



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 04:10 PM JST

PDB ID : 8ZDE / pdb\_00008zde  
Title : Crystal structure of HsmR with DNA bound  
Authors : Park, S.Y.  
Deposited on : 2024-05-02  
Resolution : 2.91 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:

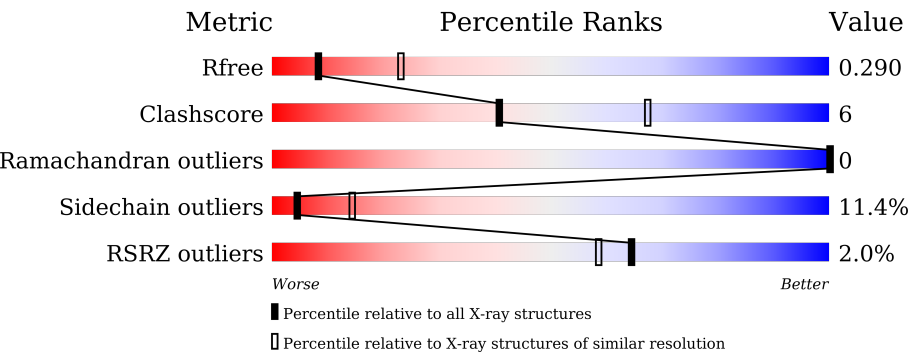
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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.







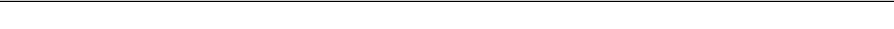
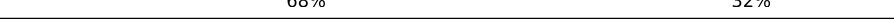
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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	167	<div><div>%</div><div><div></div><div>59%</div><div>20%</div><div>•</div><div>17%</div></div></div>
1	B	167	<div><div></div><div>74%</div><div>13%</div><div>•</div><div>12%</div></div>
1	C	167	<div><div></div><div>65%</div><div>17%</div><div>•</div><div>17%</div></div>
1	D	167	<div><div></div><div>62%</div><div>19%</div><div>•</div><div>17%</div></div>
1	E	167	<div><div>3%</div><div></div><div>65%</div><div>16%</div><div>•</div><div>18%</div></div>
1	F	167	<div><div>7%</div><div></div><div>58%</div><div>22%</div><div>•</div><div>19%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	22	 64% 36%
2	I	22	 5% 55% 45%
2	K	22	 5% 45% 55%
3	H	22	 64% 36%
3	J	22	 68% 32%
3	L	22	 59% 41%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9524 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 MarR-family transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1136	724	187	218	7			
1	B	147	Total	C	N	O	S	0	0	0
			1202	766	200	228	8			
1	C	138	Total	C	N	O	S	0	0	0
			1124	715	186	216	7			
1	D	138	Total	C	N	O	S	0	0	0
			1127	719	186	215	7			
1	E	137	Total	C	N	O	S	0	0	0
			1115	710	185	213	7			
1	F	136	Total	C	N	O	S	0	0	0
			1106	704	183	212	7			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A9R0BIW1
A	-18	GLY	-	expression tag	UNP A0A9R0BIW1
A	-17	SER	-	expression tag	UNP A0A9R0BIW1
A	-16	SER	-	expression tag	UNP A0A9R0BIW1
A	-15	HIS	-	expression tag	UNP A0A9R0BIW1
A	-14	HIS	-	expression tag	UNP A0A9R0BIW1
A	-13	HIS	-	expression tag	UNP A0A9R0BIW1
A	-12	HIS	-	expression tag	UNP A0A9R0BIW1
A	-11	HIS	-	expression tag	UNP A0A9R0BIW1
A	-10	HIS	-	expression tag	UNP A0A9R0BIW1
A	-9	SER	-	expression tag	UNP A0A9R0BIW1
A	-8	SER	-	expression tag	UNP A0A9R0BIW1
A	-7	GLY	-	expression tag	UNP A0A9R0BIW1
A	-6	LEU	-	expression tag	UNP A0A9R0BIW1
A	-5	VAL	-	expression tag	UNP A0A9R0BIW1
A	-4	PRO	-	expression tag	UNP A0A9R0BIW1
A	-3	ARG	-	expression tag	UNP A0A9R0BIW1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A9R0BIW1
A	-1	SER	-	expression tag	UNP A0A9R0BIW1
A	0	HIS	-	expression tag	UNP A0A9R0BIW1
B	-19	MET	-	initiating methionine	UNP A0A9R0BIW1
B	-18	GLY	-	expression tag	UNP A0A9R0BIW1
B	-17	SER	-	expression tag	UNP A0A9R0BIW1
B	-16	SER	-	expression tag	UNP A0A9R0BIW1
B	-15	HIS	-	expression tag	UNP A0A9R0BIW1
B	-14	HIS	-	expression tag	UNP A0A9R0BIW1
B	-13	HIS	-	expression tag	UNP A0A9R0BIW1
B	-12	HIS	-	expression tag	UNP A0A9R0BIW1
B	-11	HIS	-	expression tag	UNP A0A9R0BIW1
B	-10	HIS	-	expression tag	UNP A0A9R0BIW1
B	-9	SER	-	expression tag	UNP A0A9R0BIW1
B	-8	SER	-	expression tag	UNP A0A9R0BIW1
B	-7	GLY	-	expression tag	UNP A0A9R0BIW1
B	-6	LEU	-	expression tag	UNP A0A9R0BIW1
B	-5	VAL	-	expression tag	UNP A0A9R0BIW1
B	-4	PRO	-	expression tag	UNP A0A9R0BIW1
B	-3	ARG	-	expression tag	UNP A0A9R0BIW1
B	-2	GLY	-	expression tag	UNP A0A9R0BIW1
B	-1	SER	-	expression tag	UNP A0A9R0BIW1
B	0	HIS	-	expression tag	UNP A0A9R0BIW1
C	-19	MET	-	initiating methionine	UNP A0A9R0BIW1
C	-18	GLY	-	expression tag	UNP A0A9R0BIW1
C	-17	SER	-	expression tag	UNP A0A9R0BIW1
C	-16	SER	-	expression tag	UNP A0A9R0BIW1
C	-15	HIS	-	expression tag	UNP A0A9R0BIW1
C	-14	HIS	-	expression tag	UNP A0A9R0BIW1
C	-13	HIS	-	expression tag	UNP A0A9R0BIW1
C	-12	HIS	-	expression tag	UNP A0A9R0BIW1
C	-11	HIS	-	expression tag	UNP A0A9R0BIW1
C	-10	HIS	-	expression tag	UNP A0A9R0BIW1
C	-9	SER	-	expression tag	UNP A0A9R0BIW1
C	-8	SER	-	expression tag	UNP A0A9R0BIW1
C	-7	GLY	-	expression tag	UNP A0A9R0BIW1
C	-6	LEU	-	expression tag	UNP A0A9R0BIW1
C	-5	VAL	-	expression tag	UNP A0A9R0BIW1
C	-4	PRO	-	expression tag	UNP A0A9R0BIW1
C	-3	ARG	-	expression tag	UNP A0A9R0BIW1
C	-2	GLY	-	expression tag	UNP A0A9R0BIW1
C	-1	SER	-	expression tag	UNP A0A9R0BIW1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0A9R0BIW1
D	-19	MET	-	initiating methionine	UNP A0A9R0BIW1
D	-18	GLY	-	expression tag	UNP A0A9R0BIW1
D	-17	SER	-	expression tag	UNP A0A9R0BIW1
D	-16	SER	-	expression tag	UNP A0A9R0BIW1
D	-15	HIS	-	expression tag	UNP A0A9R0BIW1
D	-14	HIS	-	expression tag	UNP A0A9R0BIW1
D	-13	HIS	-	expression tag	UNP A0A9R0BIW1
D	-12	HIS	-	expression tag	UNP A0A9R0BIW1
D	-11	HIS	-	expression tag	UNP A0A9R0BIW1
D	-10	HIS	-	expression tag	UNP A0A9R0BIW1
D	-9	SER	-	expression tag	UNP A0A9R0BIW1
D	-8	SER	-	expression tag	UNP A0A9R0BIW1
D	-7	GLY	-	expression tag	UNP A0A9R0BIW1
D	-6	LEU	-	expression tag	UNP A0A9R0BIW1
D	-5	VAL	-	expression tag	UNP A0A9R0BIW1
D	-4	PRO	-	expression tag	UNP A0A9R0BIW1
D	-3	ARG	-	expression tag	UNP A0A9R0BIW1
D	-2	GLY	-	expression tag	UNP A0A9R0BIW1
D	-1	SER	-	expression tag	UNP A0A9R0BIW1
D	0	HIS	-	expression tag	UNP A0A9R0BIW1
E	-19	MET	-	initiating methionine	UNP A0A9R0BIW1
E	-18	GLY	-	expression tag	UNP A0A9R0BIW1
E	-17	SER	-	expression tag	UNP A0A9R0BIW1
E	-16	SER	-	expression tag	UNP A0A9R0BIW1
E	-15	HIS	-	expression tag	UNP A0A9R0BIW1
E	-14	HIS	-	expression tag	UNP A0A9R0BIW1
E	-13	HIS	-	expression tag	UNP A0A9R0BIW1
E	-12	HIS	-	expression tag	UNP A0A9R0BIW1
E	-11	HIS	-	expression tag	UNP A0A9R0BIW1
E	-10	HIS	-	expression tag	UNP A0A9R0BIW1
E	-9	SER	-	expression tag	UNP A0A9R0BIW1
E	-8	SER	-	expression tag	UNP A0A9R0BIW1
E	-7	GLY	-	expression tag	UNP A0A9R0BIW1
E	-6	LEU	-	expression tag	UNP A0A9R0BIW1
E	-5	VAL	-	expression tag	UNP A0A9R0BIW1
E	-4	PRO	-	expression tag	UNP A0A9R0BIW1
E	-3	ARG	-	expression tag	UNP A0A9R0BIW1
E	-2	GLY	-	expression tag	UNP A0A9R0BIW1
E	-1	SER	-	expression tag	UNP A0A9R0BIW1
E	0	HIS	-	expression tag	UNP A0A9R0BIW1
F	-19	MET	-	initiating methionine	UNP A0A9R0BIW1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP A0A9R0BIW1
F	-17	SER	-	expression tag	UNP A0A9R0BIW1
F	-16	SER	-	expression tag	UNP A0A9R0BIW1
F	-15	HIS	-	expression tag	UNP A0A9R0BIW1
F	-14	HIS	-	expression tag	UNP A0A9R0BIW1
F	-13	HIS	-	expression tag	UNP A0A9R0BIW1
F	-12	HIS	-	expression tag	UNP A0A9R0BIW1
F	-11	HIS	-	expression tag	UNP A0A9R0BIW1
F	-10	HIS	-	expression tag	UNP A0A9R0BIW1
F	-9	SER	-	expression tag	UNP A0A9R0BIW1
F	-8	SER	-	expression tag	UNP A0A9R0BIW1
F	-7	GLY	-	expression tag	UNP A0A9R0BIW1
F	-6	LEU	-	expression tag	UNP A0A9R0BIW1
F	-5	VAL	-	expression tag	UNP A0A9R0BIW1
F	-4	PRO	-	expression tag	UNP A0A9R0BIW1
F	-3	ARG	-	expression tag	UNP A0A9R0BIW1
F	-2	GLY	-	expression tag	UNP A0A9R0BIW1
F	-1	SER	-	expression tag	UNP A0A9R0BIW1
F	0	HIS	-	expression tag	UNP A0A9R0BIW1

- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*TP\*TP\*AP\*GP\*TP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*CP\*AP\*AP\*AP\*CP\*CP\*AP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	22	Total	C	N	O	P	0	0	0
			447	217	77	132	21			
2	I	22	Total	C	N	O	P	0	0	0
			447	217	77	132	21			
2	K	22	Total	C	N	O	P	0	0	0
			447	217	77	132	21			

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*AP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*CP\*AP\*AP\*AP\*CP\*TP\*AP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	22	Total	C	N	O	P	0	0	0
			449	217	83	128	21			
3	J	22	Total	C	N	O	P	0	0	0
			449	217	83	128	21			
3	L	22	Total	C	N	O	P	0	0	0
			449	217	83	128	21			

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total K 1 1	0	0
4	J	1	Total K 1 1	0	0

- Molecule 5 is water.

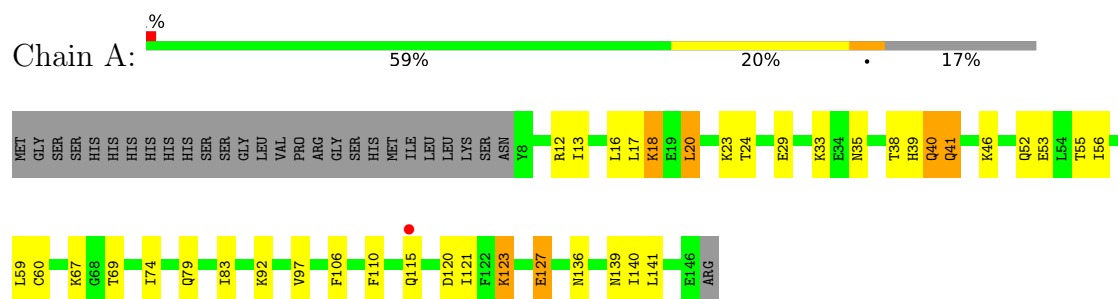
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	6	Total O 6 6	0	0
5	C	1	Total O 1 1	0	0
5	D	6	Total O 6 6	0	0
5	G	3	Total O 3 3	0	0
5	H	1	Total O 1 1	0	0
5	I	1	Total O 1 1	0	0
5	J	3	Total O 3 3	0	0
5	L	1	Total O 1 1	0	0



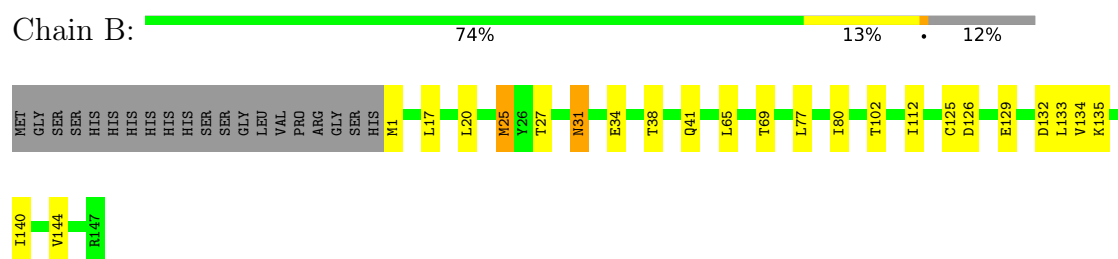
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

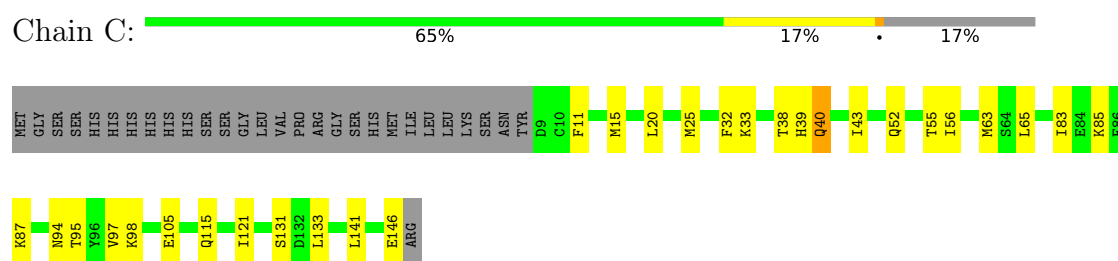
- Molecule 1: MarR-family transcriptional regulator



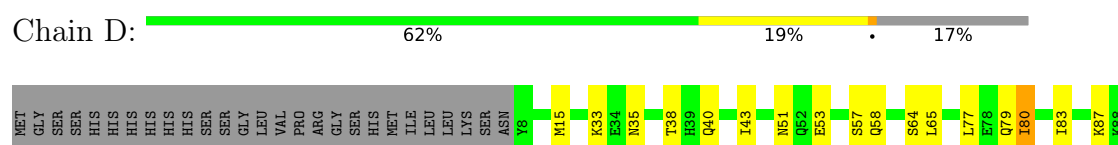
- Molecule 1: MarR-family transcriptional regulator



- Molecule 1: MarR-family transcriptional regulator

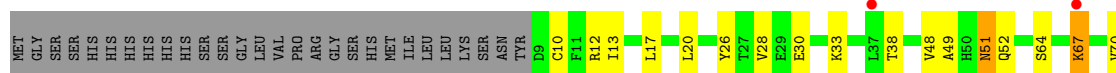


- Molecule 1: MarR-family transcriptional regulator





- Molecule 1: MarR-family transcriptional regulator



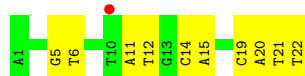
- Molecule 1: MarR-family transcriptional regulator



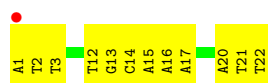
- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*AP\*GP\*TP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*CP\*AP\*AP\*AP\*CP\*CP\*AP\*TP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*AP\*GP\*TP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*CP\*AP\*AP\*AP\*CP\*CP\*AP\*TP\*T)-3')



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*AP\*GP\*TP\*TP\*TP\*GP\*TP\*AP\*TP\*GP\*CP\*AP\*AP\*AP\*CP\*CP\*AP\*TP\*T)-3')



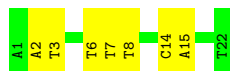
- Molecule 3: DNA (5'-D(\*AP\*AP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*CP\*AP\*AP\*AP\*CP\*TP\*AP\*AP\*T)-3')

Chain H:  64% 36%



- Molecule 3: DNA (5'-D(\*AP\*AP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*CP\*AP\*AP\*AP\*CP\*TP\*AP\*AP\*T)-3')

Chain J:  68% 32%



- Molecule 3: DNA (5'-D(\*AP\*AP\*TP\*GP\*GP\*TP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*CP\*AP\*AP\*AP\*CP\*TP\*AP\*AP\*T)-3')

Chain L:  59% 41%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	262.11Å 55.70Å 117.53Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	50.00 – 2.91 50.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.91) 99.4 (50.00-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.212 , 0.276 0.235 , 0.290	Depositor DCC
$R_{free}$ test set	1860 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 75.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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:  
K

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	0.73	0/1151	1.02	0/1541
1	B	0.77	0/1217	1.01	0/1628
1	C	0.71	0/1138	0.99	0/1523
1	D	0.79	0/1142	1.02	0/1529
1	E	0.72	0/1129	0.96	0/1511
1	F	0.76	0/1120	1.00	1/1500 (0.1%)
2	G	0.43	0/500	0.90	0/770
2	I	0.39	0/500	0.93	0/770
2	K	0.38	0/500	0.87	0/770
3	H	0.46	0/504	0.92	0/776
3	J	0.43	0/504	0.86	0/776
3	L	0.34	0/504	0.86	0/776
All	All	0.66	0/9909	0.97	1/13870 (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	F	68	GLY	N-CA-C	-5.20	106.49	112.73

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	1136	0	1152	20	0
1	B	1202	0	1234	12	0
1	C	1124	0	1143	12	0
1	D	1127	0	1146	13	0
1	E	1115	0	1137	16	0
1	F	1106	0	1124	19	0
2	G	447	0	253	6	0
2	I	447	0	253	8	0
2	K	447	0	253	8	0
3	H	449	0	251	10	0
3	J	449	0	251	4	0
3	L	449	0	251	5	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	2	0	0	0	0
5	B	6	0	0	0	0
5	C	1	0	0	0	0
5	D	6	0	0	0	0
5	G	3	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	3	0	0	0	0
5	L	1	0	0	0	0
All	All	9524	0	8448	112	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 (112) 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)
2:G:11:DA:H2''	2:G:12:DT:H5''	1.56	0.85
2:K:1:DA:H2'	2:K:2:DT:C6	2.15	0.81
2:G:12:DT:H2''	2:G:13:DG:C8	2.17	0.79
1:E:123:LYS:H	1:F:143:LYS:HD2	1.51	0.76
1:D:38:THR:HG21	2:I:12:DT:OP1	1.89	0.71
1:E:48:VAL:O	1:E:49:ALA:C	2.39	0.65
3:H:12:DT:H2''	3:H:13:DA:C8	2.35	0.62
2:G:12:DT:H2''	2:G:13:DG:H8	1.68	0.59
3:H:3:DT:H2''	3:H:4:DG:C8	2.38	0.59
2:K:12:DT:H2''	2:K:13:DG:C8	2.38	0.58
2:G:14:DC:H2'	2:G:15:DA:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD13	1:B:17:LEU:HD11	1.87	0.56
1:F:125:CYS:SG	1:F:126:ASP:N	2.77	0.56
2:I:11:DA:H2'	2:I:12:DT:C6	2.39	0.56
1:A:29:GLU:HG2	1:A:39:HIS:HB3	1.86	0.56
3:H:10:DC:H2'	3:H:11:DA:C8	2.40	0.55
3:J:14:DC:H2''	3:J:15:DA:C8	2.41	0.55
1:B:31:ASN:N	1:B:31:ASN:HD22	2.05	0.54
3:J:2:DA:H2''	3:J:3:DT:O5'	2.07	0.54
1:E:48:VAL:O	1:E:51:ASN:N	2.41	0.54
2:K:2:DT:H2''	2:K:3:DT:H5''	1.90	0.53
2:I:11:DA:H2''	2:I:12:DT:C5'	2.39	0.53
1:E:17:LEU:HD11	1:F:20:LEU:HD23	1.91	0.53
2:K:16:DA:H2'	2:K:17:DA:C8	2.44	0.53
1:C:25:MET:HB3	1:C:39:HIS:CD2	2.44	0.53
3:L:1:DA:H2'	3:L:2:DA:C8	2.44	0.52
2:I:14:DC:H2'	2:I:15:DA:C8	2.44	0.52
1:E:80:ILE:HG22	1:E:80:ILE:O	2.10	0.52
1:F:54:LEU:HD22	1:F:58:GLN:HG2	1.91	0.52
1:C:55:THR:O	1:C:56:ILE:C	2.52	0.52
2:K:14:DC:H2'	2:K:15:DA:C8	2.45	0.52
1:A:17:LEU:O	1:A:18:LYS:C	2.54	0.50
2:G:2:DT:H4'	2:G:3:DT:OP1	2.11	0.50
1:A:60:CYS:SG	1:A:67:LYS:HA	2.52	0.50
1:C:133:LEU:HD22	1:D:140:ILE:HD13	1.93	0.50
1:E:38:THR:HG21	3:L:11:DA:O3'	2.13	0.49
1:A:13:ILE:O	1:A:17:LEU:HD12	2.13	0.49
1:C:83:ILE:HD12	1:C:83:ILE:C	2.38	0.49
2:K:20:DA:H2'	2:K:21:DT:C6	2.48	0.49
1:A:59:LEU:HD13	1:A:74:ILE:HD11	1.95	0.48
3:J:6:DT:H2''	3:J:7:DT:H5'	1.95	0.48
1:D:40:GLN:HA	1:D:43:ILE:HD12	1.95	0.48
1:E:10:CYS:HB2	1:F:119:ASP:OD1	2.14	0.48
3:L:14:DC:H2'	3:L:15:DA:C8	2.48	0.48
3:J:7:DT:H1'	3:J:8:DT:H5'	1.96	0.47
1:D:133:LEU:O	1:D:134:VAL:C	2.57	0.47
1:D:140:ILE:O	1:D:144:VAL:HG23	2.14	0.47
2:I:11:DA:H2''	2:I:12:DT:O5'	2.14	0.47
3:L:12:DT:H2'	3:L:13:DA:C8	2.49	0.47
1:E:144:VAL:HG13	1:F:121:ILE:HG23	1.96	0.47
3:H:1:DA:H2''	3:H:2:DA:O5'	2.14	0.47
1:C:87:LYS:HE2	1:C:94:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1:DA:H4'	3:H:2:DA:OP1	2.14	0.47
1:B:65:LEU:HD22	1:B:69:THR:HG21	1.98	0.46
1:C:87:LYS:HE3	1:C:95:THR:OG1	2.15	0.46
1:A:38:THR:HB	1:A:40:GLN:HE21	1.80	0.46
1:F:120:ASP:C	1:F:122:PHE:N	2.72	0.46
1:F:110:PHE:HB2	1:F:114:MET:HE2	1.98	0.45
3:H:11:DA:H2''	3:H:12:DT:H5''	1.98	0.45
1:F:120:ASP:O	1:F:121:ILE:C	2.58	0.45
1:A:13:ILE:CD1	1:B:134:VAL:HG22	2.47	0.45
1:A:136:ASN:HD21	1:B:132:ASP:HB3	1.81	0.45
1:C:43:ILE:HD13	1:D:15:MET:HE1	1.99	0.45
1:E:17:LEU:HD11	1:F:20:LEU:CD2	2.47	0.44
1:C:63:MET:HE2	1:C:65:LEU:CD2	2.47	0.44
3:H:12:DT:H2''	3:H:13:DA:H8	1.81	0.44
2:I:21:DT:H2'	2:I:22:DT:H71	1.99	0.44
1:A:83:ILE:HD13	1:A:97:VAL:HG13	1.98	0.44
1:C:38:THR:HB	1:C:40:GLN:HE21	1.83	0.44
2:K:21:DT:H2'	2:K:22:DT:C6	2.52	0.44
2:K:21:DT:H2'	2:K:22:DT:C5	2.53	0.44
1:C:11:PHE:CZ	1:C:15:MET:HE3	2.53	0.44
1:A:127:GLU:CD	1:A:127:GLU:H	2.24	0.43
1:D:80:ILE:C	1:D:80:ILE:HD12	2.43	0.43
1:E:67:LYS:O	1:E:70:VAL:N	2.51	0.43
1:D:134:VAL:O	1:D:135:LYS:C	2.61	0.43
1:E:20:LEU:HD22	1:F:17:LEU:HD13	2.00	0.43
1:B:25:MET:HE3	1:B:25:MET:HA	2.01	0.43
1:D:51:ASN:O	1:D:53:GLU:N	2.51	0.43
3:L:7:DT:H1'	3:L:8:DT:H5'	2.00	0.43
1:A:139:ASN:HD21	1:B:129:GLU:HG2	1.84	0.42
1:B:38:THR:OG1	1:B:41:GLN:HG3	2.19	0.42
1:E:51:ASN:O	1:E:52:GLN:HB2	2.19	0.42
1:B:1:MET:HE2	1:C:85:LYS:HB2	2.01	0.42
1:B:140:ILE:O	1:B:144:VAL:HG13	2.19	0.42
1:A:141:LEU:HD13	1:B:20:LEU:HB2	2.00	0.42
1:E:138:ARG:HB2	1:F:16:LEU:HD13	2.01	0.42
1:A:24:THR:HG22	1:A:121:ILE:HG21	2.01	0.41
1:A:55:THR:O	1:A:56:ILE:C	2.62	0.41
1:F:120:ASP:O	1:F:122:PHE:N	2.53	0.41
3:H:11:DA:H2''	3:H:12:DT:C5'	2.50	0.41
1:C:32:PHE:O	1:C:33:LYS:C	2.63	0.41
1:D:35:ASN:OD1	1:D:113:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LYS:O	1:D:136:ASN:C	2.63	0.41
2:I:19:DC:H2'	2:I:20:DA:C8	2.55	0.41
1:D:57:SER:O	1:D:58:GLN:C	2.64	0.41
1:E:13:ILE:HD12	1:F:134:VAL:HG22	2.03	0.41
1:A:41:GLN:NE2	3:H:12:DT:OP1	2.54	0.41
1:E:111:LYS:HG3	1:E:114:MET:HE3	2.03	0.41
1:A:120:ASP:O	1:A:123:LYS:HG2	2.21	0.41
1:F:130:LEU:O	1:F:134:VAL:HG23	2.20	0.41
1:D:137:LEU:O	1:D:141:LEU:HB2	2.21	0.41
1:F:70:VAL:O	1:F:71:SER:C	2.64	0.41
1:A:53:GLU:HA	1:A:97:VAL:O	2.21	0.40
1:A:67:LYS:HG3	2:G:6:DT:H71	2.02	0.40
1:B:25:MET:HA	1:B:25:MET:CE	2.51	0.40
1:F:21:TYR:CE1	1:F:25:MET:HG3	2.56	0.40
3:H:1:DA:H2'	3:H:2:DA:C8	2.55	0.40
1:E:64:SER:CB	1:F:19:GLU:HA	2.51	0.40
2:I:5:DG:C8	2:I:6:DT:H72	2.56	0.40
1:A:106:PHE:CE2	1:A:110:PHE:CD2	3.09	0.40
1:F:54:LEU:O	1:F:97:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	137/167 (82%)	132 (96%)	5 (4%)	0	100	100
1	B	145/167 (87%)	135 (93%)	10 (7%)	0	100	100
1	C	136/167 (81%)	128 (94%)	8 (6%)	0	100	100
1	D	136/167 (81%)	128 (94%)	8 (6%)	0	100	100
1	E	135/167 (81%)	118 (87%)	17 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	134/167 (80%)	124 (92%)	10 (8%)	0	100	100
All	All	823/1002 (82%)	765 (93%)	58 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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	129/154 (84%)	111 (86%)	18 (14%)	3	8
1	B	137/154 (89%)	125 (91%)	12 (9%)	8	25
1	C	128/154 (83%)	117 (91%)	11 (9%)	8	26
1	D	128/154 (83%)	111 (87%)	17 (13%)	3	9
1	E	127/154 (82%)	115 (91%)	12 (9%)	7	22
1	F	126/154 (82%)	108 (86%)	18 (14%)	2	8
All	All	775/924 (84%)	687 (89%)	88 (11%)	4	14

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	16	LEU
1	A	18	LYS
1	A	20	LEU
1	A	23	LYS
1	A	33	LYS
1	A	35	ASN
1	A	40	GLN
1	A	41	GLN
1	A	46	LYS
1	A	52	GLN
1	A	69	THR
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	92	LYS
1	A	115	GLN
1	A	123	LYS
1	A	127	GLU
1	A	140	ILE
1	B	25	MET
1	B	27	THR
1	B	31	ASN
1	B	34	GLU
1	B	77	LEU
1	B	80	ILE
1	B	102	THR
1	B	112	ILE
1	B	125	CYS
1	B	126	ASP
1	B	133	LEU
1	B	135	LYS
1	C	20	LEU
1	C	40	GLN
1	C	52	GLN
1	C	97	VAL
1	C	98	LYS
1	C	105	GLU
1	C	115	GLN
1	C	121	ILE
1	C	131	SER
1	C	141	LEU
1	C	146	GLU
1	D	33	LYS
1	D	64	SER
1	D	65	LEU
1	D	77	LEU
1	D	79	GLN
1	D	80	ILE
1	D	83	ILE
1	D	87	LYS
1	D	89	SER
1	D	97	VAL
1	D	112	ILE
1	D	121	ILE
1	D	125	CYS
1	D	127	GLU

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Mol	Chain	Res	Type
1	D	128	ASN
1	D	141	LEU
1	D	143	LYS
1	E	12	ARG
1	E	26	TYR
1	E	28	VAL
1	E	30	GLU
1	E	33	LYS
1	E	51	ASN
1	E	67	LYS
1	E	79	GLN
1	E	86	PHE
1	E	112	ILE
1	E	115	GLN
1	E	141	LEU
1	F	13	ILE
1	F	22	SER
1	F	34	GLU
1	F	53	GLU
1	F	78	GLU
1	F	79	GLN
1	F	84	GLU
1	F	88	LYS
1	F	92	LYS
1	F	93	ARG
1	F	95	THR
1	F	100	THR
1	F	108	THR
1	F	126	ASP
1	F	133	LEU
1	F	135	LYS
1	F	140	ILE
1	F	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	52	GLN
1	A	128	ASN
1	A	139	ASN
1	B	31	ASN

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Mol	Chain	Res	Type
1	B	52	GLN
1	B	90	ASN
1	B	94	ASN
1	B	115	GLN
1	C	39	HIS
1	C	40	GLN
1	C	90	ASN
1	C	94	ASN
1	C	115	GLN
1	C	128	ASN
1	C	136	ASN
1	D	39	HIS
1	D	52	GLN
1	D	79	GLN
1	D	94	ASN
1	D	109	ASN
1	D	115	GLN
1	E	39	HIS
1	E	51	ASN
1	E	58	GLN
1	E	109	ASN
1	E	124	ASN
1	F	35	ASN
1	F	109	ASN
1	F	136	ASN
1	F	139	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	139/167 (83%)	-0.24	1 (0%) 84 81	49, 76, 110, 150	0
1	B	147/167 (88%)	-0.32	0 100 100	46, 70, 109, 146	0
1	C	138/167 (82%)	-0.23	0 100 100	52, 78, 123, 141	0
1	D	138/167 (82%)	-0.34	0 100 100	46, 69, 120, 134	0
1	E	137/167 (82%)	0.44	5 (3%) 46 40	107, 156, 192, 224	0
1	F	136/167 (81%)	0.64	11 (8%) 19 17	30, 146, 182, 200	0
2	G	22/22 (100%)	-0.43	0 100 100	20, 69, 87, 91	0
2	I	22/22 (100%)	-0.01	1 (4%) 39 33	20, 62, 81, 85	0
2	K	22/22 (100%)	0.28	1 (4%) 39 33	81, 104, 116, 118	0
3	H	22/22 (100%)	-0.19	0 100 100	48, 64, 88, 92	0
3	J	22/22 (100%)	-0.31	0 100 100	20, 63, 85, 98	0
3	L	22/22 (100%)	0.46	0 100 100	86, 104, 111, 115	0
All	All	967/1134 (85%)	-0.02	19 (1%) 64 58	20, 86, 172, 224	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	118	PHE	6.2
1	F	68	GLY	5.6
1	E	67	LYS	3.5
1	F	93	ARG	3.4
1	F	67	LYS	2.9
2	I	10	DT	2.5
1	F	95	THR	2.5
1	E	125	CYS	2.5
1	A	115	GLN	2.4
1	F	119	ASP	2.4
1	F	137	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	140	ILE	2.4
2	K	1	DA	2.4
1	F	69	THR	2.3
1	F	54	LEU	2.3
1	F	82	TYR	2.3
1	E	37	LEU	2.2
1	E	97	VAL	2.1
1	E	82	TYR	2.1

## 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, 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.

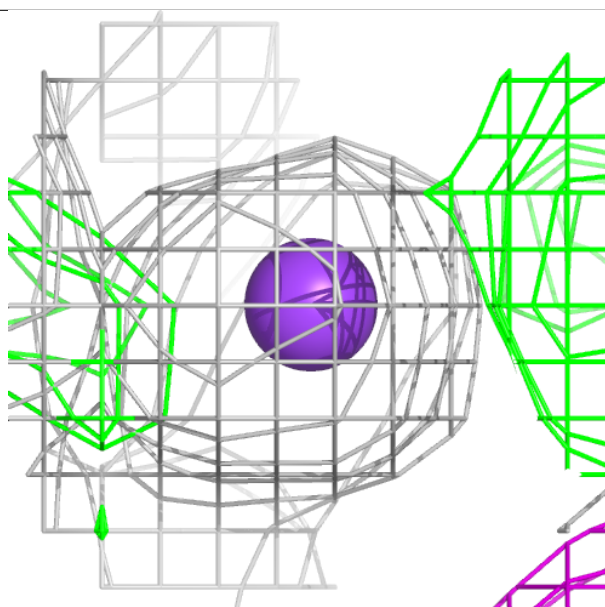
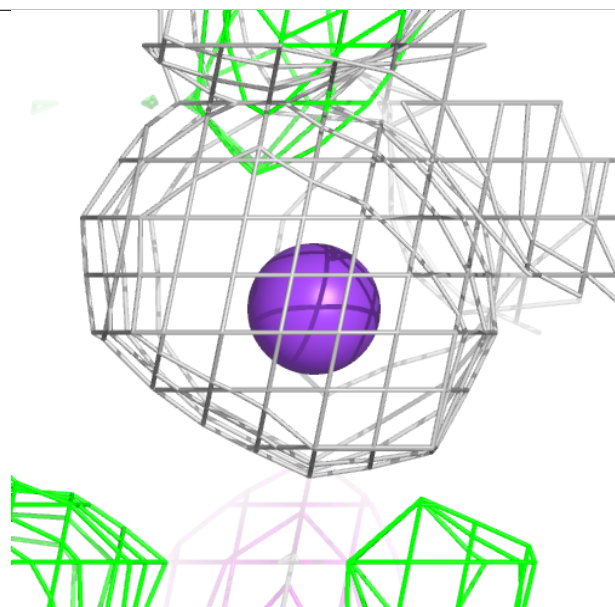
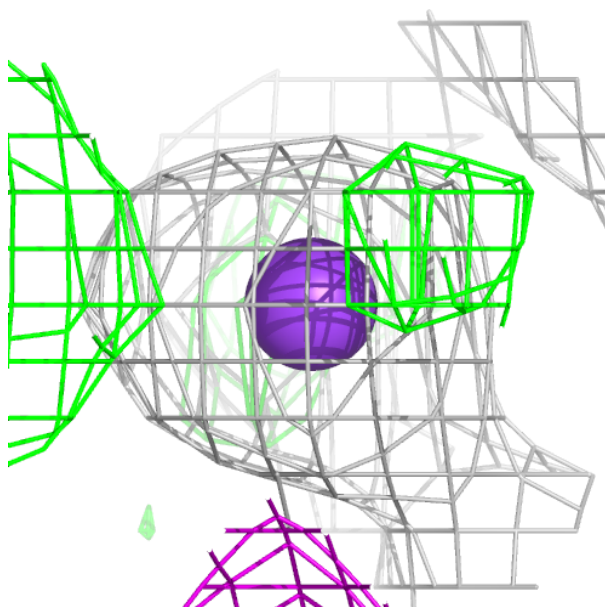
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	K	J	101	1/1	0.92	0.19	82,82,82,82	0
4	K	G	101	1/1	0.95	0.13	77,77,77,77	0

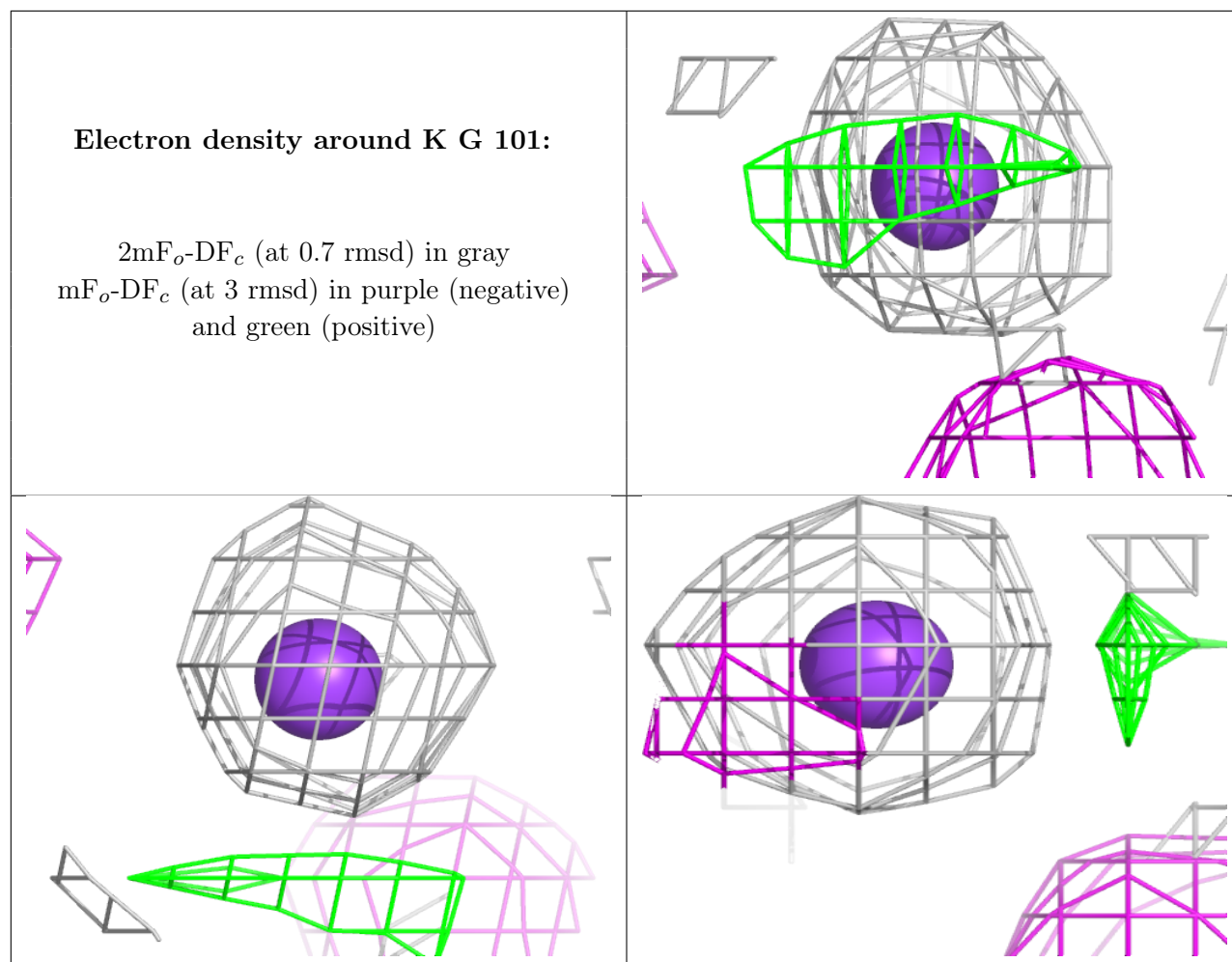
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around K J 101:**

$2mF_o-DF_c$  (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.