



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2022 – 06:24 PM JST

PDB ID : 7VVA
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 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

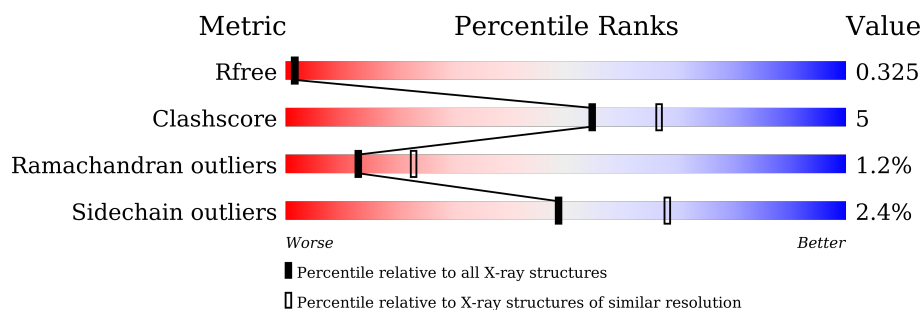
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	313	84% 12% . .
1	B	313	78% 17% . .
1	C	313	81% 13% . 5%
1	D	313	82% 14% . .
1	E	313	80% 15% . .
1	F	313	75% 8% . 16%
1	G	313	53% 11% 36%

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Mol	Chain	Length	Quality of chain
1	H	313	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment representing 37%, a yellow segment representing 7%, and a grey segment representing 55%. The percentages are labeled below the corresponding segments.

2 Entry composition

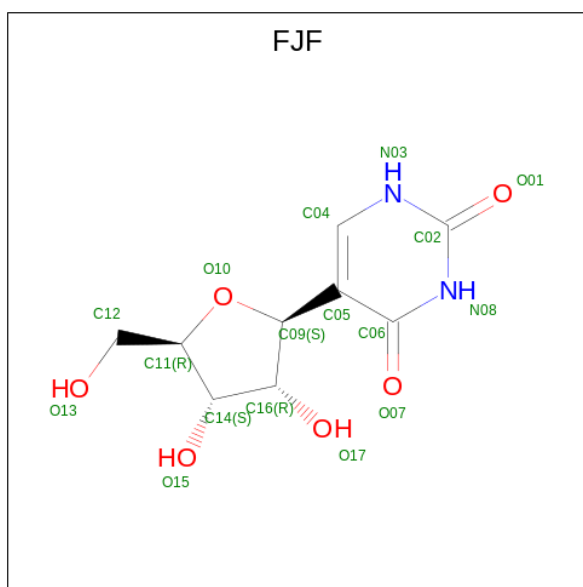
There are 3 unique types of molecules in this entry. The entry contains 15761 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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: 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		

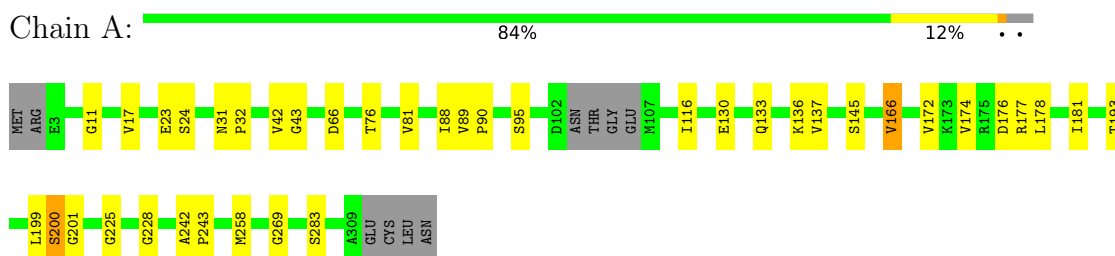
- Molecule 3 is water.

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		

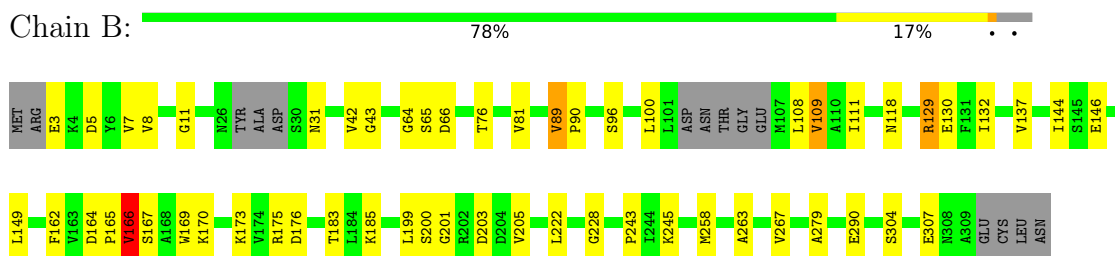
3 Residue-property plots [i](#)

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. 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. 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.

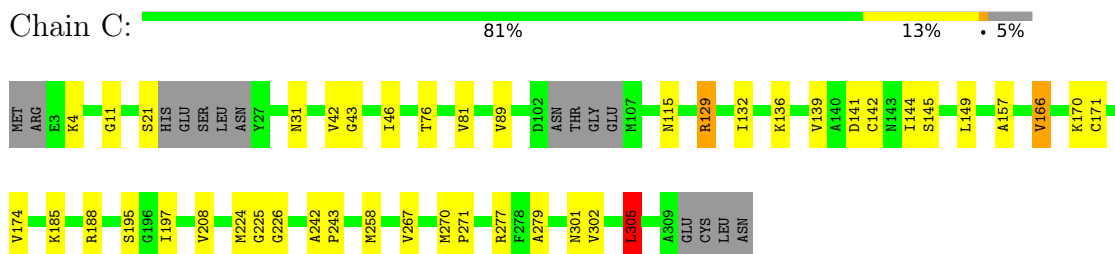
- Molecule 1: Pseudouridine kinase



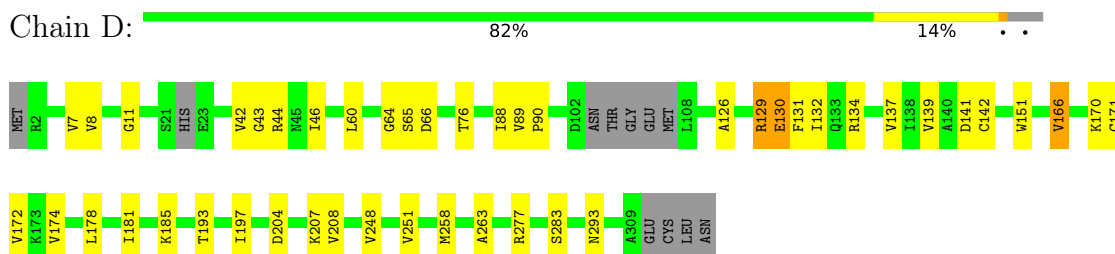
- Molecule 1: Pseudouridine kinase



- Molecule 1: Pseudouridine kinase

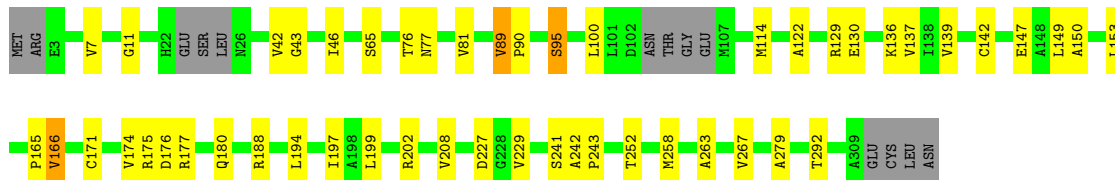


- Molecule 1: Pseudouridine kinase



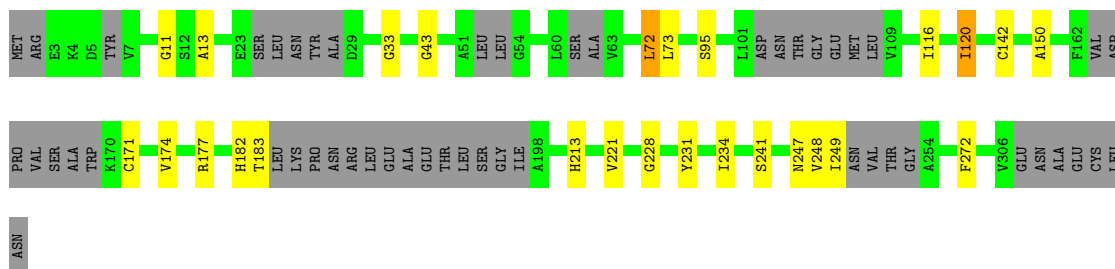
- Molecule 1: Pseudouridine kinase

Chain E: 80% 15% . .



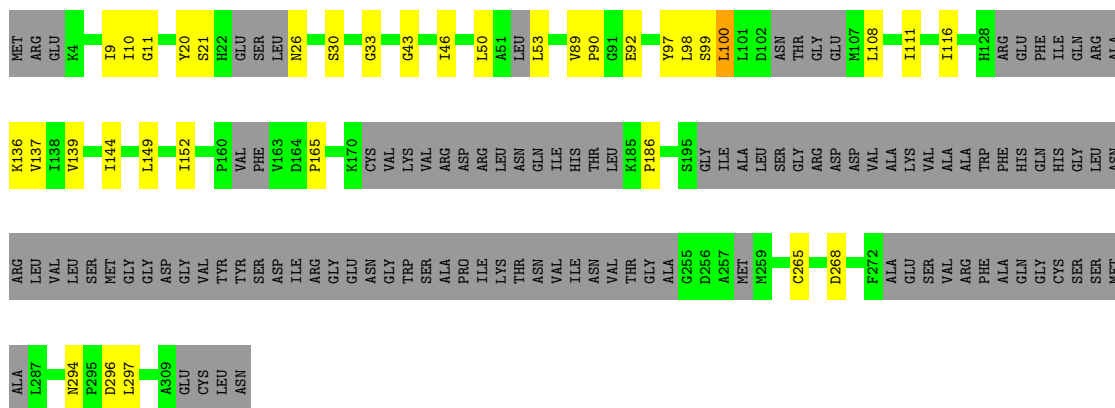
- Molecule 1: Pseudouridine kinase

Chain F: 75% 8% • 16%

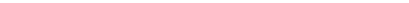


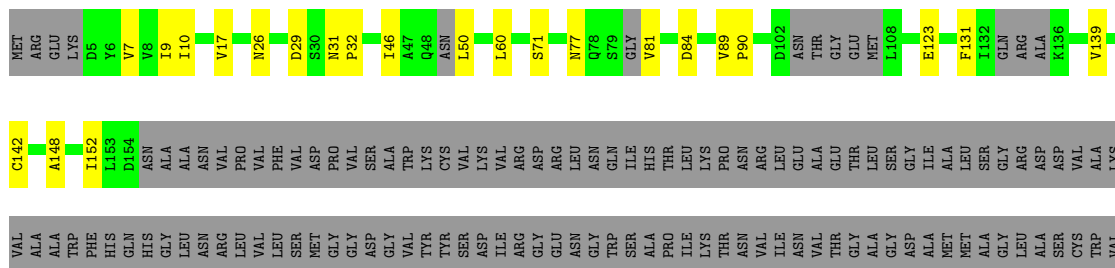
- Molecule 1: Pseudouridine kinase

Chain G:  53% 11% 36%



- Molecule 1: Pseudouridine kinase

Chain H:  37% 7% 55%



ASP
GLY
MET
PRO
PHE
ALA
GLU
SER
VAL
ARG
PHE
ALA
GLN
GLY
CYS
SER
SER
MET
MET
ALA
LEU
SER
CYS
GLU
TYR
THR
ASN
ASN
PRO
ASP
LEU
SER
ILE
ALA
ASN
VAL
ILE
SER
SER
LEU
VAL
GLU
ASN
ASN
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)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.296 , 0.325 0.300 , 0.325	Depositor DCC
R_{free} test set	1993 reflections (2.16%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.410 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15761	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage'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	0.23	0/2313	0.45	0/3149
1	B	0.25	0/2281	0.45	0/3101
1	C	0.23	0/2269	0.47	1/3086 (0.0%)
1	D	0.23	0/2295	0.45	0/3124
1	E	0.29	0/2262	0.49	0/3084
1	F	0.24	0/1945	0.46	0/2643
1	G	0.20	0/1487	0.37	0/2027
1	H	0.20	0/1064	0.39	0/1446
All	All	0.24	0/15916	0.45	1/21660 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	305	LEU	CA-CB-CG	8.03	133.78	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	2272	0	2216	22	0
1	B	2243	0	2210	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2231	0	2193	22	0
1	D	2256	0	2202	28	0
1	E	2222	0	2149	29	0
1	F	1917	0	1807	13	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	162	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.

The worst 5 of 162 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%)	12	21
1	B	293/313 (94%)	271 (92%)	14 (5%)	8 (3%)	5	7
1	C	292/313 (93%)	269 (92%)	20 (7%)	3 (1%)	15	27
1	D	296/313 (95%)	277 (94%)	15 (5%)	4 (1%)	11	19
1	E	294/313 (94%)	272 (92%)	18 (6%)	4 (1%)	11	19
1	F	244/313 (78%)	233 (96%)	10 (4%)	1 (0%)	34	53
1	G	181/313 (58%)	167 (92%)	13 (7%)	1 (1%)	25	42
1	H	130/313 (42%)	119 (92%)	11 (8%)	0	100	100
All	All	2029/2504 (81%)	1884 (93%)	120 (6%)	25 (1%)	13	23

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 ⓘ

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%)	236 (98%)	5 (2%)	53	71
1	B	240/255 (94%)	233 (97%)	7 (3%)	42	62
1	C	237/255 (93%)	232 (98%)	5 (2%)	53	71
1	D	238/255 (93%)	235 (99%)	3 (1%)	69	81
1	E	231/255 (91%)	227 (98%)	4 (2%)	60	76
1	F	197/255 (77%)	193 (98%)	4 (2%)	55	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	155/255 (61%)	150 (97%)	5 (3%)	39 59
1	H	112/255 (44%)	106 (95%)	6 (5%)	22 38
All	All	1651/2040 (81%)	1612 (98%)	39 (2%)	49 68

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	26	ASN
1	H	84	ASP
1	G	53	LEU
1	G	100	LEU
1	H	131	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	301	ASN
1	F	31	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	401	-	17,18,18	4.36	7 (41%)	20,26,26	3.35	6 (30%)
2	FJF	C	401	-	17,18,18	4.36	7 (41%)	20,26,26	3.41	7 (35%)
2	FJF	A	401	-	17,18,18	4.34	7 (41%)	20,26,26	3.35	7 (35%)
2	FJF	D	401	-	17,18,18	4.36	7 (41%)	20,26,26	3.43	8 (40%)

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	B	401	-	-	5/6/22/22	0/2/2/2
2	FJF	C	401	-	-	6/6/22/22	0/2/2/2
2	FJF	A	401	-	-	6/6/22/22	0/2/2/2
2	FJF	D	401	-	-	3/6/22/22	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FJF	O10-C09	-11.35	1.27	1.44
2	C	401	FJF	O10-C09	-11.30	1.27	1.44
2	D	401	FJF	O10-C09	-11.19	1.27	1.44
2	A	401	FJF	O10-C09	-11.03	1.28	1.44
2	A	401	FJF	C14-C11	-9.42	1.28	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FJF	N08-C02-N03	-10.35	120.20	128.43
2	C	401	FJF	N08-C02-N03	-10.32	120.22	128.43
2	A	401	FJF	N08-C02-N03	-10.22	120.31	128.43
2	B	401	FJF	N08-C02-N03	-10.18	120.33	128.43
2	A	401	FJF	C02-N08-C06	6.68	120.78	115.14

There are no chirality outliers.

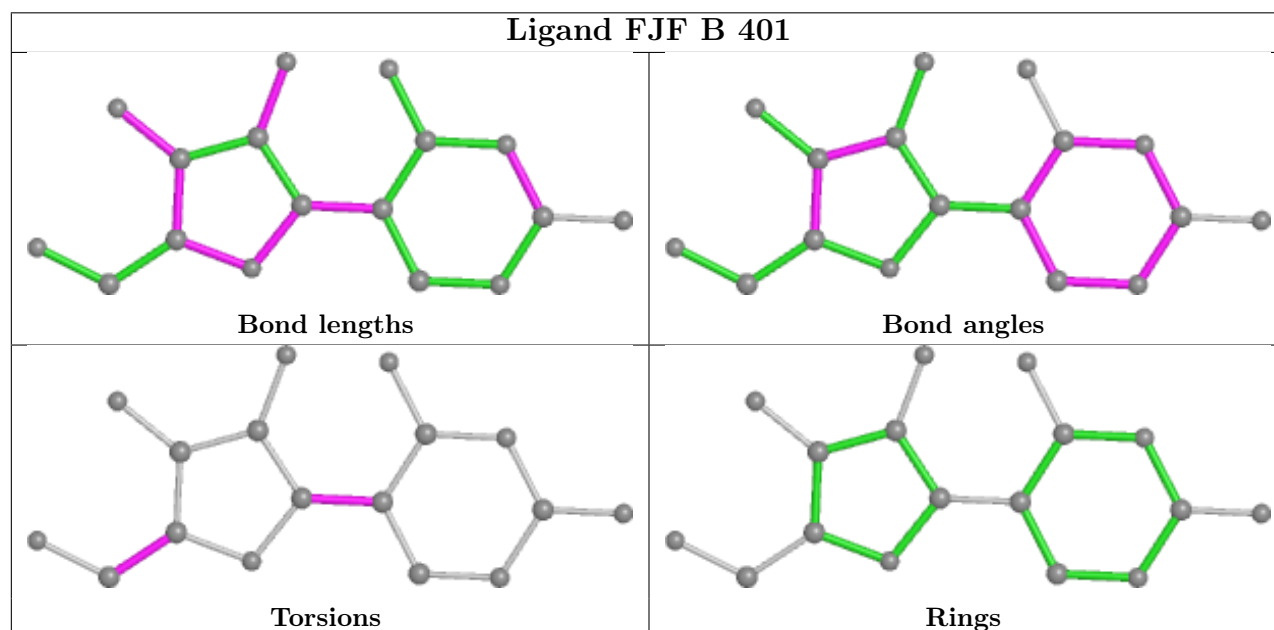
5 of 20 torsion outliers are listed below:

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	A	401	FJF	O10-C11-C12-O13

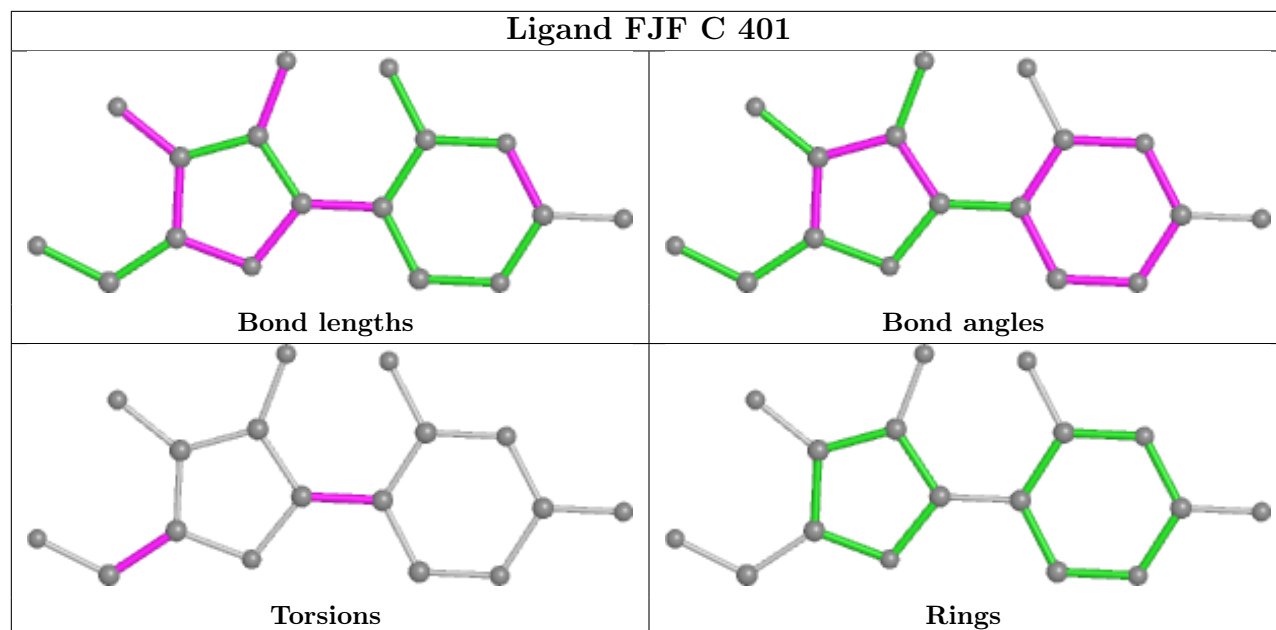
There are no ring outliers.

No monomer is involved in short contacts.

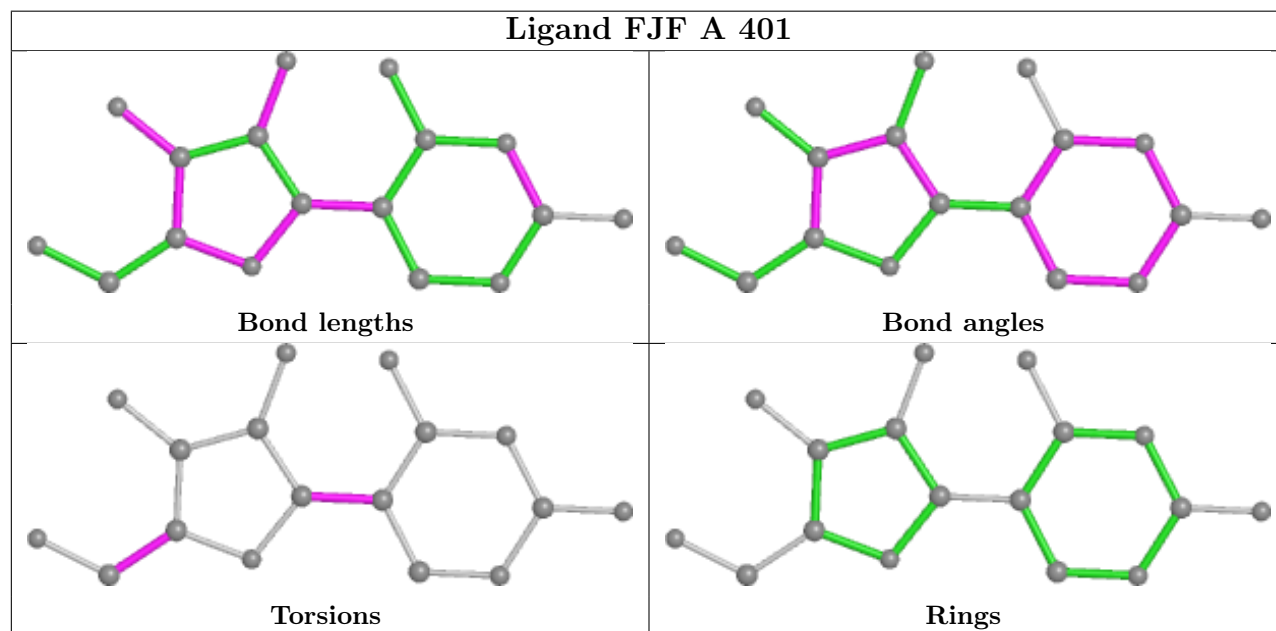
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

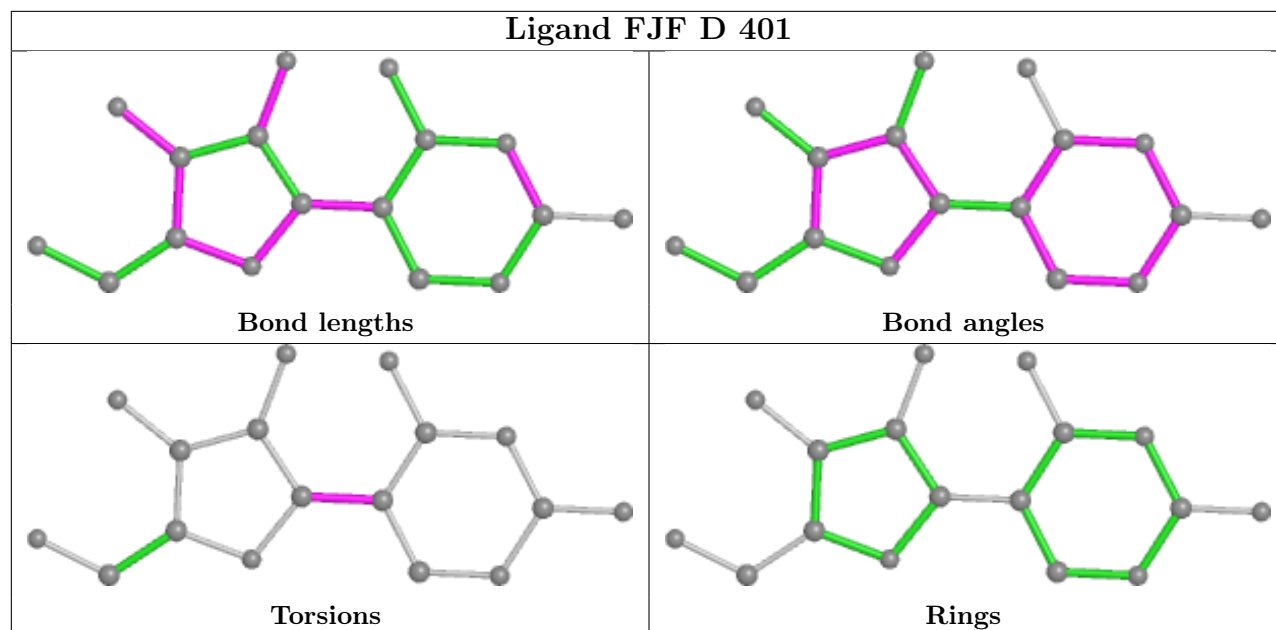


Ligand FJF C 401



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

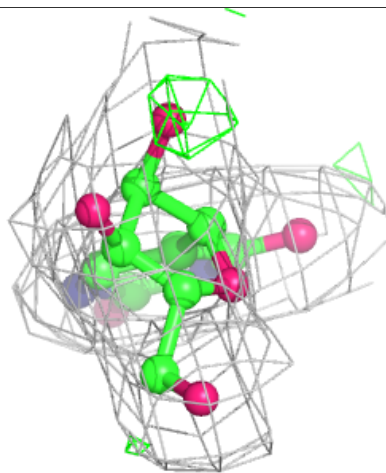
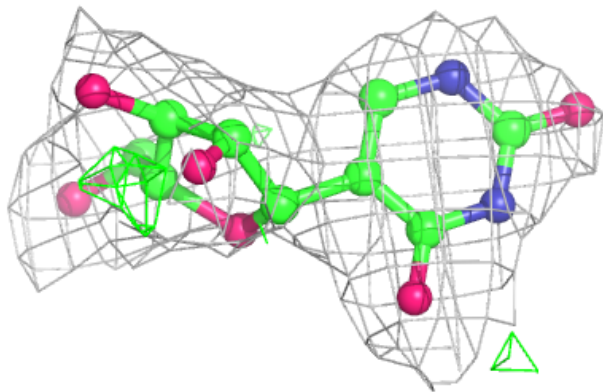
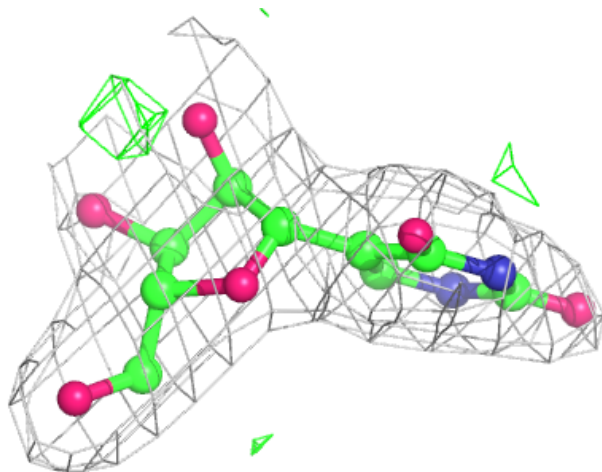
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

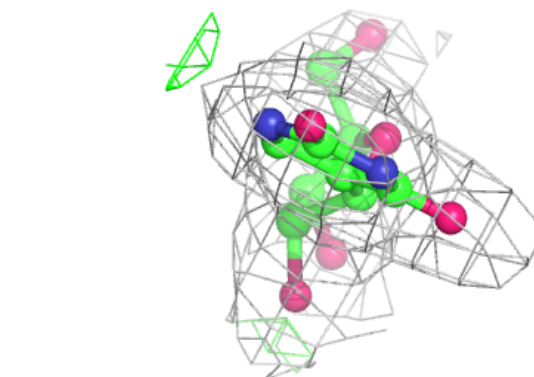
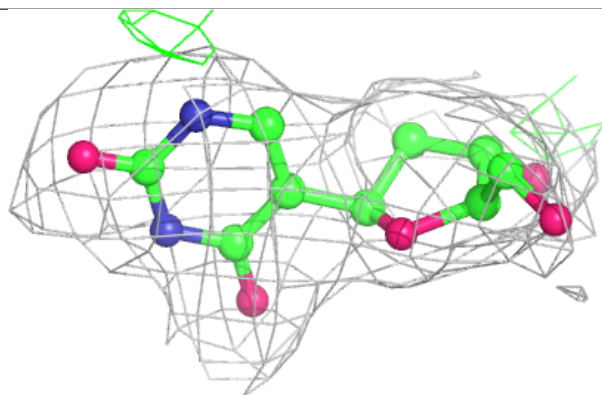
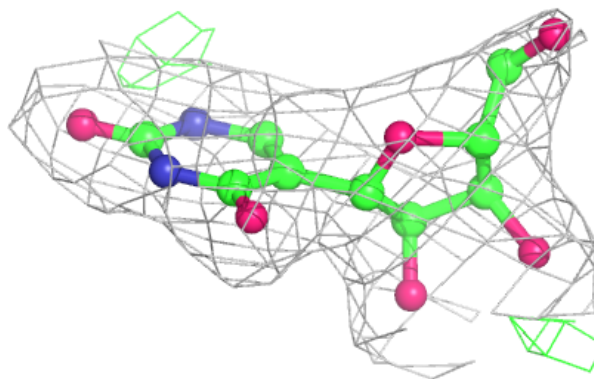
Electron density around FJF A 401:

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

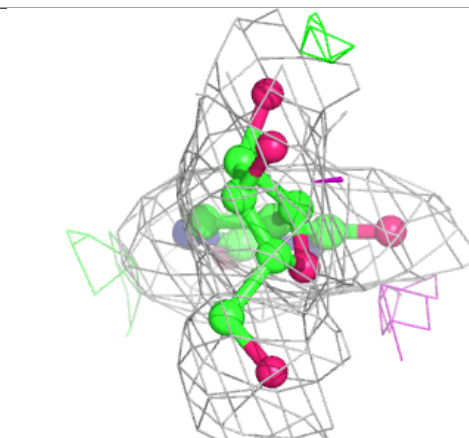
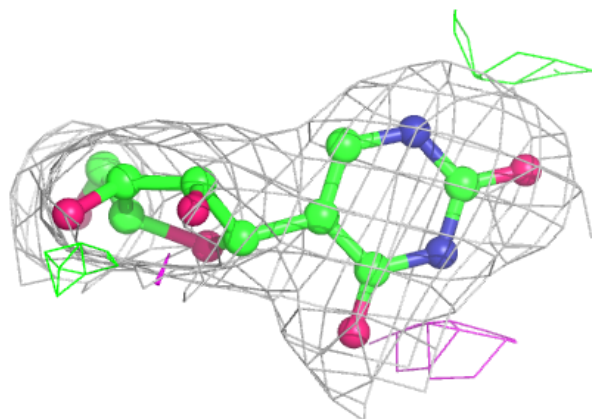
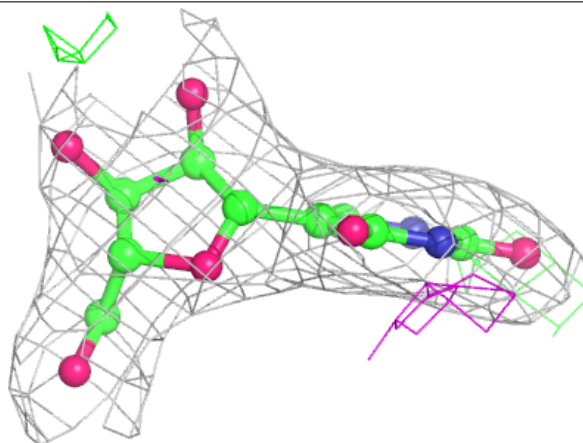


Electron density around FJF B 401:

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

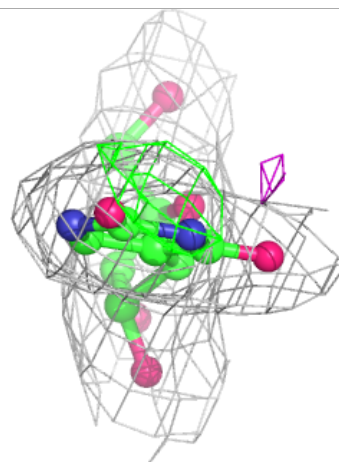
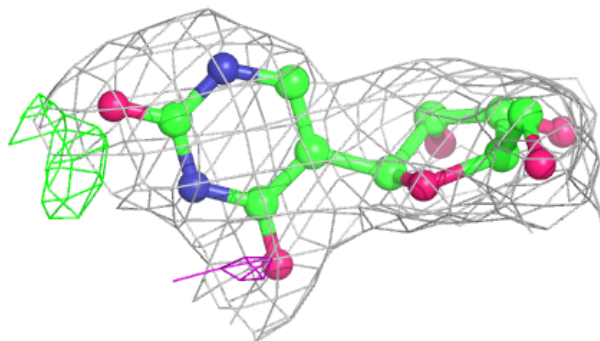
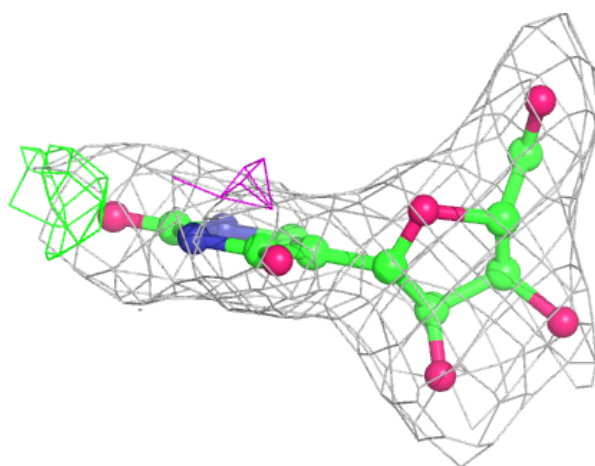
**Electron density around FJF C 401:**

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



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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.