



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 11:33 am GMT

PDB ID : 8RS7 / pdb_00008rs7
Title : Crystal structure of Zika Virus NS2B-NS3 protease in complex with an allosteric inhibitor
Authors : Ontario, J.M.; Torrente, E.
Deposited on : 2024-01-24
Resolution : 3.18 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (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

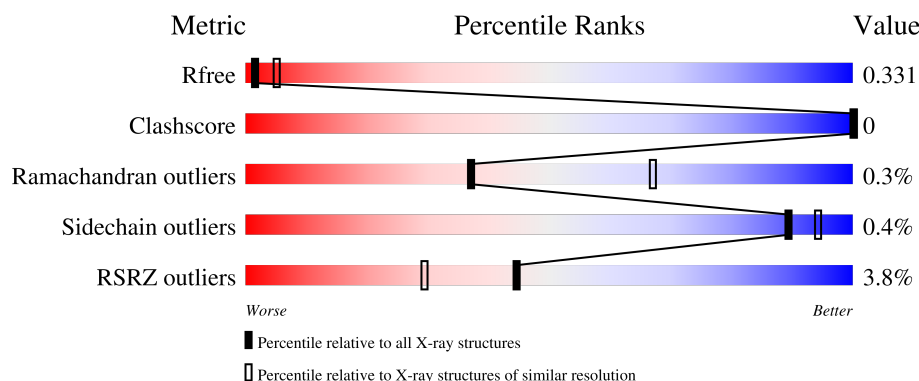
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	230	 3% 70% 30%
1	B	230	 2% 68% . 31%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2520 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	42	0	0
			1226	775	213	231	7			
1	B	158	Total	C	N	O	S	43	0	0
			1201	759	208	228	6			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	expression tag	UNP A0A140DLX4
A	46	SER	-	expression tag	UNP A0A140DLX4
A	47	HIS	-	expression tag	UNP A0A140DLX4
A	48	MET	-	expression tag	UNP A0A140DLX4
A	?	-	ARG	deletion	UNP A0A140DLX4
A	?	-	GLU	deletion	UNP A0A140DLX4
A	?	-	ILE	deletion	UNP A0A140DLX4
A	?	-	ILE	deletion	UNP A0A140DLX4
A	?	-	LEU	deletion	UNP A0A140DLX4
A	?	-	LYS	deletion	UNP A0A140DLX4
A	?	-	VAL	deletion	UNP A0A140DLX4
A	?	-	VAL	deletion	UNP A0A140DLX4
A	?	-	LEU	deletion	UNP A0A140DLX4
A	?	-	MET	deletion	UNP A0A140DLX4
A	?	-	THR	deletion	UNP A0A140DLX4
A	?	-	ILE	deletion	UNP A0A140DLX4
A	?	-	CYS	deletion	UNP A0A140DLX4
A	?	-	GLY	deletion	UNP A0A140DLX4
A	?	-	MET	deletion	UNP A0A140DLX4
A	?	-	ASN	deletion	UNP A0A140DLX4
A	?	-	PRO	deletion	UNP A0A140DLX4
A	?	-	ILE	deletion	UNP A0A140DLX4
A	?	-	ALA	deletion	UNP A0A140DLX4
A	?	-	ILE	deletion	UNP A0A140DLX4
A	?	-	PRO	deletion	UNP A0A140DLX4

Continued on next page...

Continued from previous page...

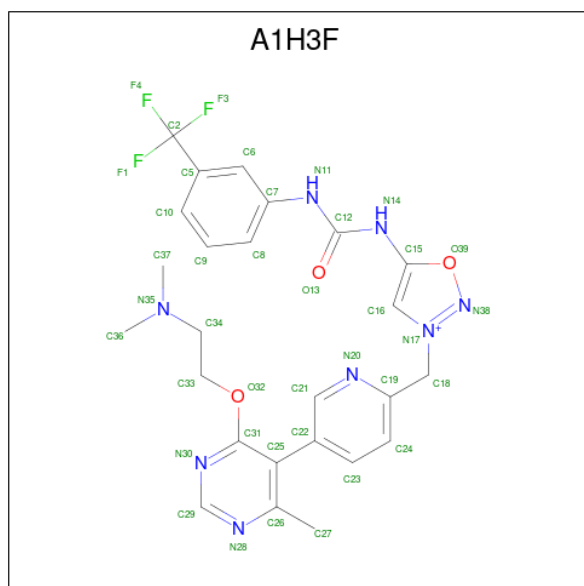
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP A0A140DLX4
A	992	GLY	ALA	linker	UNP A0A140DLX4
A	994	GLY	ALA	linker	UNP A0A140DLX4
A	995	GLY	TRP	linker	UNP A0A140DLX4
A	?	-	TYR	deletion	UNP A0A140DLX4
A	?	-	VAL	deletion	UNP A0A140DLX4
A	?	-	TYR	deletion	UNP A0A140DLX4
A	?	-	VAL	deletion	UNP A0A140DLX4
A	996	SER	LYS	linker	UNP A0A140DLX4
A	997	GLY	THR	linker	UNP A0A140DLX4
A	999	GLY	LYS	linker	UNP A0A140DLX4
A	1000	GLY	ARG	linker	UNP A0A140DLX4
A	1029	GLY	ARG	conflict	UNP A0A140DLX4
B	45	GLY	-	expression tag	UNP A0A140DLX4
B	46	SER	-	expression tag	UNP A0A140DLX4
B	47	HIS	-	expression tag	UNP A0A140DLX4
B	48	MET	-	expression tag	UNP A0A140DLX4
B	?	-	ARG	deletion	UNP A0A140DLX4
B	?	-	GLU	deletion	UNP A0A140DLX4
B	?	-	ILE	deletion	UNP A0A140DLX4
B	?	-	ILE	deletion	UNP A0A140DLX4
B	?	-	LEU	deletion	UNP A0A140DLX4
B	?	-	LYS	deletion	UNP A0A140DLX4
B	?	-	VAL	deletion	UNP A0A140DLX4
B	?	-	VAL	deletion	UNP A0A140DLX4
B	?	-	LEU	deletion	UNP A0A140DLX4
B	?	-	MET	deletion	UNP A0A140DLX4
B	?	-	THR	deletion	UNP A0A140DLX4
B	?	-	ILE	deletion	UNP A0A140DLX4
B	?	-	CYS	deletion	UNP A0A140DLX4
B	?	-	GLY	deletion	UNP A0A140DLX4
B	?	-	MET	deletion	UNP A0A140DLX4
B	?	-	ASN	deletion	UNP A0A140DLX4
B	?	-	PRO	deletion	UNP A0A140DLX4
B	?	-	ILE	deletion	UNP A0A140DLX4
B	?	-	ALA	deletion	UNP A0A140DLX4
B	?	-	ILE	deletion	UNP A0A140DLX4
B	?	-	PRO	deletion	UNP A0A140DLX4
B	?	-	PHE	deletion	UNP A0A140DLX4
B	992	GLY	ALA	linker	UNP A0A140DLX4
B	994	GLY	ALA	linker	UNP A0A140DLX4
B	995	GLY	TRP	linker	UNP A0A140DLX4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP A0A140DLX4
B	?	-	VAL	deletion	UNP A0A140DLX4
B	?	-	TYR	deletion	UNP A0A140DLX4
B	?	-	VAL	deletion	UNP A0A140DLX4
B	996	SER	LYS	linker	UNP A0A140DLX4
B	997	GLY	THR	linker	UNP A0A140DLX4
B	999	GLY	LYS	linker	UNP A0A140DLX4
B	1000	GLY	ARG	linker	UNP A0A140DLX4
B	1029	GLY	ARG	conflict	UNP A0A140DLX4

- Molecule 2 is 1-[3-[[5-[4-[2-(dimethylamino)ethoxy]-6-methyl-pyrimidin-5-yl]pyridin-2-yl]methyl]-1,2,3-oxadiazol-3-ium-5-yl]-3-[3-(trifluoromethyl)phenyl]urea (CCD ID: A1H3F) (formula: C₂₅H₂₆F₃N₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			39	25	3	8	3		
2	B	1	Total	C	F	N	O	0	0
			39	25	3	8	3		

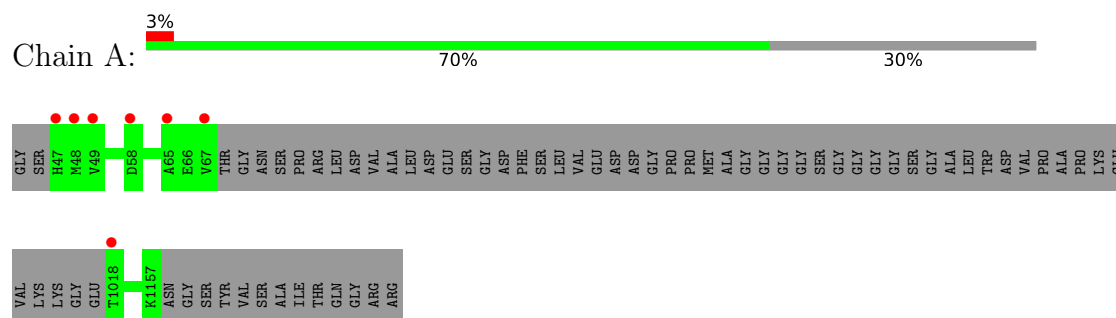
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	4	Total	O	0	0
			4	4		

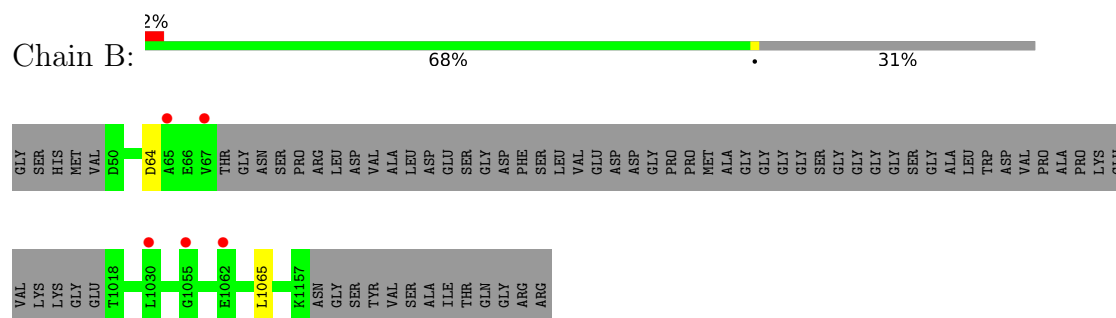
3 Residue-property plots [i](#)

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: Genome polyprotein



• Molecule 1: Genome polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.69Å 90.35Å 96.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.86 – 3.18 65.86 – 3.18	Depositor EDS
% Data completeness (in resolution range)	59.6 (65.86-3.18) 59.8 (65.86-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.281 , 0.330 0.281 , 0.331	Depositor DCC
R_{free} test set	230 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2520	wwPDB-VP
Average B, all atoms (Å ²)	73.0	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 45.02 % 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 1.4026e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1H3F

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	0.57	0/1253	0.70	0/1699
1	B	0.61	0/1227	0.73	0/1664
All	All	0.59	0/2480	0.72	0/3363

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

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	1226	0	1203	0	0
1	B	1201	0	1178	0	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
3	A	11	0	0	0	0
3	B	4	0	0	0	0
All	All	2520	0	2381	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/230 (68%)	147 (94%)	10 (6%)	0	100	100
1	B	154/230 (67%)	144 (94%)	9 (6%)	1 (1%)	22	55
All	All	311/460 (68%)	291 (94%)	19 (6%)	1 (0%)	37	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASP

5.3.2 Protein sidechains [i](#)

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	128/176 (73%)	128 (100%)	0	100	100
1	B	125/176 (71%)	124 (99%)	1 (1%)	79	89
All	All	253/352 (72%)	252 (100%)	1 (0%)	89	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1065	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1051	HIS
1	B	1051	HIS
1	B	1092	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](#)

2 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	A1H3F	B	1201	-	38,42,42	0.87	3 (7%)	48,59,59	1.73	11 (22%)
2	A1H3F	A	1201	-	38,42,42	0.88	2 (5%)	48,59,59	1.72	11 (22%)

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	A1H3F	B	1201	-	-	1/26/28/28	0/4/4/4
2	A1H3F	A	1201	-	-	0/26/28/28	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A1H3F	F4-C2	2.11	1.40	1.32
2	B	1201	A1H3F	F3-C2	2.10	1.40	1.32
2	B	1201	A1H3F	F4-C2	2.09	1.40	1.32
2	B	1201	A1H3F	F1-C2	2.04	1.40	1.32
2	A	1201	A1H3F	F3-C2	2.02	1.40	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	A1H3F	N30-C29-N28	-4.36	121.78	128.60
2	A	1201	A1H3F	N30-C29-N28	-4.33	121.83	128.60
2	B	1201	A1H3F	C25-C31-N30	-3.77	118.36	124.08
2	B	1201	A1H3F	C21-N20-C19	3.76	122.65	117.82
2	A	1201	A1H3F	C25-C31-N30	-3.69	118.48	124.08
2	A	1201	A1H3F	C21-N20-C19	3.64	122.49	117.82
2	B	1201	A1H3F	C15-N14-C12	-3.55	125.43	130.41
2	A	1201	A1H3F	C15-N14-C12	-3.47	125.53	130.41
2	B	1201	A1H3F	C29-N30-C31	3.30	121.41	115.88
2	A	1201	A1H3F	C29-N30-C31	3.29	121.39	115.88
2	B	1201	A1H3F	N14-C12-N11	3.23	118.14	112.49
2	A	1201	A1H3F	C19-C18-N17	-2.95	107.88	112.13
2	A	1201	A1H3F	N14-C12-N11	2.94	117.62	112.49
2	A	1201	A1H3F	C22-C25-C31	-2.62	119.33	122.57
2	B	1201	A1H3F	C19-C18-N17	-2.58	108.41	112.13
2	B	1201	A1H3F	C22-C21-N20	-2.44	120.30	124.32
2	B	1201	A1H3F	C22-C25-C31	-2.37	119.64	122.57
2	A	1201	A1H3F	C22-C21-N20	-2.37	120.42	124.32
2	B	1201	A1H3F	O32-C31-N30	2.24	122.57	119.23
2	A	1201	A1H3F	F3-C2-C5	-2.13	108.25	112.93
2	A	1201	A1H3F	O13-C12-N14	-2.04	120.17	123.62
2	B	1201	A1H3F	F3-C2-C5	-2.03	108.48	112.93

There are no chirality outliers.

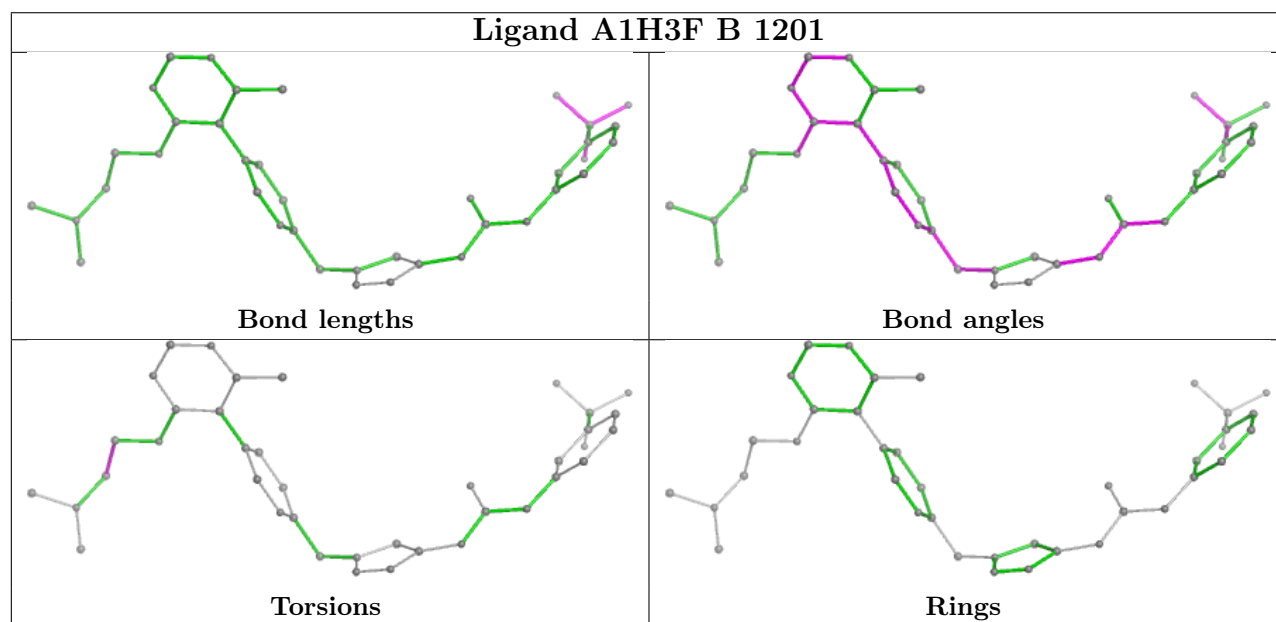
All (1) torsion outliers are listed below:

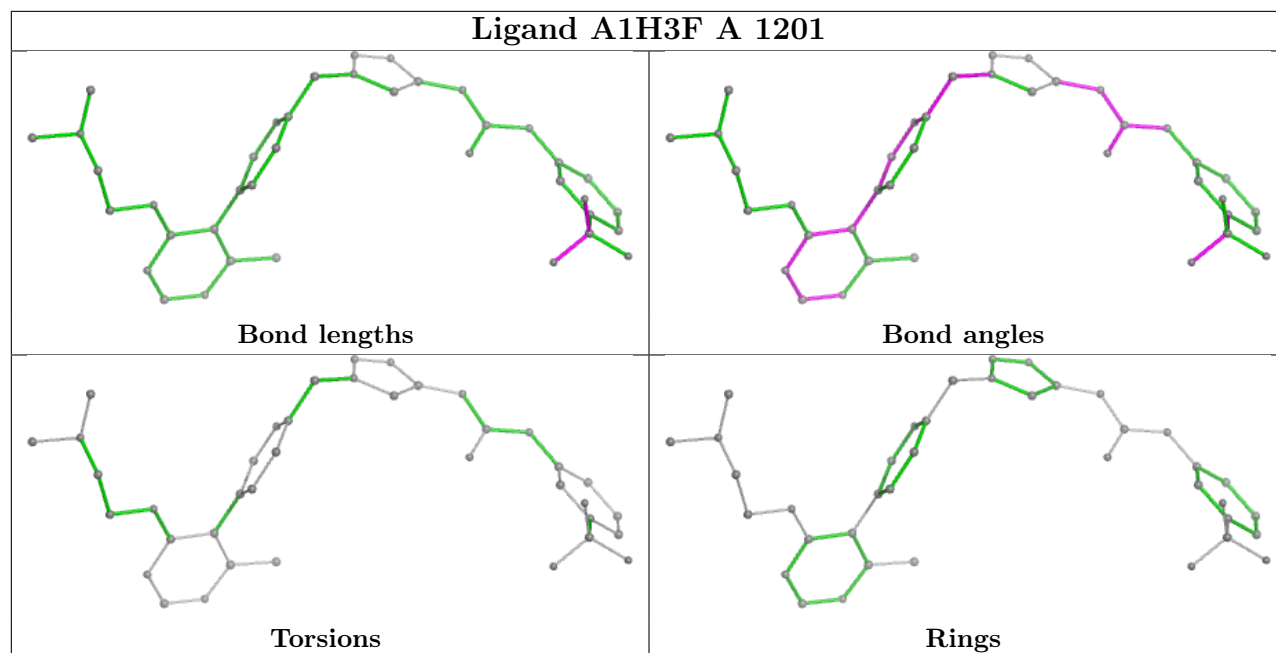
Mol	Chain	Res	Type	Atoms
2	B	1201	A1H3F	O32-C33-C34-N35

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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q < 0.9
1	A	161/230 (70%)	0.35	7 (4%)	40	26	41, 68, 112, 144	15 (9%)
1	B	158/230 (68%)	0.33	5 (3%)	50	34	38, 66, 104, 119	15 (9%)
All	All	319/460 (69%)	0.34	12 (3%)	44	29	38, 67, 108, 144	30 (9%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	HIS	3.7
1	B	65	ALA	3.0
1	A	67	VAL	2.9
1	A	48	MET	2.8
1	A	49	VAL	2.7
1	B	67	VAL	2.6
1	A	1018	THR	2.4
1	A	65	ALA	2.4
1	B	1030	LEU	2.3
1	A	58	ASP	2.1
1	B	1062	GLU	2.0
1	B	1055	GLY	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 ⓘ

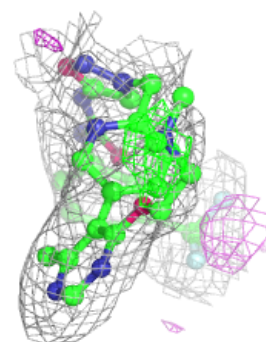
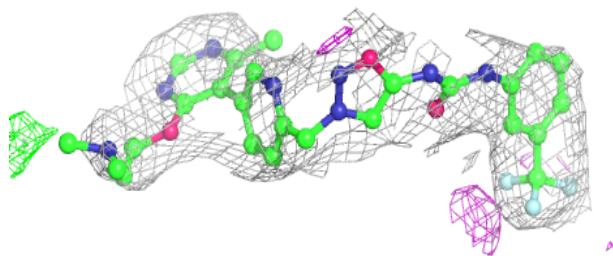
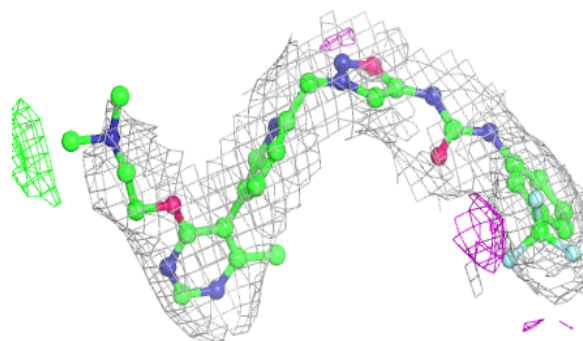
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1H3F	A	1201	39/39	0.83	0.14	64,71,80,80	0
2	A1H3F	B	1201	39/39	0.88	0.13	62,66,72,72	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.

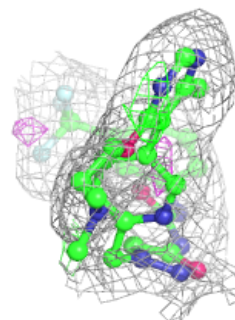
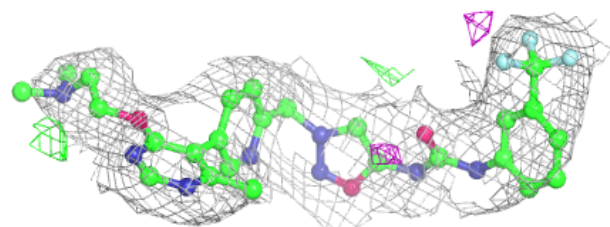
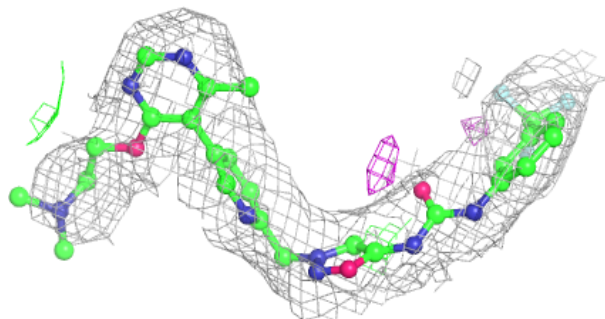
Electron density around A1H3F A 1201:

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 A1H3F B 1201:

$2mF_o-DF_c$ (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.