



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:59 PM UTC

PDB ID : 7VVA / pdb_00007vva
Title : Pseudouridine bound structure of Pseudouridine kinase (PUKI) from Escherichia coli strain B
Authors : Kim, S.H.; Rhee, S.
Deposited on : 2021-11-05
Resolution : 2.75 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

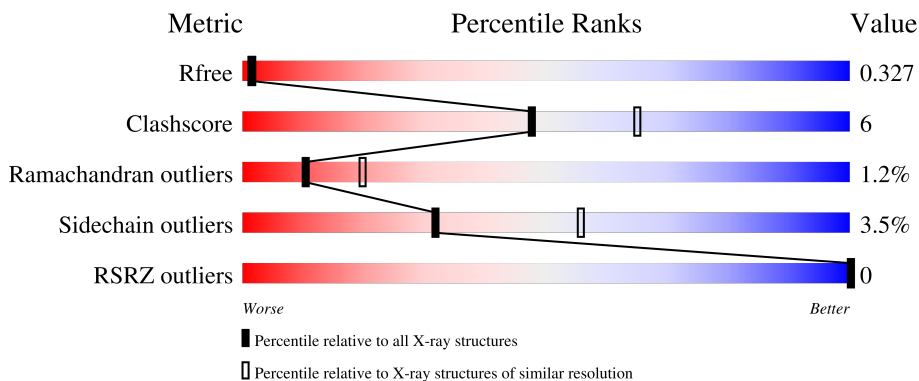
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	 83% 12% . .
1	B	313	 77% 17% . .
1	C	313	 80% 14% . 5%
1	D	313	 80% 14% . .
1	E	313	 76% 18% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	313	 <p>73% 10% 16%</p>
1	G	313	 <p>52% 11% 36%</p>
1	H	313	 <p>35% 9% 55%</p>

2 Entry composition [i](#)

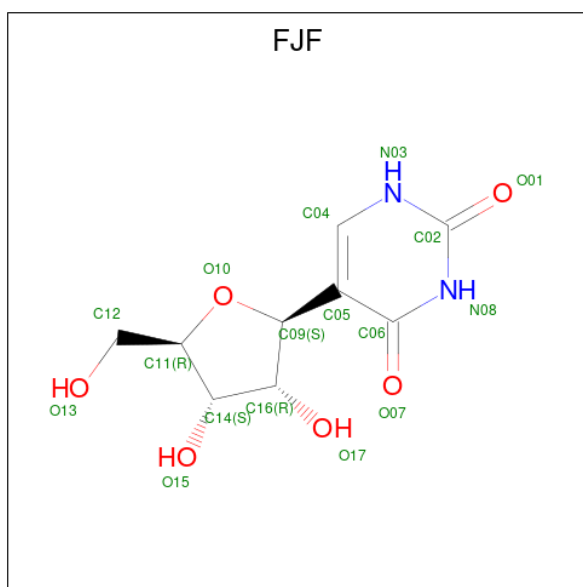
There are 3 unique types of molecules in this entry. The entry contains 15761 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	303	2272	1428	392	440	12	0	0	0
1	B	299	2243	1410	389	432	12	0	0	0
1	C	298	2231	1404	385	430	12	0	0	0
1	D	302	2256	1421	387	436	12	0	0	0
1	E	300	2222	1400	384	426	12	0	0	0
1	F	262	1917	1205	326	375	11	0	0	0
1	G	201	1468	926	240	296	6	0	0	0
1	H	140	1050	670	172	205	3	0	0	0

- 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 (CCD ID: FJF) (formula: C₉H₁₂N₂O₆) (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		

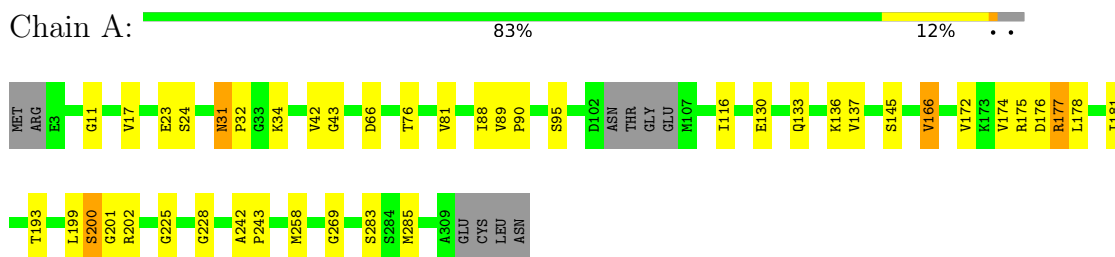
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	11	Total	O	0	0
			11	11		
3	C	4	Total	O	0	0
			4	4		
3	D	5	Total	O	0	0
			5	5		
3	E	3	Total	O	0	0
			3	3		
3	G	1	Total	O	0	0
			1	1		
3	H	3	Total	O	0	0
			3	3		

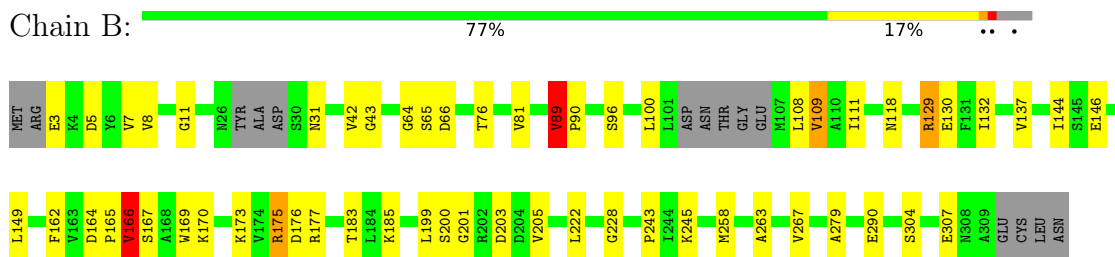
3 Residue-property plots

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.

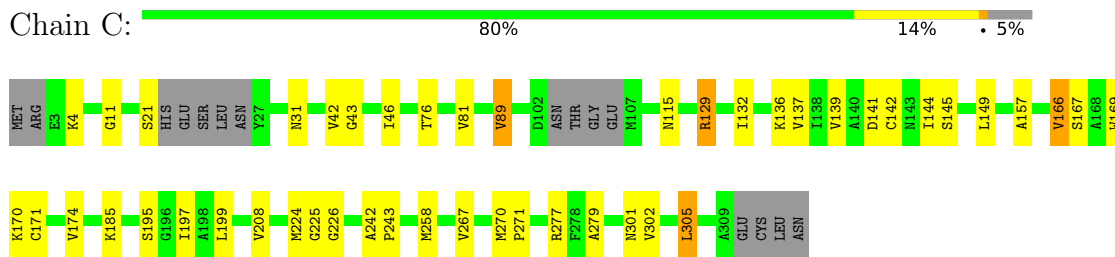
- Molecule 1: Pseudouridine kinase



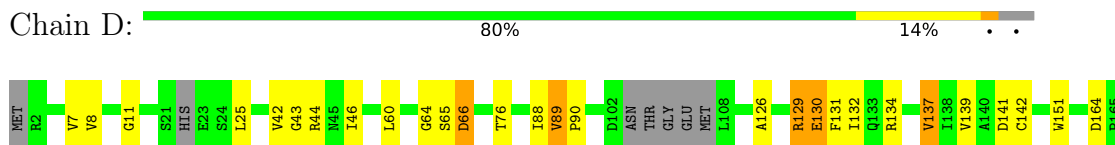
- Molecule 1: Pseudouridine kinase



- Molecule 1: Pseudouridine kinase



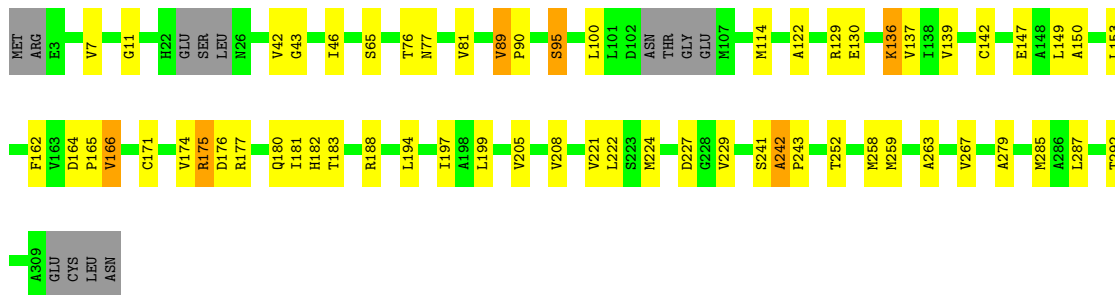
- Molecule 1: Pseudouridine kinase





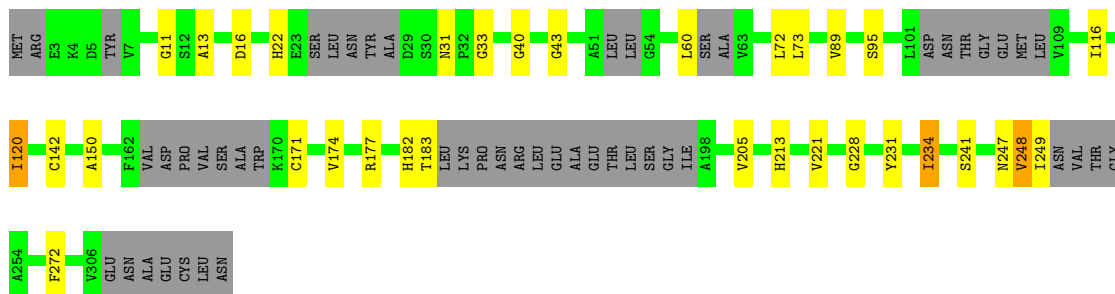
- Molecule 1: Pseudouridine kinase

Chain E: 76% 18%



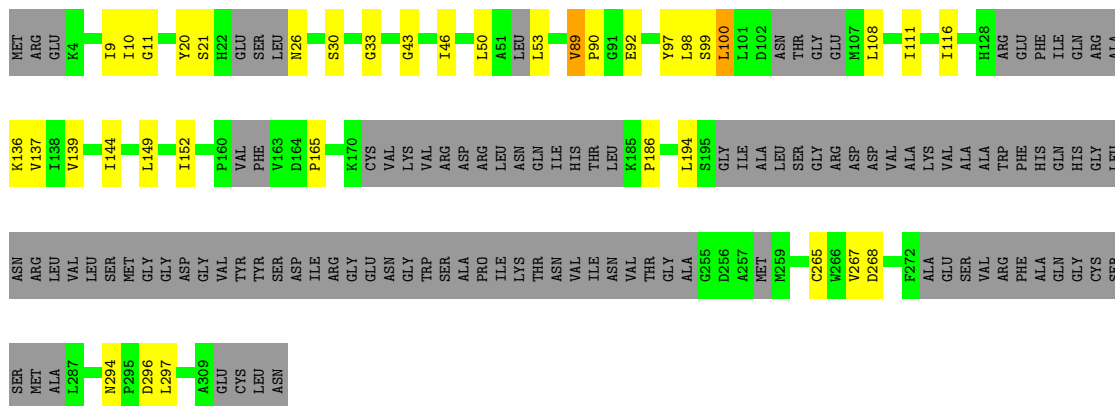
- Molecule 1: Pseudouridine kinase

Chain F: 73% 10% 16%



- Molecule 1: Pseudouridine kinase

Chain G: 52% 11% 36%



- Molecule 1: Pseudouridine kinase

Chain H: 35% 9% 55%

MET	ARG	GLU	LYS	D5	Y6	V7	V8	I9	I10	V17	M26	D29	S30	N31	P32	I46	A47	Q48	ASN	L50	L60	S71	N77	Q78	S79	V81	D84	V89	P90	D102	ASN	THR	GLY	GLU	MET	L108	V109	M114	I120	E123	F131	I132	GLN	ARG																								
ALA	K136	V137	I138	V139	C142	A148	I152	L153	D154	ASN	ALA	ALA	ASN	ASN	VAL	PRO	VAL	PHE	VAL	ASP	PRO	VAL	SER	ALA	TRP	LYS	CYS	VAL	LYS	VAL	VAL	ARG	GLY	ARG	GLN	ILE	HIS	THR	LEU	LYS	PRO	ASN	ARG	ARG	LEU	LEU	ALA	GLU	GLU	ALA	THR	GLY	THR	LEU	SER	GLY	ILE	ALA	LEU	SER	GLY							
ARG	ASP	ASP	VAL	ALA	LYS	VAL	ALA	ALA	TRP	PHE	HIS	GLN	HIS	GLY	LEU	ARG	PHE	ALA	ALA	GLN	LEU	VAL	LEU	CYS	SER	SER	MET	GLY	ALA	GLY	ASP	GLY	VAL	TYR	TYR	SER	ASP	ILE	ILE	ARG	GLY	ASP	LEU	LEU	SER	ASN	ILE	ALA	TRP	ASN	SER	ILE	VAL	ILE	SER	LEU	VAL	THR	ASN	ASN	GLU	ALA	ALA	GLU	GLU	CYS	LEU	ASN
LEU	ALA	SER	CYS	TRP	VAL	ASP	GLY	MET	PRO	PHE	ALA	GLU	SER	VAL	ARG	PHE	ALA	ALA	GLN	GLY	CYS	SER	SER	MET	ALA	LEU	SER	CYS	GLU	TYR	THR	ASN	ASN	PRO	ASP	LEU	SER	ILE	ALA	ASN	VAL	ILE	SER	LEU	VAL	THR	ASN	ASN	GLU	ALA	ALA	GLU	CYS	LEU	ASN													

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.95Å 271.89Å 101.20Å 90.00° 110.91° 90.00°	Depositor
Resolution (Å)	33.64 – 2.75 33.64 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.2 (33.64-2.75) 91.7 (33.64-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.76Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.296 , 0.325 0.302 , 0.327	Depositor DCC
R_{free} test set	1993 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.210	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.410 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15761	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/2313	0.79	3/3149 (0.1%)
1	B	0.32	0/2281	0.78	1/3101 (0.0%)
1	C	0.31	0/2269	0.81	1/3086 (0.0%)
1	D	0.31	0/2295	0.81	7/3124 (0.2%)
1	E	0.37	0/2262	0.88	6/3084 (0.2%)
1	F	0.32	0/1945	0.85	3/2643 (0.1%)
1	G	0.26	0/1487	0.71	1/2027 (0.0%)
1	H	0.26	0/1064	0.73	1/1446 (0.1%)
All	All	0.31	0/15916	0.81	23/21660 (0.1%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	31	ASN	CA-C-N	6.71	126.70	119.78
1	F	31	ASN	C-N-CA	6.71	126.70	119.78
1	B	89	VAL	N-CA-C	6.70	114.53	107.76
1	C	89	VAL	N-CA-C	6.48	113.45	107.56
1	D	89	VAL	N-CA-C	6.22	113.22	107.56

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	2272	0	2216	24	0
1	B	2243	0	2210	29	0
1	C	2231	0	2193	23	0
1	D	2256	0	2202	29	0
1	E	2222	0	2149	34	0
1	F	1917	0	1807	14	0
1	G	1468	0	1387	20	0
1	H	1050	0	1027	9	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	7	0	0	0	0
3	B	11	0	0	0	0
3	C	4	0	0	1	0
3	D	5	0	0	0	0
3	E	3	0	0	0	0
3	G	1	0	0	0	0
3	H	3	0	0	0	0
All	All	15761	0	15191	173	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.

The worst 5 of 173 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:F:213:HIS:HB3	1:F:234:ILE:HD13	1.57	0.85
1:E:129:ARG:NH1	1:E:130:GLU:OE2	2.21	0.73
1:E:188:ARG:HG2	1:E:199:LEU:HD22	1.71	0.72
1:F:11:GLY:HA3	1:F:43:GLY:HA3	1.75	0.68
1:D:129:ARG:O	1:D:132:ILE:N	2.28	0.66

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	299/313 (96%)	276 (92%)	19 (6%)	4 (1%)	9	18
1	B	293/313 (94%)	271 (92%)	14 (5%)	8 (3%)	4	7
1	C	292/313 (93%)	269 (92%)	20 (7%)	3 (1%)	12	24
1	D	296/313 (95%)	277 (94%)	15 (5%)	4 (1%)	9	17
1	E	294/313 (94%)	272 (92%)	18 (6%)	4 (1%)	9	17
1	F	244/313 (78%)	233 (96%)	10 (4%)	1 (0%)	30	50
1	G	181/313 (58%)	167 (92%)	13 (7%)	1 (1%)	21	38
1	H	130/313 (42%)	119 (92%)	11 (8%)	0	100	100
All	All	2029/2504 (81%)	1884 (93%)	120 (6%)	25 (1%)	10	20

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ARG
1	B	130	GLU
1	D	65	SER
1	D	129	ARG
1	D	130	GLU

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	241/255 (94%)	235 (98%)	6 (2%)	42	64
1	B	240/255 (94%)	233 (97%)	7 (3%)	37	61
1	C	237/255 (93%)	231 (98%)	6 (2%)	42	64
1	D	238/255 (93%)	232 (98%)	6 (2%)	42	64
1	E	231/255 (91%)	225 (97%)	6 (3%)	40	63
1	F	197/255 (77%)	189 (96%)	8 (4%)	27	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	155/255 (61%)	148 (96%)	7 (4%)	24 46
1	H	112/255 (44%)	100 (89%)	12 (11%)	6 12
All	All	1651/2040 (81%)	1593 (96%)	58 (4%)	32 56

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	136	LYS
1	H	131	PHE
1	F	174	VAL
1	H	123	GLU
1	H	71	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	180	GLN
1	F	55	ASN
1	H	127	GLN
1	F	31	ASN
1	F	238	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 oligosaccharides 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	A	401	-	18,18,18	4.32	10 (55%)	22,26,26	1.94	6 (27%)
2	FJF	B	401	-	18,18,18	4.35	10 (55%)	22,26,26	2.01	6 (27%)
2	FJF	D	401	-	18,18,18	4.34	9 (50%)	22,26,26	2.06	7 (31%)
2	FJF	C	401	-	18,18,18	4.34	9 (50%)	22,26,26	2.03	6 (27%)

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

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FJF	O10-C09	-11.70	1.27	1.43
2	C	401	FJF	O10-C09	-11.65	1.27	1.43
2	D	401	FJF	O10-C09	-11.53	1.27	1.43
2	A	401	FJF	O10-C09	-11.35	1.28	1.43
2	A	401	FJF	C14-C11	-9.49	1.28	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FJF	N03-C02-N08	4.90	120.33	115.17
2	A	401	FJF	N03-C02-N08	4.87	120.31	115.17
2	C	401	FJF	N03-C02-N08	4.79	120.22	115.17
2	D	401	FJF	N03-C02-N08	4.77	120.20	115.17
2	B	401	FJF	C06-N08-C02	-4.20	120.59	126.37

There are no chirality outliers.

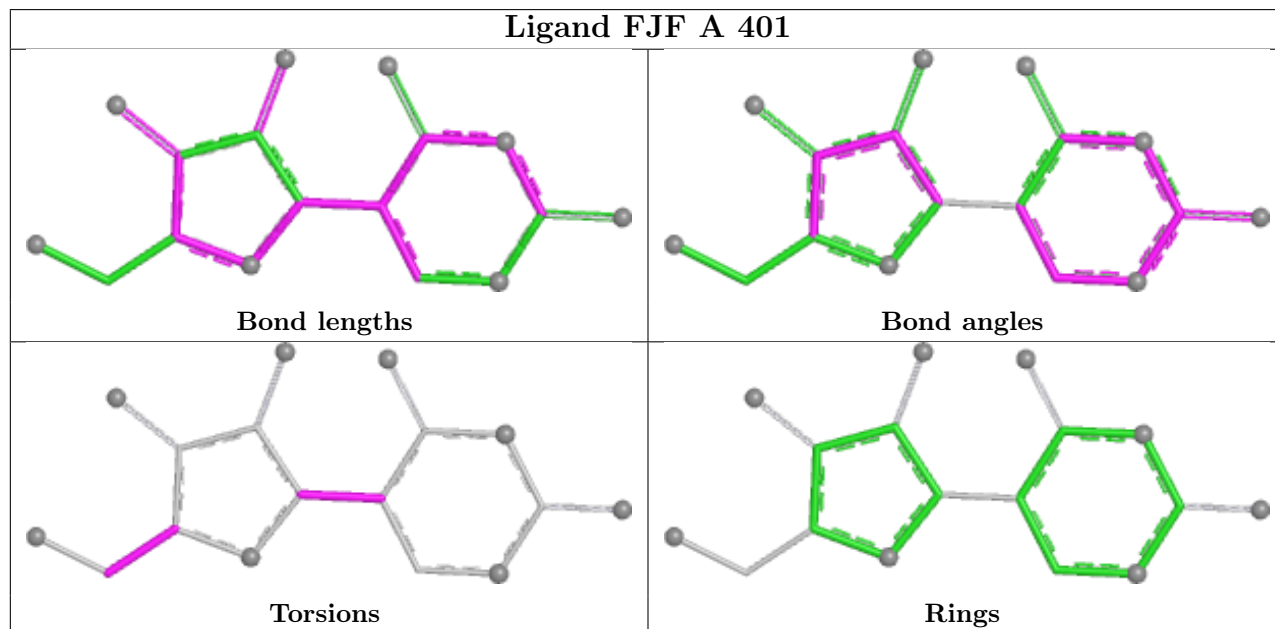
5 of 18 torsion outliers are listed below:

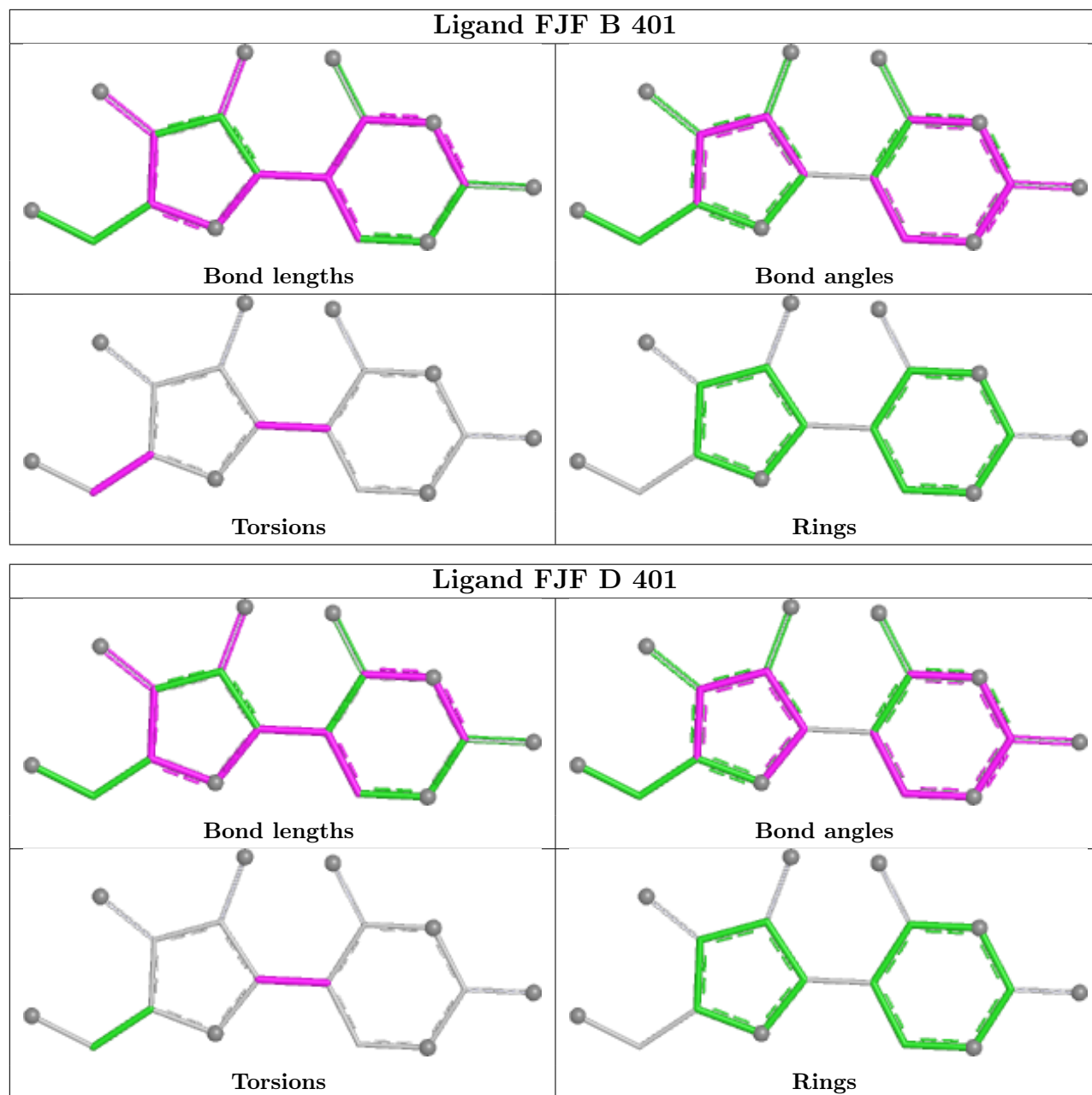
Mol	Chain	Res	Type	Atoms
2	A	401	FJF	C04-C05-C09-C16
2	A	401	FJF	C06-C05-C09-C16
2	A	401	FJF	O10-C11-C12-O13
2	B	401	FJF	C04-C05-C09-C16
2	B	401	FJF	C06-C05-C09-O10

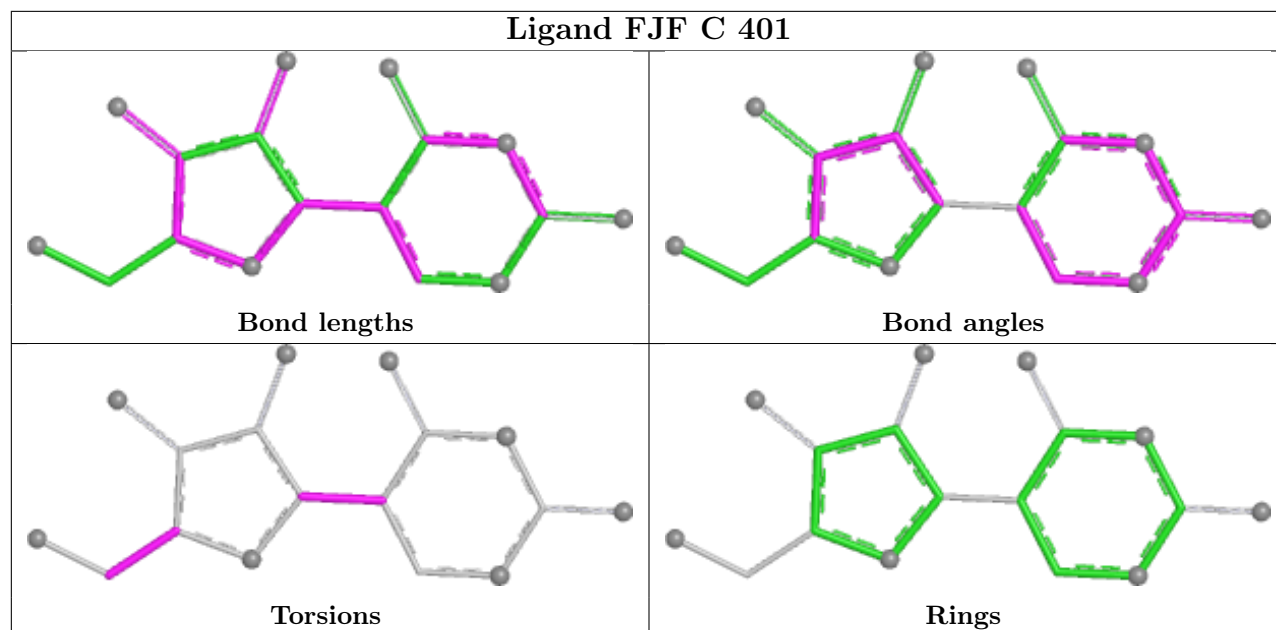
There are no ring outliers.

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.







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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/313 (96%)	-1.47	0 100 100	26, 48, 84, 132	0
1	B	299/313 (95%)	-1.48	0 100 100	38, 53, 87, 122	0
1	C	298/313 (95%)	-1.45	0 100 100	24, 48, 80, 131	0
1	D	302/313 (96%)	-1.45	0 100 100	28, 54, 94, 130	0
1	E	300/313 (95%)	-1.29	0 100 100	47, 83, 112, 126	0
1	F	262/313 (83%)	-1.20	0 100 100	50, 96, 121, 138	0
1	G	201/313 (64%)	-1.21	0 100 100	39, 88, 118, 132	0
1	H	140/313 (44%)	-1.26	0 100 100	48, 80, 110, 139	0
All	All	2105/2504 (84%)	-1.37	0 100 100	24, 65, 112, 139	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

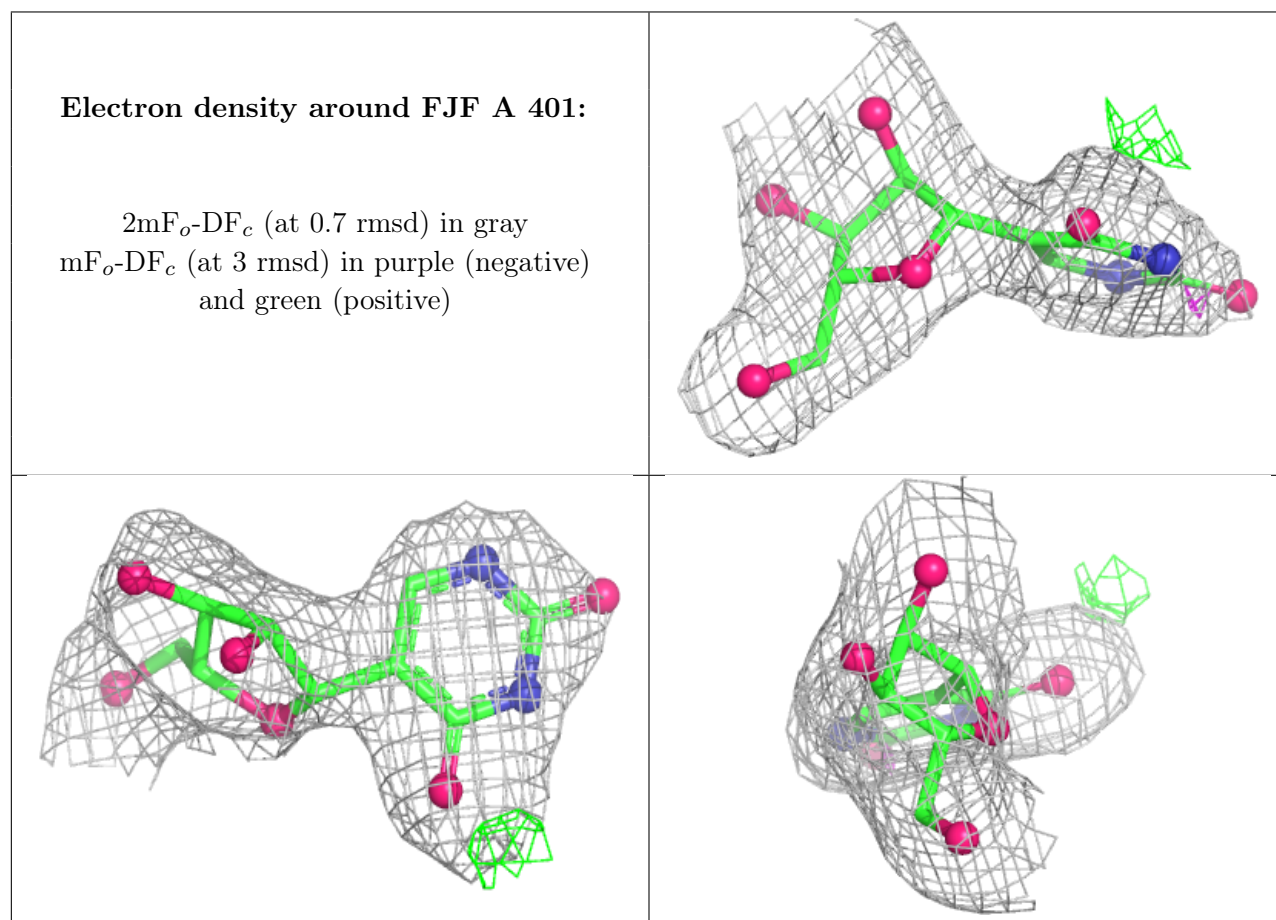
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

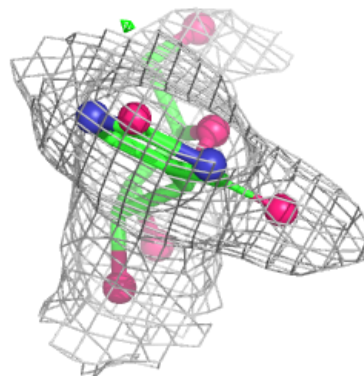
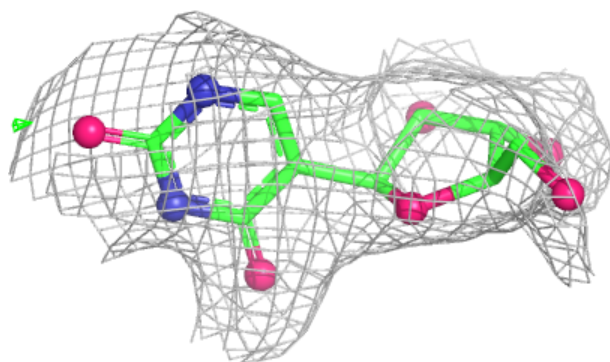
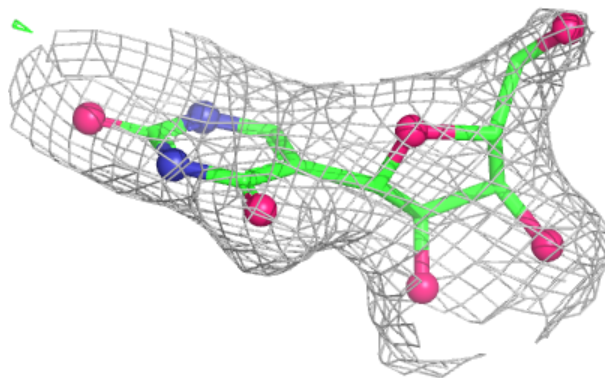
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FJF	A	401	17/17	0.99	0.04	32,52,85,86	0
2	FJF	B	401	17/17	0.99	0.03	33,48,65,79	0
2	FJF	C	401	17/17	0.99	0.04	32,49,67,67	0
2	FJF	D	401	17/17	0.99	0.03	45,52,60,60	0

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.



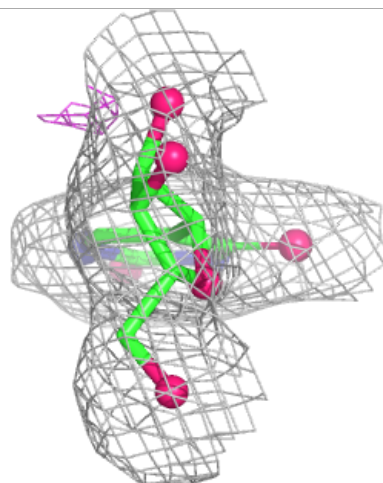
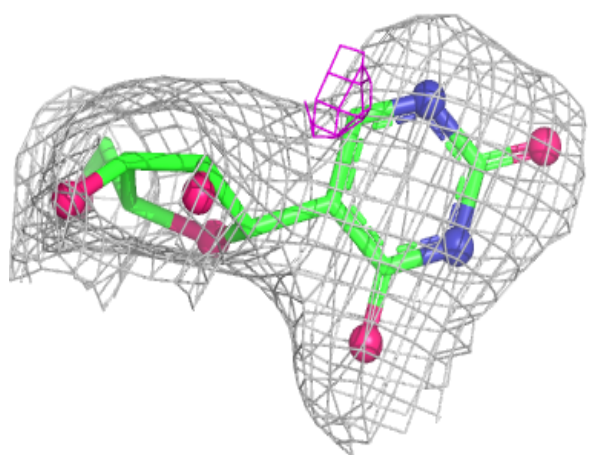
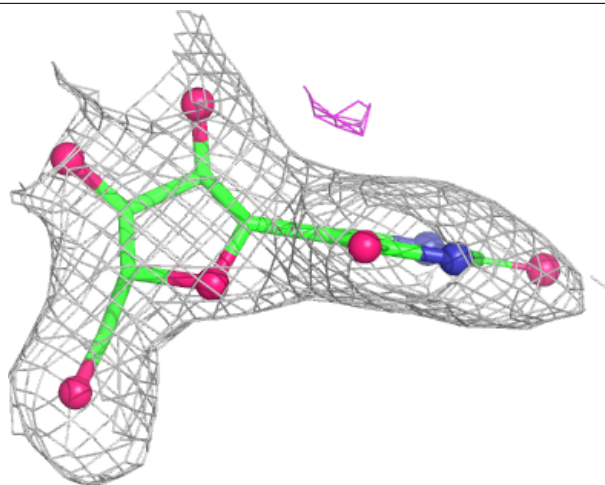
Electron density around FJF B 401:

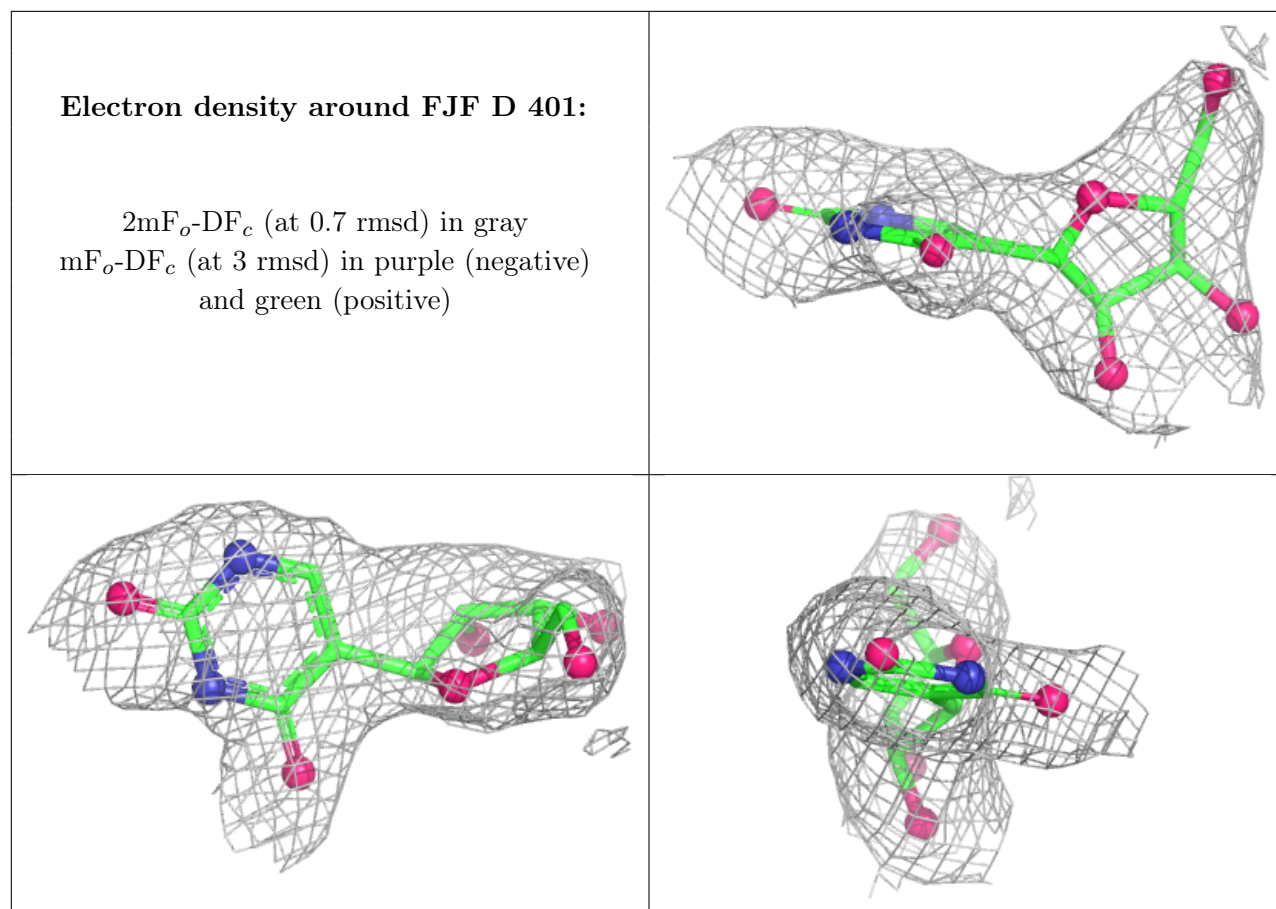
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FJF C 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.