



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 8RS6 / pdb_00008rs6
Title : Crystal structure of Zika Virus NS2B-NS3 protease in complex with compound 1
Authors : Ontoria, J.M.; Torrente, E.
Deposited on : 2024-01-24
Resolution : 2.30 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

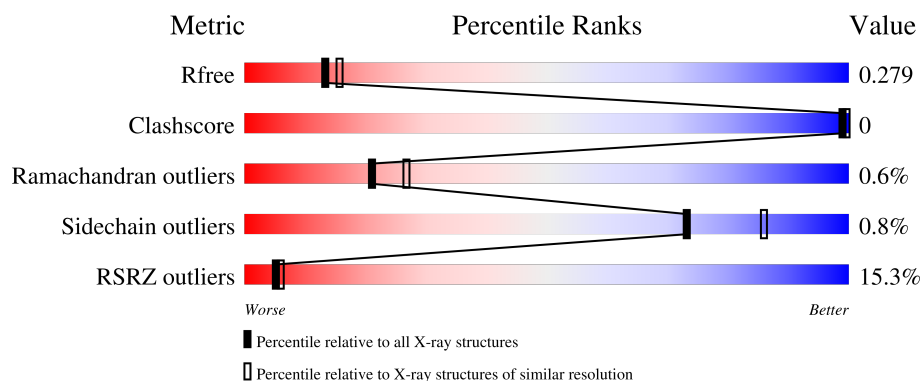
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	227	13% 72% 26%
1	B	227	10% 71% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2657 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 polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	33	0	0
			1267	798	221	242	6			
1	B	166	Total	C	N	O	S	22	1	0
			1268	798	222	242	6			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	MET	SER	conflict	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
A	?	-	PHE	deletion	UNP A0A140DLX4
A	?	-	ALA	deletion	UNP A0A140DLX4
A	?	-	ALA	deletion	UNP A0A140DLX4

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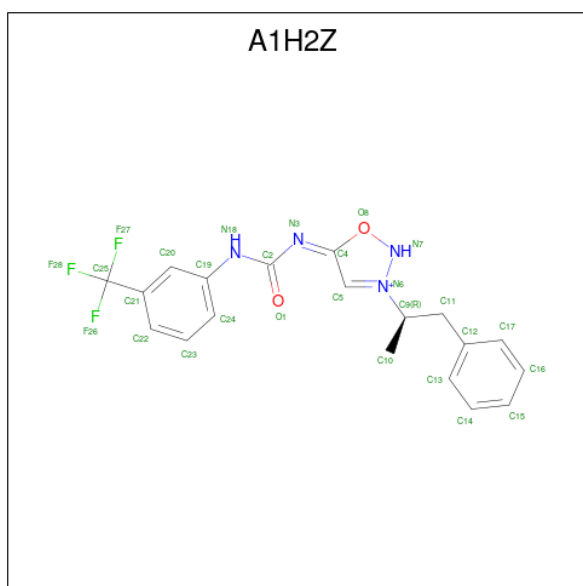
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP A0A140DLX4
A	?	-	ALA	deletion	UNP A0A140DLX4
A	991	ALA	TRP	linker	UNP A0A140DLX4
A	992	GLY	TYR	linker	UNP A0A140DLX4
A	993	GLY	VAL	linker	UNP A0A140DLX4
A	994	GLY	TYR	linker	UNP A0A140DLX4
A	995	GLY	VAL	linker	UNP A0A140DLX4
A	996	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	48	MET	SER	conflict	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	?	-	ALA	deletion	UNP A0A140DLX4
B	?	-	ALA	deletion	UNP A0A140DLX4
B	?	-	GLY	deletion	UNP A0A140DLX4
B	?	-	ALA	deletion	UNP A0A140DLX4
B	991	ALA	TRP	linker	UNP A0A140DLX4
B	992	GLY	TYR	linker	UNP A0A140DLX4
B	993	GLY	VAL	linker	UNP A0A140DLX4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	994	GLY	TYR	linker	UNP A0A140DLX4
B	995	GLY	VAL	linker	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 {E})-1-[3-[(2 {R})-1-phenylpropan-2-yl]-2 {H}-1,2,3-oxadiazol-3-ium-5-ylidene]-3-[3-(trifluoromethyl)phenyl]urea (CCD ID: A1H2Z) (formula: C₁₉H₁₈F₃N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	19	3	4	2		
2	B	1	Total	C	F	N	O	0	0
			28	19	3	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	36	Total	O	0	0
			36	36		

- Molecule 1: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.93Å 91.90Å 58.44Å 90.00° 97.97° 90.00°	Depositor
Resolution (Å)	57.87 – 2.30 57.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	56.4 (57.87-2.30) 56.3 (57.87-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.225 , 0.270 (Not available) , 0.279	Depositor DCC
R_{free} test set	666 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2657	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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: A1H2Z

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	0.81	0/1294	0.87	0/1756
1	B	0.80	0/1296	0.91	0/1760
All	All	0.81	0/2590	0.89	0/3516

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	1267	0	1243	1	0
1	B	1268	0	1236	1	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
3	A	30	0	0	0	0
3	B	36	0	0	0	0
All	All	2657	0	2479	2	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.

All (2) 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)
1:B:67:VAL:HG11	1:B:73:ARG:NH1	2.34	0.43
1:A:1111:THR:HG21	1:A:1126:VAL:HG13	2.03	0.41

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	163/227 (72%)	155 (95%)	7 (4%)	1 (1%)	21	27
1	B	163/227 (72%)	155 (95%)	7 (4%)	1 (1%)	21	27
All	All	326/454 (72%)	310 (95%)	14 (4%)	2 (1%)	21	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	LEU
1	B	1031	LEU

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	133/174 (76%)	132 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	133/174 (76%)	132 (99%)	1 (1%)	73	86
All	All	266/348 (76%)	264 (99%)	2 (1%)	73	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1126	VAL
1	B	1142	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	A1H2Z	B	1201	-	23,30,30	1.14	3 (13%)	30,42,42	1.46	4 (13%)
2	A1H2Z	A	1201	-	23,30,30	1.13	3 (13%)	30,42,42	1.44	5 (16%)

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	A1H2Z	B	1201	-	-	1/17/22/22	0/3/3/3
2	A1H2Z	A	1201	-	-	2/17/22/22	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	A1H2Z	C2-N3	-2.53	1.34	1.38
2	A	1201	A1H2Z	C2-N3	-2.53	1.34	1.38
2	B	1201	A1H2Z	F26-C25	2.08	1.40	1.33
2	A	1201	A1H2Z	F26-C25	2.03	1.40	1.33
2	A	1201	A1H2Z	F27-C25	2.02	1.40	1.33
2	B	1201	A1H2Z	F27-C25	2.02	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	A1H2Z	C10-C9-C11	-3.64	107.14	111.73
2	A	1201	A1H2Z	C10-C9-C11	-3.37	107.48	111.73
2	B	1201	A1H2Z	O1-C2-N3	-2.88	119.48	125.65
2	A	1201	A1H2Z	O1-C2-N3	-2.78	119.68	125.65
2	A	1201	A1H2Z	C20-C21-C25	2.64	123.06	119.57
2	B	1201	A1H2Z	N18-C2-N3	2.64	116.00	111.22
2	A	1201	A1H2Z	N18-C2-N3	2.60	115.94	111.22
2	B	1201	A1H2Z	C12-C11-C9	-2.18	108.28	113.68
2	A	1201	A1H2Z	C12-C11-C9	-2.17	108.32	113.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

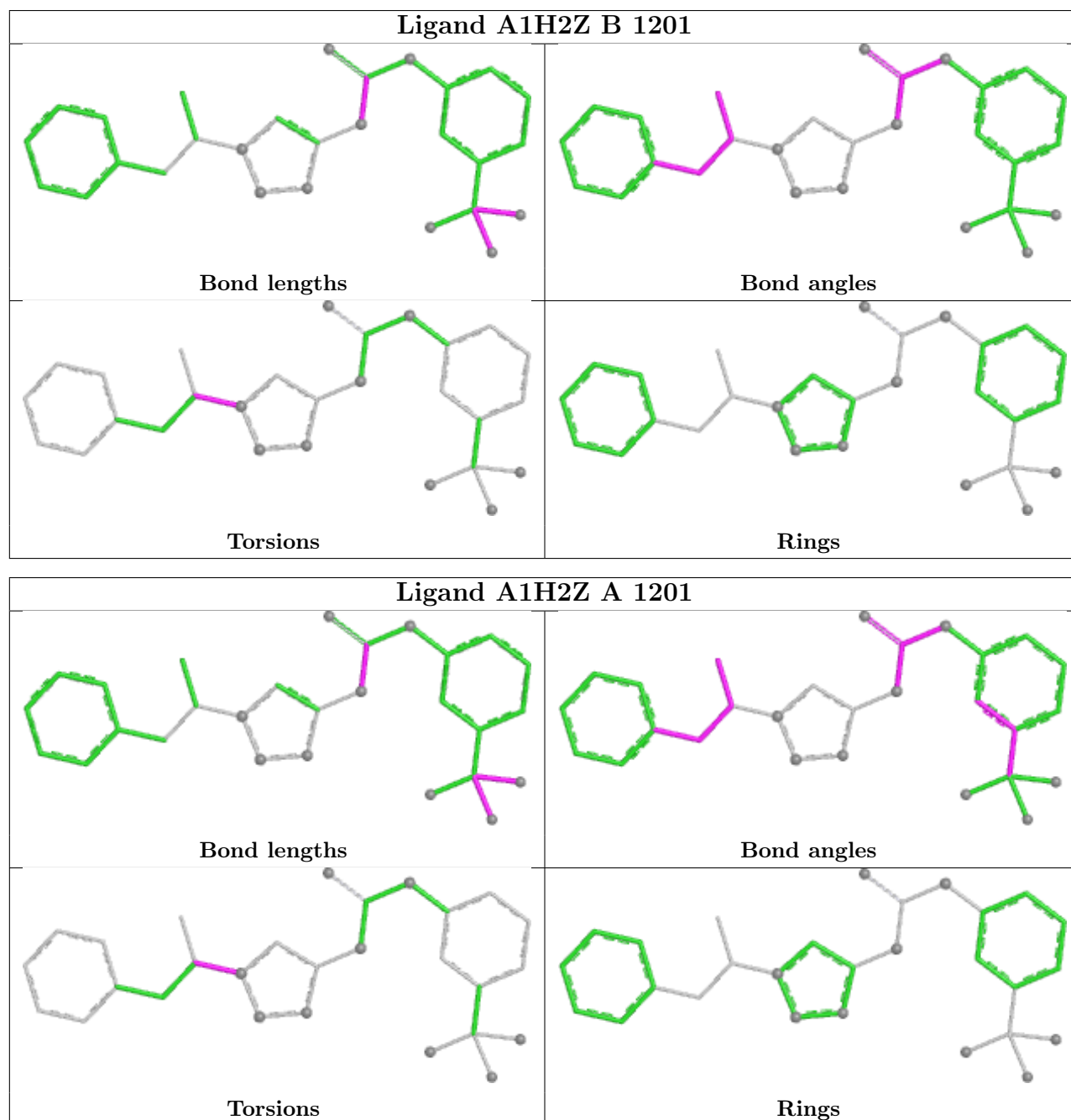
Mol	Chain	Res	Type	Atoms
2	A	1201	A1H2Z	C10-C9-N6-N7
2	B	1201	A1H2Z	C10-C9-N6-N7
2	A	1201	A1H2Z	C10-C9-N6-C5

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

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, 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	167/227 (73%)	1.02	29 (17%)	4 4	30, 53, 91, 117	11 (6%)
1	B	166/227 (73%)	1.02	22 (13%)	7 8	29, 53, 83, 102	9 (5%)
All	All	333/454 (73%)	1.02	51 (15%)	5 6	29, 53, 89, 117	20 (6%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	VAL	6.0
1	A	1031	LEU	5.9
1	A	1030	LEU	5.7
1	B	1018	THR	5.3
1	A	1032	GLY	4.9
1	B	1092[A]	HIS	4.9
1	A	1132	ALA	4.7
1	A	1018	THR	4.5
1	B	1062	GLU	4.5
1	B	76	VAL	4.3
1	B	1031	LEU	3.9
1	B	1061	GLY	3.9
1	A	1120	ASP	3.8
1	B	1064	ARG	3.8
1	A	1063	GLY	3.4
1	B	1132	ALA	3.2
1	A	1156	ILE	3.1
1	B	1118	THR	3.1
1	B	1029	GLY	2.9
1	B	1142	LYS	2.9
1	B	1030	LEU	2.8
1	B	1050	TRP	2.7
1	B	1143	CYS	2.7
1	A	1087	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1062	GLU	2.5
1	B	1086	ASP	2.5
1	B	1119	LYS	2.4
1	B	1063	GLY	2.4
1	A	1044	GLY	2.4
1	A	1157	LYS	2.4
1	A	1050	TRP	2.4
1	A	1152	ASN	2.4
1	A	50	ASP	2.3
1	A	67	VAL	2.3
1	A	1143	CYS	2.3
1	A	1123	ILE	2.3
1	B	1156	ILE	2.3
1	A	62	GLU	2.3
1	A	1034	THR	2.3
1	B	1123	ILE	2.2
1	A	1061	GLY	2.2
1	A	1019	THR	2.2
1	A	52	TYR	2.2
1	B	1093	SER	2.2
1	A	1092	HIS	2.2
1	A	1033	SER	2.2
1	A	1056	SER	2.2
1	A	1029	GLY	2.1
1	A	1145	ARG	2.1
1	B	1044	GLY	2.1
1	B	1032	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 [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,

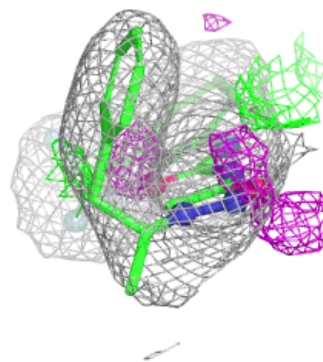
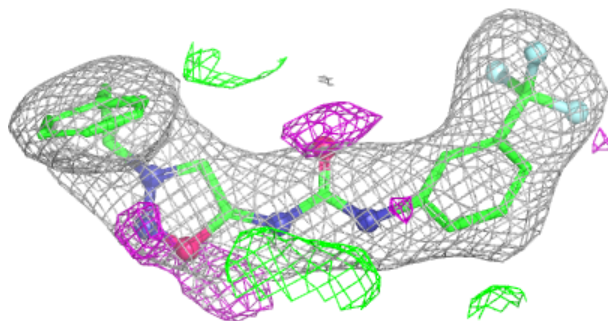
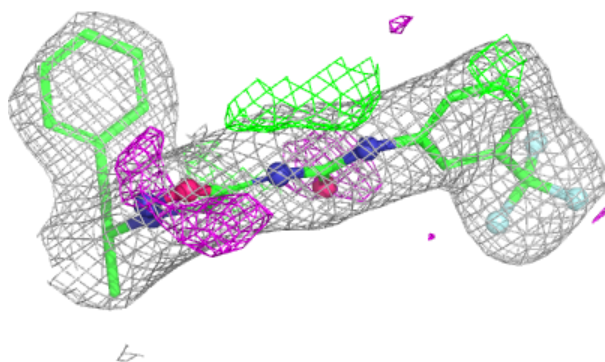
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1H2Z	A	1201	28/28	0.92	0.12	41,52,60,63	0
2	A1H2Z	B	1201	28/28	0.93	0.10	36,45,53,55	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.

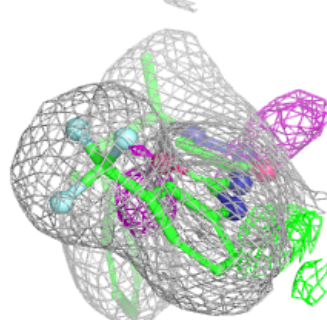
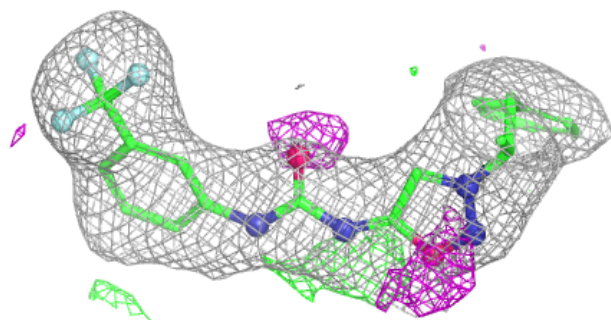
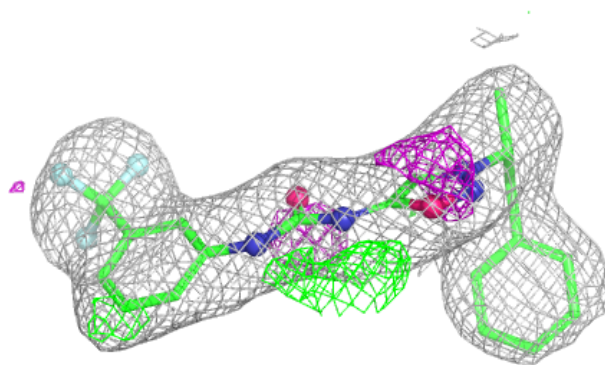
Electron density around A1H2Z A 1201:

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 A1H2Z 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.