



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 05:43 pm BST

PDB ID : 9S2V / pdb\_00009s2v  
Title : NSP14 IN COMPLEX WITH LIGAND TDI-014925-CL-2 (compound 58)  
Authors : Steinbacher, S.; Huggins, D.J.  
Deposited on : 2025-07-22  
Resolution : 2.38 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

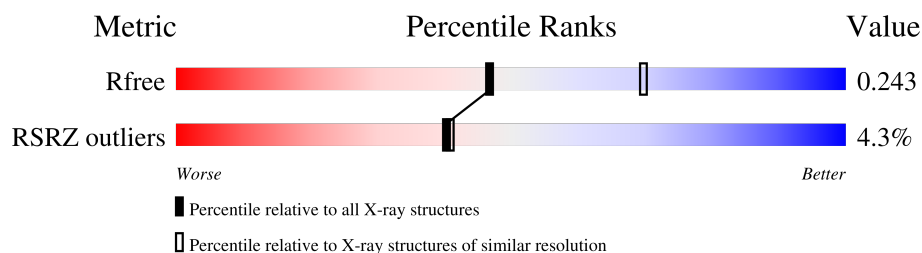
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	6699 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7391 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 Guanine-N7 methyltransferase nsp14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	24	0	0
			3561	2293	604	631	33			
1	B	433	Total	C	N	O	S	21	0	0
			3482	2242	593	614	33			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0DTD1
A	90	ALA	ASP	engineered mutation	UNP P0DTD1
A	92	ALA	GLU	engineered mutation	UNP P0DTD1
B	0	SER	-	expression tag	UNP P0DTD1
B	90	ALA	ASP	engineered mutation	UNP P0DTD1
B	92	ALA	GLU	engineered mutation	UNP P0DTD1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

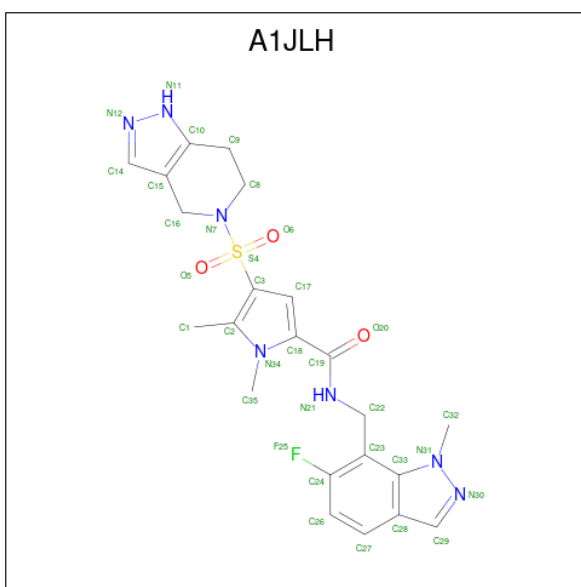
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is {N}-[(6-fluoranyl-1-methyl-indazol-7-yl)methyl]-1,5-dimethyl-4-(1,4,6,7-tetrahydropyrazolo[4,3-c]pyridin-5-ylsulfonyl)pyrrole-2-carboxamide (CCD ID: A1JLH) (formula: C<sub>22</sub>H<sub>24</sub>FN<sub>7</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			34	22	1	7	3	1		

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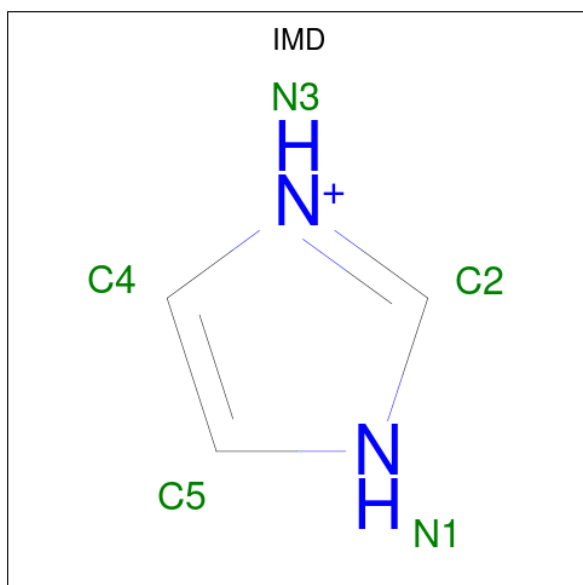
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	S	
			34	22	1	7	3	1	
								0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl		
			3	3	0	0
5	B	2	Total	Cl		
			2	2	0	0

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N		
			5	3	2	0	0
6	B	1	Total	C	N		
			5	3	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	119	Total	O		
			119	119	0	0
7	B	88	Total	O		
			88	88	0	0

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### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.46Å 100.96Å 90.43Å 90.00° 108.33° 90.00°	Depositor
Resolution (Å)	64.12 – 2.38 64.12 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.2 (64.12-2.38) 98.3 (64.12-2.38)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.193 , 0.245 0.195 , 0.243	Depositor DCC
$R_{free}$ test set	1125 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7391	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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.

## 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](#)

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#### 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](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z  > 2$
4	A1JLH	A	605	-	34,38,38	1.38	7 (20%)	31,58,58	2.04	9 (29%)
6	IMD	B	608	-	3,5,5	0.39	0	4,5,5	0.76	0
6	IMD	A	609	-	3,5,5	0.44	0	4,5,5	0.82	0
4	A1JLH	B	605	-	34,38,38	1.33	6 (17%)	31,58,58	2.06	9 (29%)
3	SAH	A	604	-	24,28,28	0.74	1 (4%)	25,40,40	1.06	3 (12%)
3	SAH	B	604	-	24,28,28	0.72	0	25,40,40	0.94	2 (8%)

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
4	A1JLH	A	605	-	-	3/12/30/30	0/5/5/5
6	IMD	B	608	-	-	-	0/1/1/1
6	IMD	A	609	-	-	-	0/1/1/1
4	A1JLH	B	605	-	-	3/12/30/30	0/5/5/5
3	SAH	A	604	-	-	4/11/31/31	0/3/3/3
3	SAH	B	604	-	-	2/11/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	A1JLH	C9-C10	-2.91	1.46	1.50
4	B	605	A1JLH	C10-N11	-2.87	1.30	1.34
4	A	605	A1JLH	C10-N11	-2.71	1.30	1.34
4	A	605	A1JLH	N12-N11	2.62	1.43	1.37
4	A	605	A1JLH	C29-C28	2.61	1.46	1.40
4	A	605	A1JLH	C2-N34	-2.55	1.37	1.39
4	B	605	A1JLH	S4-N7	2.39	1.66	1.63
4	B	605	A1JLH	C29-C28	2.34	1.45	1.40
4	B	605	A1JLH	N12-N11	2.22	1.42	1.37
3	A	604	SAH	OXT-C	-2.21	1.23	1.30
4	A	605	A1JLH	C2-C3	-2.21	1.36	1.39
4	B	605	A1JLH	C2-C3	-2.17	1.36	1.39
4	A	605	A1JLH	C3-S4	-2.05	1.75	1.78
4	B	605	A1JLH	C23-C33	-2.04	1.40	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	A1JLH	C29-N30-N31	6.24	110.73	104.23
4	A	605	A1JLH	C29-N30-N31	5.18	109.62	104.23
4	B	605	A1JLH	C35-N34-C2	4.08	128.09	124.09
4	A	605	A1JLH	C1-C2-C3	-3.86	125.46	129.47
4	A	605	A1JLH	O6-S4-N7	3.61	109.98	106.69
4	B	605	A1JLH	C1-C2-C3	-3.45	125.89	129.47
4	A	605	A1JLH	C14-C15-C10	3.35	108.42	104.71
3	A	604	SAH	OXT-C-O	-3.23	116.76	124.09
4	A	605	A1JLH	F25-C24-C23	3.22	121.53	117.65
4	A	605	A1JLH	C1-C2-N34	3.12	126.43	122.44
3	A	604	SAH	C5-C6-N6	2.70	124.45	120.35
4	A	605	A1JLH	C8-C9-C10	-2.70	108.03	113.00
4	B	605	A1JLH	F25-C24-C23	2.55	120.73	117.65
4	B	605	A1JLH	C14-C15-C10	2.54	107.53	104.71
4	B	605	A1JLH	C23-C22-N21	-2.52	105.75	109.94
4	A	605	A1JLH	C35-N34-C2	2.45	126.49	124.09
4	B	605	A1JLH	O6-S4-N7	2.35	108.83	106.69
4	B	605	A1JLH	C1-C2-N34	2.31	125.39	122.44
4	B	605	A1JLH	C16-N7-S4	2.30	120.62	116.94
3	B	604	SAH	OXT-C-CA	2.28	121.15	113.38
3	B	604	SAH	OXT-C-O	-2.17	119.17	124.09
4	A	605	A1JLH	C8-N7-S4	2.06	120.79	117.05
3	A	604	SAH	OXT-C-CA	2.04	120.33	113.38

There are no chirality outliers.

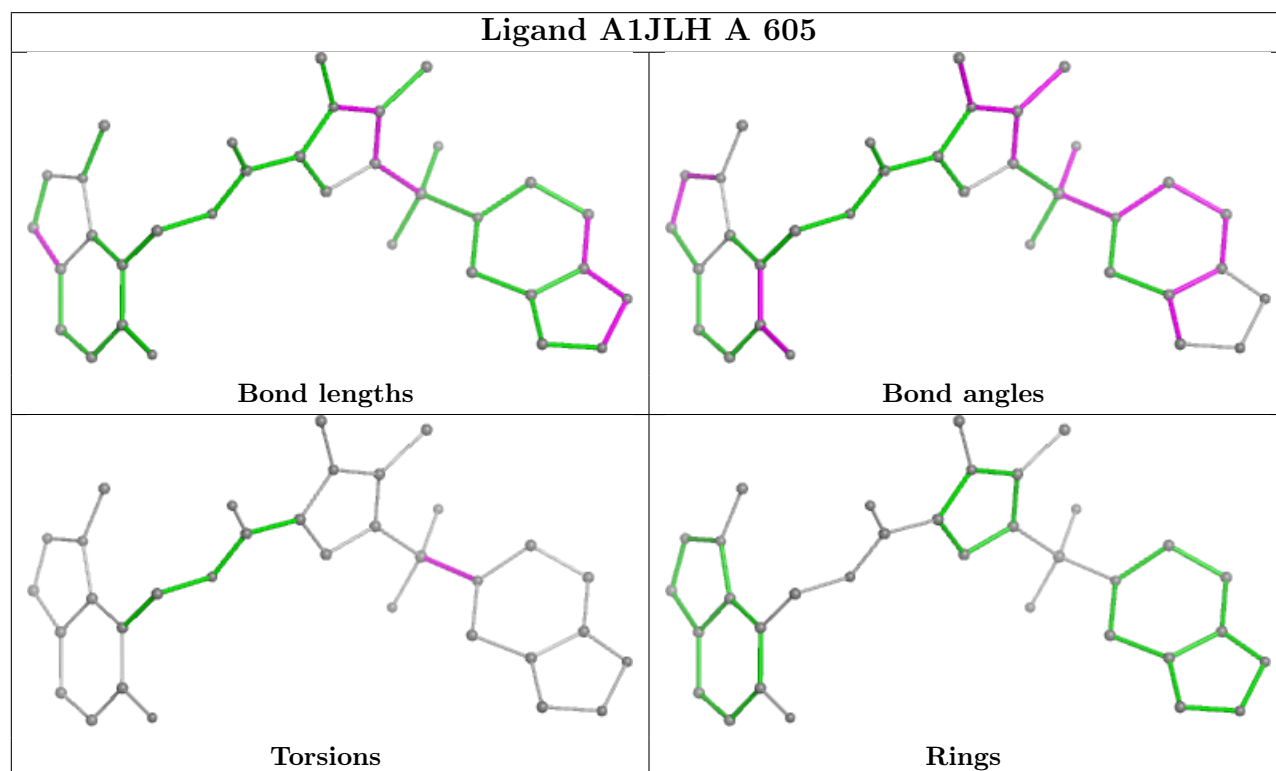
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	SAH	N-CA-CB-CG
3	A	604	SAH	C-CA-CB-CG
3	B	604	SAH	N-CA-CB-CG
3	B	604	SAH	C-CA-CB-CG
4	A	605	A1JLH	C8-N7-S4-O6
4	B	605	A1JLH	C8-N7-S4-O6
4	A	605	A1JLH	C8-N7-S4-O5
4	B	605	A1JLH	C8-N7-S4-O5
3	A	604	SAH	OXT-C-CA-CB
4	A	605	A1JLH	C8-N7-S4-C3
3	A	604	SAH	O-C-CA-CB
4	B	605	A1JLH	C8-N7-S4-C3

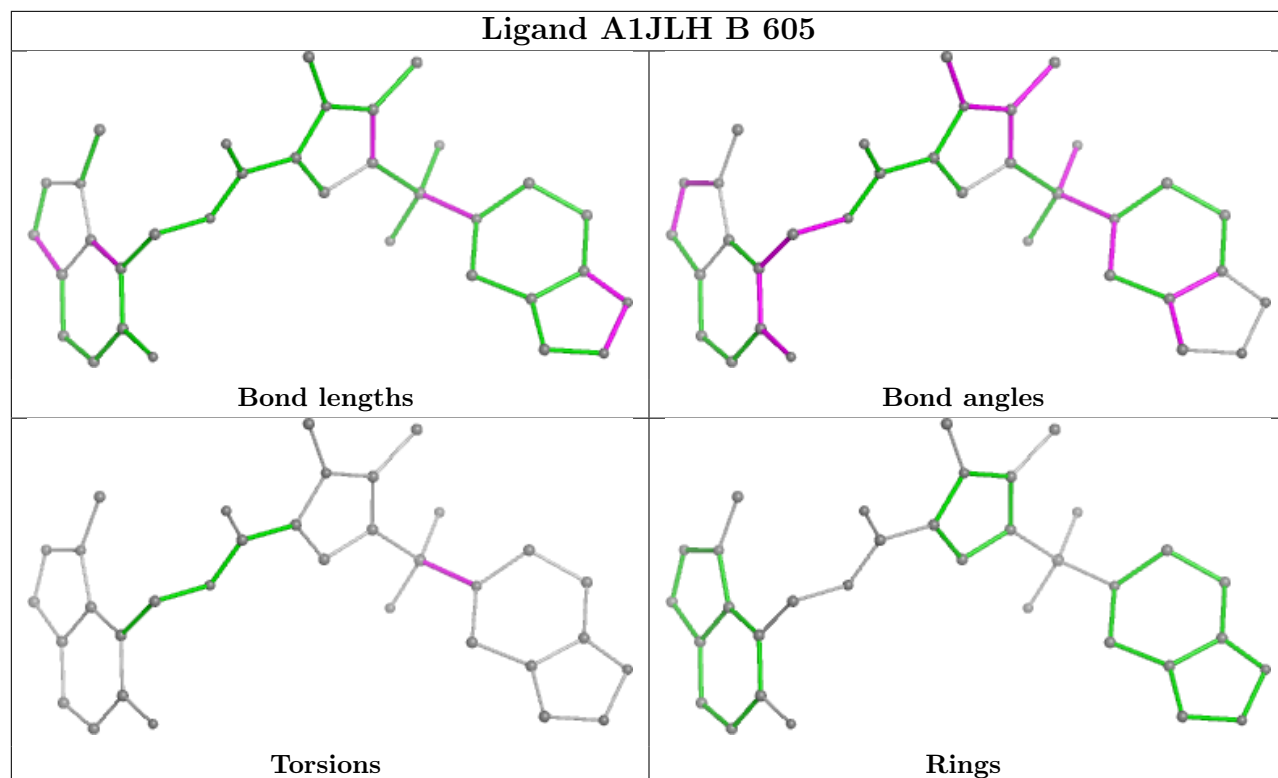
There are no ring outliers.

No monomer is involved in short contacts.

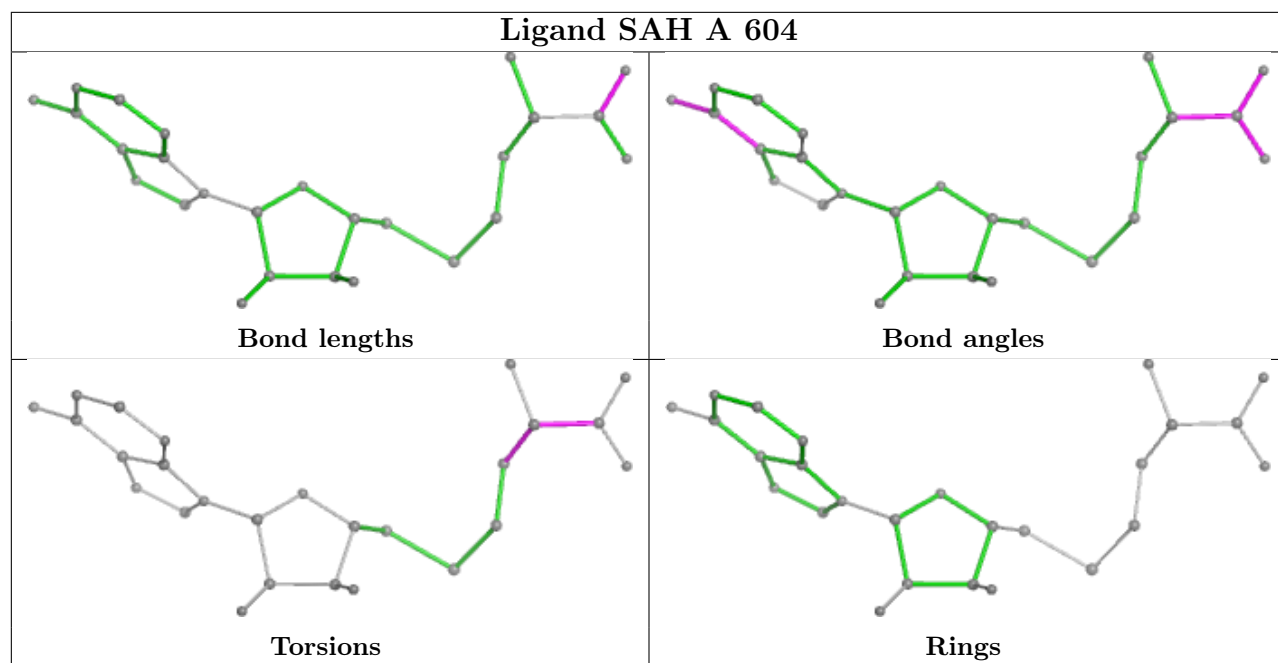
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

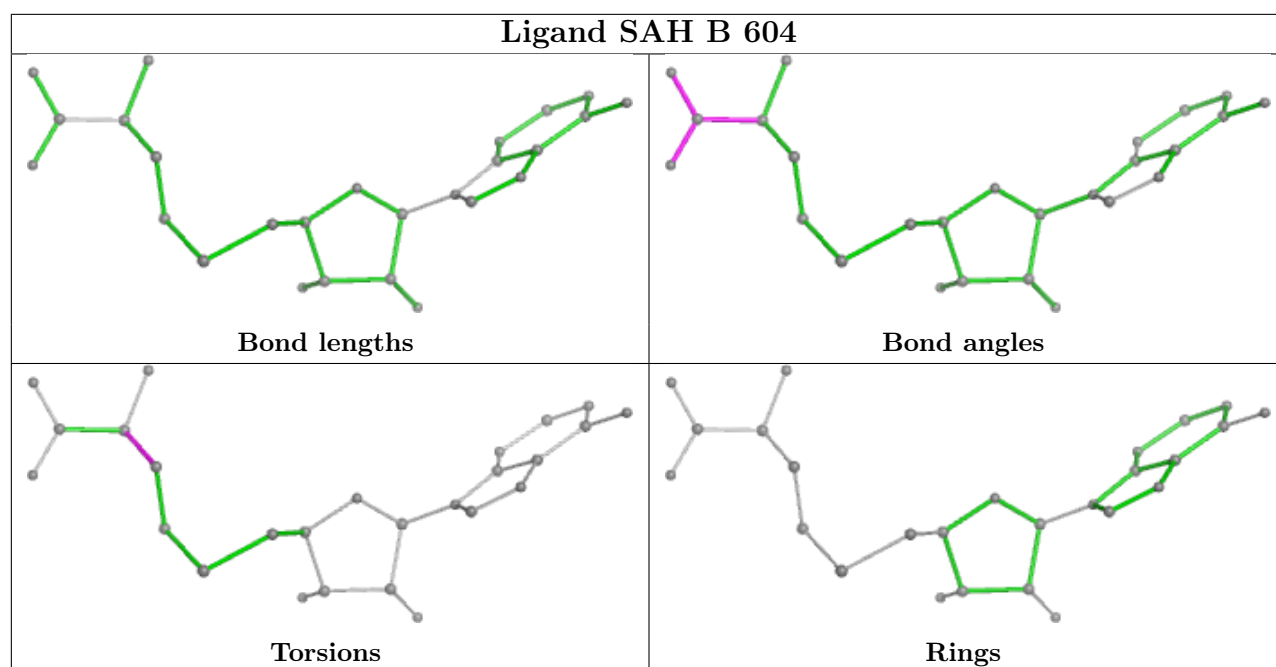


## Ligand A1JLH B 605



## Ligand SAH A 604





#### 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	445/528 (84%)	0.15	18 (4%)	43 43	33, 59, 107, 171	10 (2%)
1	B	433/528 (82%)	0.18	20 (4%)	38 38	38, 65, 114, 146	9 (2%)
All	All	878/1056 (83%)	0.17	38 (4%)	40 41	33, 63, 112, 171	19 (2%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	VAL	5.2
1	A	45	ILE	5.1
1	B	66	VAL	4.4
1	B	106	PRO	4.2
1	A	466	VAL	4.0
1	B	121	PRO	3.8
1	A	105	LEU	3.7
1	B	92	ALA	3.4
1	A	40	VAL	3.4
1	B	120	VAL	3.3
1	B	65	GLN	3.2
1	B	108	GLN	3.1
1	B	39	CYS	3.1
1	B	267	ALA	3.1
1	A	44	GLY	3.1
1	B	107	LEU	3.0
1	A	41	ASP	2.9
1	A	43	PRO	2.8
1	B	190	PHE	2.6
1	A	48	ASP	2.6
1	B	61	LYS	2.5
1	A	454	SER	2.4
1	A	42	ILE	2.3
1	B	68	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	481	GLY	2.2
1	A	268	HIS	2.2
1	A	467	PRO	2.2
1	B	109	LEU	2.1
1	A	64	TYR	2.1
1	A	46	PRO	2.1
1	A	57	MET	2.1
1	A	26	HIS	2.1
1	B	117	LEU	2.1
1	A	66	VAL	2.0
1	B	268	HIS	2.0
1	B	62	MET	2.0
1	B	273	ASP	2.0
1	A	58	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.

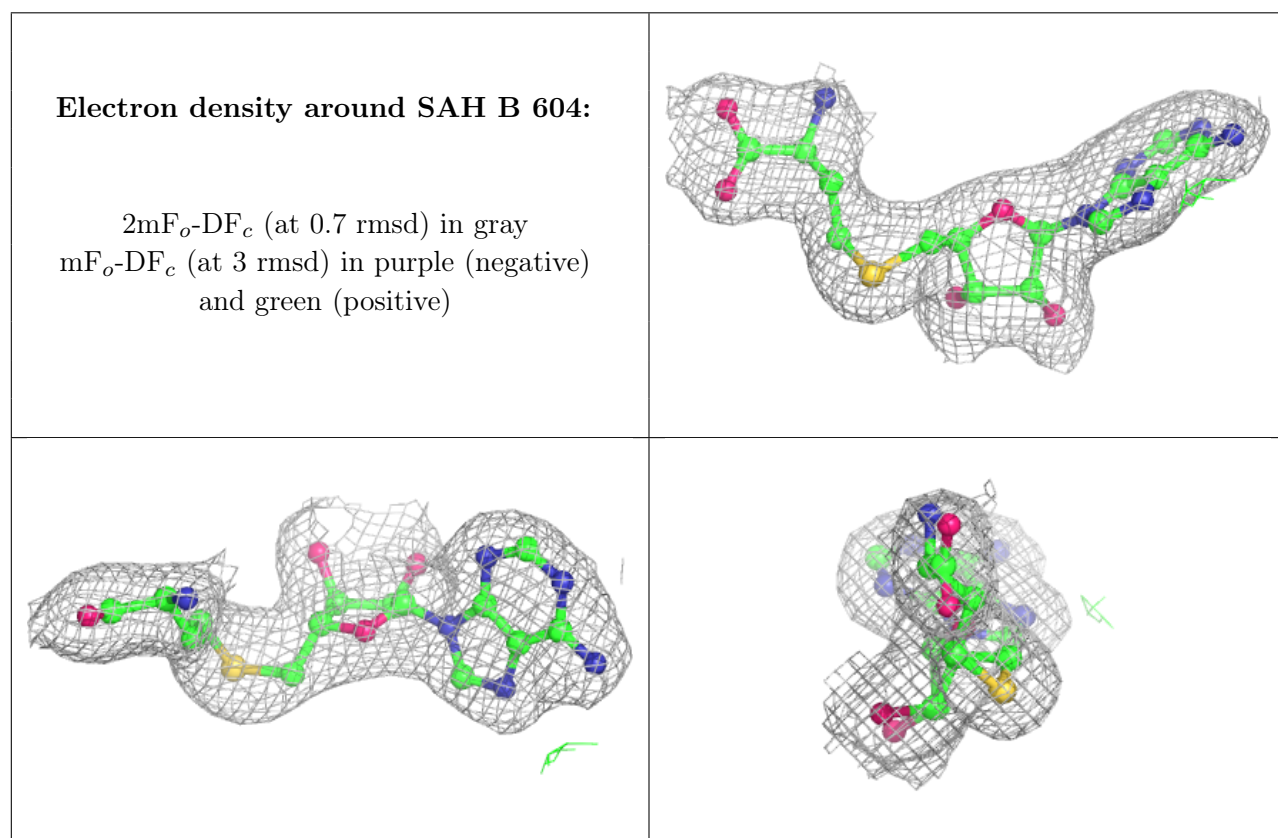
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	A	606	1/1	0.90	0.12	87,87,87,87	0
5	CL	B	607	1/1	0.91	0.16	88,88,88,88	0
6	IMD	A	609	5/5	0.91	0.14	69,77,77,79	0
5	CL	B	606	1/1	0.92	0.13	97,97,97,97	0
5	CL	A	607	1/1	0.93	0.12	80,80,80,80	0
5	CL	A	608	1/1	0.95	0.10	85,85,85,85	0
6	IMD	B	608	5/5	0.95	0.18	57,62,64,67	0
3	SAH	B	604	26/26	0.97	0.06	41,49,52,52	0
3	SAH	A	604	26/26	0.97	0.06	44,49,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	A1JLH	B	605	34/34	0.98	0.06	38,46,50,51	0
4	A1JLH	A	605	34/34	0.98	0.06	38,47,53,56	0
2	ZN	B	603	1/1	0.99	0.03	69,69,69,69	0
2	ZN	A	603	1/1	0.99	0.03	77,77,77,77	0
2	ZN	B	601	1/1	0.99	0.03	65,65,65,65	0
2	ZN	B	602	1/1	0.99	0.02	61,61,61,61	0
2	ZN	A	602	1/1	1.00	0.01	51,51,51,51	0
2	ZN	A	601	1/1	1.00	0.02	51,51,51,51	0

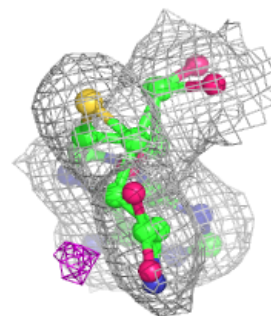
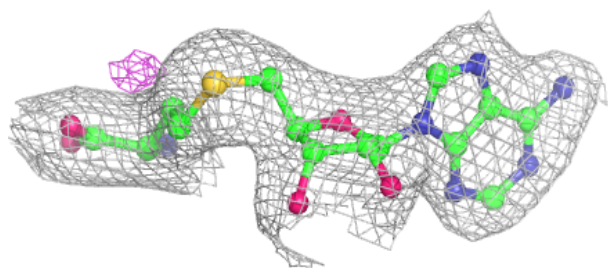
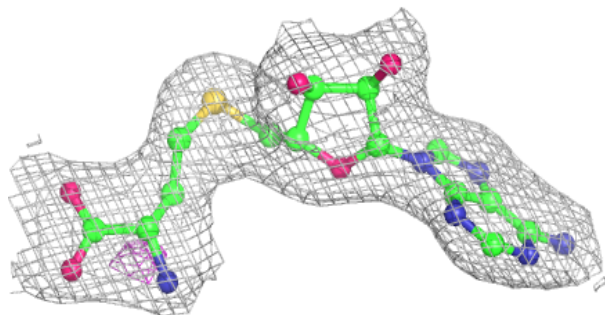
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



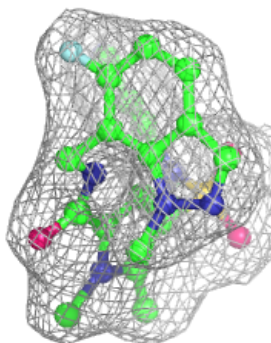
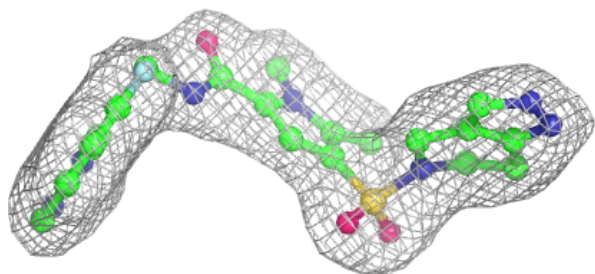
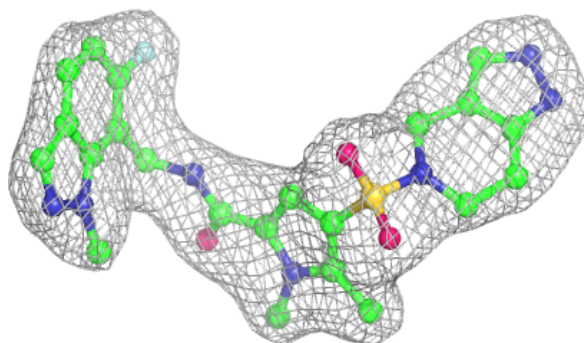


**Electron density around SAH A 604:**

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

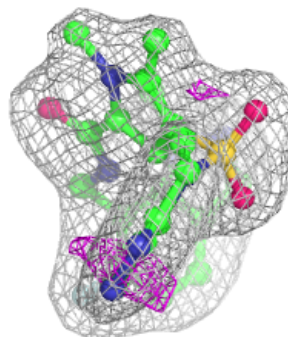
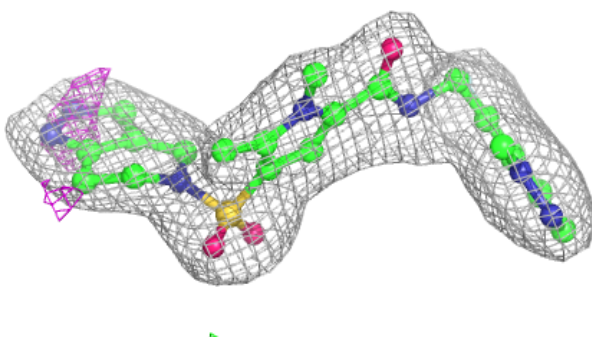
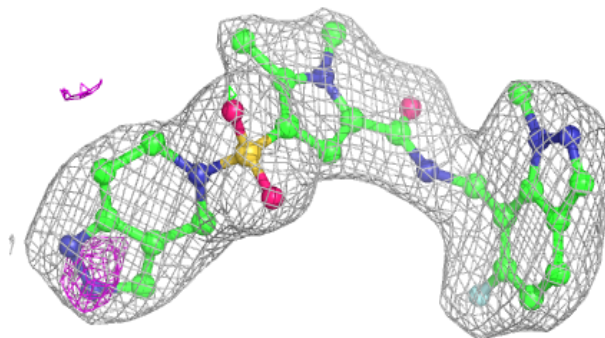
**Electron density around A1JLH B 605:**

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



**Electron density around A1JLH A 605:**

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



## 5.5 Other polymers ⓘ

There are no such residues in this entry.