



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 02:22 pm BST

PDB ID : 9RLS / pdb\_00009rls  
Title : PARP10 catalytic domain in complex with OUL499  
Authors : Alaviuhkola, J.; Lehtio, L.  
Deposited on : 2025-06-17  
Resolution : 2.75 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.

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 ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

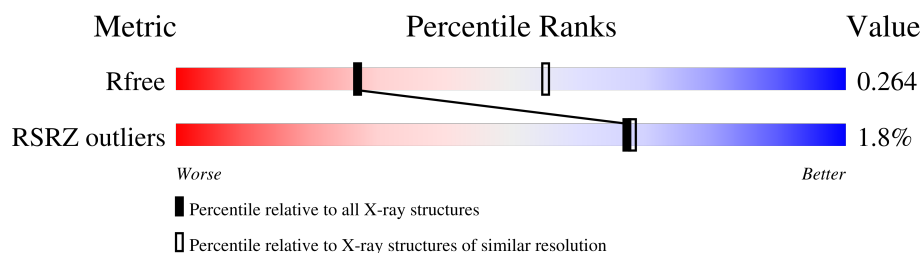
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	164625	1606 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24184 atoms, of which 11963 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 Poly [ADP-ribose] polymerase 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	189	Total	C	H	N	O	S	50	0	0
			2982	940	1482	284	270	6			
1	B	189	Total	C	H	N	O	S	51	0	0
			2992	942	1488	285	271	6			
1	C	188	Total	C	H	N	O	S	50	0	0
			2981	939	1483	284	270	5			
1	D	189	Total	C	H	N	O	S	51	0	0
			2992	942	1488	285	271	6			
1	E	188	Total	C	H	N	O	S	51	0	0
			2973	937	1479	283	269	5			
1	F	186	Total	C	H	N	O	S	51	1	0
			2970	937	1478	283	266	6			
1	G	189	Total	C	H	N	O	S	51	0	0
			2992	942	1488	285	271	6			
1	H	189	Total	C	H	N	O	S	51	0	0
			2992	942	1489	284	270	7			

There are 16 discrepancies between the modelled and reference sequences:

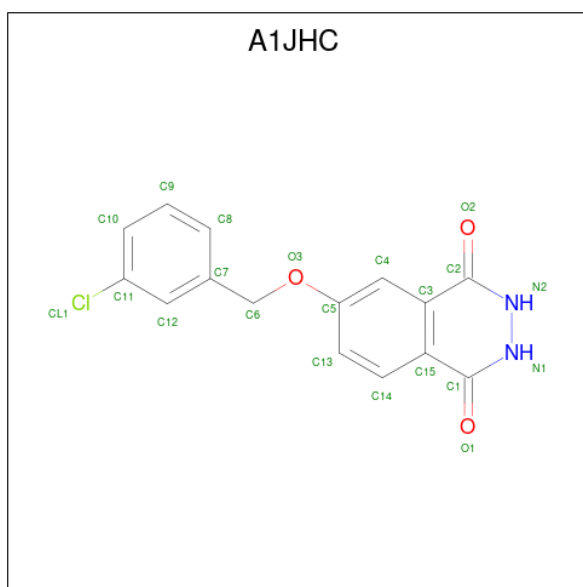
Chain	Residue	Modelled	Actual	Comment	Reference
A	817	SER	-	expression tag	UNP Q53GL7
A	818	MET	-	expression tag	UNP Q53GL7
B	817	SER	-	expression tag	UNP Q53GL7
B	818	MET	-	expression tag	UNP Q53GL7
C	817	SER	-	expression tag	UNP Q53GL7
C	818	MET	-	expression tag	UNP Q53GL7
D	817	SER	-	expression tag	UNP Q53GL7
D	818	MET	-	expression tag	UNP Q53GL7
E	817	SER	-	expression tag	UNP Q53GL7
E	818	MET	-	expression tag	UNP Q53GL7
F	817	SER	-	expression tag	UNP Q53GL7
F	818	MET	-	expression tag	UNP Q53GL7
G	817	SER	-	expression tag	UNP Q53GL7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	818	MET	-	expression tag	UNP Q53GL7
H	817	SER	-	expression tag	UNP Q53GL7
H	818	MET	-	expression tag	UNP Q53GL7

- Molecule 2 is 6-[(3-chlorophenyl)methoxy]-2,3-dihydrophthalazine-1,4-dione (CCD ID: A1JHC) (formula: C<sub>15</sub>H<sub>11</sub>ClN<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		
2	B	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		
2	C	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		
2	D	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		
2	E	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		
2	F	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		
2	G	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		
2	H	1	Total	C	Cl	H	N	O	0	0
			32	15	1	11	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	9	Total O 9 9	0	0
3	C	8	Total O 8 8	0	0
3	D	9	Total O 9 9	0	0
3	E	3	Total O 3 3	0	0
3	F	3	Total O 3 3	0	0
3	G	7	Total O 7 7	0	0
3	H	7	Total O 7 7	0	0

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.59Å 71.65Å 131.46Å 102.57° 96.38° 90.01°	Depositor
Resolution (Å)	48.32 – 2.75 48.32 – 2.75	Depositor EDS
% Data completeness (in resolution range)	90.9 (48.32-2.75) 90.9 (48.32-2.75)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.214 , 0.265 0.214 , 0.264	Depositor DCC
$R_{free}$ test set	2032 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2963e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

8 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	A1JHC	A	1101	-	22,23,23	1.42	5 (22%)	32,32,32	0.84	0
2	A1JHC	E	1101	-	22,23,23	1.63	5 (22%)	32,32,32	0.71	1 (3%)
2	A1JHC	G	1101	-	22,23,23	1.17	1 (4%)	32,32,32	0.80	2 (6%)
2	A1JHC	B	1101	-	22,23,23	1.48	4 (18%)	32,32,32	0.67	0
2	A1JHC	H	1101	-	22,23,23	1.60	5 (22%)	32,32,32	0.72	0
2	A1JHC	F	1101	-	22,23,23	1.33	4 (18%)	32,32,32	0.73	1 (3%)
2	A1JHC	D	1101	-	22,23,23	1.43	5 (22%)	32,32,32	0.63	0
2	A1JHC	C	1101	-	22,23,23	1.54	6 (27%)	32,32,32	0.85	0

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	A1JHC	A	1101	-	-	2/5/5/5	0/3/3/3
2	A1JHC	E	1101	-	-	0/5/5/5	0/3/3/3
2	A1JHC	G	1101	-	-	0/5/5/5	0/3/3/3
2	A1JHC	B	1101	-	-	0/5/5/5	0/3/3/3
2	A1JHC	H	1101	-	-	2/5/5/5	0/3/3/3
2	A1JHC	F	1101	-	-	0/5/5/5	0/3/3/3
2	A1JHC	D	1101	-	-	2/5/5/5	0/3/3/3
2	A1JHC	C	1101	-	-	3/5/5/5	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	A1JHC	C15-C1	-4.26	1.40	1.47
2	G	1101	A1JHC	C3-C2	-4.24	1.40	1.47
2	H	1101	A1JHC	C2-N2	4.14	1.40	1.33
2	E	1101	A1JHC	C1-N1	3.91	1.40	1.33
2	E	1101	A1JHC	C15-C1	-3.66	1.41	1.47
2	C	1101	A1JHC	C3-C2	-3.50	1.41	1.47
2	B	1101	A1JHC	C3-C2	-3.40	1.41	1.47
2	F	1101	A1JHC	C15-C1	-3.33	1.41	1.47
2	A	1101	A1JHC	C1-N1	3.32	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	A1JHC	C2-N2	3.27	1.39	1.33
2	F	1101	A1JHC	C3-C2	-3.26	1.41	1.47
2	H	1101	A1JHC	C1-N1	3.25	1.38	1.33
2	E	1101	A1JHC	C2-N2	3.13	1.38	1.33
2	D	1101	A1JHC	C2-N2	3.10	1.38	1.33
2	E	1101	A1JHC	C3-C2	-2.89	1.42	1.47
2	H	1101	A1JHC	C4-C3	2.89	1.44	1.39
2	D	1101	A1JHC	C1-N1	2.87	1.38	1.33
2	D	1101	A1JHC	C3-C2	-2.79	1.42	1.47
2	D	1101	A1JHC	C15-C1	-2.78	1.42	1.47
2	A	1101	A1JHC	C15-C1	-2.69	1.42	1.47
2	C	1101	A1JHC	C15-C1	-2.69	1.42	1.47
2	C	1101	A1JHC	C1-N1	2.68	1.38	1.33
2	A	1101	A1JHC	C2-N2	2.66	1.38	1.33
2	E	1101	A1JHC	C13-C5	2.43	1.43	1.38
2	A	1101	A1JHC	C3-C2	-2.42	1.43	1.47
2	C	1101	A1JHC	C4-C3	2.41	1.43	1.39
2	H	1101	A1JHC	O2-C2	2.39	1.28	1.23
2	A	1101	A1JHC	C4-C3	2.29	1.43	1.39
2	F	1101	A1JHC	C2-N2	2.26	1.37	1.33
2	F	1101	A1JHC	C4-C3	2.21	1.43	1.39
2	B	1101	A1JHC	C1-N1	2.20	1.37	1.33
2	C	1101	A1JHC	C13-C5	2.20	1.43	1.38
2	D	1101	A1JHC	C4-C3	2.13	1.43	1.39
2	H	1101	A1JHC	C3-C2	-2.06	1.43	1.47
2	B	1101	A1JHC	C2-N2	2.05	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1101	A1JHC	O1-C1-N1	-2.34	117.69	120.76
2	G	1101	A1JHC	C15-C3-C2	2.32	121.77	119.52
2	F	1101	A1JHC	O1-C1-N1	-2.27	117.79	120.76
2	E	1101	A1JHC	C15-C3-C2	2.15	121.61	119.52

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1101	A1JHC	C4-C5-O3-C6
2	H	1101	A1JHC	C13-C5-O3-C6
2	A	1101	A1JHC	C13-C5-O3-C6

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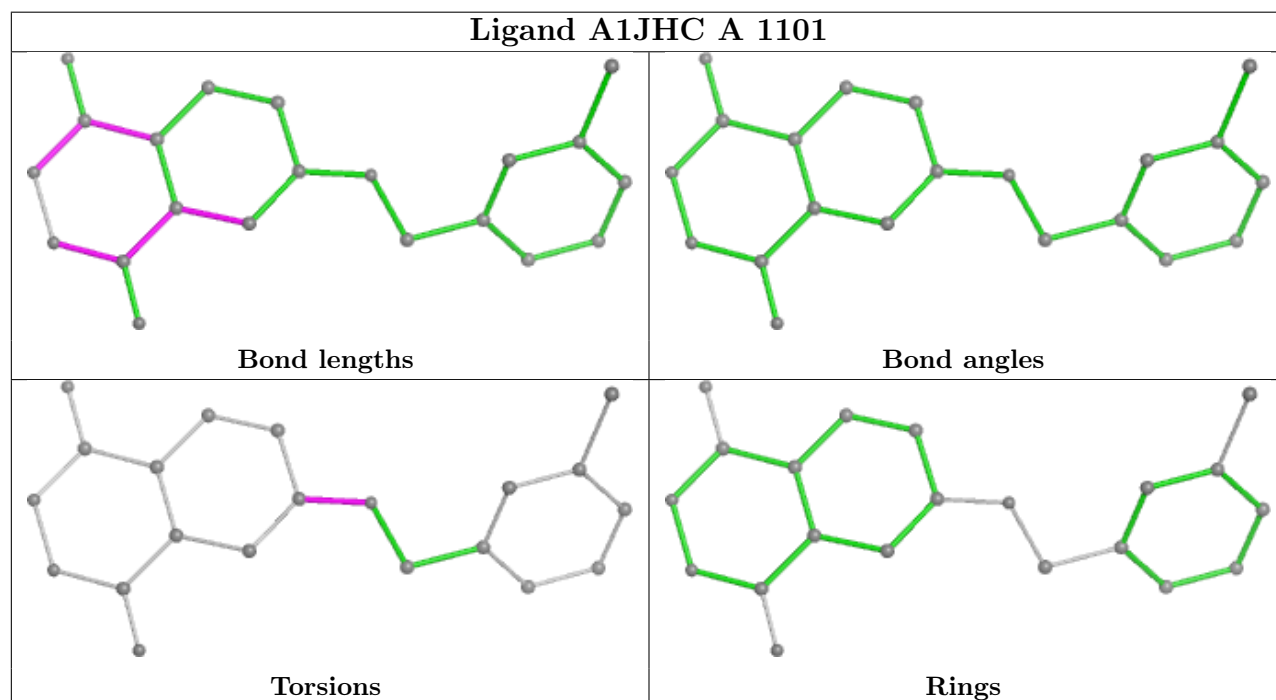
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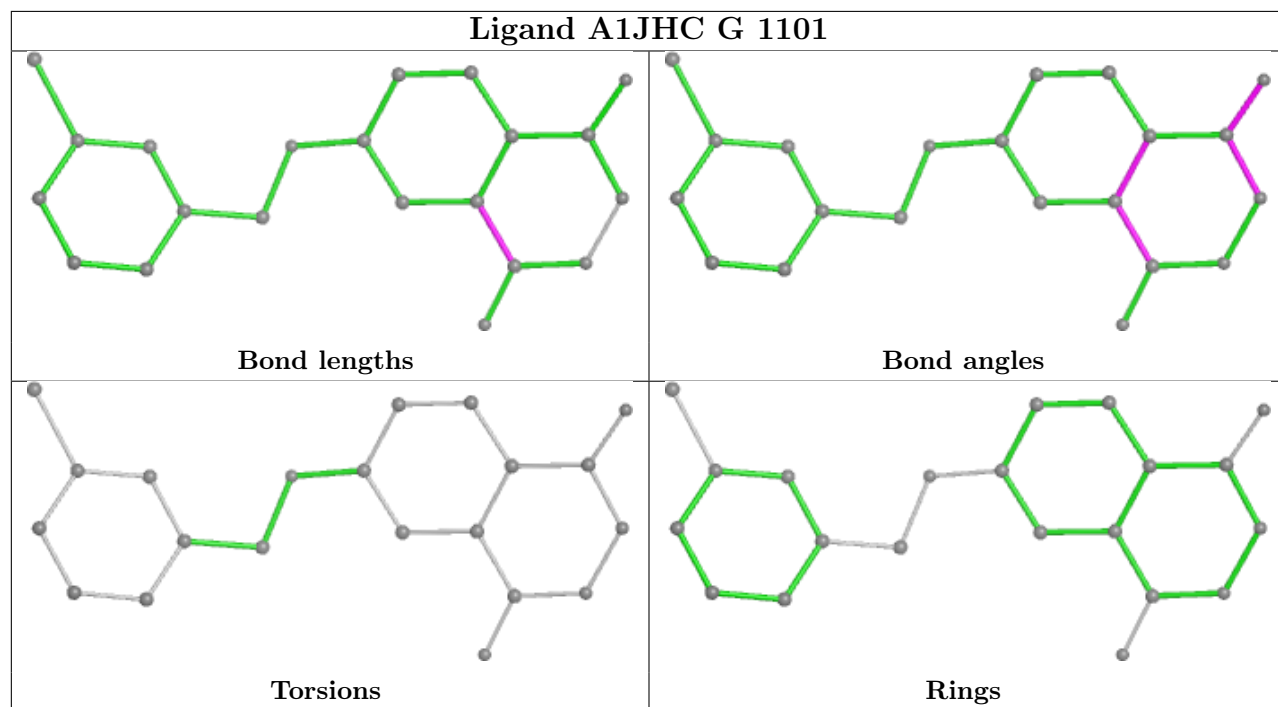
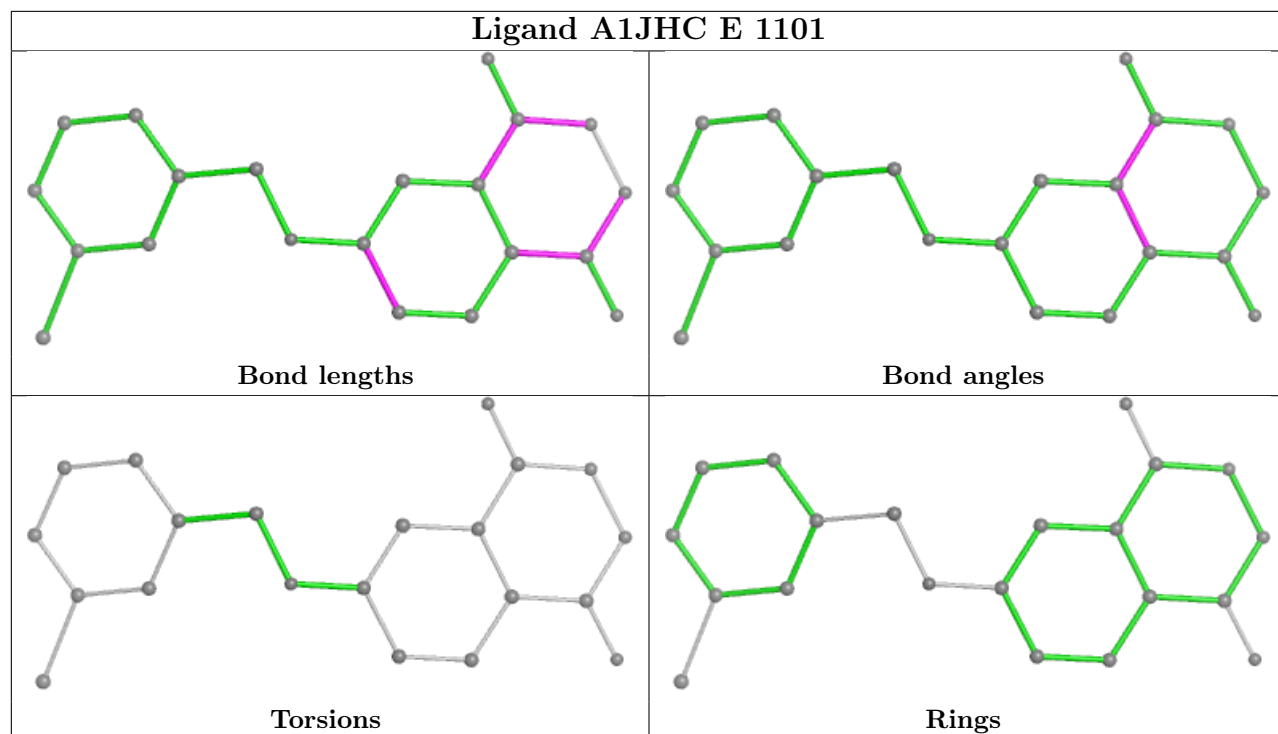
Mol	Chain	Res	Type	Atoms
2	A	1101	A1JHC	C4-C5-O3-C6
2	D	1101	A1JHC	C7-C6-O3-C5
2	C	1101	A1JHC	C4-C5-O3-C6
2	D	1101	A1JHC	C4-C5-O3-C6
2	C	1101	A1JHC	C7-C6-O3-C5
2	C	1101	A1JHC	C13-C5-O3-C6

There are no ring outliers.

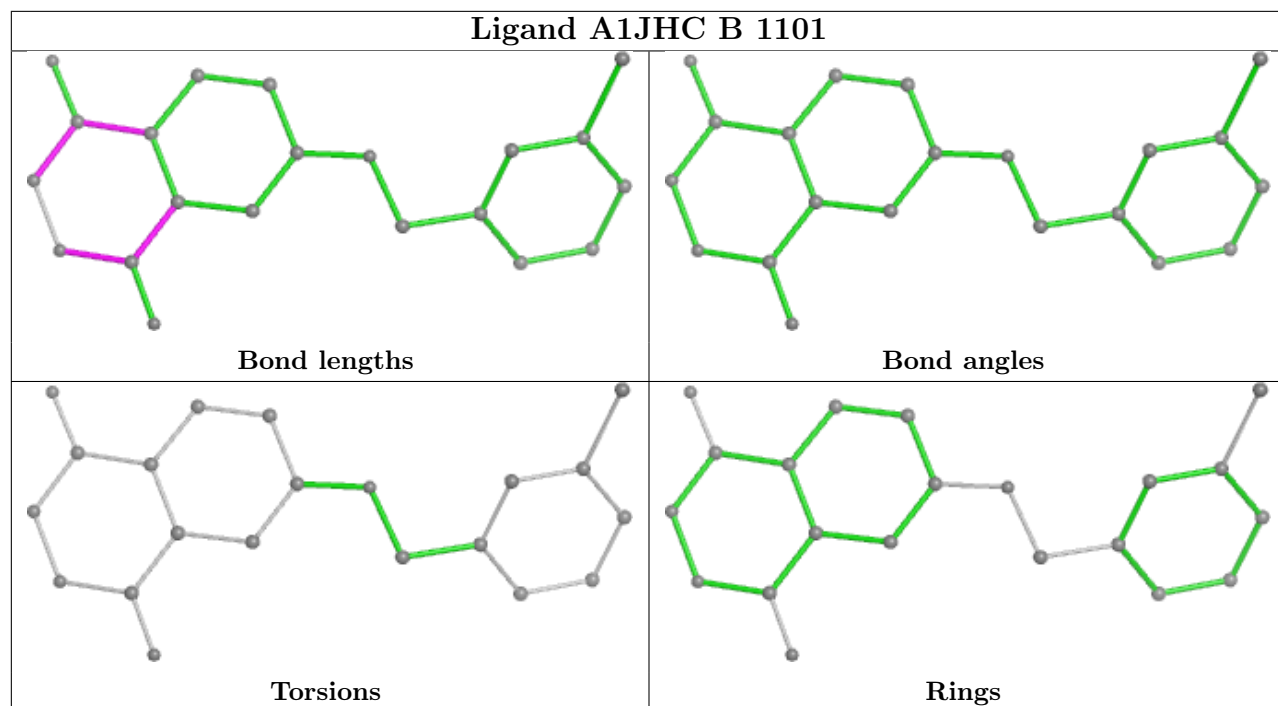
No monomer is involved in short contacts.

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.

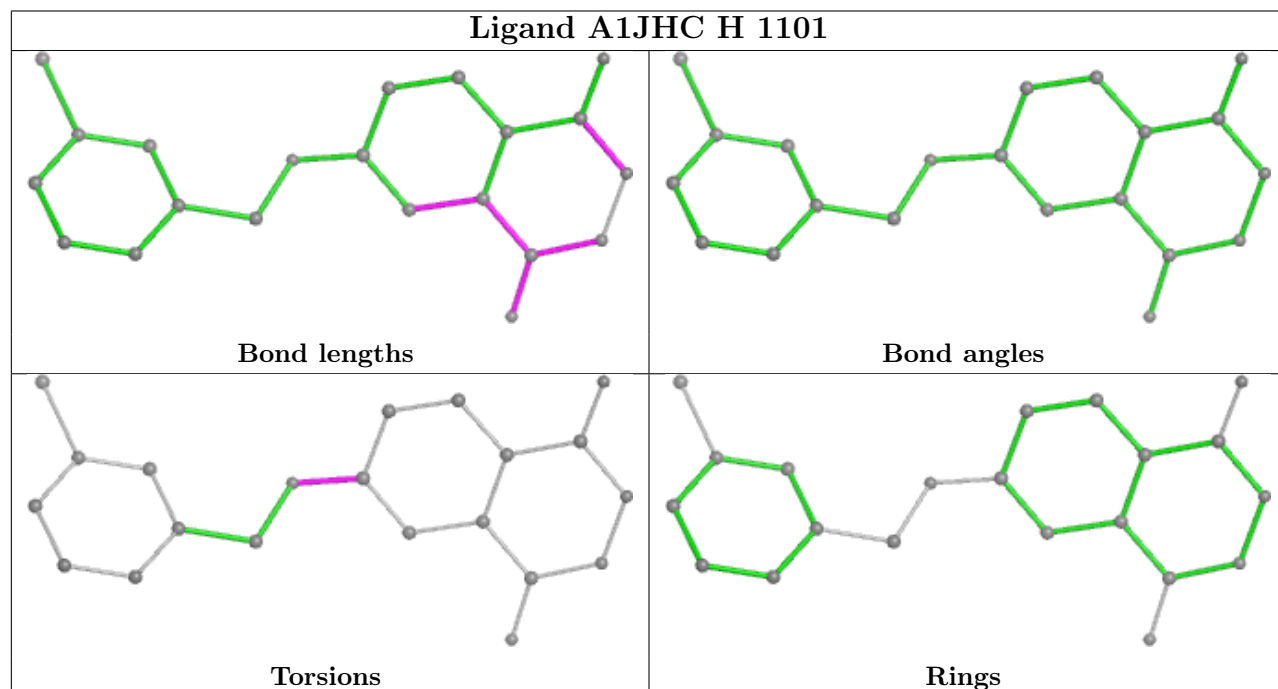




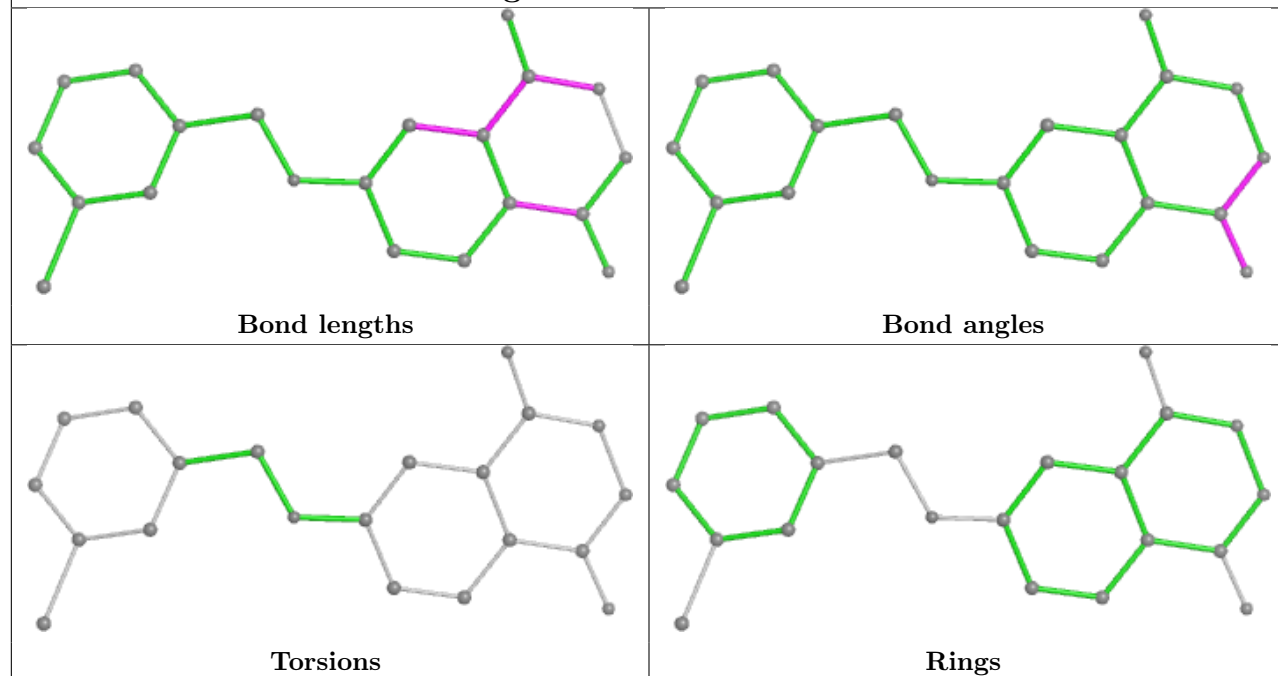
## Ligand A1JHC B 1101



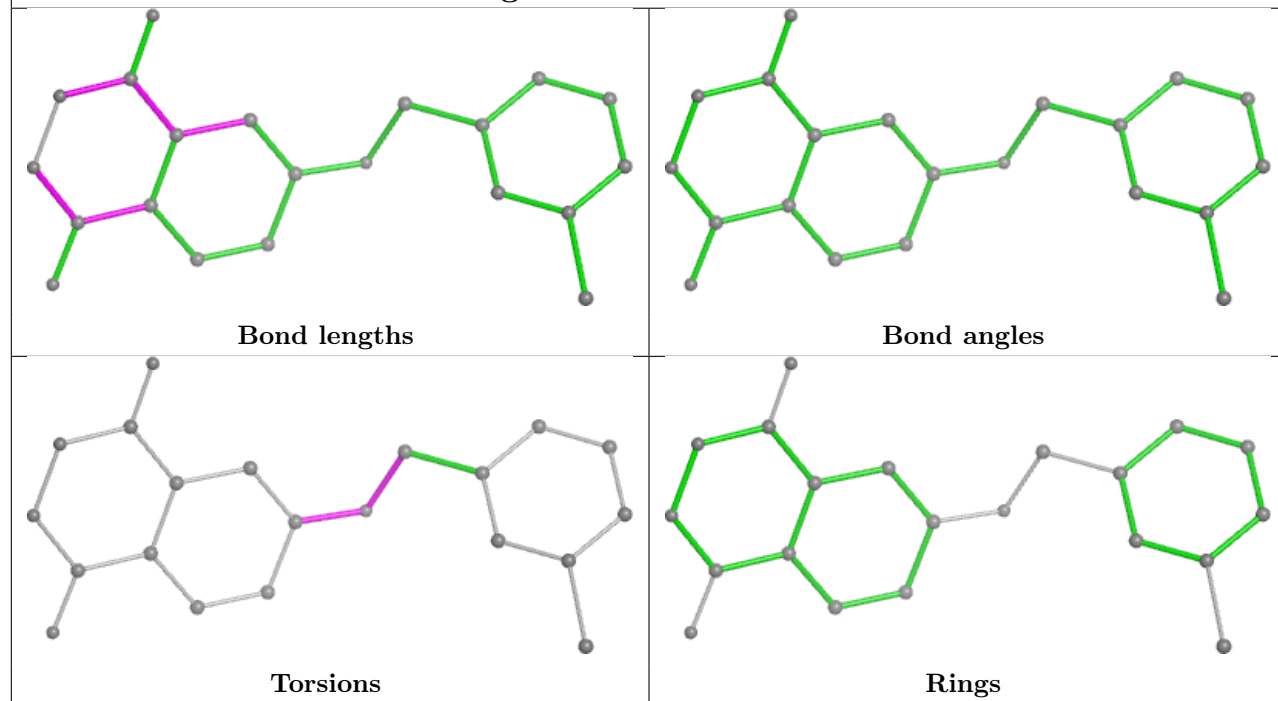
## Ligand A1JHC H 1101

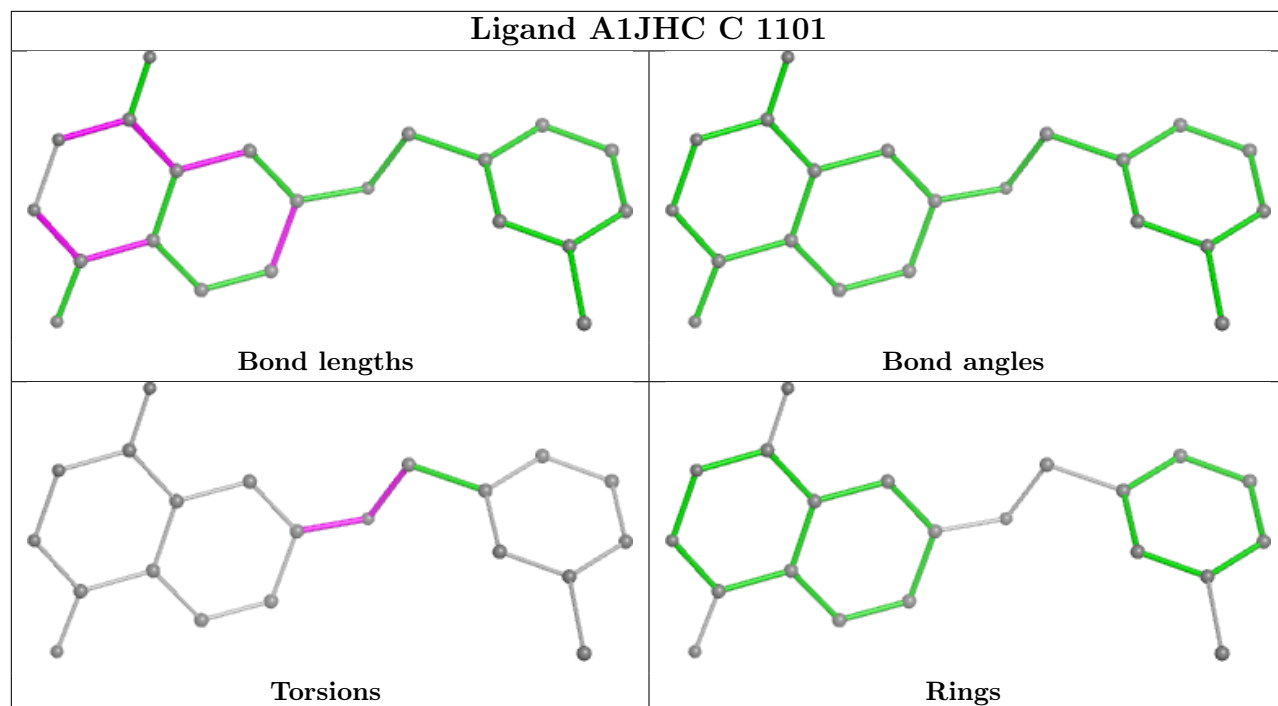


## Ligand A1JHC F 1101



## Ligand A1JHC D 1101





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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	189/191 (98%)	-0.17	2 (1%) 77 80	26, 43, 73, 84	0
1	B	189/191 (98%)	-0.02	2 (1%) 77 80	26, 47, 75, 85	0
1	C	188/191 (98%)	-0.13	1 (0%) 87 89	25, 44, 73, 91	0
1	D	189/191 (98%)	-0.10	2 (1%) 77 80	27, 48, 78, 88	0
1	E	188/191 (98%)	0.25	7 (3%) 45 47	31, 57, 85, 102	0
1	F	186/191 (97%)	0.12	4 (2%) 62 62	24, 53, 80, 92	1 (0%)
1	G	189/191 (98%)	0.19	4 (2%) 63 64	32, 55, 83, 98	0
1	H	189/191 (98%)	0.04	5 (2%) 57 58	32, 49, 77, 118	0
All	All	1507/1528 (98%)	0.02	27 (1%) 67 68	24, 50, 80, 118	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	843	ALA	3.6
1	G	843	ALA	3.5
1	C	818	MET	3.4
1	G	907	CYS	3.4
1	F	907	CYS	3.2
1	B	818	MET	3.2
1	E	843	ALA	3.1
1	H	818	MET	3.1
1	A	907	CYS	2.9
1	B	907	CYS	2.9
1	H	819	ASN	2.8
1	H	843	ALA	2.5
1	G	1006	HIS	2.5
1	D	817	SER	2.5
1	E	819	ASN	2.4
1	F	987	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	970[A]	HIS	2.3
1	E	987	ILE	2.2
1	H	987	ILE	2.2
1	H	880	PRO	2.1
1	E	982	ILE	2.1
1	E	984	GLN	2.1
1	G	945	VAL	2.1
1	F	838	TYR	2.1
1	E	817	SER	2.1
1	E	979	VAL	2.1
1	D	818	MET	2.0

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

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

## 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.4 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.

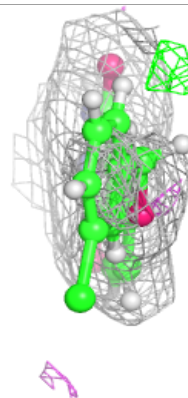
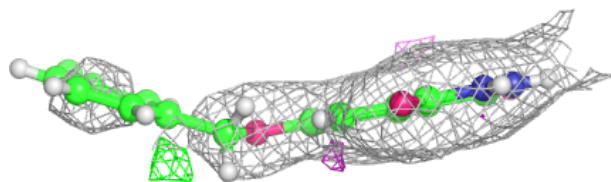
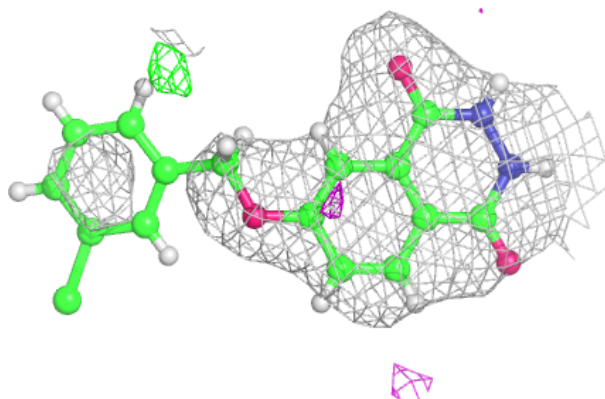
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1JHC	E	1101	21/21	0.89	0.13	44,57,104,114	0
2	A1JHC	D	1101	21/21	0.92	0.10	36,52,95,101	0
2	A1JHC	F	1101	21/21	0.92	0.11	42,55,92,102	0
2	A1JHC	G	1101	21/21	0.92	0.10	42,51,78,85	0
2	A1JHC	A	1101	21/21	0.93	0.09	29,39,75,84	0
2	A1JHC	C	1101	21/21	0.93	0.12	39,50,99,105	0
2	A1JHC	B	1101	21/21	0.94	0.09	34,49,81,94	0
2	A1JHC	H	1101	21/21	0.95	0.09	35,47,71,88	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.

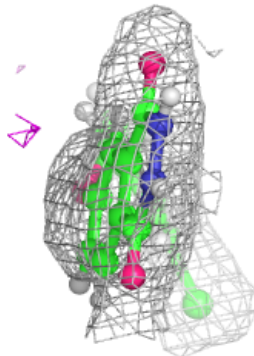
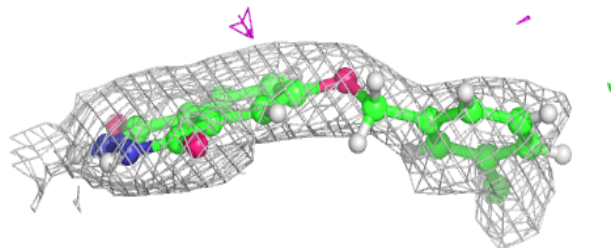
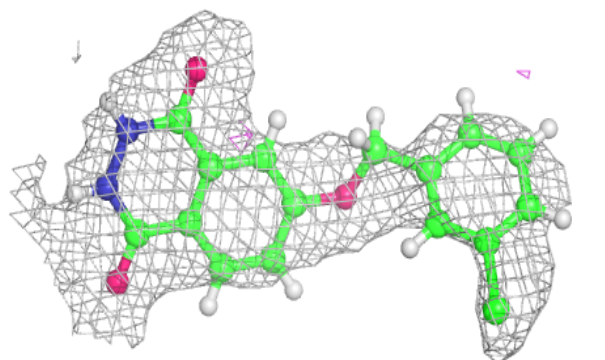


**Electron density around A1JHC E 1101:**

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

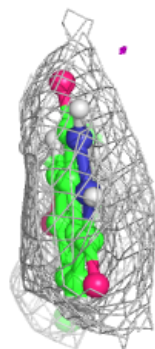
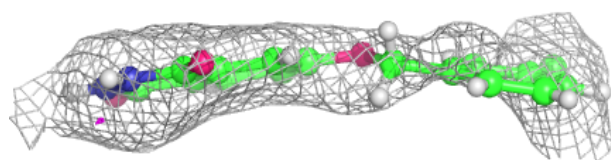
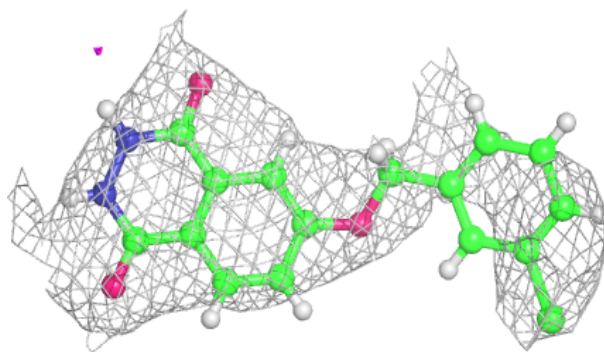
**Electron density around A1JHC D 1101:**

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

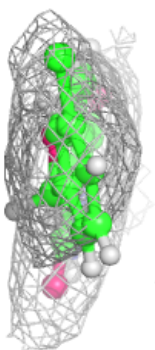
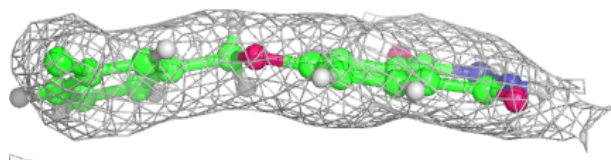
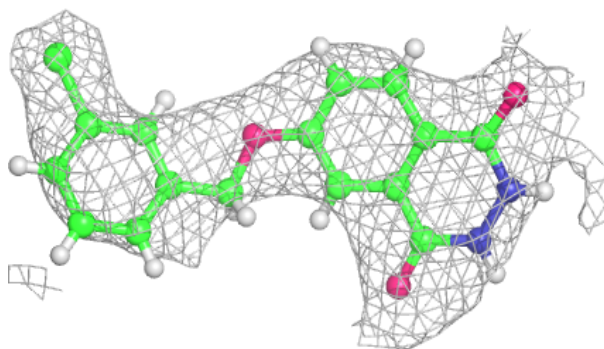


**Electron density around A1JHC F 1101:**

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

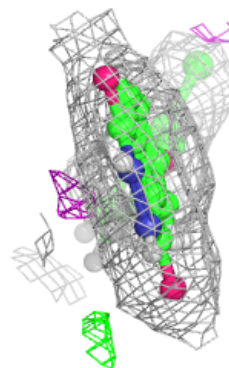
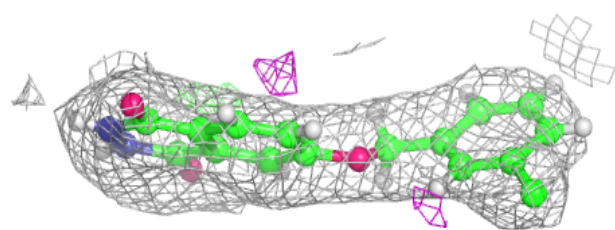
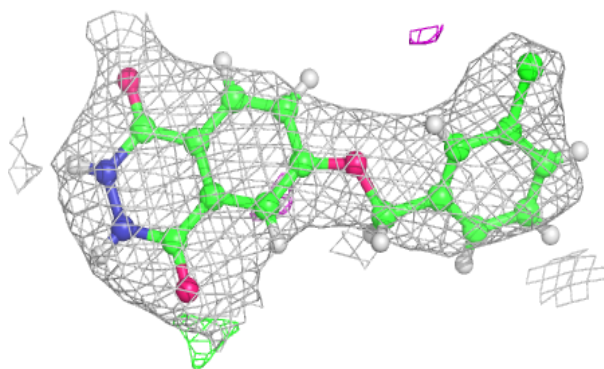
**Electron density around A1JHC G 1101:**

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

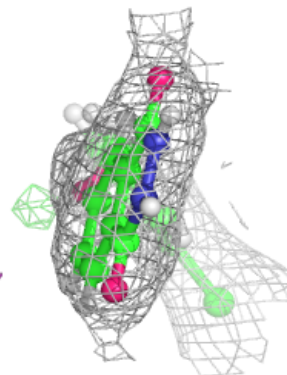
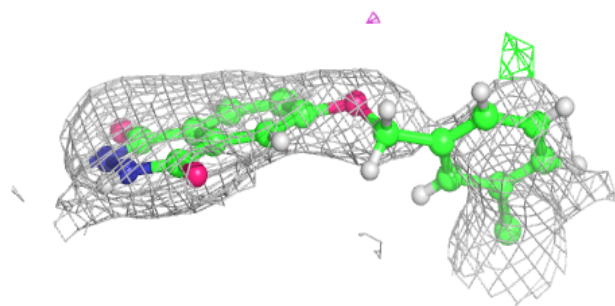
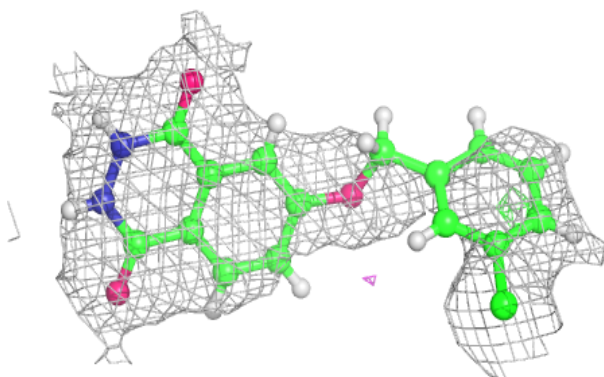


**Electron density around A1JHC A 1101:**

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

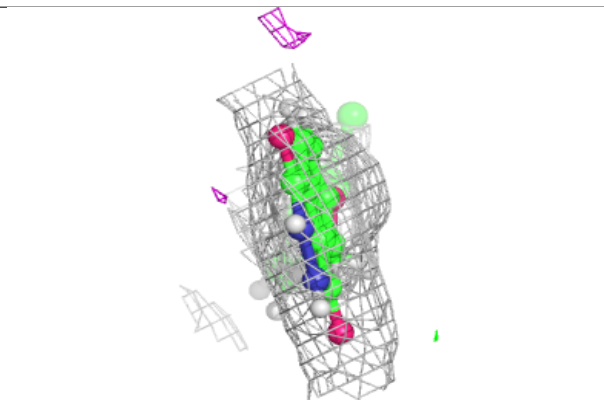
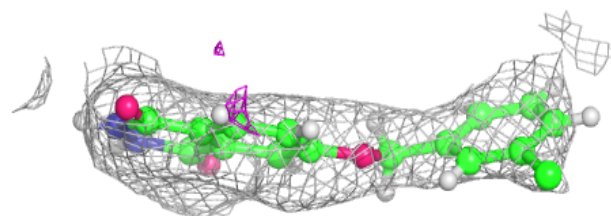
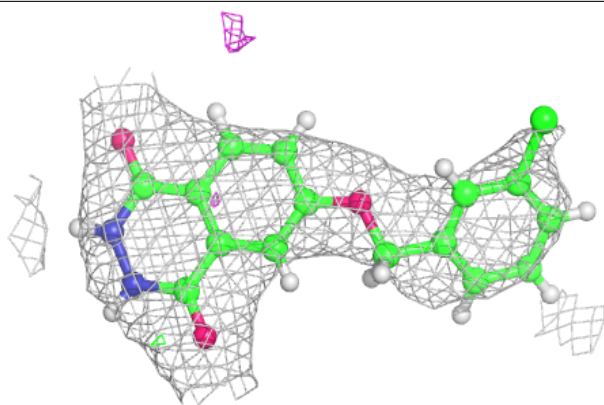
**Electron density around A1JHC C 1101:**

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

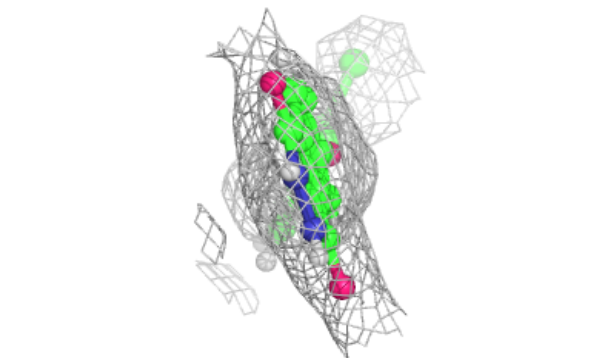
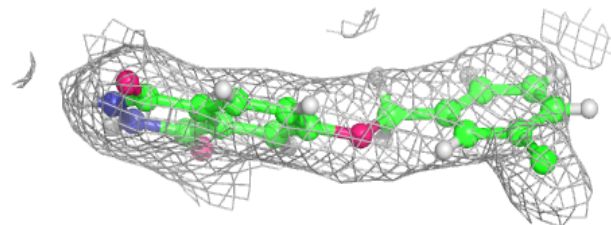
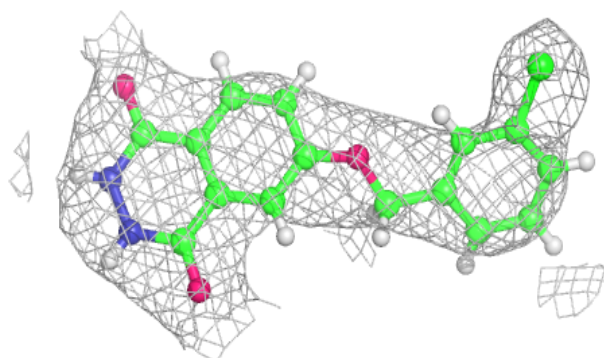


**Electron density around A1JHC B 1101:**

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

**Electron density around A1JHC H 1101:**

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



## 5.5 Other polymers [i](#)

There are no such residues in this entry.