



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2025 – 11:32 am BST

PDB ID : 9R5T / pdb\_00009r5t  
Title : NSP14 IN COMPLEX WITH LIGAND TDI-016037-NX-1  
Authors : Steinbacher, S.; Meyer, C.  
Deposited on : 2025-05-09  
Resolution : 1.89 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 Phenix2.0rc1  
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

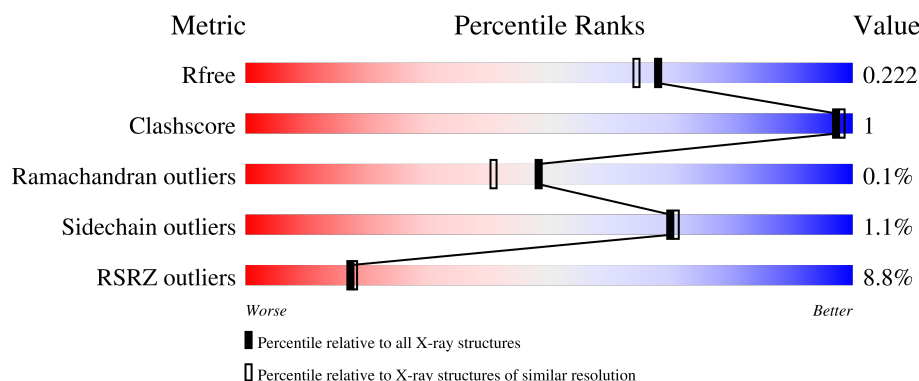
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	528	<div> <div>9%</div> <div>79%</div> <div>19%</div> </div>
1	B	528	<div> <div>6%</div> <div>80%</div> <div>18%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	B	610	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7501 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	428	Total	C	N	O	S	38	0	0
			3443	2217	585	608	33			
1	B	432	Total	C	N	O	S	40	0	0
			3475	2239	591	612	33			

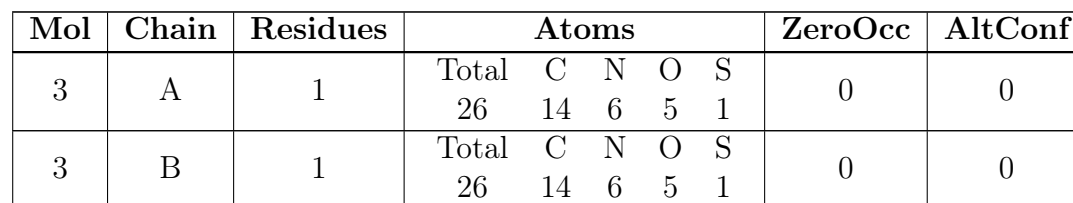
There are 6 discrepancies between the modelled and reference sequences:

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	4	Total	Zn	0	0
			4	4		

- 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).



- # A1JDF

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			37	26	1	6	3	1		

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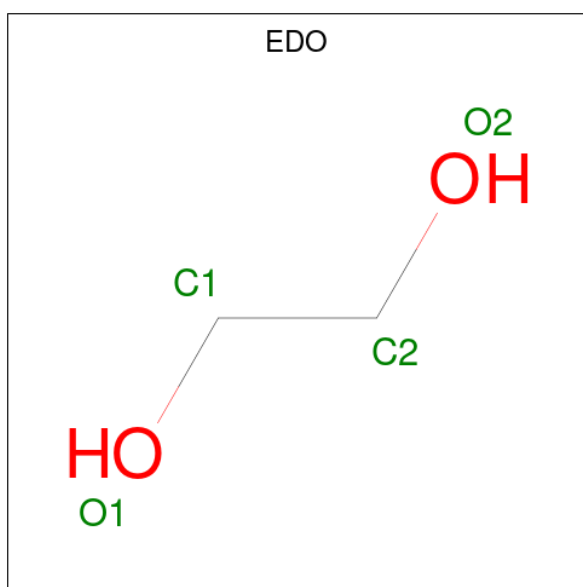
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	S	
			37	26	1	6	3	1	
								0	0

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

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



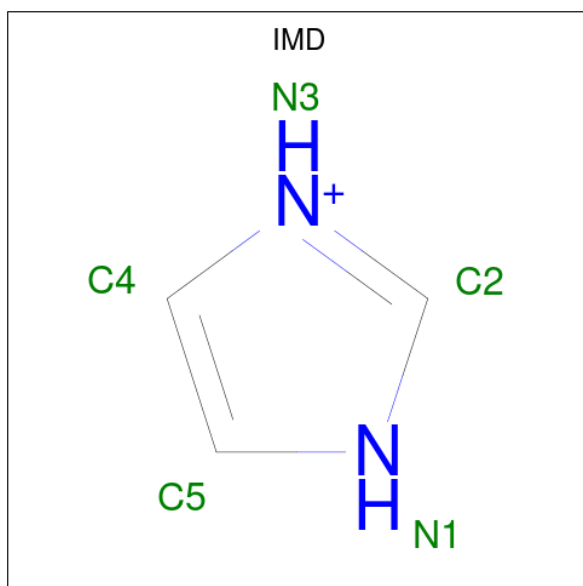
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O		
			4	2	2	0	0
6	A	1	Total	C	O		
			4	2	2	0	0
6	A	1	Total	C	O		
			4	2	2	0	0
6	A	1	Total	C	O		
			4	2	2	0	0
6	A	1	Total	C	O		
			4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is IMIDAZOLE (CCD ID: IMD) (formula:  $C_3H_5N_2$ ).



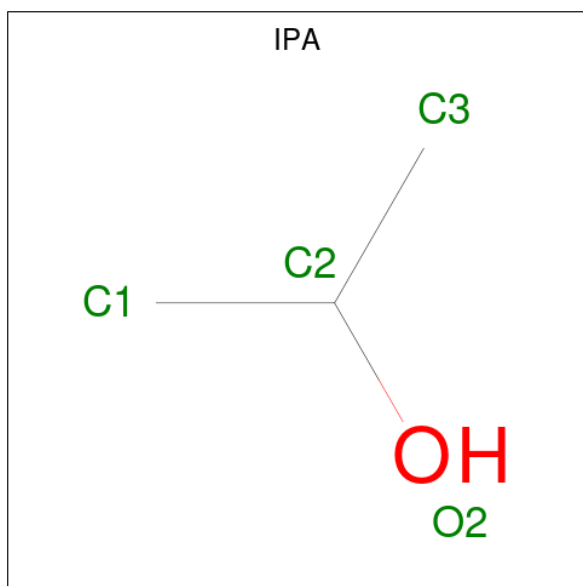
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			5	3	2		
7	B	1	Total	C	N	0	0
			5	3	2		
7	B	1	Total	C	N	0	0
			5	3	2		
7	B	1	Total	C	N	0	0
			5	3	2		

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

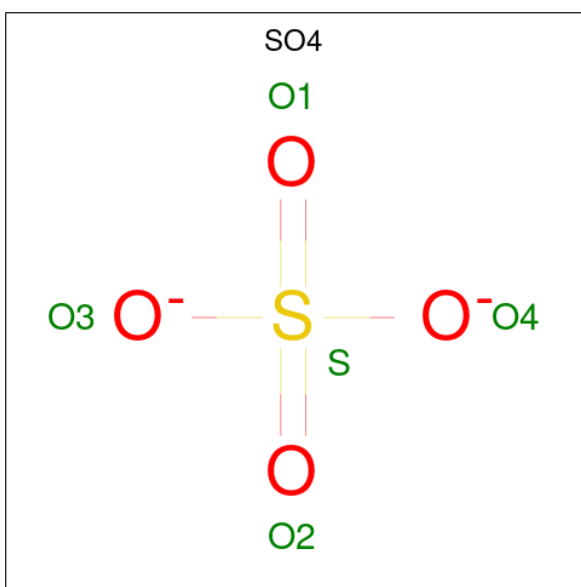
- Molecule 8 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	3	1		
8	B	1	Total	C	O	0	0
			4	3	1		
8	B	1	Total	C	O	0	0
			4	3	1		
8	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	156	Total	O	0	0
			156	156		
10	B	187	Total	O	0	2
			187	187		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.24Å 100.95Å 90.25Å 90.00° 108.12° 90.00°	Depositor
Resolution (Å)	54.05 – 1.89 54.05 – 1.89	Depositor EDS
% Data completeness (in resolution range)	64.2 (54.05-1.89) 64.2 (54.05-1.89)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.189 , 0.227 0.190 , 0.222	Depositor DCC
$R_{free}$ test set	1444 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IPA, SAH, SO4, A1JDF, IMD, CL, EDO

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	1.01	0/3537	1.37	0/4795
1	B	1.00	0/3572	1.38	0/4845
All	All	1.00	0/7109	1.37	0/9640

There are no bond length outliers.

There are no bond angle outliers.

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	3443	0	3331	3	0
1	B	3475	0	3369	7	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
4	A	37	0	0	0	0
4	B	37	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	2	0
6	A	28	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	24	0	36	0	0
7	A	5	0	5	0	0
7	B	20	0	17	2	0
8	B	16	0	32	0	0
9	B	10	0	0	0	0
10	A	156	0	0	1	0
10	B	187	0	0	2	0
All	All	7501	0	6870	11	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 1.

All (11) 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)
5:B:610:CL:CL	10:B:875:HOH:O	2.19	0.97
1:B:406:LEU:HD23	5:B:610:CL:CL	2.37	0.62
1:A:361:TYR:CE2	1:A:362:LYS:HG2	2.45	0.51
1:B:445:PHE:CD2	7:B:618:IMD:H2	2.51	0.46
1:B:522:THR:HB	10:B:851:HOH:O	2.15	0.45
1:A:375:ASP:HB2	10:A:807:HOH:O	2.16	0.45
1:B:329:LEU:HD22	1:B:348:TRP:CE2	2.52	0.45
1:B:466:VAL:O	1:B:466:VAL:HG13	2.18	0.44
1:A:91:VAL:HG11	1:A:107:LEU:HD22	1.99	0.43
1:B:249:PHE:HZ	1:B:284:GLU:HG3	1.83	0.43
1:B:312:VAL:HG13	7:B:618:IMD:H4	2.00	0.43

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	416/528 (79%)	405 (97%)	10 (2%)	1 (0%)	44	36
1	B	422/528 (80%)	412 (98%)	10 (2%)	0	100	100
All	All	838/1056 (79%)	817 (98%)	20 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	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	374/461 (81%)	368 (98%)	6 (2%)	58	56
1	B	378/461 (82%)	376 (100%)	2 (0%)	86	88
All	All	752/922 (82%)	744 (99%)	8 (1%)	70	71

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	77	GLU
1	A	222	ASP
1	A	454	SER
1	A	479	LEU
1	A	500	MET
1	B	359	LYS
1	B	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	266	ASN

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Mol	Chain	Res	Type
1	A	386	ASN
1	B	256	ASN
1	B	266	ASN
1	B	386	ASN
1	B	486	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 11 are monoatomic - leaving 28 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$
6	EDO	A	609	-	3,3,3	0.03	0	2,2,2	0.31	0
6	EDO	A	611	-	3,3,3	0.06	0	2,2,2	0.23	0
6	EDO	B	616	-	3,3,3	0.09	0	2,2,2	0.19	0
6	EDO	B	613	-	3,3,3	0.08	0	2,2,2	0.11	0
6	EDO	B	612	-	3,3,3	0.15	0	2,2,2	0.07	0
3	SAH	A	604	-	24,28,28	0.65	0	25,40,40	0.94	1 (4%)
6	EDO	B	615	-	3,3,3	0.11	0	2,2,2	0.24	0
4	A1JDF	A	605	-	36,42,42	1.30	5 (13%)	34,65,65	1.81	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	612	-	3,3,3	0.09	0	2,2,2	0.25	0
8	IPA	B	622	-	3,3,3	0.37	0	3,3,3	0.20	0
6	EDO	B	614	-	3,3,3	0.08	0	2,2,2	0.33	0
3	SAH	B	604	-	24,28,28	0.66	0	25,40,40	0.98	3 (12%)
6	EDO	A	610	-	3,3,3	0.24	0	2,2,2	0.32	0
6	EDO	A	614	-	3,3,3	0.03	0	2,2,2	0.17	0
7	IMD	B	618	-	3,5,5	0.37	0	4,5,5	0.72	0
7	IMD	A	615	-	3,5,5	0.43	0	4,5,5	0.79	0
8	IPA	B	621	-	3,3,3	0.27	0	3,3,3	0.25	0
8	IPA	B	619	-	3,3,3	0.16	0	3,3,3	0.19	0
7	IMD	B	606	2	3,5,5	0.27	0	4,5,5	0.73	0
8	IPA	B	620	-	3,3,3	0.39	0	3,3,3	0.14	0
9	SO4	B	623	-	4,4,4	0.37	0	6,6,6	0.08	0
4	A1JDF	B	608	-	36,42,42	1.35	4 (11%)	34,65,65	2.35	8 (23%)
6	EDO	A	613	-	3,3,3	0.09	0	2,2,2	0.20	0
6	EDO	A	608	-	3,3,3	0.16	0	2,2,2	0.38	0
7	IMD	B	605	2	3,5,5	0.34	0	4,5,5	0.68	0
9	SO4	B	624	-	4,4,4	0.35	0	6,6,6	0.09	0
7	IMD	B	607	2	3,5,5	0.35	0	4,5,5	0.71	0
6	EDO	B	617	-	3,3,3	0.13	0	2,2,2	0.17	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
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	A	611	-	-	1/1/1/1	-
6	EDO	B	616	-	-	0/1/1/1	-
6	EDO	B	613	-	-	1/1/1/1	-
6	EDO	B	612	-	-	1/1/1/1	-
3	SAH	A	604	-	-	4/11/31/31	0/3/3/3
6	EDO	B	615	-	-	1/1/1/1	-
4	A1JDF	A	605	-	-	0/12/27/27	0/6/6/6
6	EDO	A	612	-	-	1/1/1/1	-
6	EDO	B	614	-	-	0/1/1/1	-
3	SAH	B	604	-	-	4/11/31/31	0/3/3/3
6	EDO	A	610	-	-	1/1/1/1	-
6	EDO	A	614	-	-	1/1/1/1	-
7	IMD	B	618	-	-	-	0/1/1/1
7	IMD	A	615	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IMD	B	606	2	-	-	0/1/1/1
4	A1JDF	B	608	-	-	0/12/27/27	0/6/6/6
6	EDO	A	613	-	-	0/1/1/1	-
6	EDO	A	608	-	-	1/1/1/1	-
7	IMD	B	605	2	-	-	0/1/1/1
7	IMD	B	607	2	-	-	0/1/1/1
6	EDO	B	617	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	A1JDF	C36-C35	-4.55	1.35	1.42
4	A	605	A1JDF	C36-C35	-3.30	1.37	1.42
4	B	608	A1JDF	C21-N23	-2.76	1.37	1.39
4	A	605	A1JDF	C21-N23	-2.42	1.37	1.39
4	B	608	A1JDF	C21-C20	-2.30	1.36	1.39
4	A	605	A1JDF	C31-C30	2.29	1.45	1.40
4	A	605	A1JDF	C6-C5	2.28	1.45	1.40
4	B	608	A1JDF	C20-S25	-2.23	1.75	1.78
4	A	605	A1JDF	C9-N8	-2.13	1.46	1.49

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	608	A1JDF	C37-C36-C35	-7.82	112.45	120.03
4	B	608	A1JDF	C28-S25-C20	6.39	114.30	105.28
4	A	605	A1JDF	C28-S25-C20	6.15	113.96	105.28
4	A	605	A1JDF	C37-C36-C35	-3.54	116.60	120.03
4	B	608	A1JDF	C37-C36-C38	3.53	125.90	120.74
3	B	604	SAH	OXT-C-O	-3.06	117.14	124.09
4	A	605	A1JDF	C24-N23-C21	3.06	127.09	124.09
4	B	608	A1JDF	O26-S25-C28	-3.00	104.59	107.97
4	A	605	A1JDF	C13-C14-N15	-2.72	105.42	109.94
4	B	608	A1JDF	C14-C13-C2	-2.70	117.19	121.96
4	B	608	A1JDF	C22-C21-C20	-2.53	126.84	129.47
4	B	608	A1JDF	O26-S25-C20	-2.26	104.19	107.96
3	A	604	SAH	OXT-C-CA	2.17	120.78	113.38
3	B	604	SAH	C5-C6-N6	2.16	123.64	120.35
4	A	605	A1JDF	C22-C21-C20	-2.08	127.31	129.47
4	B	608	A1JDF	C29-C28-C38	-2.08	118.72	120.97
3	B	604	SAH	OXT-C-CA	2.07	120.42	113.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

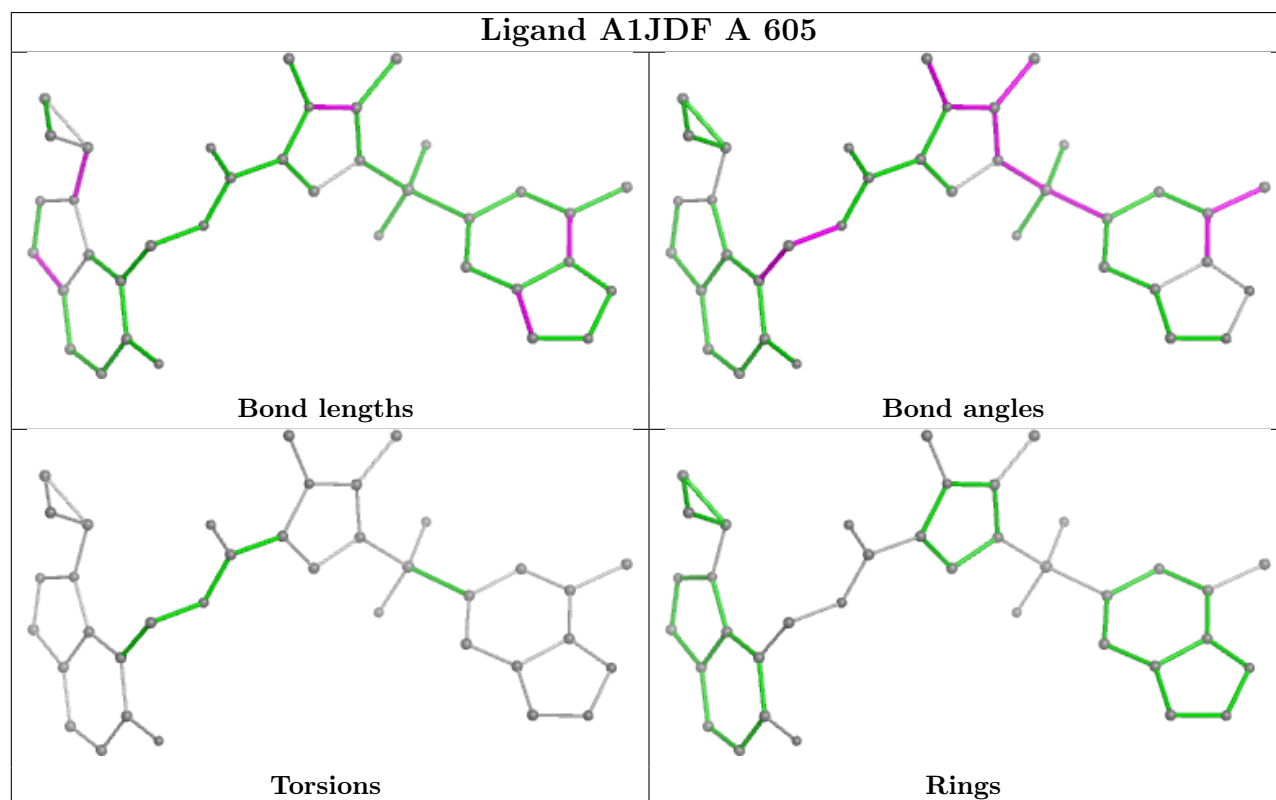
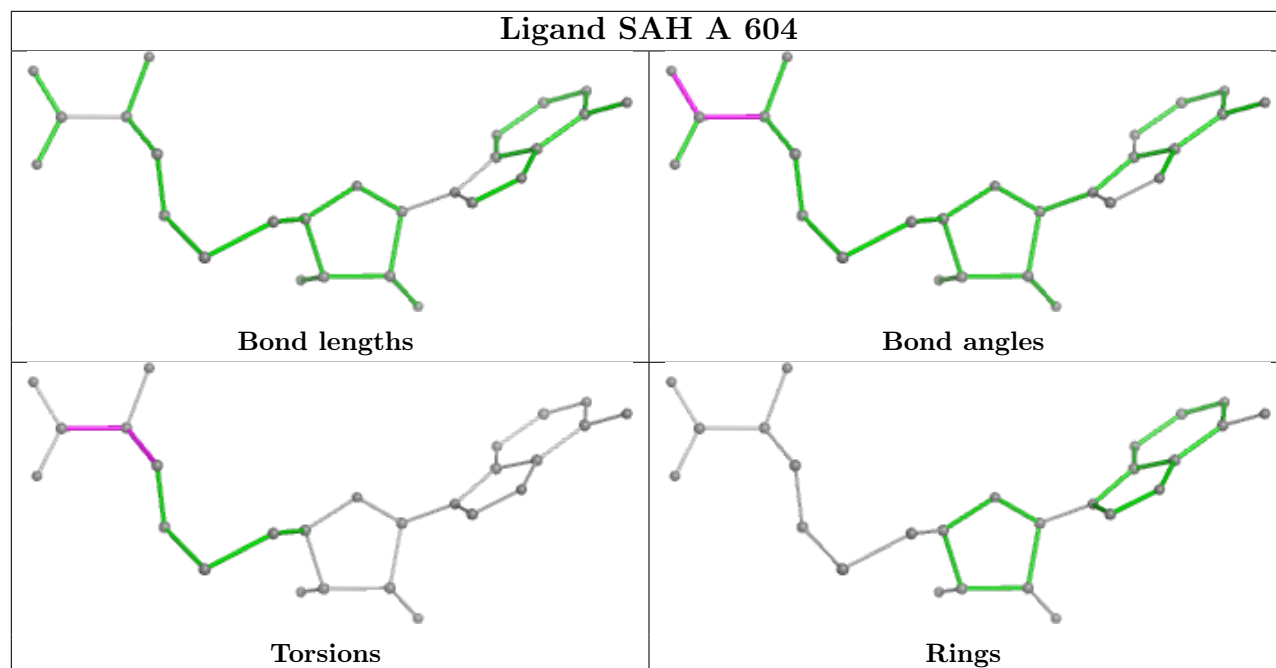
Mol	Chain	Res	Type	Atoms
3	A	604	SAH	N-CA-CB-CG
3	A	604	SAH	C-CA-CB-CG
3	B	604	SAH	C-CA-CB-CG
6	B	612	EDO	O1-C1-C2-O2
6	B	615	EDO	O1-C1-C2-O2
6	B	617	EDO	O1-C1-C2-O2
6	A	608	EDO	O1-C1-C2-O2
6	A	610	EDO	O1-C1-C2-O2
3	B	604	SAH	N-CA-CB-CG
3	B	604	SAH	O-C-CA-CB
6	A	612	EDO	O1-C1-C2-O2
3	B	604	SAH	OXT-C-CA-CB
6	A	614	EDO	O1-C1-C2-O2
3	A	604	SAH	OXT-C-CA-CB
6	B	613	EDO	O1-C1-C2-O2
3	A	604	SAH	O-C-CA-CB
6	A	611	EDO	O1-C1-C2-O2

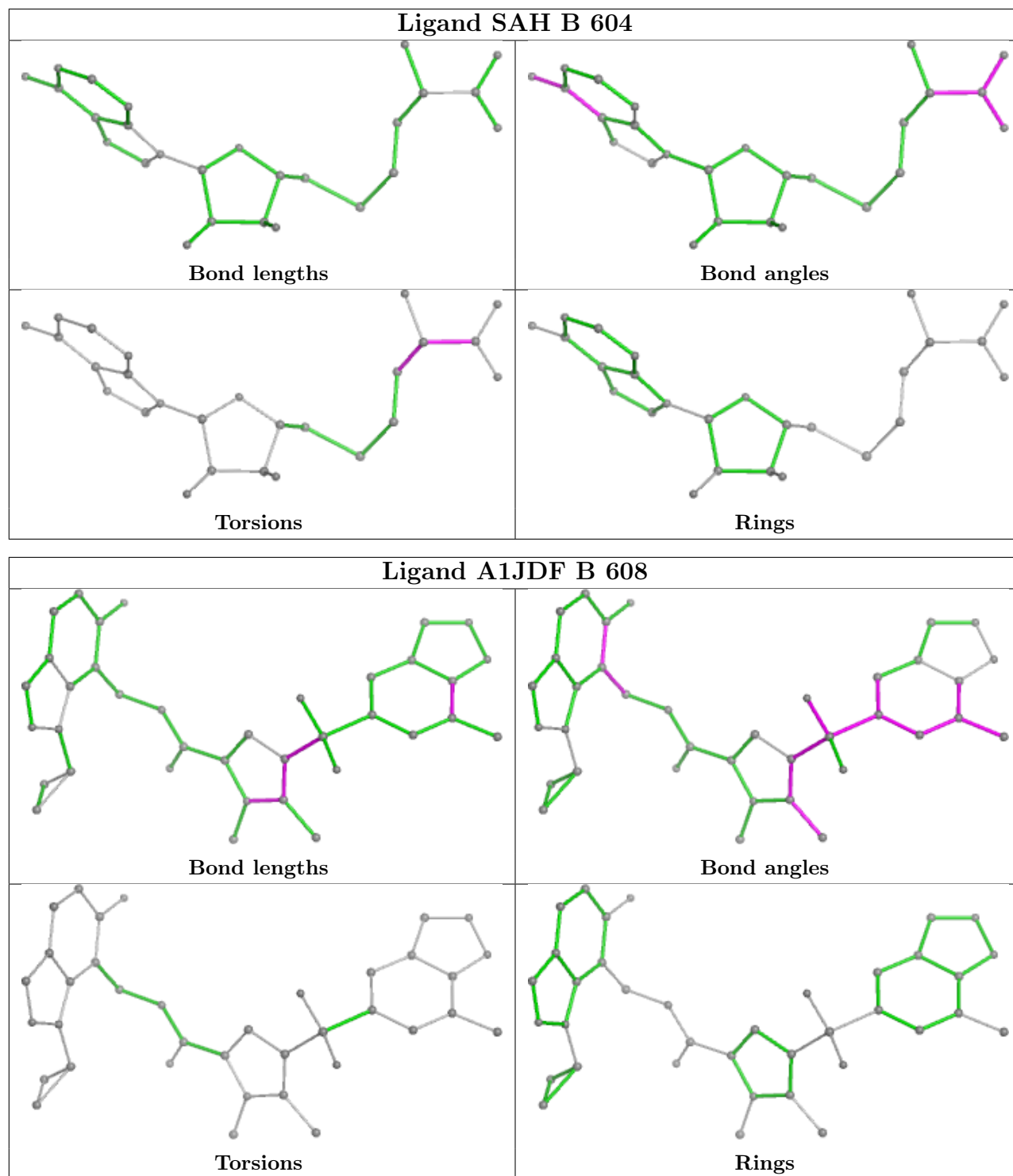
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	618	IMD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

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	428/528 (81%)	0.70	45 (10%)	13 13	34, 56, 102, 137	15 (3%)
1	B	432/528 (81%)	0.47	31 (7%)	23 24	26, 48, 86, 123	13 (3%)
All	All	860/1056 (81%)	0.59	76 (8%)	17 18	26, 52, 96, 137	28 (3%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	ALA	5.3
1	A	466	VAL	5.1
1	A	120	VAL	4.5
1	B	106	PRO	4.4
1	B	453	GLU	4.4
1	A	118	VAL	4.4
1	B	466	VAL	4.2
1	A	68	GLY	4.2
1	A	38	LEU	3.9
1	A	107	LEU	3.9
1	B	38	LEU	3.8
1	A	190	PHE	3.8
1	A	91	VAL	3.6
1	A	109	LEU	3.6
1	B	120	VAL	3.5
1	A	268	HIS	3.5
1	B	66	VAL	3.5
1	A	250	THR	3.5
1	A	57	MET	3.5
1	A	267	ALA	3.4
1	A	231	ILE	3.4
1	B	467	PRO	3.3
1	A	29	VAL	3.3
1	A	454	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	PHE	3.3
1	A	62	MET	3.2
1	B	483	VAL	3.2
1	B	188	HIS	3.1
1	A	188	HIS	3.1
1	A	467	PRO	3.1
1	A	25	THR	3.1
1	B	39	CYS	3.0
1	A	159	TRP	2.9
1	A	69	TYR	2.9
1	A	27	LEU	2.9
1	B	523	PHE	2.9
1	B	65	GLN	2.8
1	B	121	PRO	2.8
1	A	485	ARG	2.8
1	B	155	LYS	2.8
1	B	288	LYS	2.7
1	B	517	TYR	2.7
1	A	58	MET	2.6
1	B	406	LEU	2.6
1	A	156	GLY	2.6
1	A	269	VAL	2.6
1	A	55	ILE	2.6
1	A	108	GLN	2.6
1	A	249	PHE	2.5
1	A	56	SER	2.5
1	A	117	LEU	2.5
1	A	51	TYR	2.4
1	B	156	GLY	2.4
1	A	119	ALA	2.4
1	A	61	LYS	2.4
1	A	523	PHE	2.4
1	A	266	ASN	2.3
1	B	338	ILE	2.3
1	A	157	LEU	2.3
1	B	29	VAL	2.3
1	A	479	LEU	2.3
1	B	268	HIS	2.2
1	B	107	LEU	2.2
1	A	59	GLY	2.2
1	B	25	THR	2.2
1	A	483	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	345	ASP	2.1
1	B	61	LYS	2.1
1	B	57	MET	2.1
1	A	65	GLN	2.1
1	B	209	LEU	2.1
1	B	32	LYS	2.1
1	B	482	ALA	2.1
1	A	288	LYS	2.0
1	B	516	THR	2.0
1	B	157	LEU	2.0

## 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
6	EDO	B	613	4/4	0.36	0.17	106,108,108,110	0
8	IPA	B	620	4/4	0.73	0.36	67,70,70,75	0
6	EDO	B	615	4/4	0.74	0.27	91,101,102,105	0
6	EDO	A	612	4/4	0.76	0.28	96,96,98,100	0
8	IPA	B	621	4/4	0.78	0.33	92,93,94,96	0
9	SO4	B	624	5/5	0.78	0.14	96,101,106,109	0
5	CL	B	610	1/1	0.82	0.29	116,116,116,116	0
9	SO4	B	623	5/5	0.84	0.13	99,106,116,118	0
6	EDO	A	611	4/4	0.85	0.12	82,84,87,88	0
6	EDO	A	608	4/4	0.85	0.20	70,72,73,73	0
6	EDO	A	613	4/4	0.86	0.29	83,85,87,88	0
8	IPA	B	622	4/4	0.86	0.24	58,65,67,67	0
6	EDO	A	614	4/4	0.87	0.24	80,80,80,86	0

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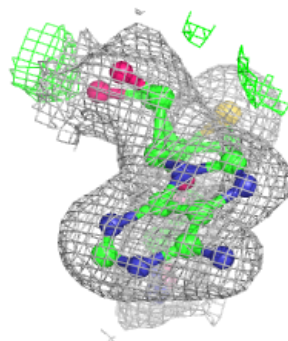
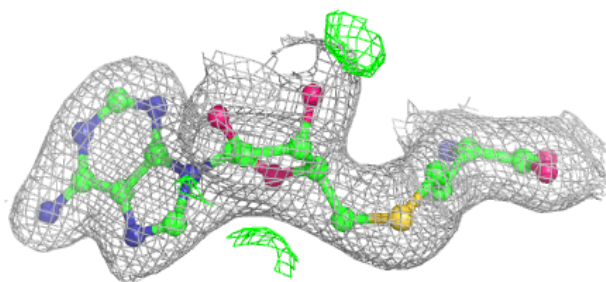
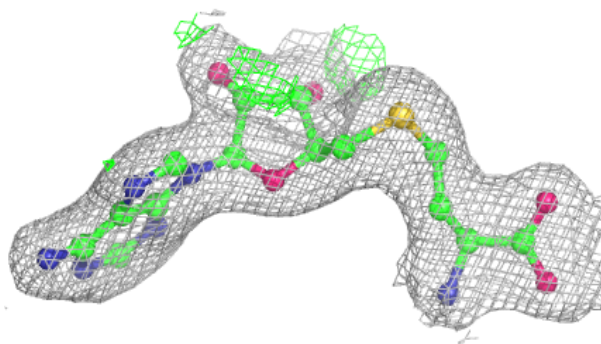
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	EDO	A	610	4/4	0.87	0.17	70,70,74,75	0
8	IPA	B	619	4/4	0.88	0.20	63,64,65,69	0
6	EDO	B	614	4/4	0.88	0.14	78,84,85,86	0
6	EDO	B	612	4/4	0.88	0.20	65,67,68,74	0
5	CL	A	607	1/1	0.89	0.18	90,90,90,90	0
7	IMD	B	607	5/5	0.89	0.20	75,83,84,87	0
6	EDO	A	609	4/4	0.90	0.09	51,51,55,57	0
5	CL	B	609	1/1	0.91	0.18	80,80,80,80	0
6	EDO	B	616	4/4	0.92	0.12	58,60,60,61	0
7	IMD	A	615	5/5	0.94	0.10	48,50,53,53	0
6	EDO	B	617	4/4	0.95	0.12	53,56,59,62	0
7	IMD	B	618	5/5	0.95	0.09	51,51,53,53	0
5	CL	A	606	1/1	0.95	0.11	80,80,80,80	0
7	IMD	B	606	5/5	0.95	0.09	42,42,44,44	0
3	SAH	B	604	26/26	0.97	0.06	35,39,40,43	0
4	A1JDF	A	605	37/37	0.97	0.06	33,36,49,54	0
7	IMD	B	605	5/5	0.97	0.06	52,52,54,56	0
2	ZN	B	603	1/1	0.97	0.05	70,70,70,70	0
3	SAH	A	604	26/26	0.98	0.05	34,38,41,42	0
4	A1JDF	B	608	37/37	0.98	0.06	32,38,47,50	0
2	ZN	A	602	1/1	0.99	0.03	58,58,58,58	0
2	ZN	A	603	1/1	0.99	0.04	65,65,65,65	0
2	ZN	A	601	1/1	0.99	0.03	57,57,57,57	0
2	ZN	B	611	1/1	0.99	0.04	47,47,47,47	0
2	ZN	B	601	1/1	1.00	0.02	38,38,38,38	0
2	ZN	B	602	1/1	1.00	0.02	42,42,42,42	0

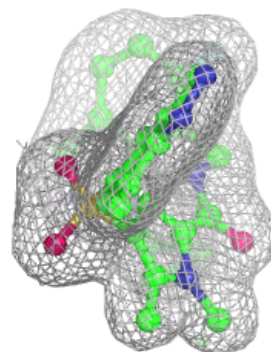
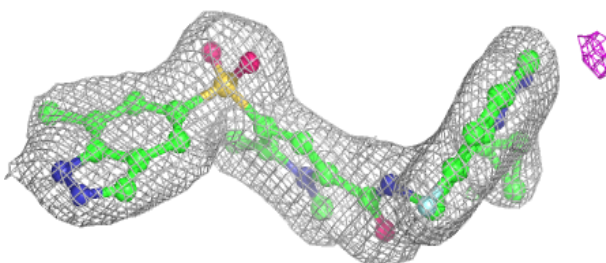
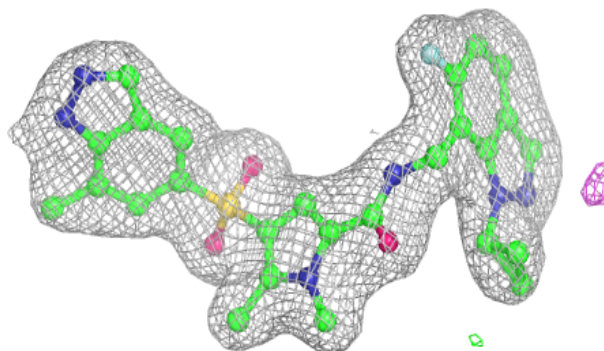
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAH B 604:**

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

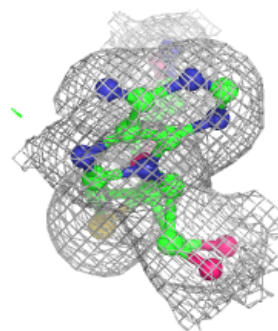
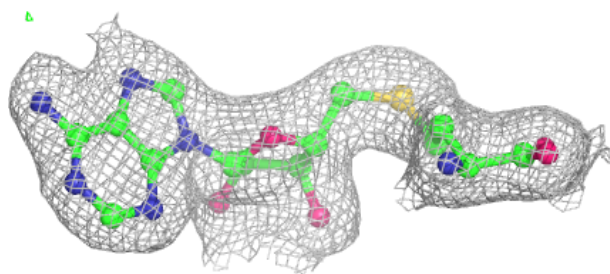
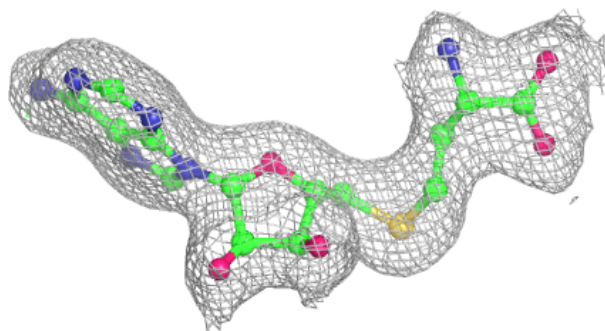
**Electron density around A1JDF A 605:**

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

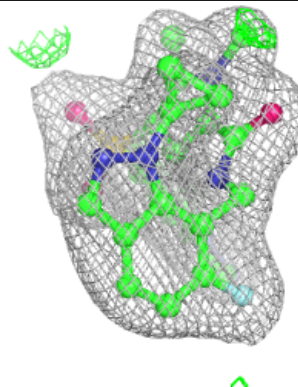
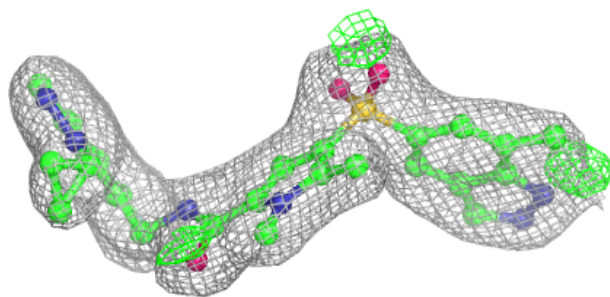
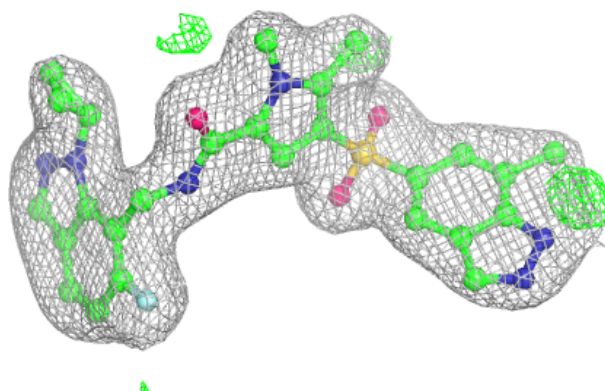


**Electron density around SAH A 604:**

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

**Electron density around A1JDF B 608:**

$2mF_o-DF_c$  (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.