



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 04:24 pm BST

PDB ID : 2VRX  
Title : Structure of Aurora B kinase in complex with ZM447439  
Authors : Girdler, F.; Sessa, F.; Patercoli, S.; Villa, F.; Ridgway, E.; Musacchio, A.; Taylor, S.S.  
Deposited on : 2008-04-16  
Resolution : 1.86 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.

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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

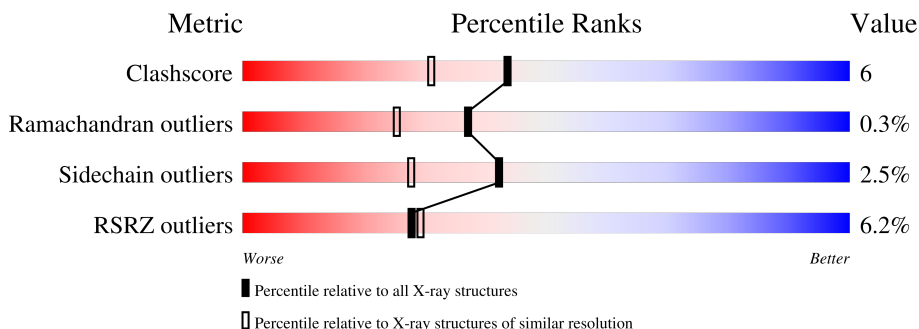
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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  $\geq 3$ , 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	285	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	285	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
2	C	43	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
2	D	43	<div> <div>26%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>



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.

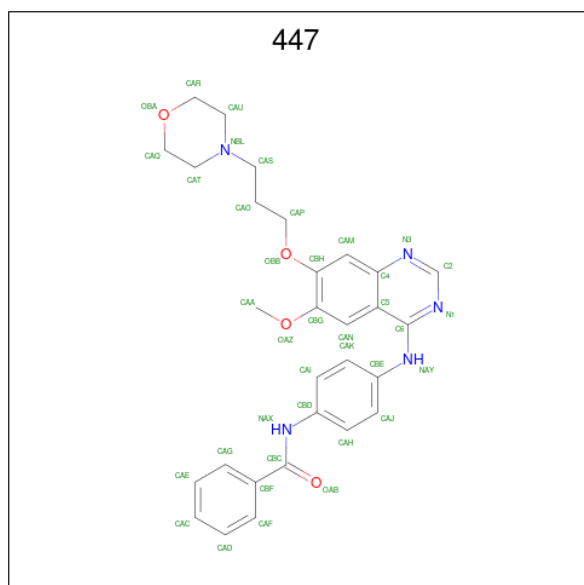
- Molecule 1 is a protein called SERINE/THREONINE-PROTEIN KINASE 12-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total 2272	C 1454	N 409	O 395	P 1	S 13	0	4	0
1	B	275	Total 2291	C 1465	N 412	O 399	P 1	S 14	0	1	0

- Molecule 2 is a protein called INNER CENTROMERE PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	41	Total 328	C 212	N 54	O 61	S 1	0	0	1
2	D	43	Total 350	C 225	N 58	O 66	S 1	0	0	0

- Molecule 3 is N-(4-{[6-methoxy-7-(3-morpholin-4-ylpropoxy)quinazolin-4-yl]amino}phenyl) benzamide (three-letter code: 447) (formula: C<sub>29</sub>H<sub>31</sub>N<sub>5</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			38	29	5	4		
3	B	1	Total	C	N	O	0	0
			38	29	5	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	267	Total	O	0	0
			267	267		
4	B	261	Total	O	0	0
			261	261		
4	C	30	Total	O	0	0
			30	30		
4	D	36	Total	O	0	0
			36	36		



- Molecule 1: SERINE/THREONINE-PROTEIN KINASE 12-A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.73Å 67.00Å 116.58Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	115.47 – 1.86 115.47 – 1.86	Depositor EDS
% Data completeness (in resolution range)	92.3 (115.47-1.86) 88.3 (115.47-1.86)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.188 , 0.243 0.190 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5911	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: TPO, 447

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	0.41	0/2322	0.56	0/3125
1	B	0.42	0/2340	0.57	0/3150
2	C	0.40	0/336	0.55	0/457
2	D	0.35	0/358	0.45	0/485
All	All	0.41	0/5356	0.56	0/7217

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	2272	0	2270	25	0
1	B	2291	0	2293	34	0
2	C	328	0	323	3	0
2	D	350	0	347	3	0
3	A	38	0	31	7	0
3	B	38	0	31	8	0
4	A	267	0	0	2	0
4	B	261	0	0	2	0
4	C	30	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	36	0	0	1	0
All	All	5911	0	5295	64	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 6.

All (64) 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:133:GLY:HA2	1:B:134:VAL:HB	1.07	1.05
1:B:133:GLY:CA	1:B:134:VAL:HB	1.94	0.97
1:B:133:GLY:HA2	1:B:134:VAL:CB	2.00	0.91
1:B:107:VAL:HG21	3:B:1356:447:HAK	1.50	0.91
1:A:211:LYS:HD3	1:A:242:PRO:HA	1.52	0.89
1:B:164:LYS:H	1:B:164:LYS:HD2	1.40	0.86
1:B:141:GLU:HB3	3:B:1356:447:HAC	1.62	0.81
1:B:223:LEU:HD11	3:B:1356:447:HAJ	1.70	0.73
1:A:150:HIS:HD2	1:A:152:ASN:H	1.37	0.72
1:B:150:HIS:HD2	1:B:152:ASN:H	1.38	0.70
1:B:229:GLU:HB3	4:B:2256:HOH:O	1.94	0.68
1:A:104:PHE:HA	1:A:128:GLN:OE1	1.94	0.67
1:B:164:LYS:HD3	1:B:165:ARG:NH2	2.11	0.65
1:B:164:LYS:HD2	1:B:164:LYS:N	2.11	0.65
1:B:98:PRO:HB3	1:B:106:ASN:HD21	1.61	0.65
1:A:152:ASN:HD21	1:A:349:ARG:HH21	1.45	0.64
1:A:150:HIS:CD2	1:A:152:ASN:H	2.16	0.63
1:B:227:LYS:NZ	2:C:816:TYR:OH	2.31	0.63
1:A:112:GLU:OE2	4:A:2024:HOH:O	2.16	0.62
1:B:126:LYS:NZ	1:B:161:HIS:HD2	1.97	0.62
1:B:150:HIS:CD2	1:B:152:ASN:H	2.18	0.61
1:B:141:GLU:HB3	3:B:1356:447:CAC	2.30	0.61
1:A:112:GLU:HG2	2:D:825:TYR:OH	2.01	0.60
1:B:234:ASP:HA	3:B:1356:447:HAF	1.85	0.59
1:B:355:TYR:HB2	2:C:818:PRO:O	2.01	0.59
1:B:152:ASN:HD21	1:B:349:ARG:HH21	1.50	0.59
1:B:143:GLU:O	1:B:147:HIS:HD2	1.86	0.59
1:A:174:PRO:O	3:A:1356:447:HAS1	2.04	0.57
1:A:237:TRP:CD2	1:A:250:CYS:HB2	2.39	0.57
1:B:132:GLU:HB2	1:B:133:GLY:HA2	1.86	0.57
1:A:136:HIS:HA	1:A:139:ARG:HG2	1.87	0.56
1:A:245:ARG:NH1	1:A:265:THR:OG1	2.39	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LYS:HZ3	1:B:161:HIS:HD2	1.53	0.55
1:B:171:GLU:O	3:B:1356:447:H2	2.06	0.55
2:D:832:LYS:O	2:D:835:GLU:HG2	2.07	0.54
1:B:122:LYS:HD3	3:B:1356:447:HAI	1.88	0.54
1:A:105:GLY:HA3	1:A:123:VAL:O	2.09	0.53
1:A:205:HIS:NE2	1:A:335:LYS:HE2	2.25	0.52
1:B:143:GLU:O	1:B:147:HIS:CD2	2.62	0.52
1:B:99:LEU:N	1:B:100:GLY:CA	2.73	0.52
1:A:143:GLU:O	1:A:147:HIS:HD2	1.93	0.51
1:A:152:ASN:ND2	1:A:349:ARG:HH21	2.09	0.51
1:A:237:TRP:CE3	1:A:250:CYS:HB2	2.47	0.50
3:A:1356:447:HAI	3:A:1356:447:OAB	2.11	0.49
1:A:277:VAL:HG13	1:A:288:PRO:HD2	1.97	0.47
1:B:152:ASN:ND2	1:B:349:ARG:HH21	2.13	0.47
1:B:132:GLU:HB2	1:B:134:VAL:HB	1.97	0.46
1:B:132:GLU:CB	1:B:133:GLY:HA2	2.44	0.46
1:A:99:LEU:HB3	3:A:1356:447:HAA3	1.97	0.46
1:A:171:GLU:O	3:A:1356:447:H2	2.16	0.46
2:D:823:ARG:O	2:D:827:THR:HG22	2.16	0.46
1:A:227:LYS:HE3	4:D:2025:HOH:O	2.14	0.46
1:B:277:VAL:HG13	1:B:288:PRO:HD2	1.97	0.46
1:B:107:VAL:CG2	3:B:1356:447:HAK	2.36	0.44
3:A:1356:447:HAA2	3:A:1356:447:OBB	2.17	0.44
1:A:309:PRO:HA	1:A:310:PRO:HD3	1.85	0.43
1:A:99:LEU:O	3:A:1356:447:HAA3	2.19	0.42
1:B:355:TYR:HA	2:C:818:PRO:HD2	2.00	0.42
1:A:90:ILE:HD11	1:A:95:ILE:HD11	2.02	0.42
1:A:349:ARG:NH1	4:A:2262:HOH:O	2.52	0.42
1:B:309:PRO:HA	1:B:310:PRO:HD3	1.93	0.41
3:A:1356:447:OAB	3:A:1356:447:CAI	2.69	0.41
1:B:209:GLU:HG2	4:B:2117:HOH:O	2.21	0.41
1:A:104:PHE:CZ	1:A:134:VAL:HG21	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	270/285 (95%)	261 (97%)	9 (3%)	0	100	100
1	B	271/285 (95%)	263 (97%)	7 (3%)	1 (0%)	30	18
2	C	39/43 (91%)	36 (92%)	2 (5%)	1 (3%)	4	0
2	D	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
All	All	621/656 (95%)	599 (96%)	20 (3%)	2 (0%)	37	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	VAL
2	C	804	GLY

### 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	246/256 (96%)	243 (99%)	3 (1%)	67	59
1	B	248/256 (97%)	242 (98%)	6 (2%)	44	29
2	C	35/38 (92%)	31 (89%)	4 (11%)	4	0
2	D	38/38 (100%)	37 (97%)	1 (3%)	41	26
All	All	567/588 (96%)	553 (98%)	14 (2%)	42	28

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLU
1	A	192	ARG
1	A	299	ARG
1	B	77	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	86	ARG
1	B	134	VAL
1	B	138	LEU
1	B	164	LYS
1	B	335	LYS
2	C	806	LEU
2	C	817	LYS
2	C	823	ARG
2	C	837	PHE
2	D	827	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	150	HIS
1	A	152	ASN
1	B	106	ASN
1	B	137	GLN
1	B	147	HIS
1	B	150	HIS
1	B	152	ASN
1	B	161	HIS
2	D	809	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	TPO	B	248	1	8,10,11	0.66	0	10,14,16	0.93	0
1	TPO	A	248	1	8,10,11	0.73	0	10,14,16	1.10	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	TPO	B	248	1	-	0/9/11/13	-
1	TPO	A	248	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	$\# Z  > 2$
3	447	A	1356	-	42,42,42	1.62	6 (14%)	56,56,56	1.82	11 (19%)
3	447	B	1356	-	42,42,42	1.66	7 (16%)	56,56,56	1.74	9 (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
3	447	A	1356	-	-	3/21/29/29	0/5/5/5
3	447	B	1356	-	-	9/21/29/29	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1356	447	C2-N3	5.18	1.40	1.32
3	B	1356	447	C2-N3	5.04	1.40	1.32
3	B	1356	447	CBF-CBC	-4.94	1.39	1.50
3	A	1356	447	CBF-CBC	-4.79	1.40	1.50
3	A	1356	447	C2-N1	3.77	1.40	1.33
3	B	1356	447	C6-C5	-3.55	1.40	1.44
3	B	1356	447	CBD-NAX	-3.52	1.34	1.41
3	B	1356	447	C2-N1	3.33	1.40	1.33
3	A	1356	447	C6-C5	-3.06	1.41	1.44
3	A	1356	447	CBD-NAX	-2.79	1.36	1.41
3	B	1356	447	CBE-NAY	-2.50	1.35	1.40
3	A	1356	447	CAM-CBH	2.15	1.40	1.36
3	B	1356	447	CAN-CBG	2.13	1.40	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1356	447	N3-C2-N1	-5.89	119.47	128.68
3	B	1356	447	N3-C2-N1	-5.82	119.58	128.68
3	A	1356	447	C6-C5-C4	5.65	119.44	115.88
3	B	1356	447	C6-C5-C4	4.97	119.01	115.88
3	B	1356	447	CBE-NAY-C6	-4.57	116.36	128.26
3	B	1356	447	C2-N1-C6	4.43	120.39	116.59
3	A	1356	447	C2-N1-C6	4.17	120.16	116.59
3	A	1356	447	OAZ-CBG-CAN	-3.99	120.07	125.24
3	B	1356	447	CAN-C5-C6	-3.90	121.36	124.88
3	A	1356	447	CAN-C5-C6	-3.88	121.38	124.88
3	A	1356	447	C2-N3-C4	3.76	120.58	115.40
3	B	1356	447	C2-N3-C4	3.40	120.08	115.40
3	A	1356	447	CBE-NAY-C6	-2.85	120.83	128.26
3	A	1356	447	OAZ-CBG-CBH	2.80	119.31	115.41
3	A	1356	447	NAY-C6-N1	2.72	122.36	118.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1356	447	C5-C4-N3	-2.59	120.08	122.83
3	A	1356	447	C5-C6-NAY	-2.15	117.36	119.73
3	B	1356	447	CAA-OAZ-CBG	-2.10	114.36	117.53
3	B	1356	447	C5-C4-N3	-2.05	120.65	122.83
3	B	1356	447	NAY-C6-N1	2.03	121.45	118.72

There are no chirality outliers.

All (12) torsion outliers are listed below:

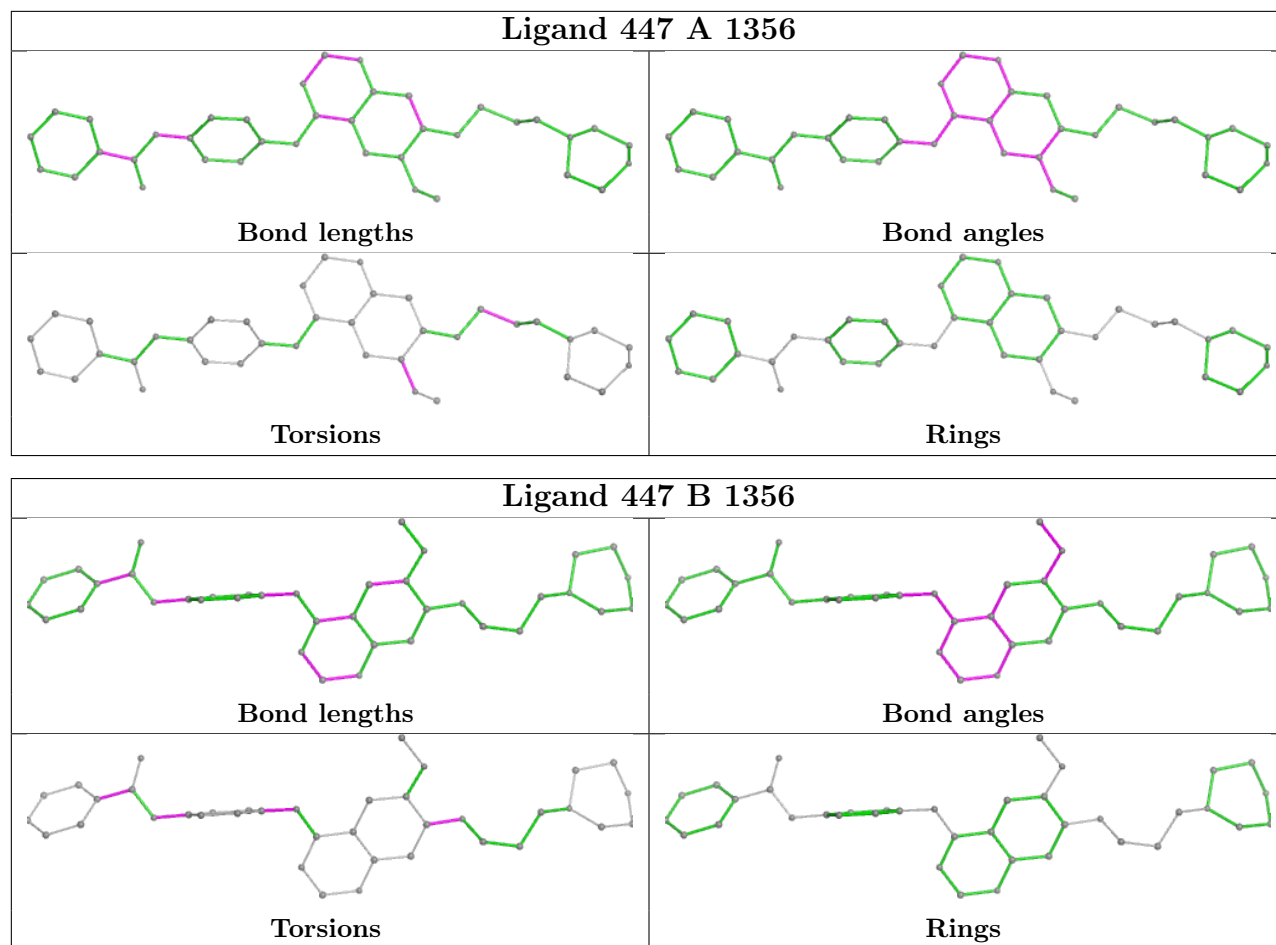
Mol	Chain	Res	Type	Atoms
3	B	1356	447	CAH-CBD-NAX-CBC
3	B	1356	447	CAI-CBD-NAX-CBC
3	A	1356	447	CAN-CBG-OAZ-CAA
3	A	1356	447	CBH-CBG-OAZ-CAA
3	B	1356	447	OAB-CBC-CBF-CAF
3	B	1356	447	NAX-CBC-CBF-CAF
3	B	1356	447	CBG-CBH-OBB-CAP
3	A	1356	447	CAS-CAO-CAP-OBB
3	B	1356	447	OAB-CBC-CBF-CAG
3	B	1356	447	NAX-CBC-CBF-CAG
3	B	1356	447	CAM-CBH-OBB-CAP
3	B	1356	447	CAK-CBE-NAY-C6

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1356	447	7	0
3	B	1356	447	8	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 ⓘ

### 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, 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	268/285 (94%)	0.09	12 (4%) 39 41	8, 21, 39, 42	4 (1%)
1	B	274/285 (96%)	0.02	15 (5%) 32 33	6, 20, 42, 55	1 (0%)
2	C	41/43 (95%)	0.73	1 (2%) 59 62	25, 29, 41, 43	0
2	D	43/43 (100%)	1.40	11 (25%) 2 2	30, 42, 54, 56	0
All	All	626/656 (95%)	0.19	39 (6%) 28 29	6, 22, 45, 56	5 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	TYR	5.3
1	B	133	GLY	4.1
1	B	134	VAL	3.9
2	D	804	GLY	3.8
1	A	244	LEU	3.7
1	B	354	VAL	3.6
1	B	105	GLY	3.5
1	A	294	HIS	3.4
2	D	837	PHE	3.2
1	A	243	SER	3.2
1	B	79	ALA	3.1
1	B	132	GLU	3.0
1	B	96	GLY	2.9
1	B	80	LEU	2.9
1	A	354	VAL	2.7
1	B	78	THR	2.6
1	A	251	GLY	2.6
2	D	808	THR	2.6
1	A	103	LYS	2.6
2	D	833	LEU	2.5
2	D	827	THR	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	355	TYR	2.4
1	A	96	GLY	2.4
2	D	836	LEU	2.4
1	A	245	ARG	2.4
1	B	136	HIS	2.4
1	B	179	TYR	2.4
2	D	840	SER	2.3
2	C	837	PHE	2.3
1	A	246	ARG	2.2
1	B	131	LYS	2.2
1	B	129	LEU	2.2
2	D	828	ILE	2.2
1	A	137	GLN	2.2
1	A	133	GLY	2.2
2	D	809	GLN	2.2
2	D	826	GLY	2.1
1	B	100	GLY	2.1
2	D	838	ASN	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	TPO	A	248	11/12	0.95	0.10	30,33,35,36	0
1	TPO	B	248	11/12	0.98	0.04	18,20,22,23	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

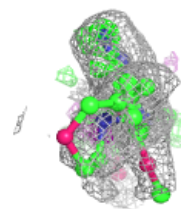
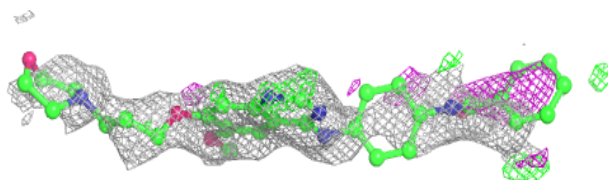
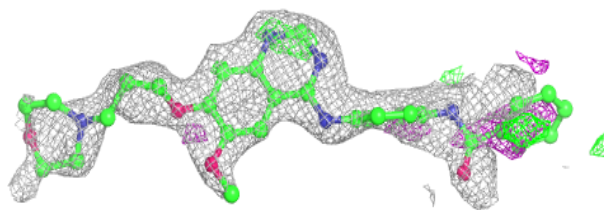
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

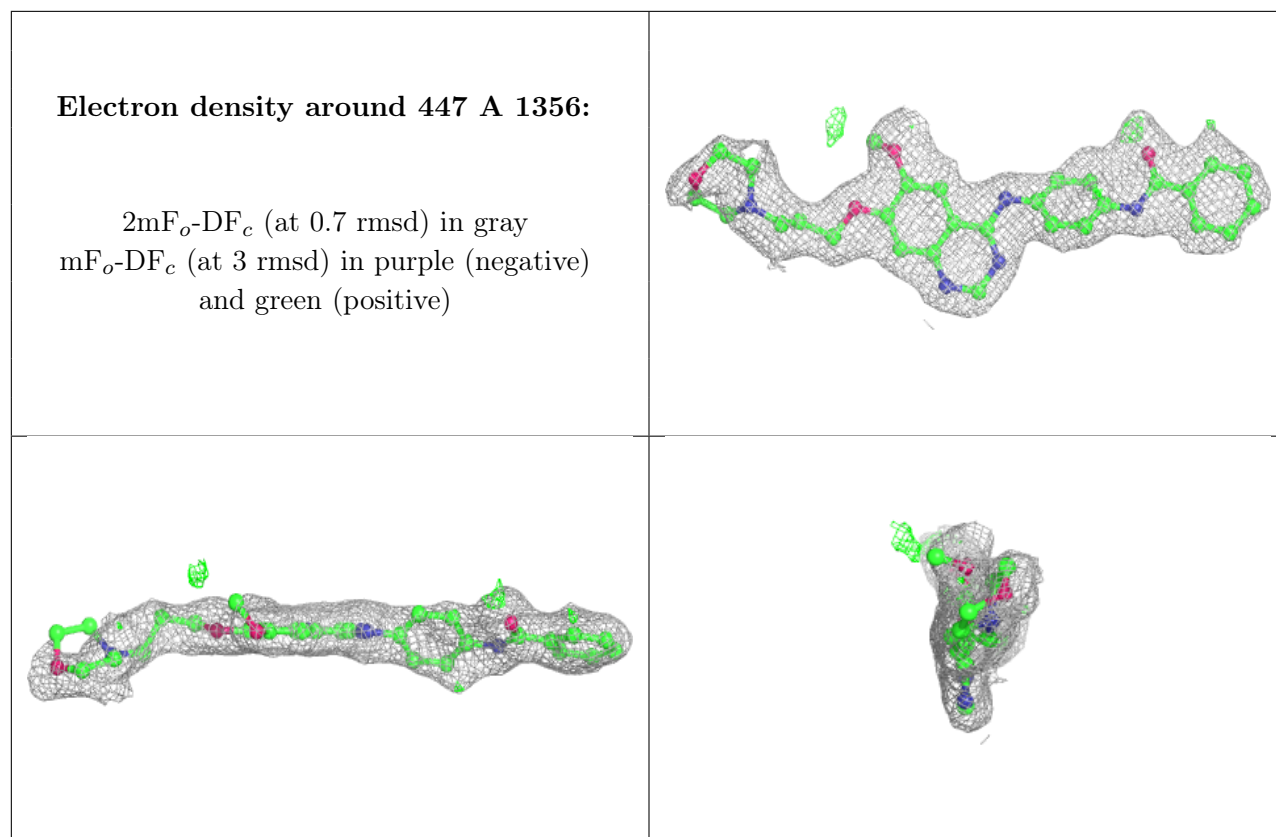
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	447	B	1356	38/38	0.69	0.20	55,58,62,62	0
3	447	A	1356	38/38	0.87	0.11	29,33,43,44	0

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 447 B 1356:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.