



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:35 PM UTC

PDB ID : 5UPF / pdb_00005upf
Title : Crystal structure of human NAMPT with isoindoline urea inhibitor compound 53
Authors : Longenecker, K.L.; Raich, D.; Korepanova, A.V.
Deposited on : 2017-02-02
Resolution : 1.69 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

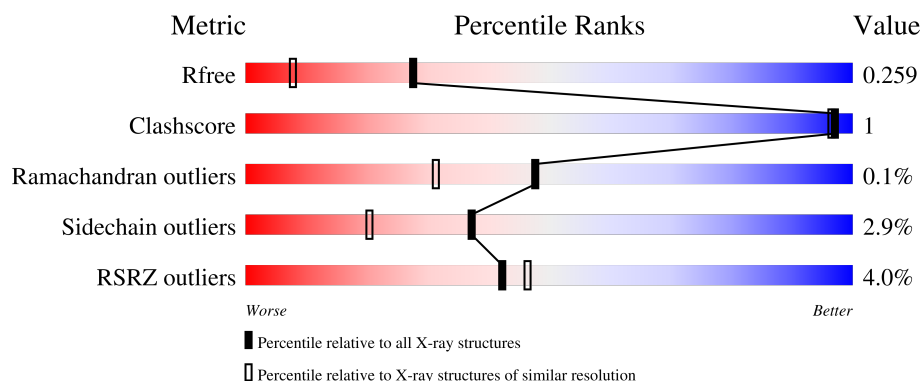
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

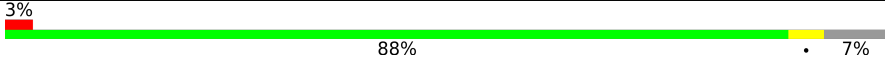
The reported resolution of this entry is 1.69 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	499	
1	B	499	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8261 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.

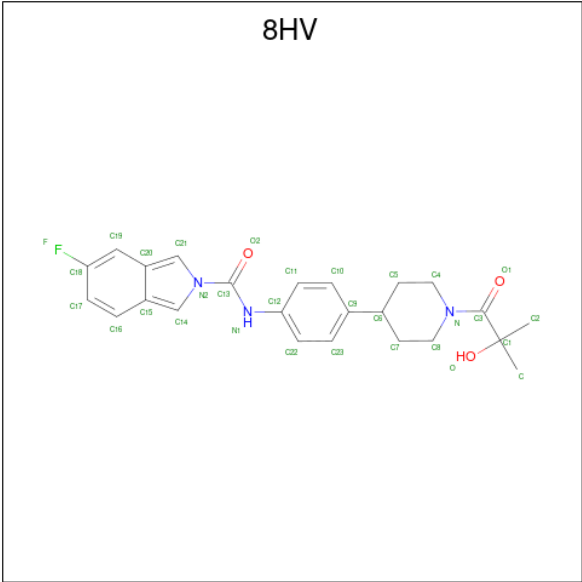
- Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	B	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	ASP	-	expression tag	UNP P43490
A	493	TYR	-	expression tag	UNP P43490
A	494	LYS	-	expression tag	UNP P43490
A	495	ASP	-	expression tag	UNP P43490
A	496	ASP	-	expression tag	UNP P43490
A	497	ASP	-	expression tag	UNP P43490
A	498	ASP	-	expression tag	UNP P43490
A	499	LYS	-	expression tag	UNP P43490
B	492	ASP	-	expression tag	UNP P43490
B	493	TYR	-	expression tag	UNP P43490
B	494	LYS	-	expression tag	UNP P43490
B	495	ASP	-	expression tag	UNP P43490
B	496	ASP	-	expression tag	UNP P43490
B	497	ASP	-	expression tag	UNP P43490
B	498	ASP	-	expression tag	UNP P43490
B	499	LYS	-	expression tag	UNP P43490

- Molecule 2 is 5-fluoro-N-{4-[1-(2-hydroxy-2-methylpropanoyl)piperidin-4-yl]phenyl}-2H-isoin-dole-2-carboxamide (CCD ID: 8HV) (formula: C₂₄H₂₆FN₃O₃).

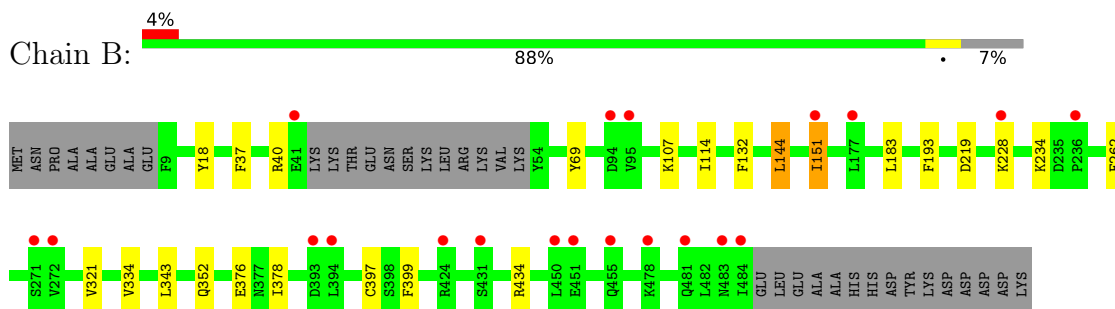


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	24	1	3	3		
2	B	1	Total	C	F	N	O	0	0
			31	24	1	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	395	Total	O	0	0
			395	395		
3	B	382	Total	O	0	0
			382	382		

- Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.10Å 106.58Å 83.34Å 90.00° 96.86° 90.00°	Depositor
Resolution (Å)	24.74 – 1.69 24.74 – 1.69	Depositor EDS
% Data completeness (in resolution range)	92.7 (24.74-1.69) 92.6 (24.74-1.69)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.69Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.215 , 0.241 (Not available) , 0.259	Depositor DCC
R_{free} test set	5497 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8261	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% 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: 8HV

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	0.83	0/3799	1.12	3/5149 (0.1%)
1	B	0.84	0/3799	1.12	6/5149 (0.1%)
All	All	0.84	0/7598	1.12	9/10298 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	262	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	193	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	192	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	399	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	399	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	132	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	40	ARG	CA-C-N	5.05	130.79	121.70
1	B	40	ARG	C-N-CA	5.05	130.79	121.70

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	3711	0	3686	7	0
1	B	3711	0	3686	7	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
3	A	395	0	0	0	0
3	B	382	0	0	0	0
All	All	8261	0	7372	14	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 (14) 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:343:LEU:HD13	1:B:376:GLU:HG3	1.78	0.66
1:A:343:LEU:HD13	1:A:376:GLU:HG3	1.77	0.64
1:A:323:LYS:HA	1:A:326:GLU:HG2	1.82	0.61
1:A:343:LEU:CD1	1:A:376:GLU:HG3	2.34	0.58
1:B:343:LEU:CD1	1:B:376:GLU:HG3	2.34	0.56
1:A:343:LEU:HD13	1:A:376:GLU:CG	2.41	0.50
1:B:343:LEU:HD13	1:B:376:GLU:CG	2.42	0.50
1:B:321:VAL:HG23	1:B:352:GLN:HE21	1.79	0.47
1:B:114:ILE:HG12	1:B:144:LEU:HD13	1.97	0.47
1:A:93:ASP:HB3	1:A:95:VAL:HG23	1.99	0.45
1:B:69:TYR:CD2	1:B:151:ILE:HD11	2.53	0.43
1:A:114:ILE:HG12	1:A:144:LEU:HD13	2.01	0.42
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.55	0.42
1:A:37:PHE:CZ	1:A:397:CYS:HB3	2.55	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	460/499 (92%)	448 (97%)	11 (2%)	1 (0%)	43	28
1	B	460/499 (92%)	450 (98%)	10 (2%)	0	100	100
All	All	920/998 (92%)	898 (98%)	21 (2%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	VAL

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	408/438 (93%)	395 (97%)	13 (3%)	34	17
1	B	408/438 (93%)	397 (97%)	11 (3%)	39	23
All	All	816/876 (93%)	792 (97%)	24 (3%)	37	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	93	ASP
1	A	95	VAL
1	A	107	LYS
1	A	144	LEU
1	A	151	ILE
1	A	183	LEU
1	A	219	ASP
1	A	228	LYS
1	A	378	ILE
1	A	434	ARG
1	A	455	GLN
1	A	484	ILE
1	B	18	TYR
1	B	107	LYS

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Mol	Chain	Res	Type
1	B	144	LEU
1	B	151	ILE
1	B	183	LEU
1	B	219	ASP
1	B	228	LYS
1	B	234	LYS
1	B	334	VAL
1	B	378	ILE
1	B	434	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	154	GLN
1	A	201	GLN
1	A	412	ASN
1	A	459	HIS
1	B	146	ASN
1	B	154	GLN
1	B	201	GLN
1	B	285	ASN
1	B	352	GLN
1	B	412	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

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	8HV	A	901	-	29,34,34	1.59	3 (10%)	40,50,50	1.41	5 (12%)
2	8HV	B	501	-	29,34,34	1.60	3 (10%)	40,50,50	1.49	5 (12%)

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	8HV	A	901	-	-	0/22/32/32	0/4/4/4
2	8HV	B	501	-	-	0/22/32/32	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	8HV	C14-N2	5.73	1.47	1.38
2	B	501	8HV	C21-N2	5.72	1.47	1.38
2	A	901	8HV	C21-N2	5.47	1.46	1.38
2	B	501	8HV	C14-N2	5.47	1.46	1.38
2	A	901	8HV	C13-N2	-2.72	1.36	1.41
2	B	501	8HV	C13-N2	-2.70	1.36	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	8HV	C20-C21-N2	-4.65	102.42	108.44
2	A	901	8HV	C20-C21-N2	-4.54	102.56	108.44
2	B	501	8HV	C15-C14-N2	-4.42	102.72	108.44
2	A	901	8HV	C15-C14-N2	-4.36	102.79	108.44
2	B	501	8HV	C21-N2-C14	4.01	113.26	108.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	8HV	C21-N2-C14	3.48	112.68	108.92
2	B	501	8HV	C15-C20-C19	-3.03	120.48	124.45
2	A	901	8HV	C15-C20-C19	-2.99	120.53	124.45
2	B	501	8HV	O1-C3-C1	-2.80	112.58	119.18
2	A	901	8HV	O1-C3-C1	-2.78	112.61	119.18

There are no chirality outliers.

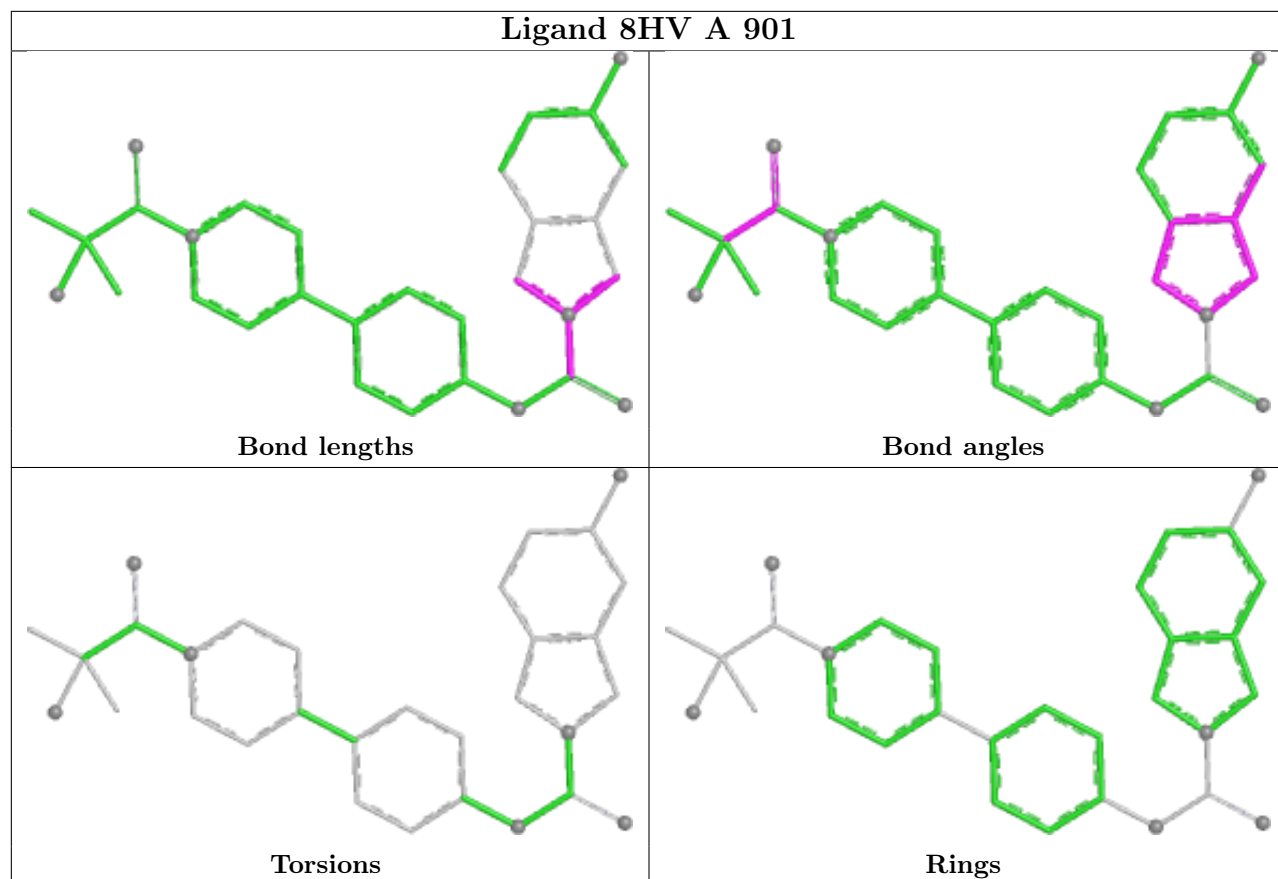
There are no torsion outliers.

There are no ring outliers.

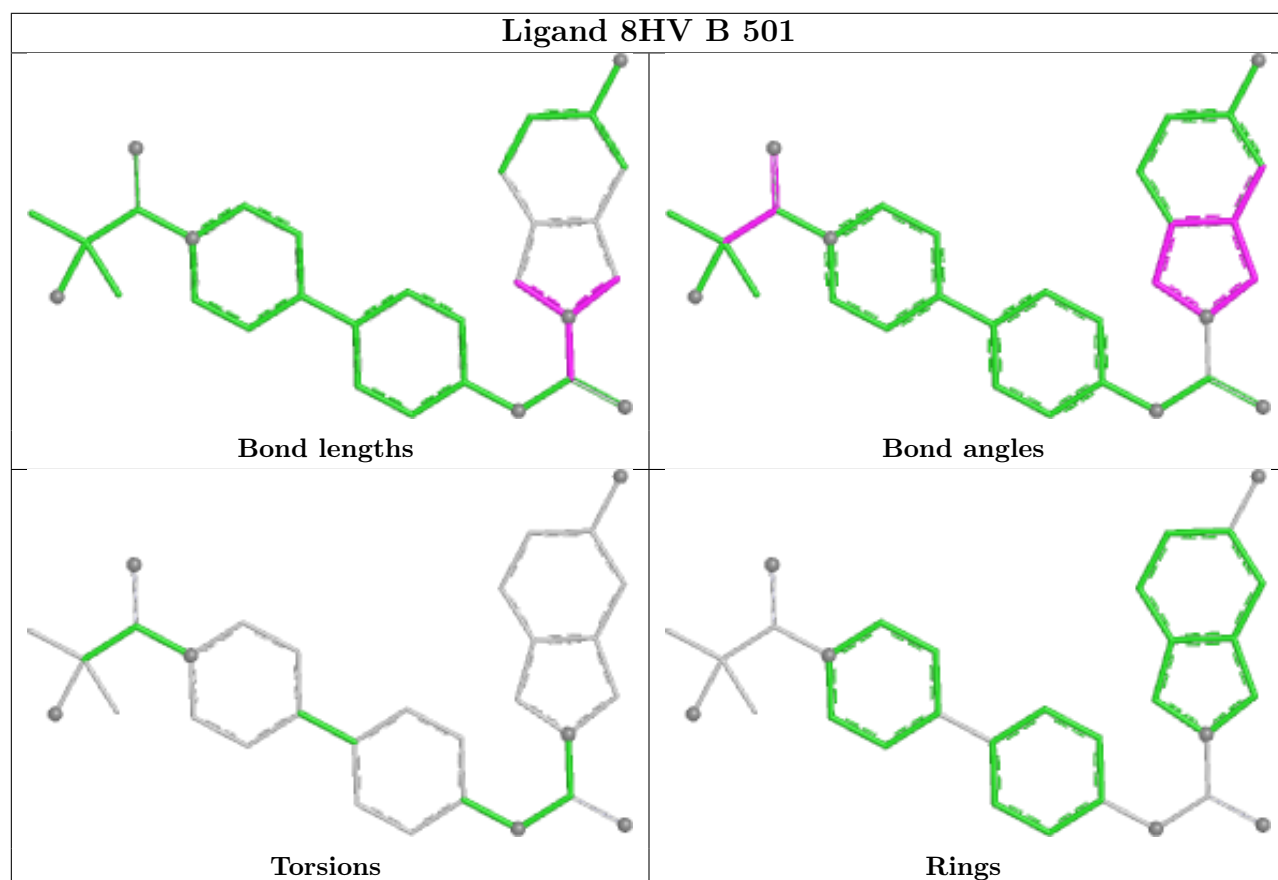
No monomer is involved in short contacts.

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 8HV A 901



Ligand 8HV B 501



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	464/499 (92%)	0.47	17 (3%) 45 49	11, 20, 36, 65	0
1	B	464/499 (92%)	0.46	20 (4%) 40 44	12, 20, 36, 77	0
All	All	928/998 (92%)	0.46	37 (3%) 42 46	11, 20, 37, 77	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	484	ILE	9.7
1	A	484	ILE	7.1
1	A	228	LYS	4.0
1	B	271	SER	3.8
1	B	450	LEU	3.5
1	A	94	ASP	3.3
1	B	41	GLU	3.2
1	A	450	LEU	3.1
1	A	95	VAL	2.9
1	A	108	TYR	2.9
1	B	228	LYS	2.8
1	A	459	HIS	2.7
1	B	451	GLU	2.7
1	A	107	LYS	2.6
1	B	151	ILE	2.6
1	B	478	LYS	2.6
1	B	483	ASN	2.6
1	A	438	GLY	2.5
1	A	93	ASP	2.5
1	B	94	ASP	2.5
1	B	177	LEU	2.5
1	A	236	PRO	2.5
1	A	483	ASN	2.4
1	B	424	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	334	VAL	2.4
1	A	467	VAL	2.4
1	B	236	PRO	2.4
1	B	95	VAL	2.4
1	B	455	GLN	2.3
1	B	393	ASP	2.3
1	A	393	ASP	2.3
1	A	271	SER	2.3
1	B	394	LEU	2.2
1	B	481	GLN	2.2
1	A	451	GLU	2.1
1	B	431	SER	2.1
1	B	272	VAL	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](#)

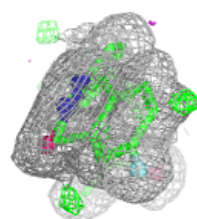
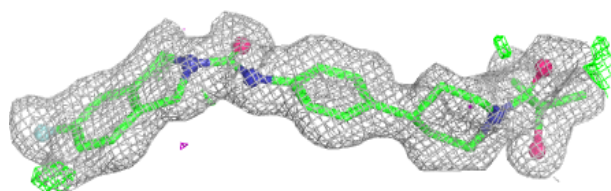
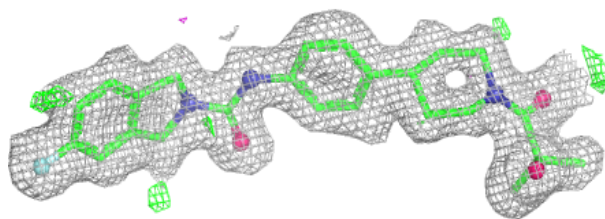
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	8HV	B	501	31/31	0.92	0.08	13,16,23,29	0
2	8HV	A	901	31/31	0.93	0.08	11,16,24,29	0

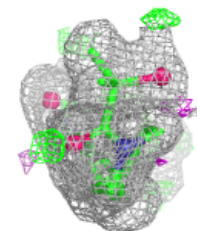
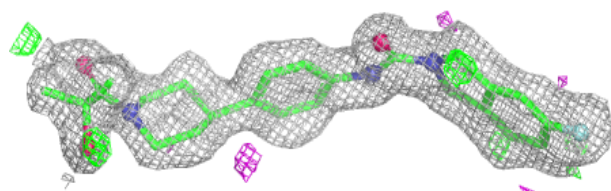
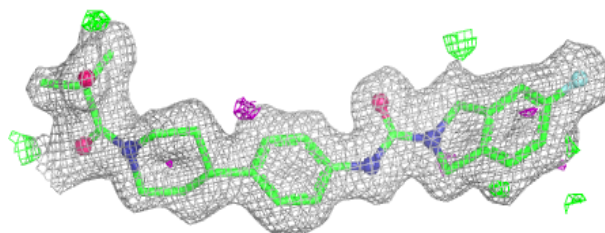
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8HV B 501:

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

**Electron density around 8HV A 901:**

$2mF_o-DF_c$ (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.