



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:33 pm BST

PDB ID : 5W86  
Title : CRYSTAL STRUCTURE OF JAK3 KINASE DOMAIN WITH A 4,6-DIAMINONICOTINAMIDE INHIBITOR (COMPOUND NUMBER 7)  
Authors : Sack, J.S.  
Deposited on : 2017-06-21  
Resolution : 2.61 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.

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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 : 2.11  
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) : 2.11

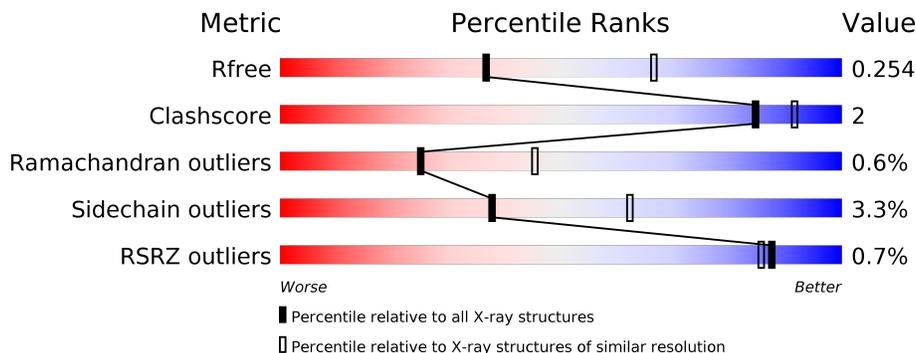
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 on 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	287	
1	B	287	
1	C	287	
1	D	287	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8915 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 Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	271	2126	1358	358	394	2	14	0	1	0
1	B	269	2116	1351	355	394	2	14	0	0	0
1	C	275	2186	1396	374	400	2	14	0	0	0
1	D	274	2196	1401	374	405	2	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	SER	CYS	engineered mutation	UNP P52333
A	1048	SER	CYS	engineered mutation	UNP P52333
B	1040	SER	CYS	engineered mutation	UNP P52333
B	1048	SER	CYS	engineered mutation	UNP P52333
C	1040	SER	CYS	engineered mutation	UNP P52333
C	1048	SER	CYS	engineered mutation	UNP P52333
D	1040	SER	CYS	engineered mutation	UNP P52333
D	1048	SER	CYS	engineered mutation	UNP P52333

- Molecule 2 is 4-(benzylamino)-6-({4-[(1-methylpiperidin-4-yl)carbamoyl]phenyl}amino)pyridine-3-carboxamide (three-letter code: 9YV) (formula: C<sub>26</sub>H<sub>30</sub>N<sub>6</sub>O<sub>2</sub>).



### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

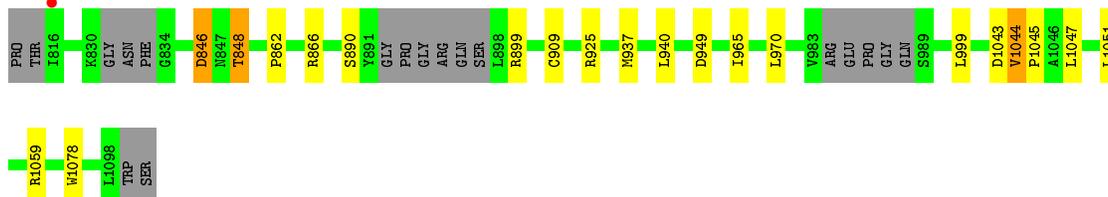
- Molecule 1: Tyrosine-protein kinase JAK3

Chain A: 



- Molecule 1: Tyrosine-protein kinase JAK3

Chain B: 



- Molecule 1: Tyrosine-protein kinase JAK3

Chain C: 



- Molecule 1: Tyrosine-protein kinase JAK3

Chain D: 



E1019	Y1023	E1033	F1034	L1035	R1036	E1041	L1047	L1051	E1055	H1071	K1075	P1082	S1089	L1095	D1096	W1099	SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.98Å 112.30Å 97.12Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	56.98 – 2.61 56.15 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.0 (56.98-2.61) 97.8 (56.15-2.61)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.209 , 0.264 0.221 , 0.254	Depositor DCC
$R_{free}$ test set	1824 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 19.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.400 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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 45.85 % 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 1.2451e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 9YV, PTR

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	0.52	0/2139	0.71	0/2895
1	B	0.53	0/2128	0.70	0/2879
1	C	0.51	0/2203	0.69	0/2978
1	D	0.50	0/2212	0.71	0/2988
All	All	0.52	0/8682	0.70	0/11740

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	2126	0	2065	4	0
1	B	2116	0	2056	12	0
1	C	2186	0	2144	10	0
1	D	2196	0	2157	14	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
2	C	34	0	0	1	0
2	D	34	0	0	0	0
3	A	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	0	0	0
3	C	40	0	0	0	0
3	D	44	0	0	0	0
All	All	8915	0	8422	40	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 2.

All (40) 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:D:1071:HIS:CE1	1:D:1075:LYS:HE2	1.90	1.05
1:C:817:PHE:HB3	1:C:822:LEU:HD11	1.60	0.83
1:B:862:PRO:HB2	1:B:866:ARG:HH21	1.49	0.77
1:D:1033:GLU:OE1	1:D:1036:ARG:NH2	2.23	0.71
1:B:937:MET:CE	1:B:965:ILE:HD13	2.20	0.71
1:D:927:LEU:HD11	1:D:1095:LEU:O	1.94	0.67
1:B:937:MET:HE3	1:B:965:ILE:HD13	1.77	0.66
1:B:846:ASP:HB3	1:B:848:THR:HB	1.78	0.66
1:B:890:SER:HB3	1:B:899:ARG:HB2	1.78	0.66
1:C:884:VAL:HG11	2:C:4000:9YV:N26	2.12	0.65
1:D:1007:GLN:HG3	1:D:1082:PRO:O	2.01	0.61
1:C:1034:PHE:HB3	1:C:1038:MET:HE3	1.85	0.58
1:D:1051:LEU:O	1:D:1055:GLU:HG3	2.06	0.56
1:A:927:LEU:HD11	1:A:1095:LEU:O	2.06	0.56
1:C:1034:PHE:O	1:C:1038:MET:HG2	2.05	0.56
1:B:937:MET:HE2	1:B:965:ILE:HD13	1.89	0.52
1:B:1044:VAL:HG22	1:B:1045:PRO:HD2	1.93	0.51
1:D:1096:ASP:O	1:D:1099:TRP:NE1	2.44	0.50
1:D:1015:VAL:O	1:D:1019:GLU:HG3	2.11	0.50
1:D:949:ASP:HB2	1:D:970:LEU:HD12	1.93	0.49
1:D:1096:ASP:O	1:D:1099:TRP:CD1	2.66	0.49
1:C:949:ASP:HB2	1:C:970:LEU:HD12	1.95	0.48
1:B:949:ASP:HB2	1:B:970:LEU:HD12	1.95	0.48
1:D:990:PRO:HG2	1:D:994:TYR:CE1	2.50	0.47
1:A:949:ASP:HB2	1:A:970:LEU:HD12	1.96	0.47
1:B:925:ARG:HA	1:B:925:ARG:HD3	1.75	0.46
1:C:883:ILE:HD11	1:C:940:LEU:HD13	1.99	0.45
1:D:1033:GLU:OE2	1:D:1036:ARG:NH1	2.50	0.45
1:C:1000:SER:HB3	1:C:1051:LEU:HD21	1.97	0.45
1:D:890:SER:HB3	1:D:899:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:GLN:HB3	1:A:899:ARG:HG2	1.99	0.44
1:B:999:LEU:HB2	1:B:1051:LEU:HD13	2.00	0.44
1:A:890:SER:HB3	1:A:899:ARG:HB2	2.00	0.44
1:C:1038:MET:HB2	1:C:1049:ARG:CG	2.48	0.44
1:C:856:GLN:HB3	1:C:899:ARG:HG2	2.00	0.43
1:D:918:ARG:HG3	1:D:1023:TYR:CG	2.54	0.43
1:C:1022:THR:HG23	1:C:1063:PRO:HB3	2.00	0.43
1:D:857:LEU:HD11	1:D:868:PHE:HB2	2.02	0.41
1:B:1059:ARG:HE	1:B:1078:TRP:HB3	1.86	0.41
1:B:862:PRO:HB2	1:B:866:ARG:NH2	2.27	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	A	261/287 (91%)	249 (95%)	9 (3%)	3 (1%)	14	27
1	B	259/287 (90%)	250 (96%)	8 (3%)	1 (0%)	34	55
1	C	267/287 (93%)	260 (97%)	6 (2%)	1 (0%)	34	55
1	D	264/287 (92%)	253 (96%)	10 (4%)	1 (0%)	34	55
All	All	1051/1148 (92%)	1012 (96%)	33 (3%)	6 (1%)	25	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	860	SER
1	A	1042	ARG
1	B	1043	ASP
1	A	862	PRO
1	C	1043	ASP

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Mol	Chain	Res	Type
1	D	845	GLY

### 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	224/249 (90%)	219 (98%)	5 (2%)	52	74
1	B	224/249 (90%)	218 (97%)	6 (3%)	44	69
1	C	232/249 (93%)	224 (97%)	8 (3%)	37	61
1	D	236/249 (95%)	225 (95%)	11 (5%)	26	49
All	All	916/996 (92%)	886 (97%)	30 (3%)	38	62

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	869	GLN
1	A	927	LEU
1	A	940	LEU
1	A	1053	LEU
1	A	1069	GLU
1	B	846	ASP
1	B	848	THR
1	B	909	CYS
1	B	940	LEU
1	B	1044	VAL
1	B	1047	LEU
1	C	869	GLN
1	C	940	LEU
1	C	997	GLU
1	C	1007	GLN
1	C	1044	VAL
1	C	1047	LEU
1	C	1053	LEU
1	C	1099	TRP
1	D	844	LEU

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Mol	Chain	Res	Type
1	D	863	ASP
1	D	869	GLN
1	D	870	ARG
1	D	875	LEU
1	D	927	LEU
1	D	940	LEU
1	D	1035	LEU
1	D	1041	GLU
1	D	1047	LEU
1	D	1089	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1007	GLN
1	D	1071	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](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PTR	D	981	1	15,16,17	0.63	0	19,22,24	0.93	0
1	PTR	A	981	1	15,16,17	0.70	0	19,22,24	0.84	1 (5%)
1	PTR	C	981	1	15,16,17	0.55	0	19,22,24	0.68	0
1	PTR	D	980	1	15,16,17	0.64	0	19,22,24	0.71	1 (5%)
1	PTR	C	980	1	15,16,17	0.75	0	19,22,24	0.37	0
1	PTR	B	980	1	15,16,17	0.62	0	19,22,24	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PTR	A	980	1	15,16,17	0.59	0	19,22,24	0.72	1 (5%)
1	PTR	B	981	1	15,16,17	0.60	0	19,22,24	0.77	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
1	PTR	D	981	1	-	0/10/11/13	0/1/1/1
1	PTR	A	981	1	-	0/10/11/13	0/1/1/1
1	PTR	C	981	1	-	1/10/11/13	0/1/1/1
1	PTR	D	980	1	-	0/10/11/13	0/1/1/1
1	PTR	C	980	1	-	0/10/11/13	0/1/1/1
1	PTR	B	980	1	-	0/10/11/13	0/1/1/1
1	PTR	A	980	1	-	0/10/11/13	0/1/1/1
1	PTR	B	981	1	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	980	PTR	O2P-P-OH	2.50	113.07	105.24
1	D	980	PTR	O2P-P-OH	2.18	112.06	105.24
1	A	981	PTR	O2P-P-OH	2.03	111.60	105.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	981	PTR	CZ-OH-P-O1P
1	B	981	PTR	CZ-OH-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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	9YV	B	4000	-	37,37,37	0.39	0	48,50,50	0.59	1 (2%)
2	9YV	D	4000	-	37,37,37	0.32	0	48,50,50	0.81	1 (2%)
2	9YV	A	4000	-	37,37,37	0.39	0	48,50,50	0.80	1 (2%)
2	9YV	C	4000	-	37,37,37	0.35	0	48,50,50	0.53	1 (2%)

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	9YV	B	4000	-	-	2/21/31/31	0/4/4/4
2	9YV	D	4000	-	-	0/21/31/31	0/4/4/4
2	9YV	A	4000	-	-	0/21/31/31	0/4/4/4
2	9YV	C	4000	-	-	0/21/31/31	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	4000	9YV	C6-C1-C8	4.51	124.63	121.72
2	A	4000	9YV	C6-C1-C8	4.40	124.56	121.72
2	B	4000	9YV	C6-C1-C8	2.54	123.36	121.72
2	C	4000	9YV	C6-C1-C8	2.24	123.17	121.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

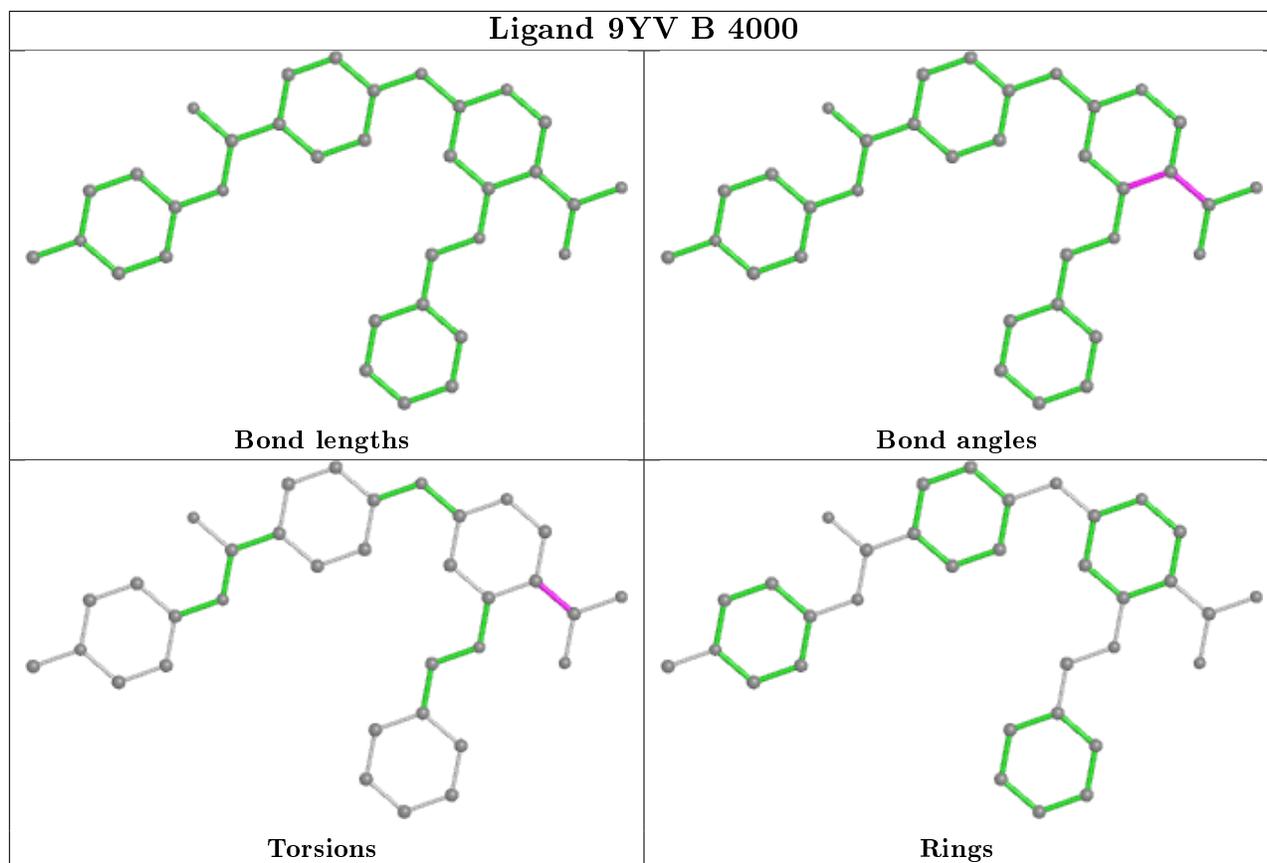
Mol	Chain	Res	Type	Atoms
2	B	4000	9YV	C6-C1-C8-N26
2	B	4000	9YV	C6-C1-C8-O27

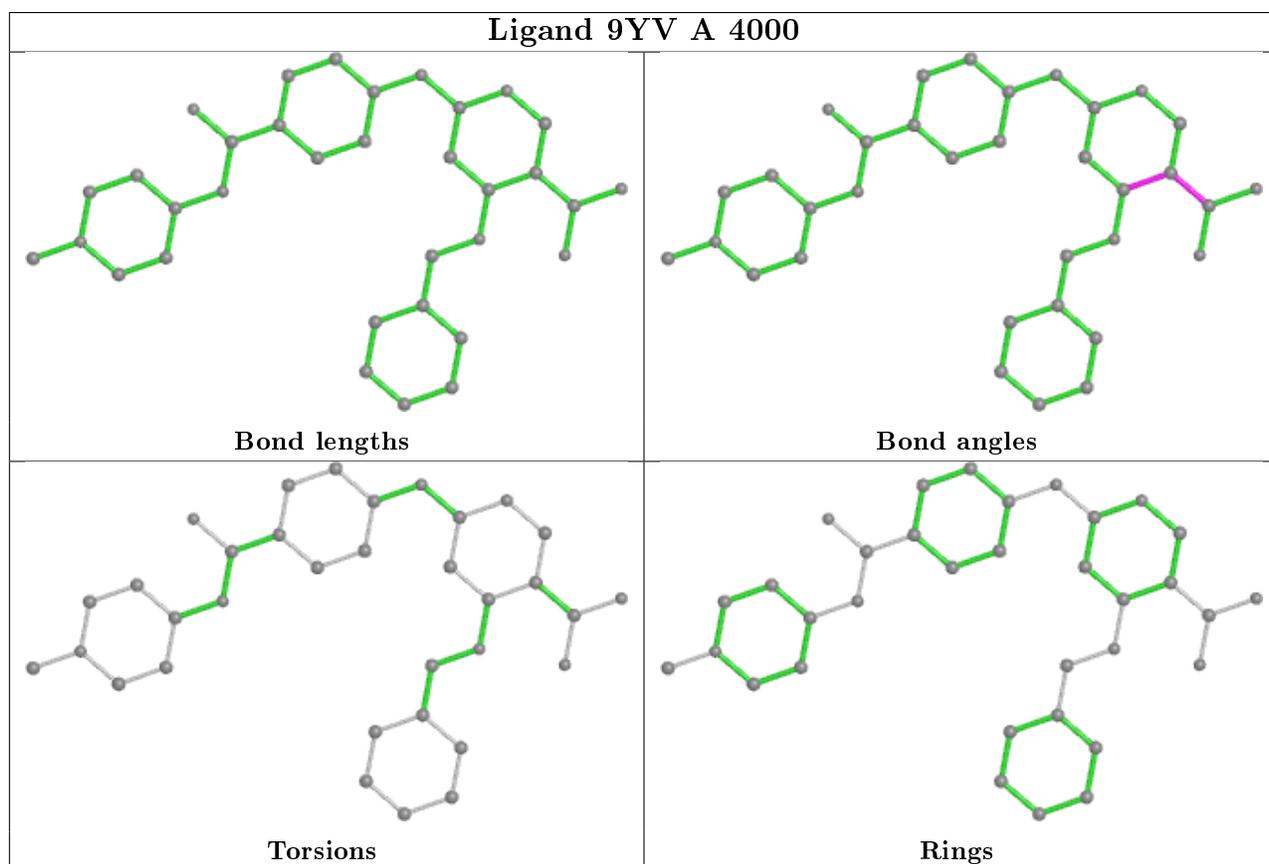
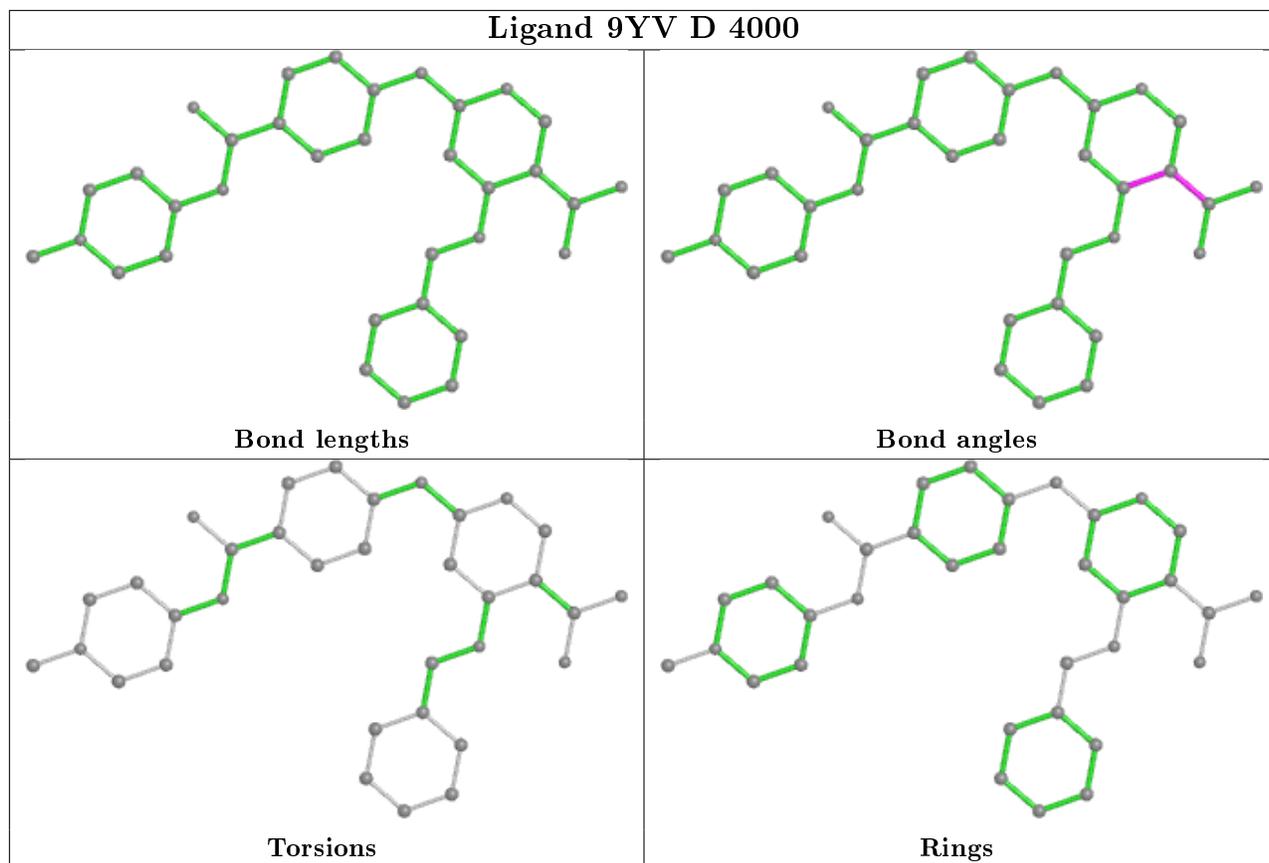
There are no ring outliers.

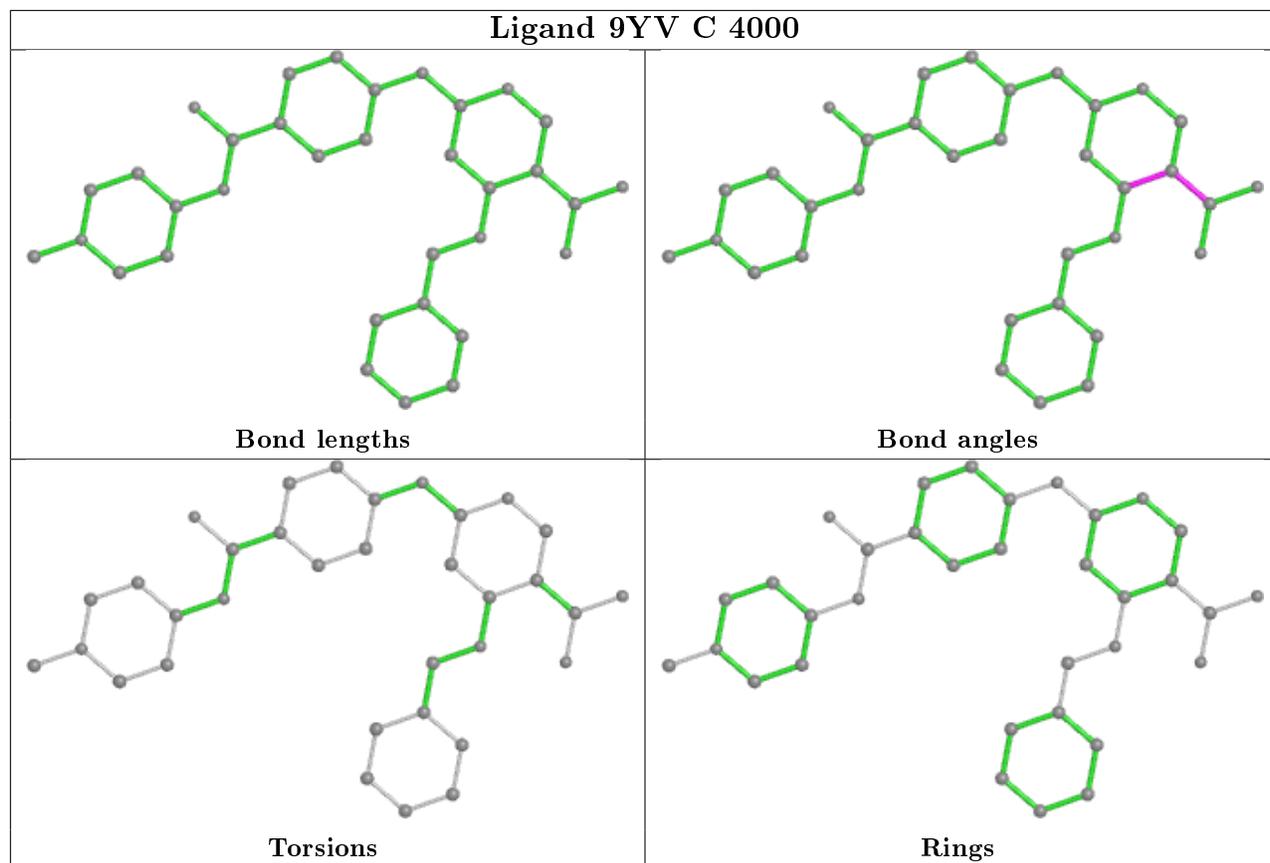
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4000	9YV	1	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 [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, 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	269/287 (93%)	-0.35	0 <b>100</b>   <b>100</b>	5, 27, 50, 64	13 (4%)
1	B	267/287 (93%)	-0.28	1 (0%) <b>92</b>   <b>91</b>	11, 30, 49, 67	3 (1%)
1	C	273/287 (95%)	-0.19	3 (1%) <b>80</b>   <b>78</b>	11, 30, 54, 75	6 (2%)
1	D	272/287 (94%)	-0.15	4 (1%) <b>73</b>   <b>70</b>	7, 28, 52, 76	6 (2%)
All	All	1081/1148 (94%)	-0.24	8 (0%) <b>87</b>   <b>85</b>	5, 29, 52, 76	28 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	834	GLY	2.9
1	C	815	THR	2.8
1	D	832	ASN	2.7
1	C	814	PRO	2.6
1	B	816	ILE	2.3
1	D	831	GLY	2.2
1	D	861	GLY	2.1
1	C	859	HIS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	PTR	B	980	16/17	0.82	0.20	38,42,43,44	4
1	PTR	C	980	16/17	0.86	0.23	36,42,43,44	4
1	PTR	D	980	16/17	0.88	0.18	25,27,31,31	4
1	PTR	A	980	16/17	0.89	0.20	23,27,29,30	4

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PTR	D	981	16/17	0.91	0.22	9,12,25,25	12
1	PTR	A	981	16/17	0.93	0.19	12,15,21,23	12
1	PTR	B	981	16/17	0.94	0.18	26,31,39,41	12
1	PTR	C	981	16/17	0.95	0.16	28,30,36,38	12

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

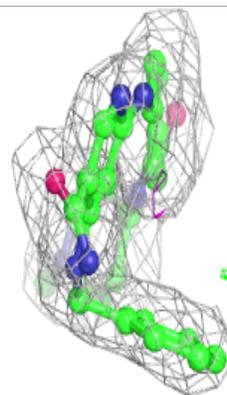
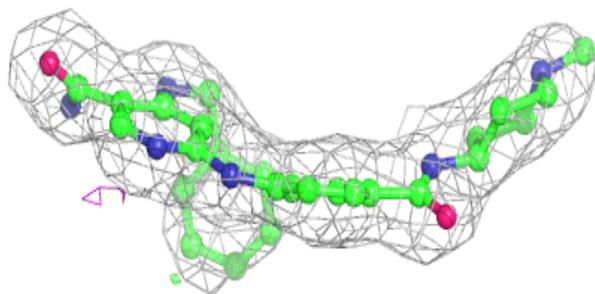
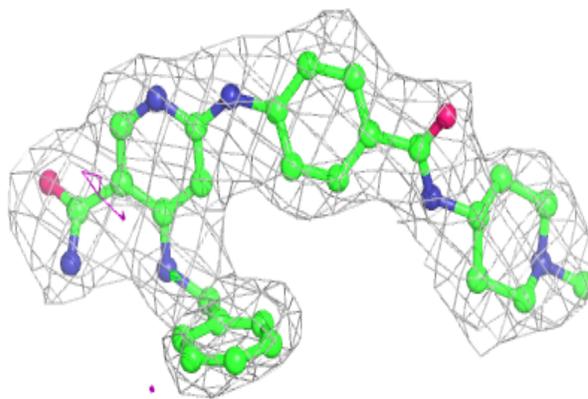
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	9YV	B	4000	34/34	0.94	0.14	10,20,40,44	0
2	9YV	D	4000	34/34	0.94	0.18	14,24,61,63	0
2	9YV	A	4000	34/34	0.95	0.15	7,15,53,54	0
2	9YV	C	4000	34/34	0.95	0.17	12,19,48,49	0

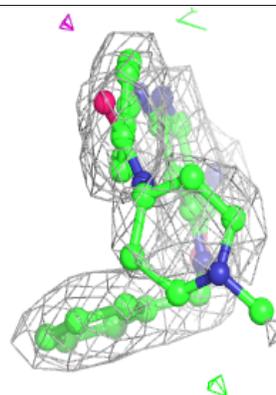
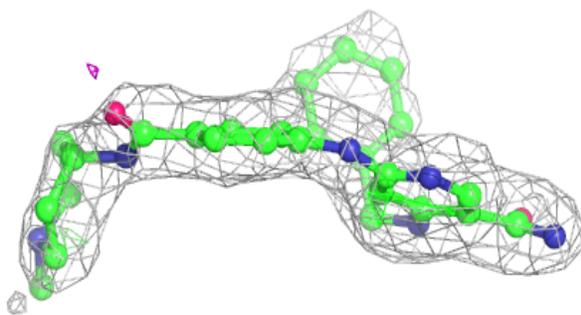
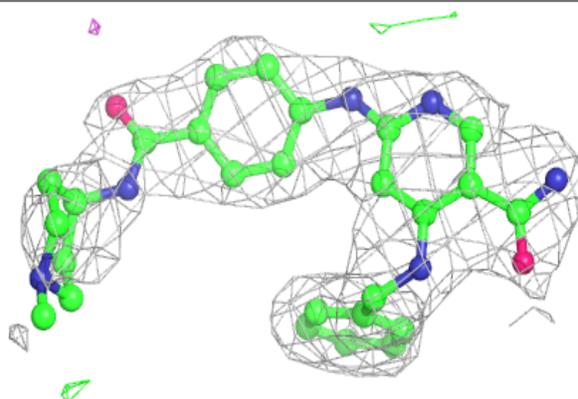
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 9YV B 4000:**

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

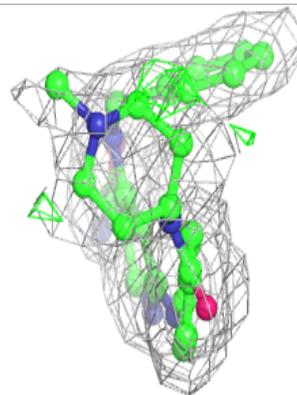
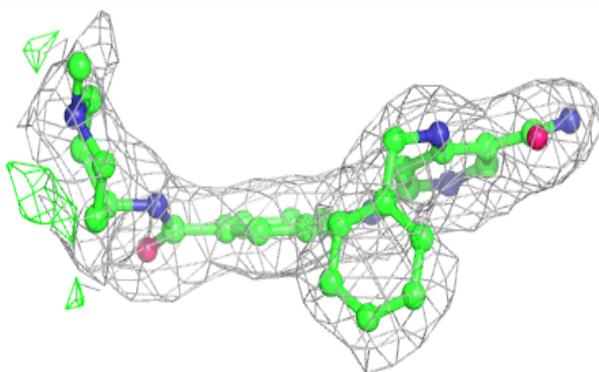
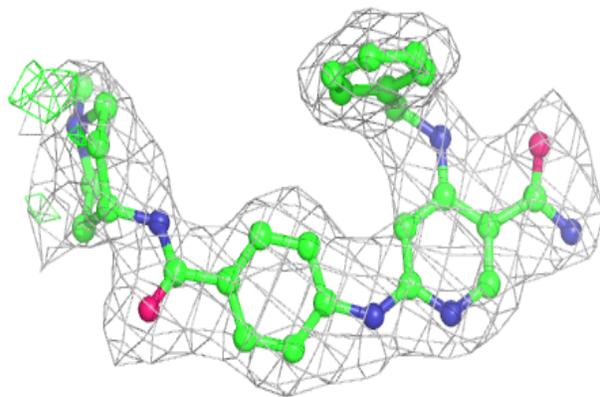
**Electron density around 9YV D 4000:**

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

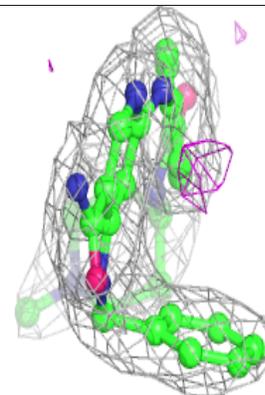
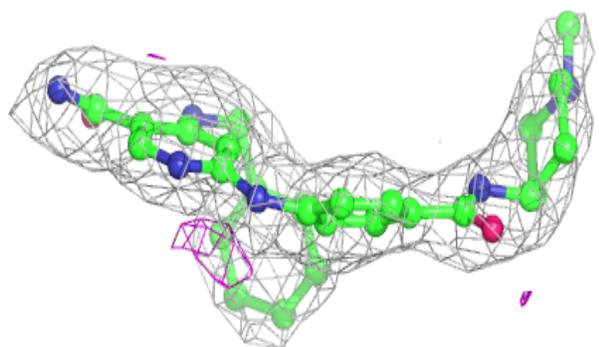
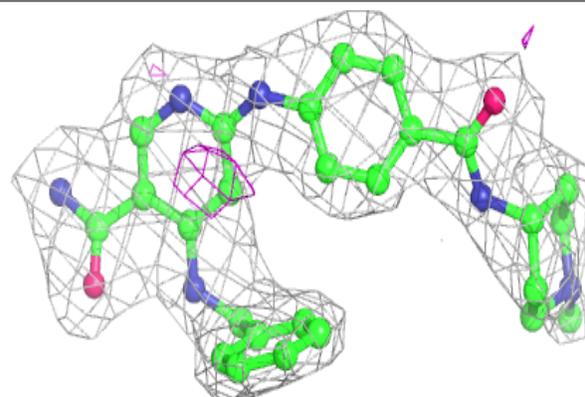


**Electron density around 9YV A 4000:**

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

**Electron density around 9YV C 4000:**

$2mF_o-DF_c$  (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.