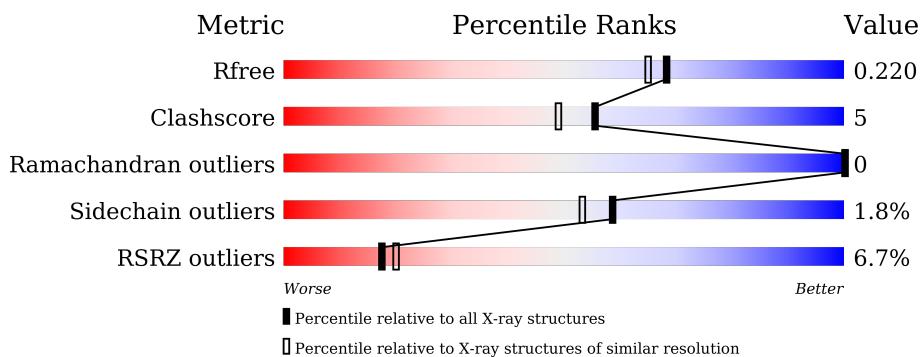
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

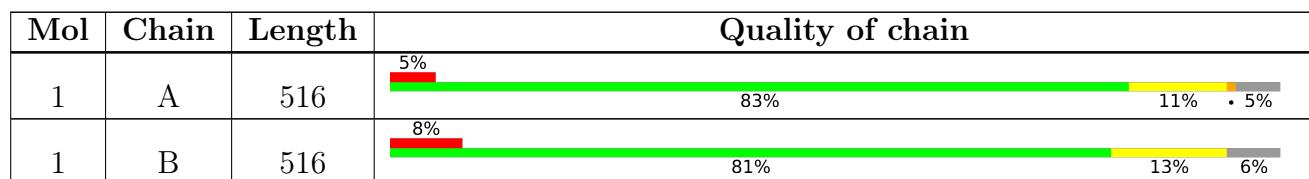
The reported resolution of this entry is 1.92 Å.

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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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.



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
3	JT4	B	602	-	X	-	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8334 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.

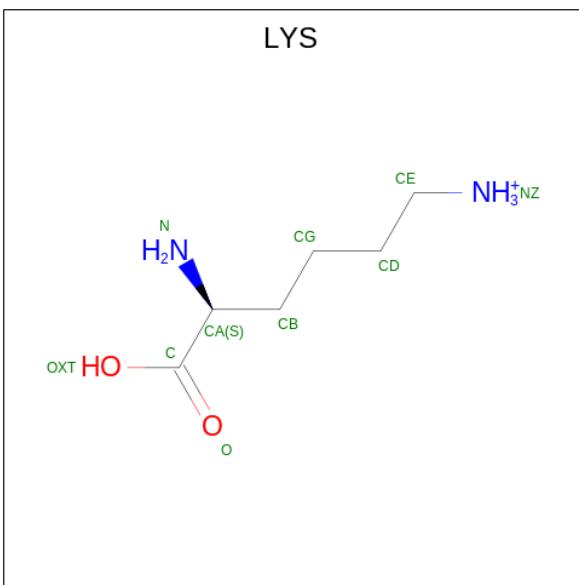
- Molecule 1 is a protein called Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C 3911	N 2524	O 652	S 718	17	0	0
1	B	484	Total	C 3867	N 2493	O 642	S 715	17	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP A0A024X378
A	584	GLY	-	expression tag	UNP A0A024X378
A	585	GLY	-	expression tag	UNP A0A024X378
A	586	HIS	-	expression tag	UNP A0A024X378
A	587	HIS	-	expression tag	UNP A0A024X378
A	588	HIS	-	expression tag	UNP A0A024X378
A	589	HIS	-	expression tag	UNP A0A024X378
A	590	HIS	-	expression tag	UNP A0A024X378
A	591	HIS	-	expression tag	UNP A0A024X378
B	76	MET	-	initiating methionine	UNP A0A024X378
B	584	GLY	-	expression tag	UNP A0A024X378
B	585	GLY	-	expression tag	UNP A0A024X378
B	586	HIS	-	expression tag	UNP A0A024X378
B	587	HIS	-	expression tag	UNP A0A024X378
B	588	HIS	-	expression tag	UNP A0A024X378
B	589	HIS	-	expression tag	UNP A0A024X378
B	590	HIS	-	expression tag	UNP A0A024X378
B	591	HIS	-	expression tag	UNP A0A024X378

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).

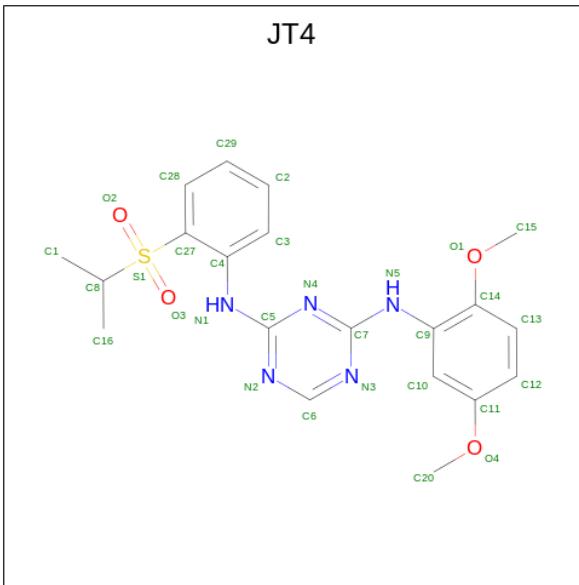


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		

Mol	Chain	Residues	Total	C	N	O	ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is {N}4-(2,5-dimethoxyphenyl)-{N}2-(2-propan-2-ylsulfonylphenyl)-1,3,5-triazine-2,4-diamine (three-letter code: JT4) (formula: C<sub>20</sub>H<sub>23</sub>N<sub>5</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



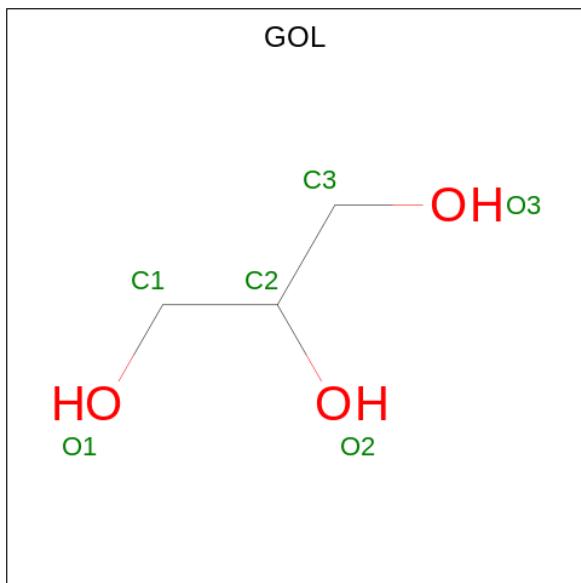
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	
			30	20	5	4	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	30	20	5	4	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

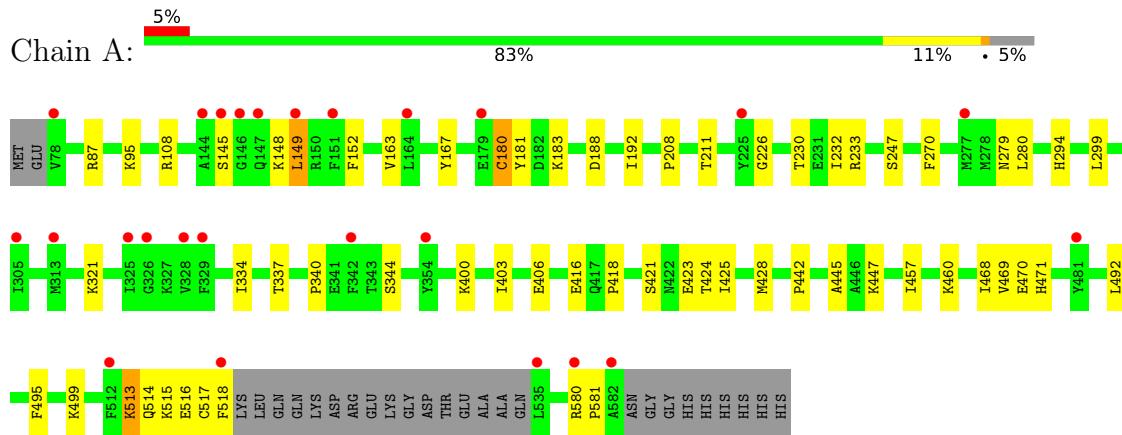
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	242	242	242	0	0
5	B	228	228	228	0	0

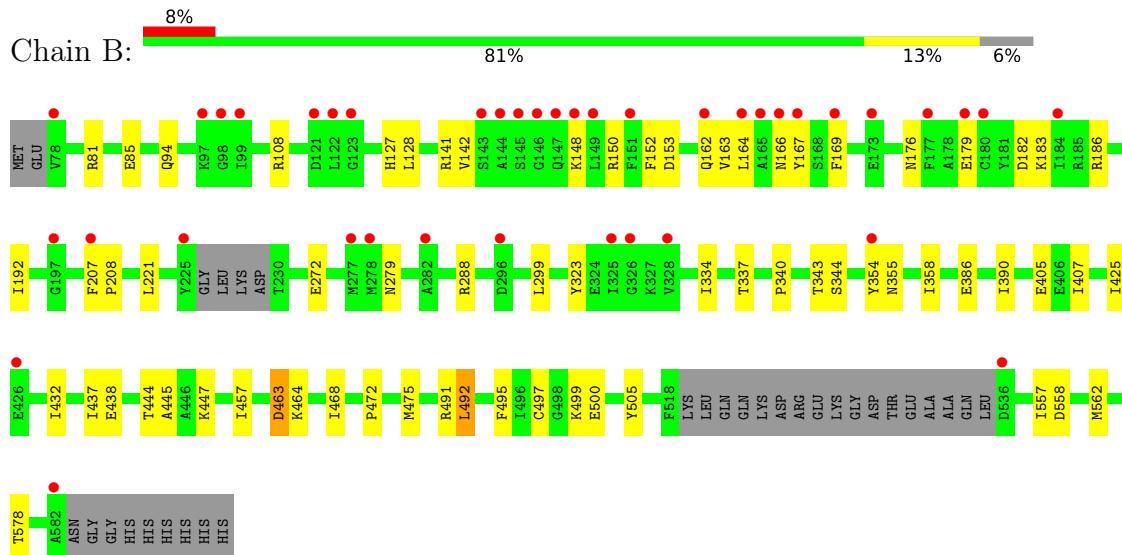
### 3 Residue-property plots [\(i\)](#)

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: Lysine-tRNA ligase



- Molecule 1: Lysine-tRNA ligase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.15Å 99.13Å 169.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 1.92 48.98 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.56-1.92) 99.9 (48.98-1.92)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.93 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
$R$ , $R_{free}$	0.186 , 0.220 0.186 , 0.220	Depositor DCC
$R_{free}$ test set	4640 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.4	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, JT4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/4009	0.64	2/5428 (0.0%)
1	B	0.39	0/3963	0.61	0/5368
All	All	0.41	0/7972	0.62	2/10796 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ILE	CG1-CB-CG2	-6.96	96.09	111.40
1	A	299	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3911	0	3814	36	0
1	B	3867	0	3748	42	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
3	A	30	0	0	0	0
3	B	30	0	0	1	0
4	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	242	0	0	8	0
5	B	228	0	0	5	0
All	All	8334	0	7594	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:N	1:A:423:GLU:OE1	2.17	0.76
4:A:603:GOL:C3	5:A:711:HOH:O	2.37	0.73
4:A:603:GOL:H31	5:A:711:HOH:O	1.93	0.68
1:A:87:ARG:NH2	1:A:188:ASP:OD1	2.26	0.68
1:B:150:ARG:NH2	1:B:182:ASP:OD1	2.23	0.67
1:B:141:ARG:HH11	1:B:141:ARG:HG2	1.59	0.66
1:A:469:VAL:HG23	1:A:470:GLU:HG3	1.77	0.65
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.80	0.64
1:A:425:ILE:HD11	1:A:445:ALA:HB2	1.80	0.63
1:A:418:PRO:HG2	1:A:421:SER:HB3	1.80	0.62
1:B:141:ARG:HG2	1:B:141:ARG:NH1	2.17	0.59
1:A:334:ILE:HG12	1:A:340:PRO:HD3	1.86	0.57
1:B:343:THR:HG22	1:B:557:ILE:HD12	1.88	0.55
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.88	0.55
1:B:94:GLN:HE22	1:B:183:LYS:NZ	2.05	0.55
1:B:166:ASN:HB3	1:B:169:PHE:HD2	1.72	0.55
1:B:186:ARG:NH1	1:B:221:LEU:O	2.40	0.54
1:B:578:THR:HB	5:B:730:HOH:O	2.06	0.54
1:A:233:ARG:HG3	5:A:701:HOH:O	2.08	0.53
1:A:580:ARG:HD2	1:A:581:PRO:HD2	1.91	0.53
1:A:406:GLU:OE2	1:A:460:LYS:HE3	2.09	0.53
1:A:192:ILE:HG23	1:A:208:PRO:HB3	1.91	0.52
1:B:166:ASN:HB3	1:B:169:PHE:CD2	2.44	0.52
1:A:108:ARG:HD2	5:A:747:HOH:O	2.08	0.52
1:A:513:LYS:O	1:A:515:LYS:N	2.43	0.52
1:A:279:ASN:HB2	5:A:726:HOH:O	2.09	0.51
1:B:334:ILE:HG12	1:B:340:PRO:HD3	1.92	0.51
1:A:400:LYS:HD2	5:A:735:HOH:O	2.10	0.51
1:A:499:LYS:HA	1:A:499:LYS:HE2	1.93	0.51
1:B:127:HIS:O	1:B:128:LEU:HD23	2.11	0.50
1:B:358:ILE:HD13	1:B:492:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:NH2	1:B:162:GLN:OE1	2.45	0.50
1:A:181:TYR:OH	1:A:211:THR:HG23	2.12	0.49
1:B:425:ILE:HD11	1:B:445:ALA:HB2	1.95	0.48
1:A:516:GLU:C	1:A:518:PHE:H	2.17	0.48
1:B:279:ASN:HB2	5:B:720:HOH:O	2.13	0.48
1:B:472:PRO:HD2	1:B:475:MET:SD	2.54	0.48
1:A:514:GLN:O	1:A:515:LYS:C	2.52	0.48
1:B:176:ASN:HB3	1:B:179:GLU:HB3	1.96	0.47
1:B:355:ASN:ND2	5:B:708:HOH:O	2.46	0.47
1:A:442:PRO:HD2	1:A:447:LYS:NZ	2.30	0.47
1:A:145:SER:HB2	1:A:149:LEU:HD23	1.96	0.47
1:A:424:THR:O	1:A:428:MET:HG3	2.15	0.47
1:A:468:ILE:HD12	1:A:495:PHE:CE1	2.49	0.47
1:B:500:GLU:HG2	3:B:602:JT4:O2	2.15	0.47
1:B:354:TYR:HD2	1:B:355:ASN:OD1	1.98	0.46
1:A:516:GLU:C	1:A:518:PHE:N	2.69	0.46
1:B:176:ASN:HA	5:B:758:HOH:O	2.15	0.46
1:A:230:THR:HG23	1:A:232:ILE:H	1.80	0.46
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.98	0.46
1:A:280:LEU:HD12	5:A:894:HOH:O	2.17	0.45
1:A:517:CYS:O	1:A:518:PHE:C	2.52	0.45
1:A:337:THR:HG21	1:A:499:LYS:HD3	1.99	0.45
1:A:294:HIS:CE1	5:B:781:HOH:O	2.70	0.45
1:B:437:ILE:HG22	1:B:438:GLU:N	2.32	0.45
1:B:141:ARG:HB3	1:B:153:ASP:HB2	1.98	0.45
1:B:390:ILE:HD11	1:B:497:CYS:SG	2.58	0.44
1:A:226:GLY:O	1:A:230:THR:HG21	2.17	0.44
1:B:148:LYS:HG3	1:B:167:TYR:HB2	2.00	0.44
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.99	0.44
1:B:272:GLU:HB2	1:B:323:TYR:CZ	2.53	0.43
1:A:460:LYS:HG3	5:A:793:HOH:O	2.19	0.42
1:B:142:VAL:HG22	1:B:152:PHE:CD1	2.55	0.42
1:A:270:PHE:CD2	1:A:321:LYS:HB3	2.54	0.42
1:B:432:ILE:HG23	1:B:437:ILE:HB	2.02	0.42
1:B:444:THR:HG23	1:B:447:LYS:H	1.84	0.42
1:B:164:LEU:HD13	1:B:207:PHE:CE2	2.55	0.42
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.87	0.41
1:A:180:CYS:HA	1:A:183:LYS:HE2	2.01	0.41
1:A:403:ILE:HG21	1:A:471:HIS:HA	2.03	0.41
1:B:444:THR:CG2	1:B:447:LYS:H	2.33	0.41
1:B:558:ASP:O	1:B:562:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:THR:HG21	1:B:499:LYS:HD2	2.03	0.41
1:A:148:LYS:HD3	1:A:167:TYR:CD2	2.56	0.41
1:A:581:PRO:HG3	1:B:299:LEU:HD21	2.02	0.41
1:B:81:ARG:O	1:B:85:GLU:HG3	2.21	0.41
1:B:491:ARG:HA	1:B:505:TYR:HB3	2.03	0.41
1:B:463:ASP:HB3	1:B:464:LYS:HG2	2.03	0.40
1:B:468:ILE:HD12	1:B:495:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	485/516 (94%)	471 (97%)	14 (3%)	0	100 100
1	B	478/516 (93%)	468 (98%)	10 (2%)	0	100 100
All	All	963/1032 (93%)	939 (98%)	24 (2%)	0	100 100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	420/464 (90%)	412 (98%)	8 (2%)	57 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	415/464 (89%)	408 (98%)	7 (2%)	60 55
All	All	835/928 (90%)	820 (98%)	15 (2%)	59 53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	149	LEU
1	A	180	CYS
1	A	247	SER
1	A	344	SER
1	A	416	GLU
1	A	492	LEU
1	A	513	LYS
1	B	108	ARG
1	B	288	ARG
1	B	344	SER
1	B	386	GLU
1	B	405	GLU
1	B	463	ASP
1	B	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	GLN

### 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)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LYS	A	601	-	8,9,9	0.82	0	9,10,10	1.30	2 (22%)
2	LYS	B	601	-	8,9,9	0.74	0	9,10,10	1.19	2 (22%)
3	JT4	B	602	-	31,32,32	4.84	24 (77%)	40,45,45	3.55	12 (30%)
4	GOL	A	603	-	5,5,5	0.20	0	5,5,5	0.26	0
3	JT4	A	602	-	31,32,32	4.69	22 (70%)	40,45,45	3.28	10 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	A	601	-	-	0/9/9/9	-
2	LYS	B	601	-	-	0/9/9/9	-
3	JT4	B	602	-	-	10/24/24/24	0/3/3/3
4	GOL	A	603	-	-	0/4/4/4	-
3	JT4	A	602	-	-	7/24/24/24	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	JT4	C28-C27	11.54	1.52	1.39
3	A	602	JT4	C28-C27	11.04	1.52	1.39
3	A	602	JT4	C10-C9	8.13	1.52	1.39
3	B	602	JT4	C3-C4	7.99	1.53	1.39
3	B	602	JT4	C10-C9	7.92	1.51	1.39
3	A	602	JT4	C3-C4	7.90	1.53	1.39
3	B	602	JT4	C12-C11	7.41	1.53	1.38
3	B	602	JT4	C7-N3	7.23	1.44	1.34
3	A	602	JT4	C12-C11	7.03	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	JT4	C5-N2	-6.61	1.25	1.34
3	A	602	JT4	C5-N2	-6.39	1.25	1.34
3	B	602	JT4	C13-C14	6.36	1.52	1.39
3	A	602	JT4	C4-C27	-6.33	1.31	1.40
3	A	602	JT4	C7-N3	6.31	1.43	1.34
3	A	602	JT4	C13-C14	6.27	1.52	1.39
3	B	602	JT4	C6-N2	6.05	1.45	1.33
3	B	602	JT4	C4-C27	-5.80	1.31	1.40
3	B	602	JT4	C29-C2	5.67	1.53	1.38
3	A	602	JT4	C29-C2	5.50	1.52	1.38
3	A	602	JT4	C6-N2	5.14	1.43	1.33
3	A	602	JT4	C6-N3	-4.84	1.24	1.33
3	B	602	JT4	C6-N3	-4.77	1.25	1.33
3	A	602	JT4	C9-C14	-4.34	1.31	1.40
3	A	602	JT4	C13-C12	-4.21	1.31	1.38
3	B	602	JT4	C5-N1	4.17	1.45	1.36
3	B	602	JT4	C7-N5	4.14	1.44	1.36
3	A	602	JT4	C10-C11	-4.12	1.31	1.38
3	B	602	JT4	C9-C14	-3.87	1.32	1.40
3	B	602	JT4	C10-C11	-3.81	1.32	1.38
3	A	602	JT4	C7-N5	3.78	1.44	1.36
3	B	602	JT4	C5-N4	3.63	1.45	1.34
3	A	602	JT4	C5-N4	3.54	1.45	1.34
3	A	602	JT4	C29-C28	-3.51	1.31	1.38
3	B	602	JT4	C29-C28	-3.43	1.31	1.38
3	A	602	JT4	C5-N1	3.39	1.43	1.36
3	B	602	JT4	C2-C3	-3.24	1.32	1.38
3	A	602	JT4	C2-C3	-3.08	1.32	1.38
3	B	602	JT4	O3-S1	3.03	1.47	1.44
3	B	602	JT4	C13-C12	-2.95	1.33	1.38
3	B	602	JT4	O1-C14	2.93	1.41	1.37
3	A	602	JT4	C7-N4	-2.84	1.26	1.34
3	B	602	JT4	C7-N4	-2.69	1.26	1.34
3	A	602	JT4	O2-S1	2.69	1.46	1.44
3	B	602	JT4	O2-S1	2.35	1.46	1.44
3	B	602	JT4	C4-N1	2.21	1.46	1.39
3	A	602	JT4	C4-N1	2.11	1.45	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	JT4	O3-S1-O2	-15.89	104.13	118.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	JT4	O3-S1-O2	-14.98	104.97	118.71
3	B	602	JT4	N2-C5-N4	-7.20	119.73	126.55
3	A	602	JT4	N2-C5-N4	-7.05	119.87	126.55
3	A	602	JT4	N3-C7-N4	-6.20	120.68	126.55
3	B	602	JT4	O3-S1-C8	-5.60	104.20	107.97
3	B	602	JT4	N3-C6-N2	-5.60	119.85	128.60
3	B	602	JT4	N3-C7-N4	-5.59	121.25	126.55
3	A	602	JT4	N3-C6-N2	-5.39	120.18	128.60
3	B	602	JT4	O2-S1-C8	5.32	111.55	107.97
3	B	602	JT4	C27-S1-C8	4.24	114.03	105.55
3	A	602	JT4	C27-C4-N1	-4.22	117.46	121.45
3	A	602	JT4	O2-S1-C8	3.84	110.55	107.97
3	B	602	JT4	C27-C4-N1	-3.40	118.24	121.45
3	A	602	JT4	C27-S1-C8	3.09	111.72	105.55
3	A	602	JT4	O3-S1-C27	2.99	113.60	107.76
3	A	602	JT4	C7-N4-C5	2.92	118.84	113.89
3	B	602	JT4	C7-N4-C5	2.81	118.66	113.89
2	A	601	LYS	OXT-C-CA	2.68	122.52	113.38
2	A	601	LYS	OXT-C-O	-2.52	118.37	124.09
3	B	602	JT4	O1-C14-C9	2.48	117.84	114.80
2	B	601	LYS	OXT-C-CA	2.31	121.24	113.38
2	B	601	LYS	OXT-C-O	-2.28	118.90	124.09
3	A	602	JT4	N5-C7-N4	2.18	124.31	116.92
3	B	602	JT4	O3-S1-C27	2.04	111.75	107.76
3	B	602	JT4	N5-C7-N4	2.04	123.86	116.92

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	JT4	C4-C27-S1-O2
3	A	602	JT4	C1-C8-S1-O2
3	A	602	JT4	C1-C8-S1-O3
3	A	602	JT4	C16-C8-S1-O3
3	B	602	JT4	C4-C27-S1-O2
3	B	602	JT4	C1-C8-S1-C27
3	B	602	JT4	C1-C8-S1-O2
3	B	602	JT4	C1-C8-S1-O3
3	B	602	JT4	C16-C8-S1-O3
3	B	602	JT4	C28-C27-S1-O2
3	A	602	JT4	C16-C8-S1-O2
3	A	602	JT4	C28-C27-S1-O2

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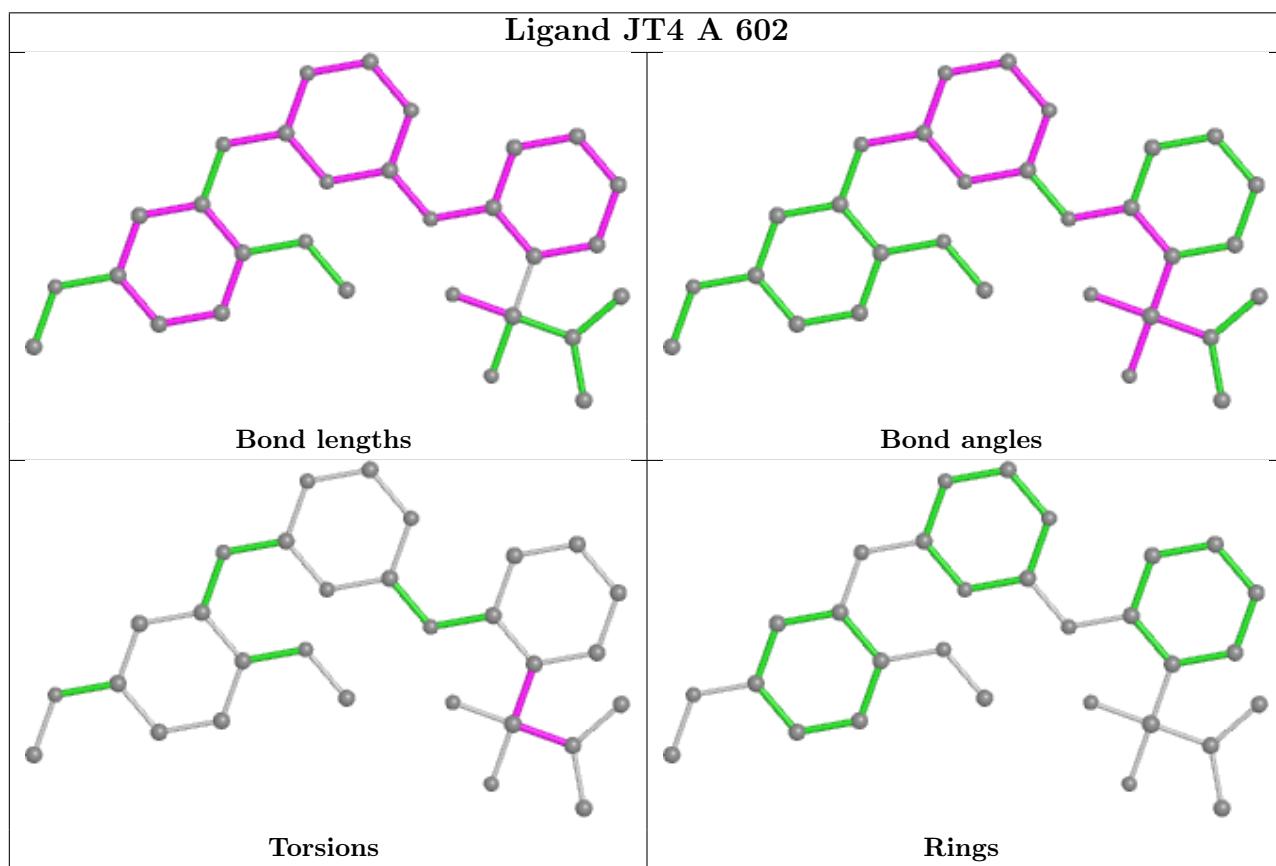
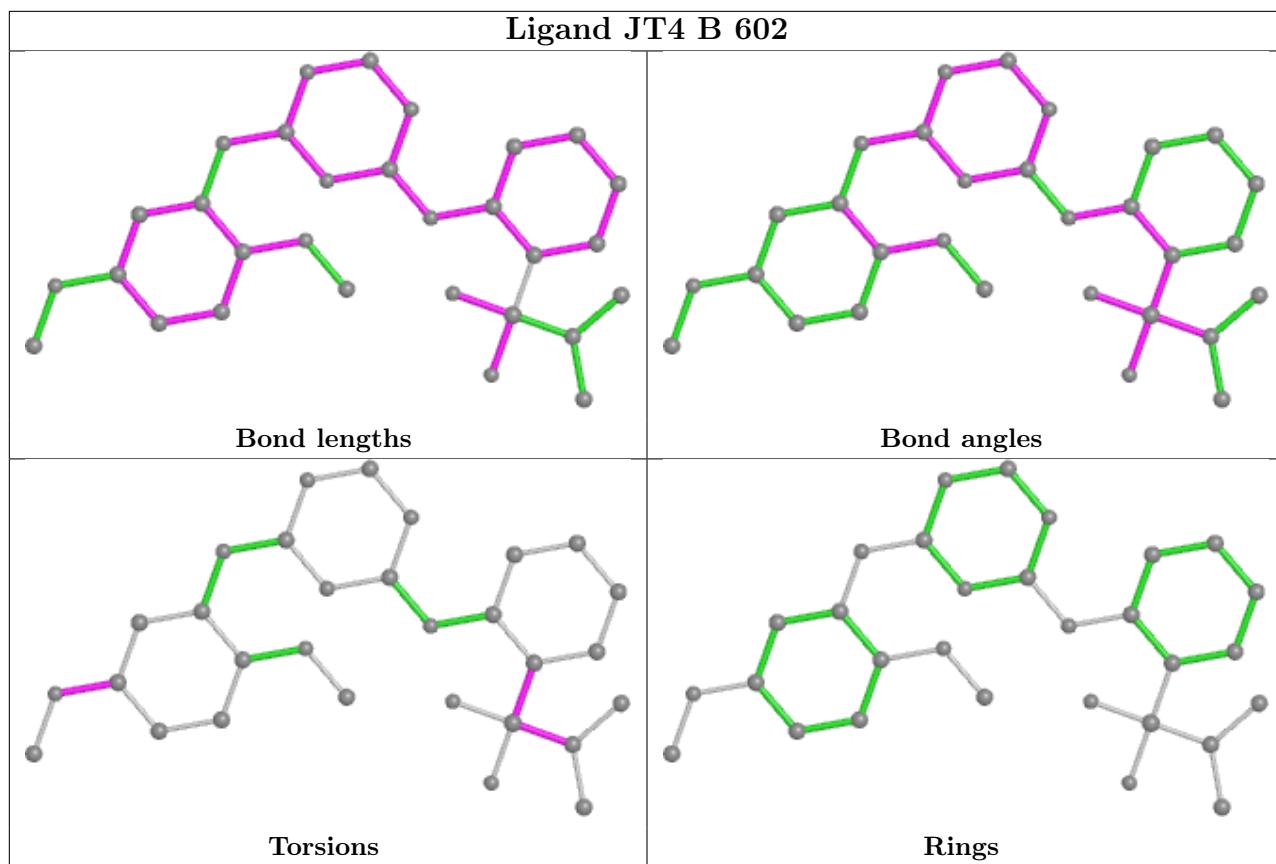
Mol	Chain	Res	Type	Atoms
3	A	602	JT4	C16-C8-S1-C27
3	B	602	JT4	C16-C8-S1-C27
3	B	602	JT4	C12-C11-O4-C20
3	B	602	JT4	C10-C11-O4-C20
3	B	602	JT4	C16-C8-S1-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	JT4	1	0
4	A	603	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	489/516 (94%)	0.43	25 (5%) 28 31	26, 43, 67, 98	0
1	B	484/516 (93%)	0.51	40 (8%) 11 13	26, 44, 79, 107	0
All	All	973/1032 (94%)	0.47	65 (6%) 17 20	26, 44, 76, 107	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	PHE	5.5
1	A	144	ALA	5.3
1	A	145	SER	5.3
1	B	122	LEU	5.3
1	A	151	PHE	4.6
1	A	535	LEU	4.5
1	B	149	LEU	4.5
1	B	164	LEU	4.5
1	A	78	VAL	4.0
1	B	582	ALA	4.0
1	B	145	SER	3.9
1	B	78	VAL	3.6
1	A	146	GLY	3.5
1	B	165	ALA	3.5
1	B	169	PHE	3.4
1	B	147	GLN	3.4
1	B	207	PHE	3.4
1	B	180	CYS	3.4
1	A	149	LEU	3.4
1	B	146	GLY	3.3
1	A	164	LEU	3.2
1	B	144	ALA	3.2
1	B	151	PHE	3.2
1	B	177	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	354	TYR	3.1
1	A	328	VAL	3.1
1	B	328	VAL	3.1
1	B	197	GLY	3.1
1	B	98	GLY	3.0
1	B	97	LYS	2.9
1	B	167	TYR	2.9
1	A	512	PHE	2.9
1	B	99	ILE	2.8
1	A	580	ARG	2.8
1	B	184	ILE	2.8
1	B	296	ASP	2.7
1	B	326	GLY	2.6
1	A	225	TYR	2.5
1	A	277	MET	2.5
1	B	123	GLY	2.5
1	B	143	SER	2.5
1	A	313	MET	2.5
1	A	582	ALA	2.4
1	A	305	ILE	2.4
1	B	148	LYS	2.3
1	A	325	ILE	2.3
1	A	326	GLY	2.2
1	B	162	GLN	2.2
1	B	173	GLU	2.2
1	B	179	GLU	2.2
1	A	481	TYR	2.2
1	B	225	TYR	2.2
1	B	354	TYR	2.2
1	A	147	GLN	2.2
1	A	329	PHE	2.2
1	B	536	ASP	2.1
1	B	325	ILE	2.1
1	B	277	MET	2.0
1	B	121	ASP	2.0
1	A	342	PHE	2.0
1	B	278	MET	2.0
1	A	179	GLU	2.0
1	B	282	ALA	2.0
1	B	426	GLU	2.0
1	B	166	ASN	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 [\(i\)](#)

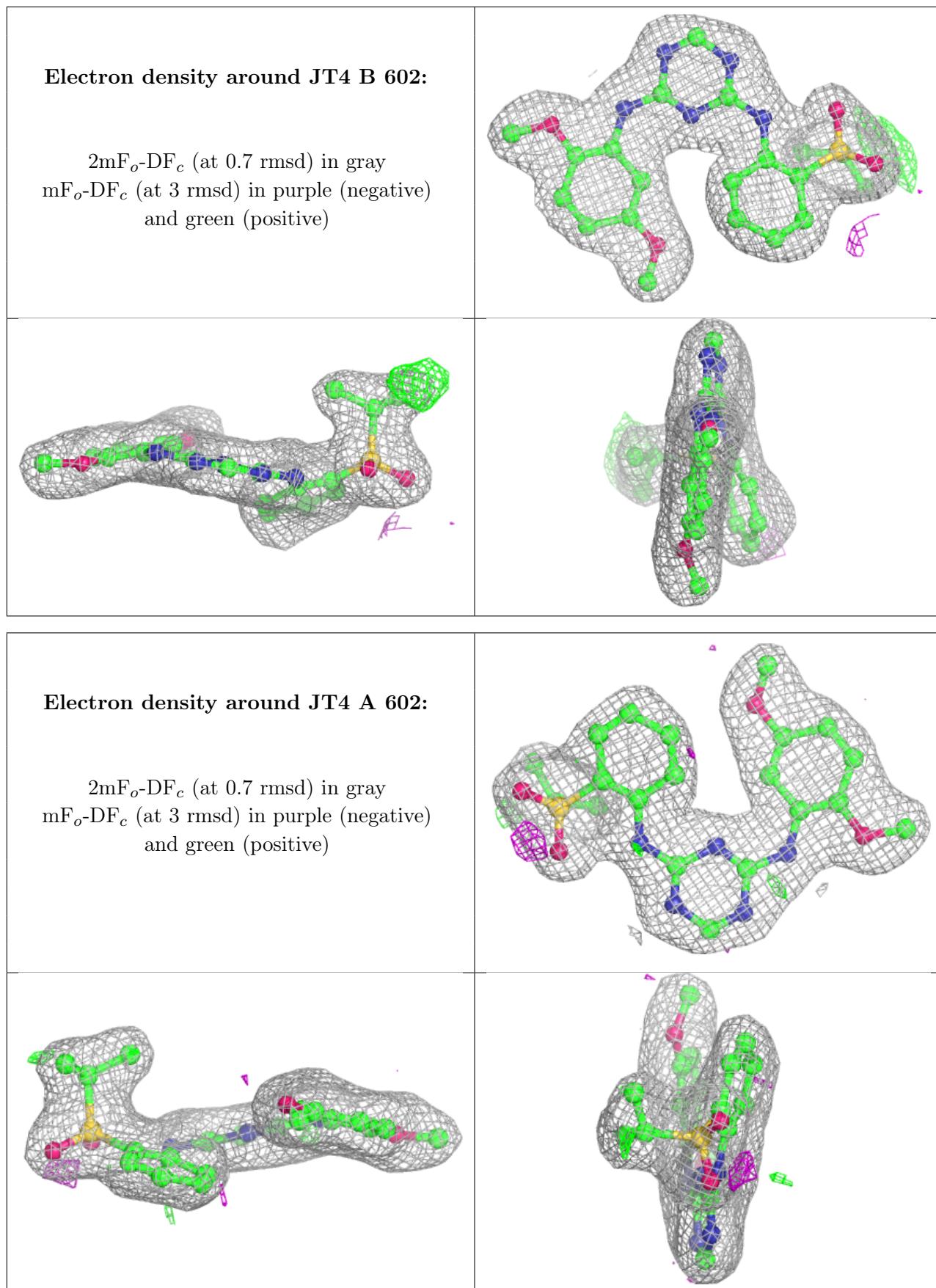
There are no monosaccharides in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	A	603	6/6	0.81	0.22	41,47,53,54	0
2	LYS	B	601	10/10	0.95	0.13	31,34,41,45	0
2	LYS	A	601	10/10	0.95	0.15	28,31,36,43	0
3	JT4	B	602	30/30	0.96	0.14	29,35,42,45	0
3	JT4	A	602	30/30	0.98	0.18	28,33,38,42	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.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.