



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:09 am BST

PDB ID : 5VQQ  
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with N-(6-cyan  
o-3-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)-4-meth  
ylnaphthalen-1-yl)-2-fluoro-N-methylacetamide (JLJ683), a Non-nucleoside  
Inhibitor  
Authors : Chan, A.H.; Anderson, K.S.  
Deposited on : 2017-05-09  
Resolution : 2.55 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

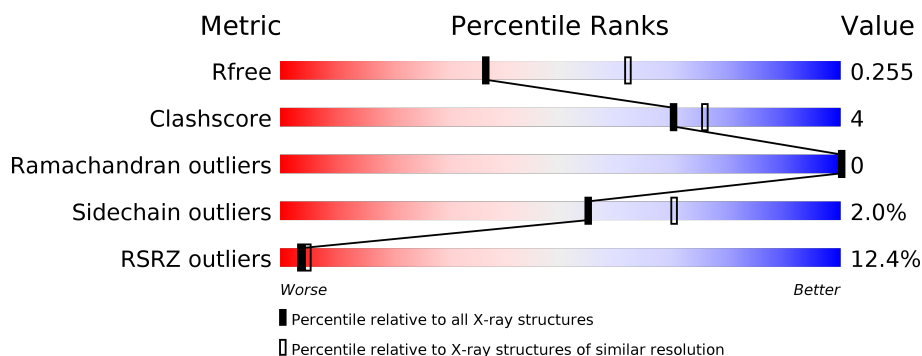
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	557	<div> <div>11%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
2	B	428	<div> <div>13%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7796 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4413	2861	726	818	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

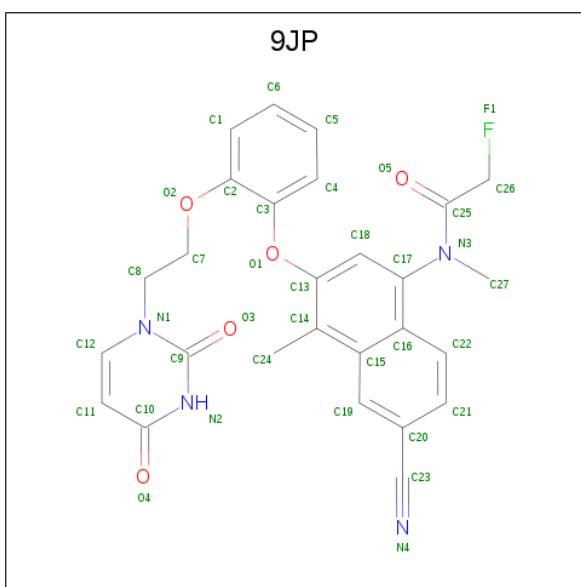
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3307	2152	547	602	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is N-(6-cyano-3-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}-4-methylnaphthalen-1-yl)-2-fluoro-N-methylacetamide (three-letter code: 9JP) (formula: C<sub>27</sub>H<sub>23</sub>FN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			37	27	1	4	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S	0	0
			5	4 1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	14	Total 14	O 14	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.40 Å   73.50 Å   108.26 Å 90.00°   99.27°   90.00°	Depositor
Resolution (Å)	43.22 – 2.55 43.22 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.22-2.55) 95.0 (43.22-2.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.54 Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, $R_{free}$	0.225   ,   0.255 0.225   ,   0.255	Depositor DCC
$R_{free}$ test set	2000 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7796	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9JP, SO4

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	0.24	0/4530	0.42	0/6169
2	B	0.24	0/3401	0.42	0/4622
All	All	0.24	0/7931	0.42	0/10791

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	4413	0	4419	36	0
2	B	3307	0	3316	24	0
3	A	37	0	0	0	0
4	A	5	0	0	0	0
5	A	20	0	0	1	0
5	B	14	0	0	0	0
All	All	7796	0	7735	56	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 4.

All (56) 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:A:544:GLY:HA2	2:B:286:THR:HG22	1.70	0.73
2:B:308:GLU:HA	2:B:311:LYS:HE2	1.76	0.68
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.76	0.67
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.75	0.67
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.77	0.65
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.32	0.62
1:A:363:ASN:HD21	1:A:366:LYS:HE3	1.68	0.58
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.38	0.56
1:A:480:GLN:NE2	5:A:702:HOH:O	2.38	0.55
1:A:252:TRP:HB2	1:A:295:LEU:HD11	1.89	0.54
2:B:203:GLU:HA	2:B:206:ARG:HG2	1.89	0.54
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.90	0.52
1:A:249:LYS:HB2	1:A:252:TRP:CE2	2.46	0.51
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.46	0.50
2:B:84:THR:HB	2:B:154:LYS:HE2	1.94	0.50
1:A:252:TRP:HD1	1:A:295:LEU:HD21	1.77	0.49
1:A:454:LYS:HZ2	1:A:552:VAL:HB	1.77	0.48
1:A:46:LYS:HE2	1:A:116:PHE:CD2	2.49	0.48
1:A:253:THR:OG1	1:A:255:ASN:OD1	2.32	0.48
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.49	0.48
1:A:80:LEU:O	1:A:84:THR:OG1	2.25	0.47
2:B:167:ILE:HG12	2:B:212:TRP:CE3	2.49	0.47
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.95	0.47
1:A:369:THR:O	1:A:373:GLN:HG2	2.14	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.47
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.15	0.46
2:B:74:LEU:HD21	2:B:409:THR:HA	1.97	0.46
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.98	0.45
1:A:363:ASN:ND2	1:A:366:LYS:HE3	2.32	0.45
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.99	0.45
1:A:366:LYS:HE2	1:A:405:TYR:OH	2.17	0.45
2:B:163:SER:O	2:B:167:ILE:HG13	2.17	0.44
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.98	0.44
1:A:105:SER:O	1:A:190:GLY:HA2	2.18	0.44
1:A:258:GLN:HA	1:A:261:VAL:HG12	1.99	0.44
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.52	0.44
1:A:28:GLU:HG2	1:A:32:LYS:HE3	1.99	0.44
1:A:195:ILE:HG13	1:A:199:ARG:HE	1.83	0.44
2:B:28:GLU:HG2	2:B:32:LYS:HD2	2.01	0.43
2:B:425:LEU:HD23	2:B:425:LEU:HA	1.89	0.43
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLU:O	2:B:339:TYR:HA	2.19	0.43
1:A:34:LEU:HD21	1:A:62:ALA:HB2	2.01	0.42
1:A:353:LYS:O	1:A:374:LYS:NZ	2.51	0.42
1:A:542:ILE:HG12	2:B:283:LEU:HD12	2.02	0.42
1:A:443:ASP:HB3	1:A:550:LYS:HD3	2.02	0.41
1:A:266:TRP:O	1:A:269:GLN:HG2	2.20	0.41
1:A:62:ALA:HA	1:A:72:ARG:O	2.21	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.41
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.94	0.41
1:A:112:GLY:HA2	1:A:185:ASP:HB2	2.02	0.41
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.52	0.40
2:B:202:ILE:HD13	2:B:202:ILE:HA	1.89	0.40
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.02	0.40
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.41	0.40
2:B:354:TYR:CE1	2:B:356:ARG:HB3	2.56	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	543/557 (98%)	527 (97%)	16 (3%)	0	100	100
2	B	394/428 (92%)	383 (97%)	11 (3%)	0	100	100
All	All	937/985 (95%)	910 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	479/495 (97%)	469 (98%)	10 (2%)	53	68
2	B	362/390 (93%)	355 (98%)	7 (2%)	57	72
All	All	841/885 (95%)	824 (98%)	17 (2%)	55	70

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	90	VAL
1	A	115	TYR
1	A	182	GLN
1	A	210	LEU
1	A	220	LYS
1	A	249	LYS
1	A	295	LEU
1	A	300	GLU
1	A	301	LEU
2	B	8	VAL
2	B	69	THR
2	B	74	LEU
2	B	232	TYR
2	B	233	GLU
2	B	414	TRP
2	B	417	VAL

Some 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 carbohydrates 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
3	9JP	A	601	-	35,40,40	0.80	1 (2%)	44,56,56	1.66	9 (20%)
4	SO4	A	602	-	4,4,4	0.15	0	6,6,6	0.06	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
3	9JP	A	601	-	-	1/21/22/22	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	9JP	C10-N2	2.20	1.36	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	9JP	C11-C10-N2	-4.45	113.52	123.31
3	A	601	9JP	C3-O1-C13	4.02	127.61	118.04
3	A	601	9JP	C11-C12-N1	3.84	124.34	121.28
3	A	601	9JP	C16-C17-N3	3.12	121.90	118.97
3	A	601	9JP	O2-C2-C3	3.04	122.00	115.73
3	A	601	9JP	O2-C2-C1	-2.92	117.64	123.97
3	A	601	9JP	C7-O2-C2	2.70	124.30	117.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	9JP	C18-C13-C14	-2.50	119.53	122.45
3	A	601	9JP	C8-N1-C12	2.00	121.80	118.11

There are no chirality outliers.

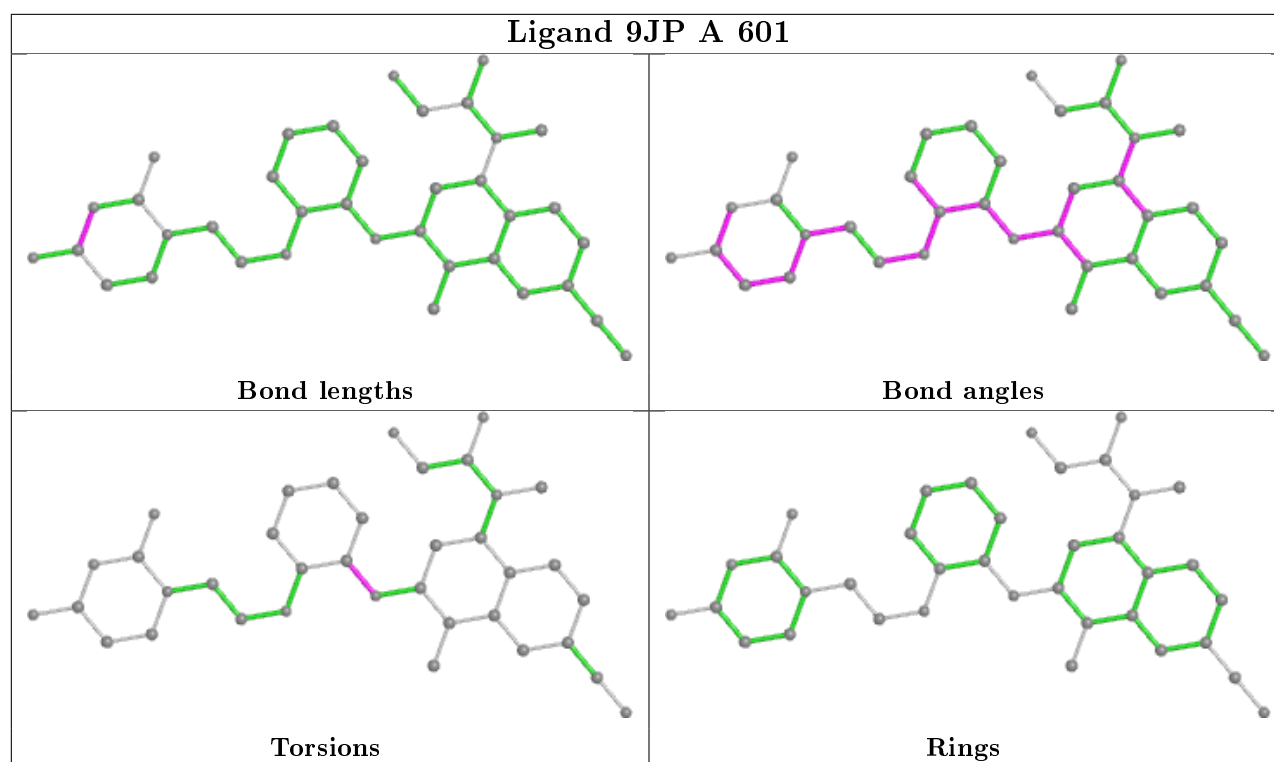
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	9JP	C2-C3-O1-C13

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, 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	547/557 (98%)	0.76	63 (11%) 4 6	39, 70, 120, 155	0
2	B	400/428 (93%)	0.84	54 (13%) 3 4	42, 67, 123, 135	0
All	All	947/985 (96%)	0.79	117 (12%) 4 5	39, 69, 121, 155	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	LEU	10.4
1	A	285	GLY	9.8
2	B	358	ARG	9.7
1	A	290	THR	9.3
1	A	221	HIS	9.1
1	A	260	LEU	8.8
1	A	288	ALA	8.6
2	B	212	TRP	7.2
2	B	207	GLN	6.6
2	B	168	LEU	6.3
1	A	286	THR	6.2
2	B	241	VAL	6.1
1	A	256	ASP	5.9
1	A	257	ILE	5.8
2	B	67	ASP	5.7
1	A	295	LEU	5.6
1	A	292	VAL	5.5
1	A	548	VAL	5.5
1	A	287	LYS	5.4
2	B	232	TYR	5.4
2	B	209	LEU	5.3
2	B	166	LYS	5.2
1	A	247	PRO	5.2
2	B	195	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	252	TRP	5.0
2	B	202	ILE	5.0
1	A	255	ASN	4.9
2	B	198	HIS	4.9
1	A	90	VAL	4.9
1	A	261	VAL	4.8
1	A	552	VAL	4.8
2	B	359	GLY	4.7
1	A	551	LEU	4.7
1	A	283	LEU	4.6
1	A	218	ASP	4.6
1	A	219	LYS	4.6
1	A	244	ILE	4.4
1	A	293	ILE	4.4
2	B	191	SER	4.3
2	B	189	VAL	4.3
2	B	211	ARG	4.1
2	B	88	TRP	3.9
2	B	210	LEU	3.8
1	A	250	ASP	3.8
1	A	263	LYS	3.7
1	A	93	GLY	3.6
1	A	245	VAL	3.6
1	A	550	LYS	3.6
1	A	291	GLU	3.6
1	A	294	PRO	3.5
2	B	107	THR	3.5
2	B	206	ARG	3.5
1	A	297	GLU	3.4
1	A	282	LEU	3.4
2	B	240	THR	3.3
1	A	116	PHE	3.3
2	B	95	PRO	3.2
2	B	199	ARG	3.2
1	A	220	LYS	3.2
2	B	169	GLU	3.2
1	A	279	LEU	3.1
1	A	15	GLY	3.0
2	B	87	PHE	3.0
2	B	238	LYS	2.9
2	B	284	ARG	2.9
2	B	357	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	356	ARG	2.8
1	A	298	GLU	2.8
2	B	234	LEU	2.8
1	A	248	GLU	2.8
1	A	246	LEU	2.7
2	B	193	LEU	2.7
1	A	284	ARG	2.7
1	A	544	GLY	2.7
2	B	196	GLY	2.7
2	B	204	GLU	2.7
2	B	197	GLN	2.7
2	B	108	VAL	2.7
2	B	208	HIS	2.7
1	A	259	LYS	2.7
2	B	239	TRP	2.7
2	B	200	THR	2.6
1	A	92	LEU	2.6
2	B	66	LYS	2.6
2	B	94	ILE	2.6
2	B	190	GLY	2.6
1	A	300	GLU	2.5
2	B	233	GLU	2.5
2	B	237	ASP	2.4
1	A	222	GLN	2.4
2	B	173	LYS	2.4
1	A	183	TYR	2.4
1	A	542	ILE	2.4
1	A	264	LEU	2.4
2	B	178	ILE	2.3
1	A	132	ILE	2.3
2	B	109	LEU	2.3
1	A	541	GLY	2.3
2	B	360	ALA	2.3
2	B	171	PHE	2.3
1	A	225	PRO	2.2
1	A	91	GLN	2.2
1	A	35	VAL	2.2
1	A	254	VAL	2.2
2	B	180	ILE	2.2
1	A	243	PRO	2.2
2	B	425	LEU	2.2
1	A	117	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	170	PRO	2.1
1	A	144	TYR	2.1
1	A	253	THR	2.1
1	A	304	ALA	2.1
2	B	69	THR	2.1
2	B	179	VAL	2.1
1	A	2	ILE	2.0
1	A	115	TYR	2.0
2	B	428	GLN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

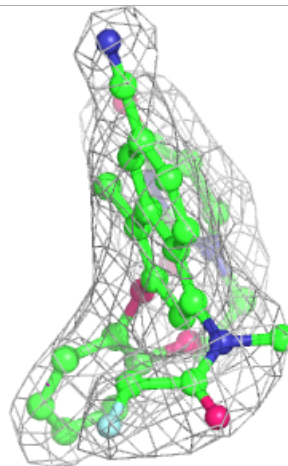
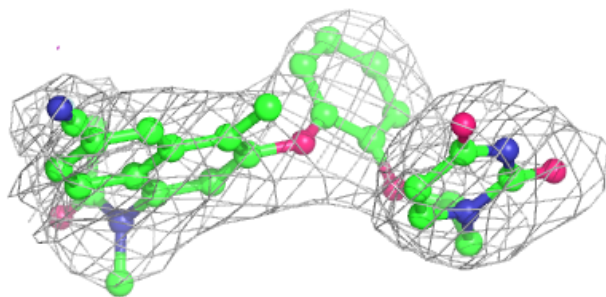
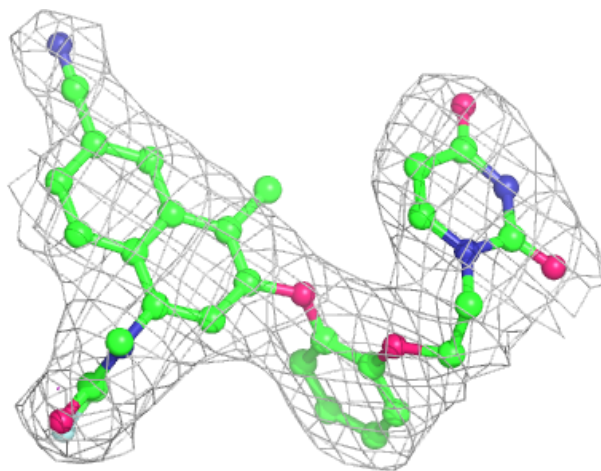
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	9JP	A	601	37/37	0.93	0.17	57,67,79,83	0
4	SO4	A	602	5/5	0.94	0.11	92,96,103,108	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 9JP A 601:**

$2mF_o-DF_c$  (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.