



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2022 – 06:23 PM JST

PDB ID : 7VTG  
Title : Pseudouridine bound structure of Pseudouridine kinase (PUKI) S30A mutant from Escherichia coli strain B  
Authors : Kim, S.H.; Rhee, S.  
Deposited on : 2021-10-29  
Resolution : 1.90 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 ⓘ symbol.

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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 : 2.27  
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) : 2.27

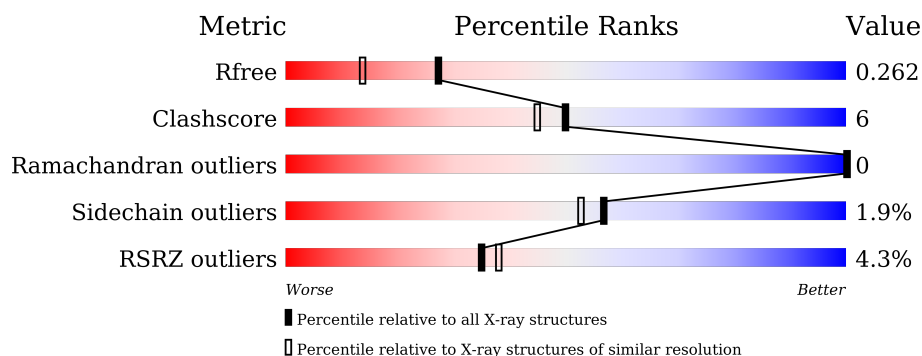
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	313	<div> <div>4%</div> <div>81% 13% 5%</div> </div>
1	B	313	<div> <div>4%</div> <div>84% 12%</div> </div>
1	C	313	<div> <div>4%</div> <div>82% 12%</div> </div>
1	D	313	<div> <div>4%</div> <div>83% 12% 5%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FJF	A	401	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9498 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.

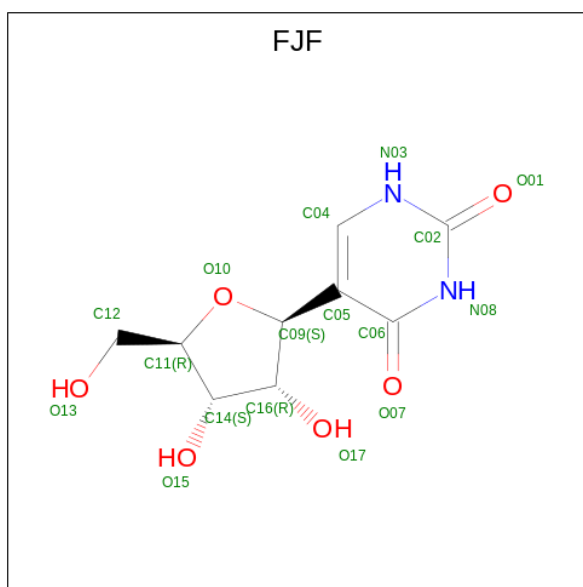
- Molecule 1 is a protein called Pseudouridine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2232	1404	383	432	13			
1	B	300	Total	C	N	O	S	0	0	0
			2260	1420	389	438	13			
1	C	299	Total	C	N	O	S	0	0	0
			2255	1417	388	437	13			
1	D	298	Total	C	N	O	S	0	0	0
			2246	1413	386	434	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	SER	engineered mutation	UNP A0A1V3W5E1
B	30	ALA	SER	engineered mutation	UNP A0A1V3W5E1
C	30	ALA	SER	engineered mutation	UNP A0A1V3W5E1
D	30	ALA	SER	engineered mutation	UNP A0A1V3W5E1

- Molecule 2 is 5-[(2 {S},3 {R},4 {S},5 {R})-5-(hydroxymethyl)-3,4-bis(oxidanyl)oxolan-2-yl]-1 {H}-pyrimidine-2,4-dione (three-letter code: FJF) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	9	2	6		
2	B	1	Total	C	N	O	0	0
			17	9	2	6		
2	C	1	Total	C	N	O	0	0
			17	9	2	6		
2	D	1	Total	C	N	O	0	0
			17	9	2	6		

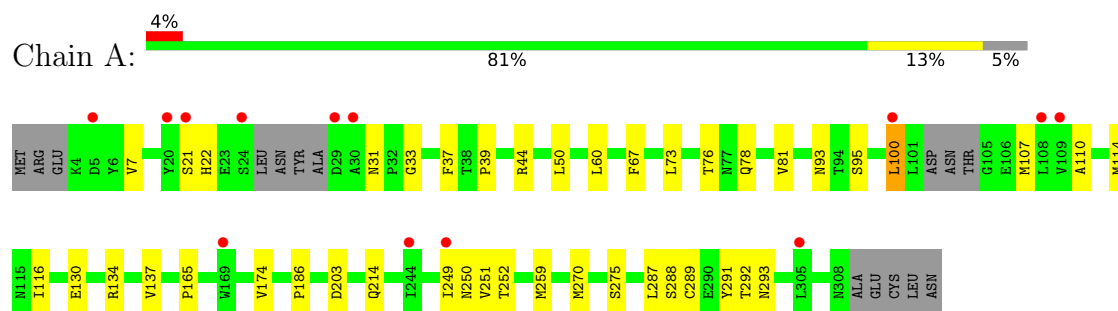
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	105	Total	O	0	0
			105	105		
3	C	113	Total	O	0	0
			113	113		
3	D	112	Total	O	0	0
			112	112		

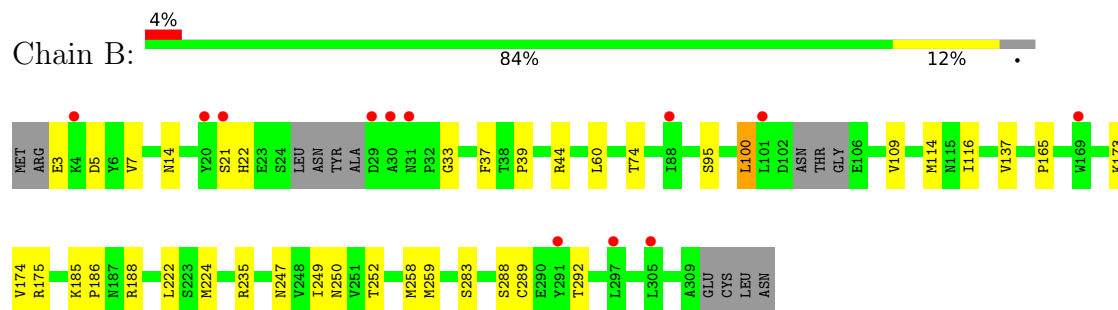
### 3 Residue-property plots

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.

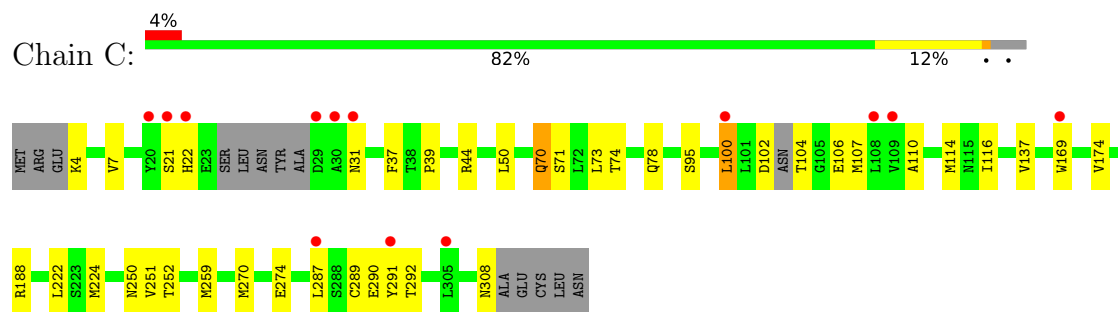
#### • Molecule 1: Pseudouridine kinase



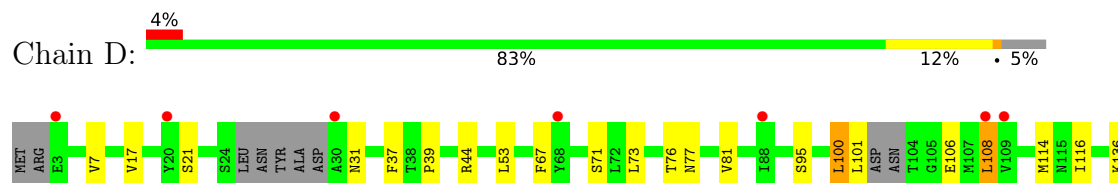
#### • Molecule 1: Pseudouridine kinase

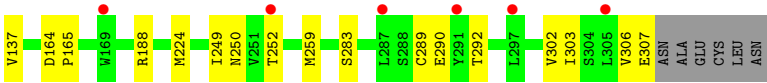


#### • Molecule 1: Pseudouridine kinase



#### • Molecule 1: Pseudouridine kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.09Å 185.09Å 51.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.72 – 1.90 33.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.72-1.90) 87.6 (33.72-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.47 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.219 , 0.262 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	2020 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.476 for -h,-k,l 0.487 for h,-h-k,-l 0.476 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.82	0/2271	0.79	1/3089 (0.0%)
1	B	0.81	0/2299	0.81	2/3125 (0.1%)
1	C	0.84	0/2294	0.81	1/3118 (0.0%)
1	D	0.81	1/2285 (0.0%)	0.80	2/3105 (0.1%)
All	All	0.82	1/9149 (0.0%)	0.80	6/12437 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	17	VAL	CB-CG1	5.64	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	D	259	MET	CG-SD-CE	-6.01	90.58	100.20
1	C	259	MET	CG-SD-CE	-5.94	90.69	100.20
1	A	259	MET	CG-SD-CE	-5.92	90.73	100.20
1	B	259	MET	CG-SD-CE	-5.80	90.92	100.20
1	D	108	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2232	0	2185	26	0
1	B	2260	0	2219	23	0
1	C	2255	0	2217	37	0
1	D	2246	0	2214	26	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0
3	A	107	0	0	3	0
3	B	105	0	0	1	0
3	C	113	0	0	1	0
3	D	112	0	0	2	0
All	All	9498	0	8835	103	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 6.

All (103) 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:B:22:HIS:CD2	1:B:33:GLY:HA2	2.08	0.88
1:C:21:SER:OG	1:C:31:ASN:ND2	2.06	0.88
1:C:70:GLN:HA	1:C:70:GLN:HE21	1.47	0.80
1:A:21:SER:OG	1:A:31:ASN:ND2	2.21	0.74
1:D:21:SER:OG	1:D:31:ASN:ND2	2.21	0.73
1:D:95:SER:HB3	1:D:116:ILE:HG22	1.71	0.71
1:A:95:SER:HB3	1:A:116:ILE:HG22	1.74	0.69
1:C:95:SER:HB3	1:C:116:ILE:HG22	1.75	0.69
1:B:95:SER:HB3	1:B:116:ILE:HG22	1.79	0.66
1:A:22:HIS:HB2	1:A:33:GLY:HA2	1.79	0.65
1:C:106:GLU:O	1:C:106:GLU:HG3	1.96	0.65
1:D:252:THR:HG22	1:D:292:THR:HG23	1.77	0.64
1:C:290:GLU:CD	1:C:290:GLU:H	2.01	0.64
1:B:235:ARG:NH1	3:B:501:HOH:O	2.30	0.64
1:A:93:ASN:ND2	3:A:501:HOH:O	2.18	0.62
1:A:130:GLU:OE2	1:A:134:ARG:NH1	2.32	0.62
1:A:252:THR:HG22	1:A:292:THR:HG23	1.80	0.62
1:D:188:ARG:HB2	1:D:224:MET:HE1	1.81	0.62
1:B:252:THR:HG22	1:B:292:THR:HG23	1.81	0.62
1:C:290:GLU:HG2	1:C:291:TYR:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:GLN:HE21	1:C:70:GLN:CA	2.13	0.61
1:C:290:GLU:HG2	1:C:291:TYR:CD2	2.36	0.61
1:C:102:ASP:O	1:C:104:THR:HB	2.01	0.60
1:C:70:GLN:O	1:C:70:GLN:NE2	2.36	0.59
1:A:95:SER:HB2	1:A:114:MET:HA	1.86	0.58
1:C:71:SER:HB2	1:D:71:SER:OG	2.04	0.58
1:C:252:THR:HG22	1:C:292:THR:HG23	1.85	0.57
1:A:39:PRO:HB2	1:A:44:ARG:CZ	2.35	0.56
1:D:95:SER:HB2	1:D:114:MET:HA	1.87	0.56
1:B:39:PRO:HB2	1:B:44:ARG:CZ	2.36	0.56
1:A:37:PHE:HE2	1:B:37:PHE:CE2	2.24	0.55
1:C:37:PHE:CE2	1:D:37:PHE:HE1	2.25	0.54
1:A:270:MET:HE1	1:A:275:SER:HA	1.88	0.54
1:C:37:PHE:HE2	1:D:37:PHE:CE1	2.25	0.54
1:C:250:ASN:HB3	1:C:289:CYS:O	2.08	0.54
1:B:95:SER:HB2	1:B:114:MET:HA	1.89	0.54
1:B:188:ARG:HB2	1:B:224:MET:HE1	1.89	0.54
1:A:37:PHE:CE2	1:B:37:PHE:HE2	2.27	0.53
1:D:39:PRO:HB2	1:D:44:ARG:CZ	2.39	0.53
1:B:188:ARG:CB	1:B:224:MET:HE1	2.38	0.53
1:C:4:LYS:O	1:C:4:LYS:HD2	2.08	0.53
1:A:7:VAL:HG22	1:A:137:VAL:HG12	1.90	0.53
1:C:70:GLN:HA	1:C:70:GLN:NE2	2.22	0.53
1:B:250:ASN:HB3	1:B:289:CYS:O	2.09	0.53
1:C:39:PRO:HB2	1:C:44:ARG:CZ	2.39	0.52
1:B:235:ARG:HH11	1:B:235:ARG:HG3	1.73	0.52
1:C:37:PHE:CE2	1:D:37:PHE:CE1	2.98	0.52
1:C:74:THR:O	1:C:78:GLN:HG2	2.10	0.51
1:C:95:SER:HB2	1:C:114:MET:HA	1.93	0.51
1:D:188:ARG:CB	1:D:224:MET:HE1	2.41	0.50
1:C:222:LEU:HD11	1:C:224:MET:HE3	1.94	0.50
1:D:76:THR:HG22	1:D:81:VAL:HB	1.92	0.50
1:D:106:GLU:O	1:D:106:GLU:HG3	2.10	0.50
1:D:303:ILE:O	1:D:307:GLU:HG2	2.11	0.50
1:D:77:ASN:ND2	3:D:503:HOH:O	2.45	0.50
1:A:37:PHE:CE2	1:B:37:PHE:CE2	3.00	0.49
1:C:21:SER:N	1:C:102:ASP:HA	2.27	0.49
1:D:250:ASN:HB3	1:D:289:CYS:O	2.13	0.49
1:C:188:ARG:HB2	1:C:224:MET:HE1	1.94	0.49
1:B:100:LEU:HD22	1:B:100:LEU:HA	1.72	0.48
1:B:7:VAL:HG22	1:B:137:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ARG:CB	1:C:224:MET:HE1	2.44	0.47
1:D:7:VAL:HG22	1:D:137:VAL:HG12	1.97	0.47
1:C:100:LEU:HD22	1:C:100:LEU:HA	1.74	0.47
1:D:136:LYS:NZ	3:D:504:HOH:O	2.47	0.47
1:D:101:LEU:HA	1:D:106:GLU:O	2.15	0.46
1:B:222:LEU:HD11	1:B:224:MET:HE3	1.96	0.46
1:C:7:VAL:HG22	1:C:137:VAL:HG12	1.98	0.46
1:C:169:TRP:HB2	3:C:601:HOH:O	2.15	0.46
1:D:302:VAL:O	1:D:306:VAL:HG23	2.16	0.46
1:C:270:MET:HE3	1:C:274:GLU:HB3	1.98	0.45
1:A:250:ASN:HB3	1:A:289:CYS:O	2.16	0.45
1:A:100:LEU:HD22	1:A:100:LEU:HA	1.73	0.45
1:B:3:GLU:HG2	1:B:5:ASP:H	1.80	0.45
1:D:249:ILE:HD11	1:D:290:GLU:N	2.30	0.45
1:A:249:ILE:HD12	1:A:288:SER:O	2.17	0.45
1:A:165:PRO:HG2	1:A:186:PRO:HA	2.00	0.44
1:A:203:ASP:HB2	3:A:574:HOH:O	2.18	0.44
1:C:21:SER:H	1:C:102:ASP:HA	1.82	0.44
1:A:7:VAL:HG11	1:A:50:LEU:HD13	1.99	0.43
1:B:165:PRO:HG2	1:B:186:PRO:HA	2.00	0.43
1:C:21:SER:HG	1:C:31:ASN:ND2	2.09	0.43
1:A:107:MET:SD	1:A:110:ALA:HB2	2.58	0.43
1:A:214:GLN:HG3	3:A:564:HOH:O	2.18	0.43
1:C:78:GLN:HG3	1:D:67:PHE:CZ	2.53	0.43
1:B:185:LYS:HD2	1:B:258:MET:HE3	2.00	0.43
1:A:291:TYR:HB2	1:A:293:ASN:O	2.19	0.42
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.78	0.42
1:C:7:VAL:HG11	1:C:50:LEU:HD13	2.02	0.42
1:B:14:ASN:OD1	1:B:95:SER:OG	2.23	0.42
1:B:173:LYS:HB3	1:B:173:LYS:HE3	1.89	0.42
1:A:76:THR:HG22	1:A:81:VAL:HB	2.00	0.42
1:D:100:LEU:HD12	1:D:108:LEU:HD22	2.01	0.42
1:A:73:LEU:HA	1:A:73:LEU:HD23	1.76	0.41
1:A:251:VAL:HA	1:A:287:LEU:HD23	2.02	0.41
1:D:73:LEU:HD23	1:D:73:LEU:HA	1.83	0.41
1:A:67:PHE:CE2	1:B:74:THR:HG22	2.56	0.41
1:C:70:GLN:CA	1:C:70:GLN:NE2	2.80	0.41
1:D:53:LEU:HD23	1:D:53:LEU:HA	1.92	0.41
1:C:107:MET:SD	1:C:110:ALA:HB2	2.60	0.41
1:D:164:ASP:HA	1:D:165:PRO:HD3	1.86	0.41
1:C:251:VAL:HA	1:C:287:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ILE:HD12	1:B:288:SER:O	2.20	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	292/313 (93%)	283 (97%)	9 (3%)	0	100	100
1	B	294/313 (94%)	285 (97%)	9 (3%)	0	100	100
1	C	293/313 (94%)	284 (97%)	9 (3%)	0	100	100
1	D	292/313 (93%)	286 (98%)	6 (2%)	0	100	100
All	All	1171/1252 (94%)	1138 (97%)	33 (3%)	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	238/254 (94%)	234 (98%)	4 (2%)	60	57
1	B	242/254 (95%)	235 (97%)	7 (3%)	42	35
1	C	242/254 (95%)	237 (98%)	5 (2%)	53	48
1	D	241/254 (95%)	239 (99%)	2 (1%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	963/1016 (95%)	945 (98%)	18 (2%)	57	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	78	GLN
1	A	100	LEU
1	A	174	VAL
1	B	21	SER
1	B	60	LEU
1	B	100	LEU
1	B	109	VAL
1	B	174	VAL
1	B	247	ASN
1	B	283	SER
1	C	22	HIS
1	C	70	GLN
1	C	100	LEU
1	C	174	VAL
1	C	308	ASN
1	D	100	LEU
1	D	283	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	C	70	GLN
1	D	93	ASN
1	D	128	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FJF	D	401	-	17,18,18	6.00	11 (64%)	20,26,26	4.31	10 (50%)
2	FJF	A	401	-	17,18,18	6.29	11 (64%)	20,26,26	4.61	13 (65%)
2	FJF	C	401	-	17,18,18	6.13	11 (64%)	20,26,26	4.82	10 (50%)
2	FJF	B	401	-	17,18,18	5.97	12 (70%)	20,26,26	4.45	11 (55%)

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	FJF	D	401	-	-	3/6/22/22	0/2/2/2
2	FJF	A	401	-	-	4/6/22/22	0/2/2/2
2	FJF	C	401	-	-	4/6/22/22	0/2/2/2
2	FJF	B	401	-	-	4/6/22/22	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FJF	C16-C09	-18.99	1.32	1.54
2	C	401	FJF	C16-C09	-18.08	1.33	1.54
2	B	401	FJF	C16-C09	-17.29	1.34	1.54
2	D	401	FJF	C16-C09	-16.90	1.34	1.54
2	A	401	FJF	C14-C11	-9.46	1.28	1.53
2	C	401	FJF	C14-C11	-9.36	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FJF	C14-C11	-8.93	1.30	1.53
2	B	401	FJF	C14-C11	-8.80	1.30	1.53
2	D	401	FJF	C16-C14	6.25	1.70	1.53
2	B	401	FJF	C16-C14	6.13	1.70	1.53
2	D	401	FJF	C04-C05	6.00	1.47	1.38
2	D	401	FJF	O10-C11	5.95	1.58	1.45
2	D	401	FJF	O10-C09	5.91	1.53	1.44
2	C	401	FJF	C16-C14	5.91	1.69	1.53
2	A	401	FJF	C16-C14	5.88	1.69	1.53
2	B	401	FJF	C04-C05	5.85	1.47	1.38
2	A	401	FJF	O10-C09	5.77	1.53	1.44
2	C	401	FJF	C04-C05	5.69	1.47	1.38
2	C	401	FJF	O10-C09	5.57	1.53	1.44
2	B	401	FJF	O10-C11	5.54	1.57	1.45
2	C	401	FJF	O10-C11	5.54	1.57	1.45
2	A	401	FJF	O10-C11	5.49	1.57	1.45
2	B	401	FJF	C06-N08	5.44	1.42	1.33
2	A	401	FJF	C06-N08	5.34	1.42	1.33
2	A	401	FJF	C04-C05	5.31	1.46	1.38
2	D	401	FJF	C06-N08	5.03	1.41	1.33
2	C	401	FJF	C06-N08	5.02	1.41	1.33
2	D	401	FJF	C02-N03	4.79	1.47	1.38
2	B	401	FJF	O10-C09	4.69	1.51	1.44
2	A	401	FJF	C02-N03	4.45	1.47	1.38
2	B	401	FJF	C02-N03	4.41	1.46	1.38
2	C	401	FJF	C02-N03	4.30	1.46	1.38
2	C	401	FJF	C04-N03	4.25	1.43	1.34
2	B	401	FJF	C04-N03	4.16	1.43	1.34
2	C	401	FJF	C02-N08	4.14	1.46	1.38
2	B	401	FJF	C02-N08	4.02	1.46	1.38
2	A	401	FJF	C04-N03	3.99	1.42	1.34
2	D	401	FJF	C04-N03	3.91	1.42	1.34
2	D	401	FJF	C02-N08	3.76	1.45	1.38
2	D	401	FJF	C05-C06	3.70	1.49	1.41
2	B	401	FJF	C05-C06	3.70	1.49	1.41
2	A	401	FJF	C05-C06	3.69	1.49	1.41
2	A	401	FJF	C02-N08	3.63	1.45	1.38
2	C	401	FJF	C05-C06	3.12	1.48	1.41
2	B	401	FJF	C12-C11	2.06	1.58	1.51

All (44) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FJF	N08-C02-N03	-15.06	116.46	128.43
2	A	401	FJF	N08-C02-N03	-14.26	117.09	128.43
2	B	401	FJF	N08-C02-N03	-14.21	117.14	128.43
2	D	401	FJF	N08-C02-N03	-13.30	117.85	128.43
2	C	401	FJF	C11-O10-C09	-8.49	98.94	109.42
2	C	401	FJF	C02-N08-C06	8.14	122.01	115.14
2	D	401	FJF	C11-O10-C09	-7.78	99.82	109.42
2	A	401	FJF	C02-N08-C06	7.53	121.50	115.14
2	A	401	FJF	C11-O10-C09	-7.37	100.33	109.42
2	D	401	FJF	C02-N08-C06	7.01	121.06	115.14
2	B	401	FJF	C02-N08-C06	6.49	120.62	115.14
2	B	401	FJF	C11-O10-C09	-6.43	101.49	109.42
2	B	401	FJF	C04-N03-C02	4.95	123.52	115.36
2	A	401	FJF	C04-N03-C02	4.77	123.23	115.36
2	C	401	FJF	C04-N03-C02	4.76	123.21	115.36
2	A	401	FJF	O10-C09-C05	-4.46	103.02	109.93
2	A	401	FJF	C05-C04-N03	-4.35	119.10	124.44
2	C	401	FJF	C05-C04-N03	-4.29	119.16	124.44
2	B	401	FJF	C05-C04-N03	-4.17	119.32	124.44
2	D	401	FJF	C04-N03-C02	4.17	122.23	115.36
2	C	401	FJF	O10-C09-C05	-4.02	103.71	109.93
2	D	401	FJF	C05-C04-N03	-3.83	119.74	124.44
2	B	401	FJF	O15-C14-C16	-3.66	99.99	111.82
2	A	401	FJF	C05-C06-N08	-3.62	120.70	125.36
2	D	401	FJF	O10-C09-C05	-3.56	104.42	109.93
2	C	401	FJF	C05-C06-N08	-3.47	120.89	125.36
2	B	401	FJF	O10-C09-C05	-3.34	104.76	109.93
2	D	401	FJF	C05-C06-N08	-3.16	121.29	125.36
2	B	401	FJF	O10-C11-C12	-2.97	102.78	109.21
2	D	401	FJF	O10-C11-C12	-2.92	102.91	109.21
2	B	401	FJF	C12-C11-C14	2.83	121.90	115.09
2	A	401	FJF	O15-C14-C16	-2.81	102.75	111.82
2	C	401	FJF	O10-C11-C12	-2.62	103.55	109.21
2	D	401	FJF	C12-C11-C14	2.57	121.27	115.09
2	C	401	FJF	O15-C14-C16	-2.48	103.81	111.82
2	B	401	FJF	C05-C06-N08	-2.47	122.18	125.36
2	A	401	FJF	O15-C14-C11	-2.29	104.42	111.05
2	D	401	FJF	O15-C14-C16	-2.27	104.47	111.82
2	C	401	FJF	C16-C14-C11	2.26	107.03	102.64
2	B	401	FJF	O10-C09-C16	-2.23	101.05	104.66
2	A	401	FJF	C16-C14-C11	2.12	106.75	102.64
2	A	401	FJF	C12-C11-C14	2.07	120.08	115.09
2	A	401	FJF	O17-C16-C09	-2.02	107.14	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FJF	O10-C11-C12	-2.02	104.85	109.21

There are no chirality outliers.

All (15) torsion outliers are listed below:

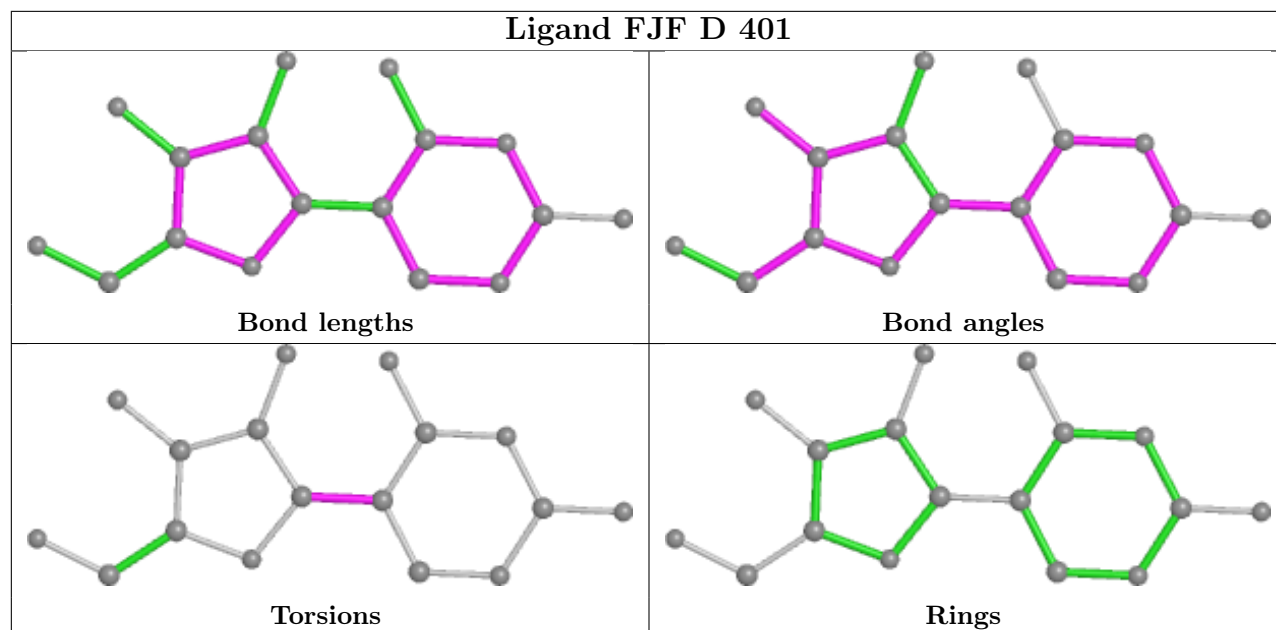
Mol	Chain	Res	Type	Atoms
2	A	401	FJF	C04-C05-C09-O10
2	A	401	FJF	C04-C05-C09-C16
2	A	401	FJF	C06-C05-C09-O10
2	A	401	FJF	C06-C05-C09-C16
2	B	401	FJF	C04-C05-C09-O10
2	B	401	FJF	C04-C05-C09-C16
2	B	401	FJF	C06-C05-C09-O10
2	C	401	FJF	C04-C05-C09-O10
2	C	401	FJF	C04-C05-C09-C16
2	C	401	FJF	C06-C05-C09-O10
2	C	401	FJF	C06-C05-C09-C16
2	D	401	FJF	C04-C05-C09-O10
2	D	401	FJF	C06-C05-C09-O10
2	D	401	FJF	C04-C05-C09-C16
2	B	401	FJF	C06-C05-C09-C16

There are no ring outliers.

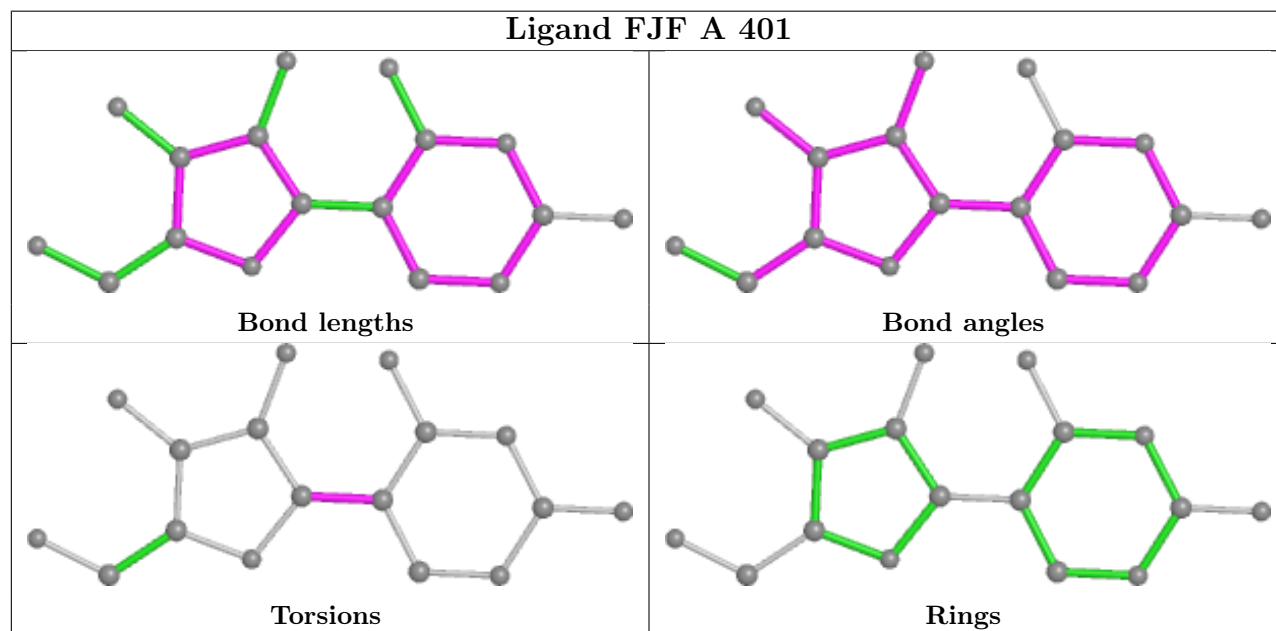
No monomer is involved in short contacts.

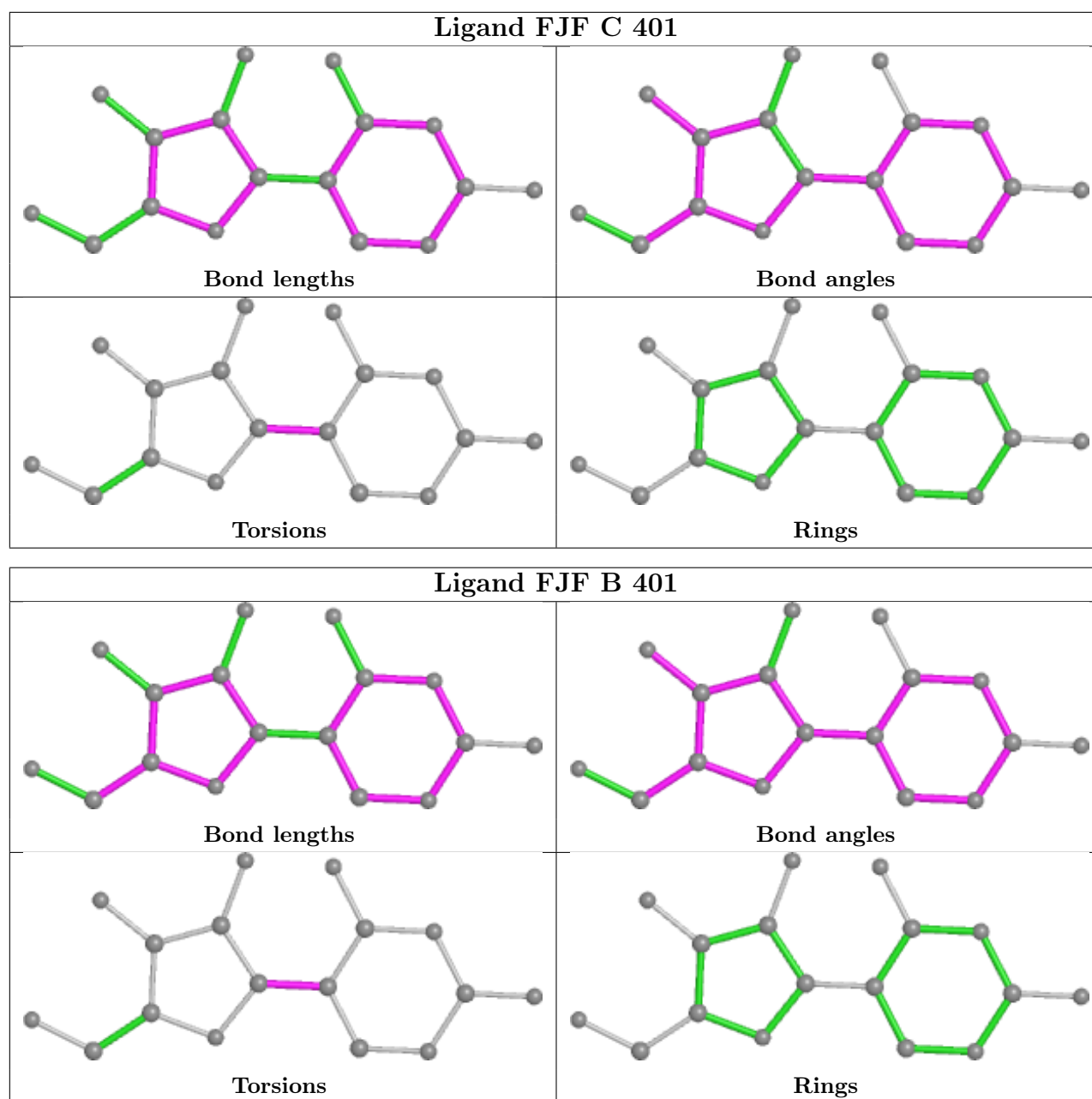
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand FJF D 401



## Ligand FJF A 401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	298/313 (95%)	0.29	13 (4%) 34 37	33, 49, 93, 138	0
1	B	300/313 (95%)	0.34	12 (4%) 38 41	32, 50, 99, 127	0
1	C	299/313 (95%)	0.29	13 (4%) 35 38	33, 49, 99, 145	0
1	D	298/313 (95%)	0.33	13 (4%) 34 37	31, 50, 100, 143	0
All	All	1195/1252 (95%)	0.32	51 (4%) 35 38	31, 50, 99, 145	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	ALA	6.3
1	A	30	ALA	4.6
1	C	30	ALA	4.6
1	C	21	SER	4.0
1	D	291	TYR	3.9
1	C	291	TYR	3.8
1	B	21	SER	3.7
1	D	109	VAL	3.7
1	B	305	LEU	3.6
1	A	29	ASP	3.6
1	A	109	VAL	3.6
1	C	22	HIS	3.3
1	A	108	LEU	3.1
1	B	297	LEU	3.1
1	D	108	LEU	3.1
1	A	249	ILE	3.1
1	A	21	SER	3.0
1	D	20	TYR	2.9
1	B	88	ILE	2.9
1	B	4	LYS	2.9
1	D	3	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	169	TRP	2.8
1	D	30	ALA	2.8
1	B	20	TYR	2.8
1	D	305	LEU	2.8
1	C	20	TYR	2.8
1	A	305	LEU	2.7
1	C	108	LEU	2.7
1	B	291	TYR	2.6
1	D	68	TYR	2.6
1	D	169	TRP	2.6
1	C	29	ASP	2.6
1	C	109	VAL	2.6
1	D	287	LEU	2.5
1	A	20	TYR	2.5
1	A	100	LEU	2.5
1	B	29	ASP	2.4
1	A	24	SER	2.4
1	C	287	LEU	2.4
1	D	252	THR	2.4
1	B	169	TRP	2.4
1	C	100	LEU	2.3
1	C	31	ASN	2.2
1	A	169	TRP	2.1
1	B	31	ASN	2.1
1	D	88	ILE	2.1
1	B	101	LEU	2.1
1	A	5	ASP	2.0
1	A	244	ILE	2.0
1	C	305	LEU	2.0
1	D	297	LEU	2.0

## 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](#)

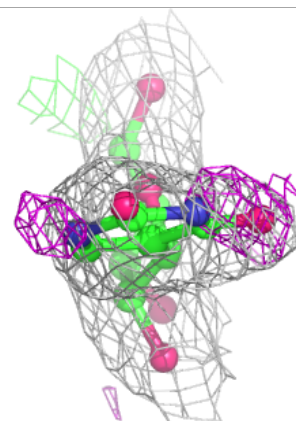
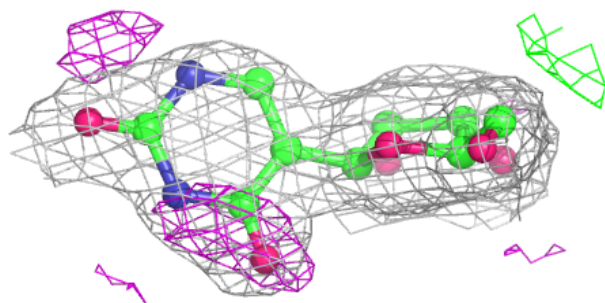
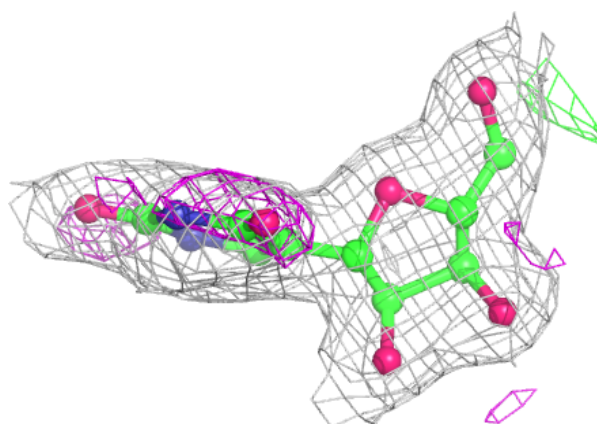
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FJF	C	401	17/17	0.94	0.09	34,41,52,57	0
2	FJF	A	401	17/17	0.95	0.09	35,42,49,59	0
2	FJF	B	401	17/17	0.96	0.09	34,40,54,58	0
2	FJF	D	401	17/17	0.97	0.10	34,40,56,59	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 FJF C 401:

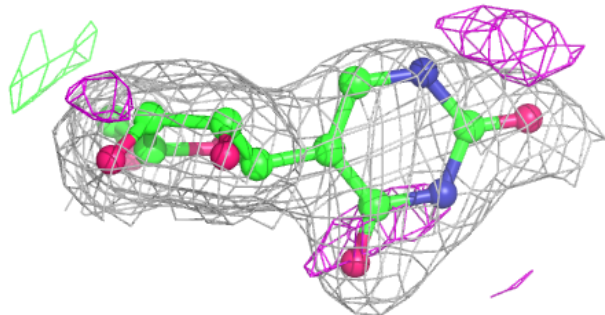
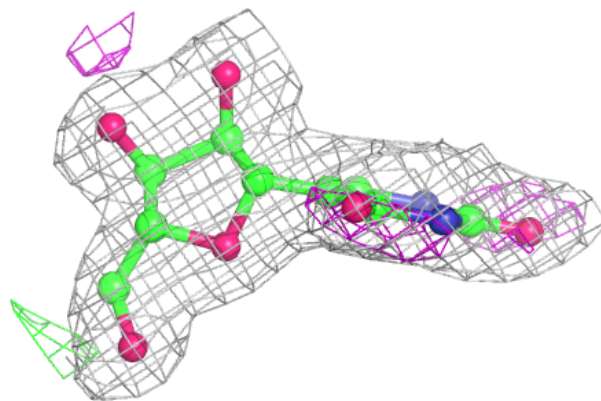
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



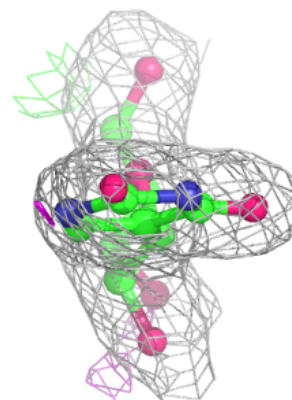
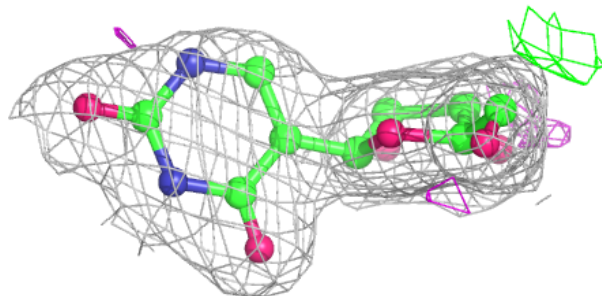
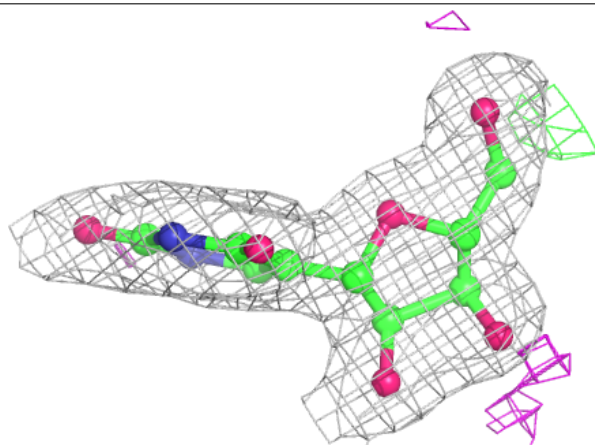


**Electron density around FJF A 401:**

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

**Electron density around FJF B 401:**

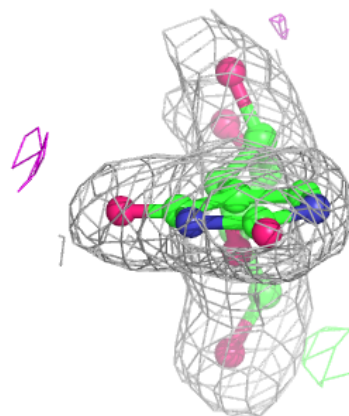
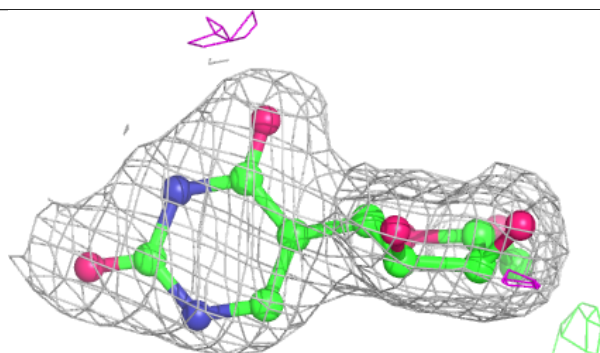
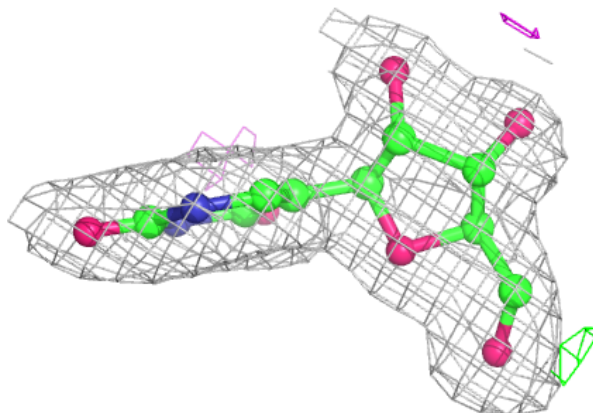
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FJF D 401:**

$2mF_o - DF_c$  (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.