



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 6, 2021 – 12:04 pm BST

PDB ID : 6YKG
Title : Structure-based exploration of selectivity for ATM inhibitors in Huntingtons disease
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Deposited on : 2020-04-06
Resolution : 3.12 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

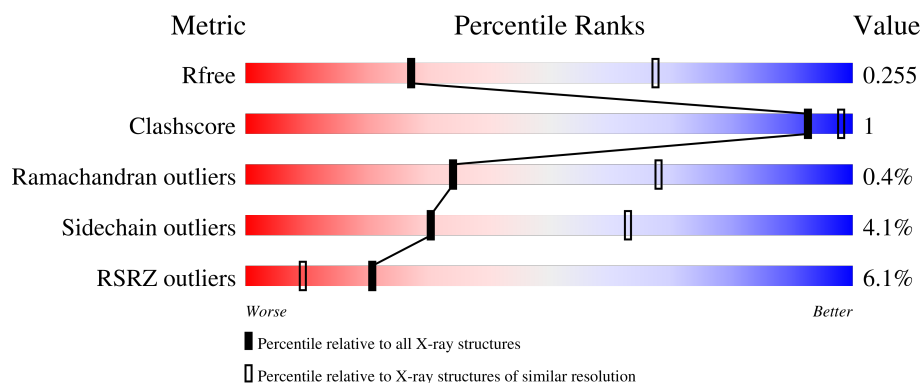
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	AAA	636	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8944 atoms, of which 4476 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 Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	559	8893	2828	4451	759	833	22	243	0	0

There are 29 discrepancies between the modelled and reference sequences:

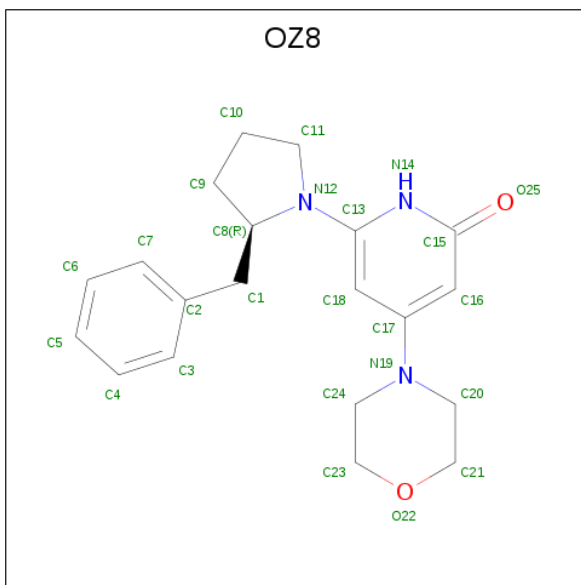
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	245	MET	-	initiating methionine	UNP Q8NEB9
AAA	246	HIS	-	expression tag	UNP Q8NEB9
AAA	247	HIS	-	expression tag	UNP Q8NEB9
AAA	248	HIS	-	expression tag	UNP Q8NEB9
AAA	249	HIS	-	expression tag	UNP Q8NEB9
AAA	250	HIS	-	expression tag	UNP Q8NEB9
AAA	251	HIS	-	expression tag	UNP Q8NEB9
AAA	252	SER	-	expression tag	UNP Q8NEB9
AAA	253	SER	-	expression tag	UNP Q8NEB9
AAA	254	GLY	-	expression tag	UNP Q8NEB9
AAA	255	VAL	-	expression tag	UNP Q8NEB9
AAA	256	ASP	-	expression tag	UNP Q8NEB9
AAA	257	LEU	-	expression tag	UNP Q8NEB9
AAA	258	GLY	-	expression tag	UNP Q8NEB9
AAA	259	THR	-	expression tag	UNP Q8NEB9
AAA	260	GLU	-	expression tag	UNP Q8NEB9
AAA	261	ASN	-	expression tag	UNP Q8NEB9
AAA	262	LEU	-	expression tag	UNP Q8NEB9
AAA	263	TYR	-	expression tag	UNP Q8NEB9
AAA	264	PHE	-	expression tag	UNP Q8NEB9
AAA	265	GLN	-	expression tag	UNP Q8NEB9
AAA	266	SER	-	expression tag	UNP Q8NEB9
AAA	267	MET	-	expression tag	UNP Q8NEB9
AAA	612	ALA	PHE	conflict	UNP Q8NEB9
AAA	616	ASN	LEU	conflict	UNP Q8NEB9
AAA	634	LEU	ILE	conflict	UNP Q8NEB9
AAA	682	LEU	MET	conflict	UNP Q8NEB9

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	684	TRP	PHE	conflict	UNP Q8NEB9
AAA	687	GLY	-	insertion	UNP Q8NEB9

- Molecule 2 is 4-morpholin-4-yl-6-[(2 {R})-2-(phenylmethyl)pyrrolidin-1-yl]-1 {H}-pyridin-2-one (three-letter code: OZ8) (formula: C₂₀H₂₅N₃O₂) (labeled as "Ligand of Interest" by depositor).

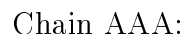


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	0	0
			50	20	25	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	O	0	0
			1	1		

- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.86Å 168.12Å 61.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.12 49.73 – 3.12	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.73-3.12) 99.8 (49.73-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.261 0.215 , 0.255	Depositor DCC
R_{free} test set	815 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8944	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OZ8

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	AAA	0.53	0/4530	0.68	1/6139 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	280	GLY	C-N-CD	-5.43	108.65	120.60

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	AAA	4442	4451	4393	13	0
2	AAA	25	25	0	0	0
3	AAA	1	0	0	0	0
All	All	4468	4476	4393	13	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 (13) 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:AAA:555:LEU:HD21	1:AAA:573:LEU:HD12	1.84	0.59
1:AAA:360:VAL:HG11	1:AAA:387:ALA:HB2	1.86	0.58
1:AAA:415:LEU:HA	1:AAA:526:GLN:HE22	1.79	0.48
1:AAA:672:VAL:HG13	1:AAA:682:LEU:HD23	1.98	0.45
1:AAA:580:ASN:OD1	1:AAA:586:SER:N	2.50	0.44
1:AAA:742:VAL:HG12	1:AAA:745:ARG:HD3	1.98	0.44
1:AAA:750:LEU:HD23	1:AAA:758:LEU:HD11	2.00	0.43
1:AAA:398:GLN:HB3	1:AAA:823:LEU:HD12	2.01	0.42
1:AAA:695:LEU:HD11	1:AAA:783:GLU:HG3	2.02	0.42
1:AAA:503:ASP:HA	1:AAA:677:THR:HG21	2.02	0.41
1:AAA:767:LEU:HD13	1:AAA:839:THR:HG23	2.02	0.41
1:AAA:737:THR:HG21	1:AAA:760:HIS:CE1	2.57	0.40
1:AAA:308:LEU:HD21	1:AAA:332:LYS:HD2	2.04	0.40

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	AAA	553/636 (87%)	535 (97%)	16 (3%)	2 (0%)	34 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	279	SER
1	AAA	626	GLU

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	AAA	482/573 (84%)	462 (96%)	20 (4%)	30	63

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	286	LEU
1	AAA	294	ASP
1	AAA	305	THR
1	AAA	328	LYS
1	AAA	355	TRP
1	AAA	375	THR
1	AAA	388	ASP
1	AAA	474	ASP
1	AAA	512	LYS
1	AAA	534	SER
1	AAA	540	SER
1	AAA	551	ARG
1	AAA	562	GLU
1	AAA	563	SER
1	AAA	567	LYS
1	AAA	584	ASN
1	AAA	591	ILE
1	AAA	634	LEU
1	AAA	804	TYR
1	AAA	841	LYS

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

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	OZ8	AAA	901	-	26,28,28	0.41	0	33,38,38	1.52	6 (18%)

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	OZ8	AAA	901	-	-	5/12/30/30	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	901	OZ8	C24-N19-C20	3.84	120.00	111.52
2	AAA	901	OZ8	N14-C13-N12	3.55	120.52	116.57
2	AAA	901	OZ8	C18-C13-N12	-2.98	118.80	122.31
2	AAA	901	OZ8	C16-C15-N14	-2.88	120.72	124.08
2	AAA	901	OZ8	C11-N12-C13	-2.44	119.67	123.46
2	AAA	901	OZ8	C9-C8-C1	-2.31	110.46	113.97

There are no chirality outliers.

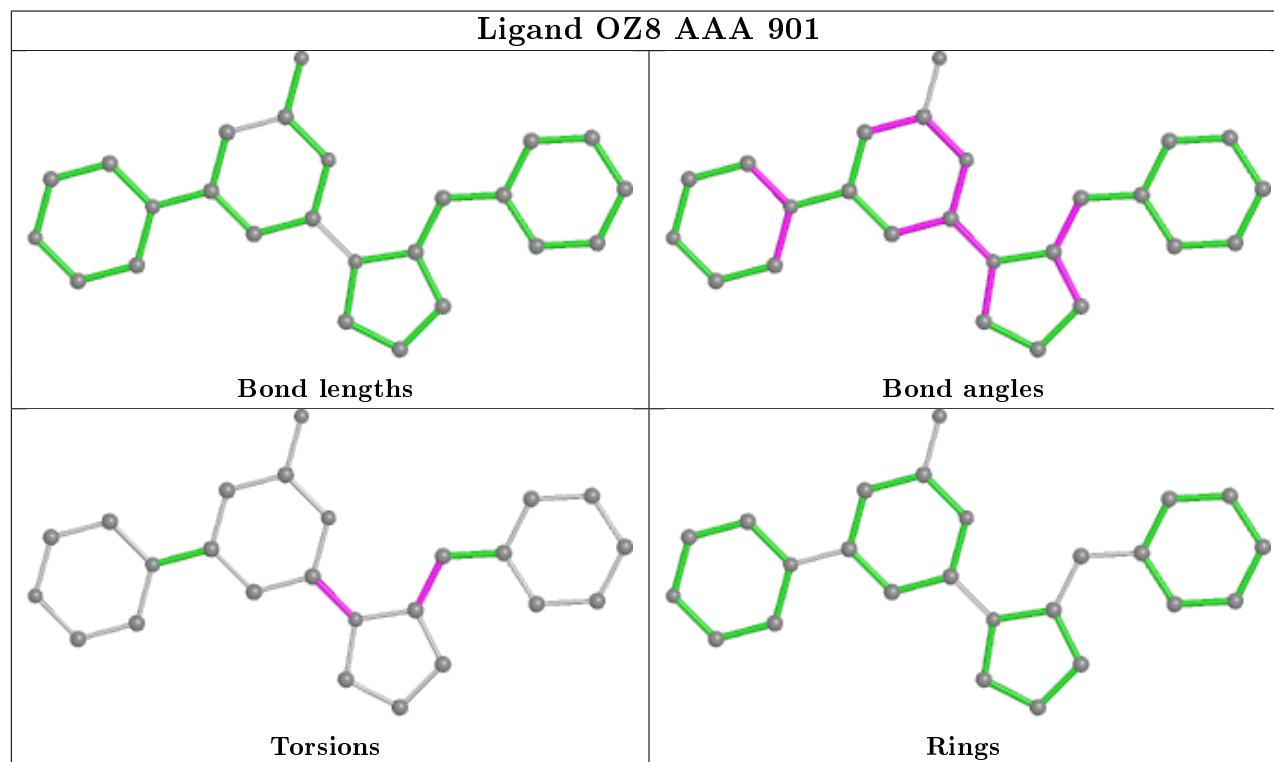
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	901	OZ8	C2-C1-C8-C9
2	AAA	901	OZ8	C2-C1-C8-N12
2	AAA	901	OZ8	N14-C13-N12-C8
2	AAA	901	OZ8	C18-C13-N12-C8
2	AAA	901	OZ8	C18-C13-N12-C11

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

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, 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	AAA	559/636 (87%)	0.42	34 (6%) 21 9	32, 57, 102, 141	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	300	VAL	5.2
1	AAA	280	GLY	3.9
1	AAA	352	LEU	3.7
1	AAA	281	PRO	3.5
1	AAA	308	LEU	3.4
1	AAA	347	GLN	3.2
1	AAA	349	LEU	2.8
1	AAA	325	ASN	2.8
1	AAA	357	PRO	2.7
1	AAA	356	LYS	2.7
1	AAA	611	LEU	2.6
1	AAA	335	LYS	2.5
1	AAA	296	LEU	2.5
1	AAA	285	ASP	2.5
1	AAA	697	THR	2.5
1	AAA	565	ASN	2.4
1	AAA	306	LYS	2.4
1	AAA	353	GLY	2.4
1	AAA	576	LEU	2.4
1	AAA	309	THR	2.2
1	AAA	561	ARG	2.2
1	AAA	297	ASN	2.2
1	AAA	351	LEU	2.2
1	AAA	305	THR	2.2
1	AAA	336	CYS	2.2
1	AAA	386	GLN	2.2
1	AAA	320	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	339	TRP	2.1
1	AAA	350	GLU	2.1
1	AAA	355	TRP	2.0
1	AAA	294	ASP	2.0
1	AAA	617	MET	2.0
1	AAA	699	GLY	2.0
1	AAA	566	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

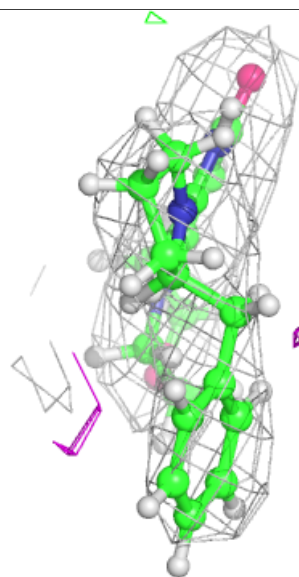
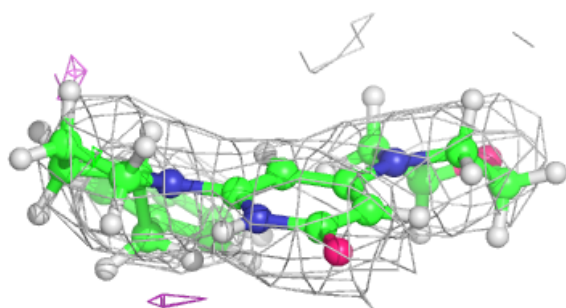
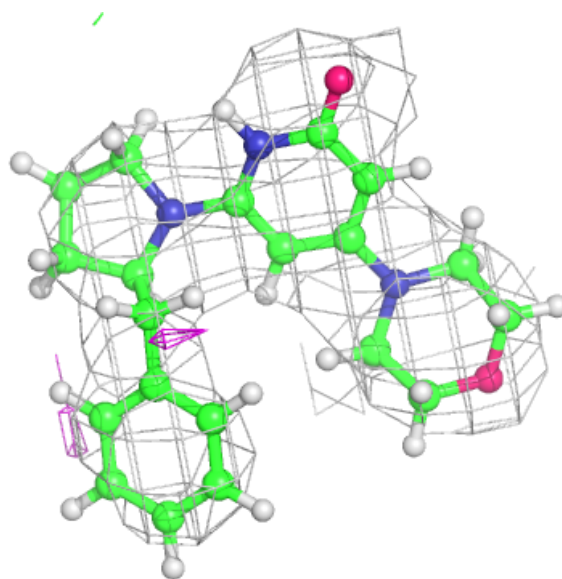
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OZ8	AAA	901	25/25	0.94	0.30	43,44,46,46	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 OZ8 AAA 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 ⓘ

There are no such residues in this entry.