



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:04 am BST

PDB ID : 4RW6
Title : Crystal Structure of HIV-1 Reverse Transcriptase (Y181C) variant in complex with (E)-3-(3-chloro-5-(4-chloro-2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)phenyl)acrylonitrile (JLJ494), a Non-nucleoside Inhibitor
Authors : Frey, K.M.; Anderson, K.S.
Deposited on : 2014-12-01
Resolution : 2.63 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 : 2.11
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

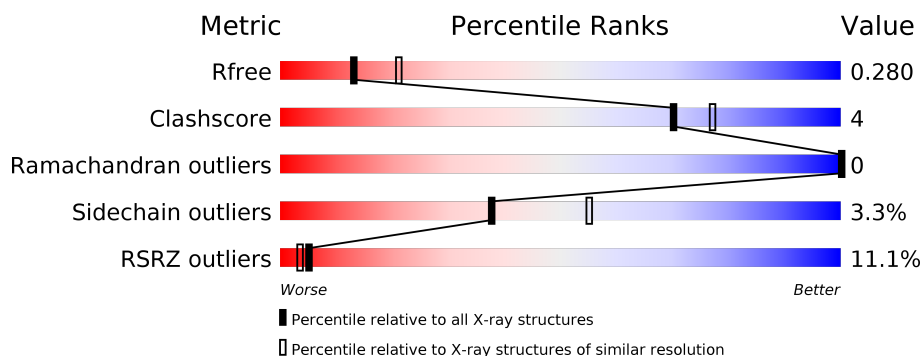
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 ≥ 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>9%</div> <div>84%</div> <div>12%</div> <div>••</div> </div>
2	B	428	<div> <div>13%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7775 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, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4360	2825	721	805	9			

There are 6 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	181	CYS	TYR	ENGINEERED MUTATION	UNP P03366
A	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

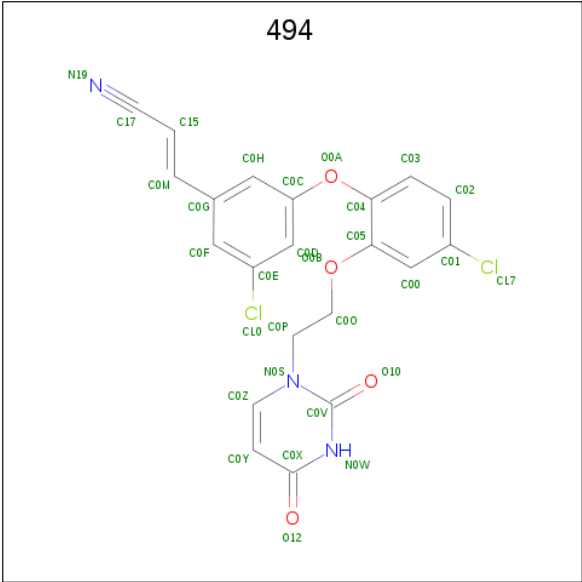
- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3356	2184	556	610	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 (2E)-3-(3-chloro-5-{4-chloro-2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}phenyl)prop-2-enenitrile (three-letter code: 494) (formula: C₂₁H₁₅Cl₂N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			30	21	2	3	4		

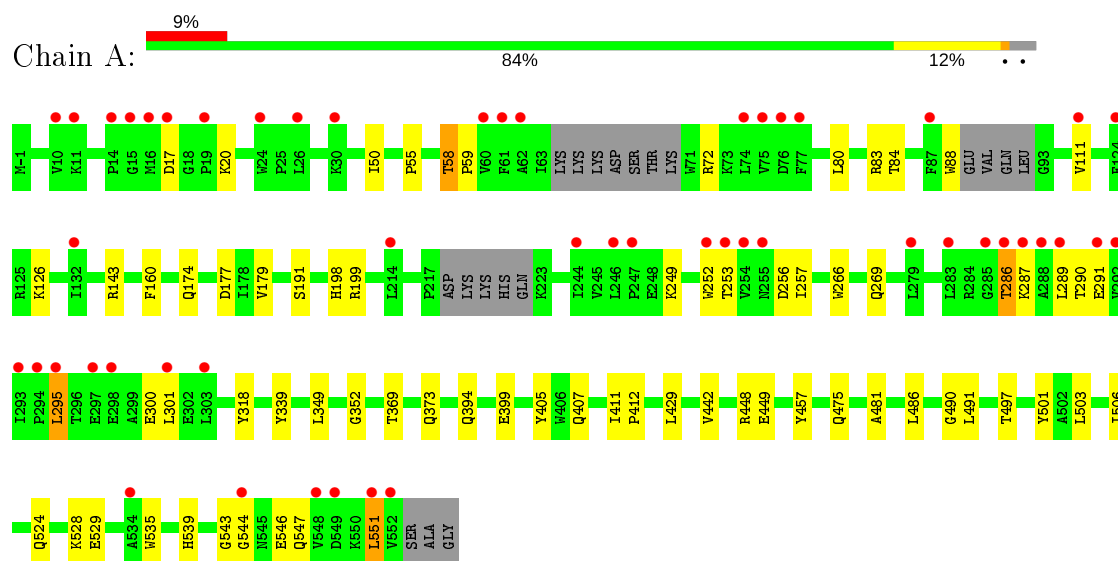
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	9	Total	O	0	0
			9	9		

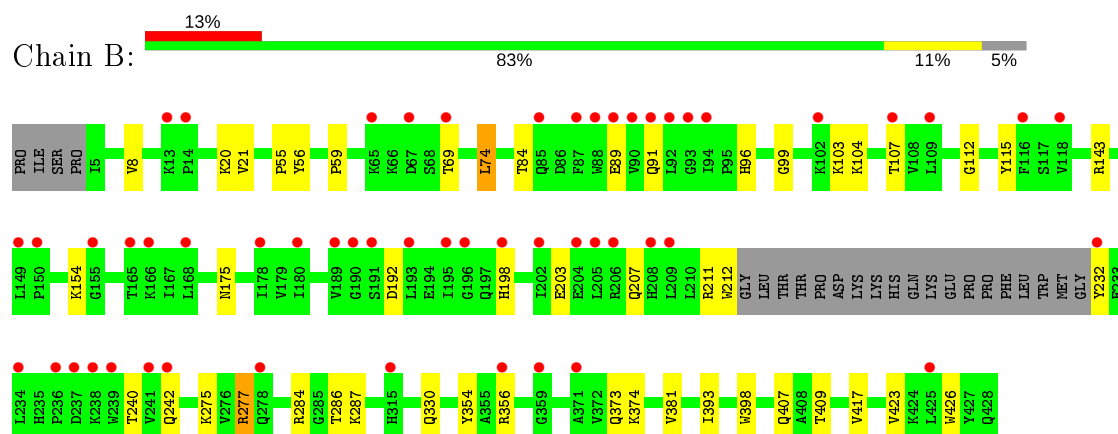
3 Residue-property plots [i](#)

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: Reverse transcriptase/ribonuclease H, p66 subunit



- Molecule 2: Reverse transcriptase/ribonuclease H, p51 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.32Å 73.94Å 107.60Å 90.00° 99.76° 90.00°	Depositor
Resolution (Å)	43.08 – 2.63 43.07 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.08-2.63) 99.5 (43.07-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.280 0.234 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7775	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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:
494

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	0.22	0/4473	0.42	0/6083
2	B	0.22	0/3451	0.42	0/4687
All	All	0.22	0/7924	0.42	0/10770

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	4360	0	4397	34	0
2	B	3356	0	3387	25	0
3	A	30	0	15	3	0
4	A	20	0	0	0	0
4	B	9	0	0	0	0
All	All	7775	0	7799	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:539:HIS:HE1	1:A:547:GLN:HG2	1.55	0.71
2:B:89:GLU:HB2	2:B:91:GLN:HG2	1.71	0.70
2:B:373:GLN:HE22	2:B:407:GLN:H	1.44	0.65
1:A:17:ASP:O	1:A:83:ARG:NE	2.28	0.64
2:B:96:HIS:NE2	2:B:381:VAL:O	2.28	0.63
1:A:295:LEU:HD13	1:A:300:GLU:HB2	1.81	0.62
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.82	0.62
2:B:373:GLN:HE22	2:B:407:GLN:N	2.01	0.57
1:A:191:SER:OG	1:A:198:HIS:ND1	2.28	0.57
1:A:111:VAL:HG11	1:A:160:PHE:HZ	1.70	0.56
2:B:74:LEU:HD21	2:B:409:THR:HA	1.86	0.56
2:B:56:TYR:O	2:B:143:ARG:NH2	2.26	0.56
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.43	0.53
1:A:369:THR:O	1:A:373:GLN:HG2	2.09	0.53
2:B:20:LYS:HE2	2:B:55:PRO:HB2	1.92	0.51
2:B:354:TYR:CE1	2:B:356:ARG:HB3	2.44	0.51
1:A:249:LYS:NZ	1:A:256:ASP:OD2	2.43	0.51
1:A:490:GLY:O	1:A:528:LYS:NZ	2.36	0.51
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.94	0.49
1:A:318:TYR:CE2	3:A:601:494:H11	2.48	0.49
1:A:318:TYR:CZ	3:A:601:494:H11	2.49	0.48
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.29	0.47
1:A:547:GLN:O	1:A:551:LEU:HB2	2.14	0.47
2:B:275:LYS:HE3	2:B:277:ARG:HB3	1.96	0.47
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.96	0.46
2:B:112:GLY:HA2	2:B:115:TYR:HD1	1.81	0.46
2:B:423:VAL:HA	2:B:426:TRP:CE3	2.51	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.98	0.46
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.51	0.46
2:B:211:ARG:HG3	2:B:212:TRP:HD1	1.81	0.46
2:B:240:THR:O	2:B:242:GLN:NE2	2.48	0.46
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.97	0.45
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.99	0.45
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.98	0.45
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.99	0.45
1:A:177:ASP:OD1	1:A:177:ASP:N	2.48	0.44
2:B:84:THR:HB	2:B:154:LYS:HE2	2.00	0.44
2:B:356:ARG:HE	2:B:374:LYS:NZ	2.16	0.44
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.00	0.43
1:A:486:LEU:HB3	1:A:524:GLN:HB3	2.01	0.43
1:A:491:LEU:HB3	1:A:529:GLU:CG	2.49	0.43
1:A:286:THR:HB	1:A:287:LYS:H	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HE2	1:A:55:PRO:HB2	2.02	0.42
1:A:253:THR:HA	1:A:291:GLU:O	2.20	0.42
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.54	0.42
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.55	0.41
1:A:411:ILE:HG22	1:A:412:PRO:O	2.20	0.41
1:A:543:GLY:HA3	2:B:284:ARG:HA	2.03	0.41
2:B:286:THR:OG1	2:B:286:THR:O	2.37	0.41
1:A:253:THR:O	1:A:257:ILE:HG13	2.20	0.41
1:A:179:VAL:HB	3:A:601:494:CL7	2.56	0.41
2:B:203:GLU:OE2	2:B:207:GLN:NE2	2.53	0.41
1:A:266:TRP:O	1:A:269:GLN:HG2	2.21	0.41
1:A:80:LEU:O	1:A:84:THR:OG1	2.27	0.41
2:B:99:GLY:O	2:B:103:LYS:HG2	2.21	0.41
1:A:58:THR:HG22	1:A:59:PRO:HD2	2.03	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	530/557 (95%)	513 (97%)	17 (3%)	0	100	100
2	B	401/428 (94%)	393 (98%)	8 (2%)	0	100	100
All	All	931/985 (94%)	906 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	477/495 (96%)	458 (96%)	19 (4%)	31	47
2	B	369/390 (95%)	360 (98%)	9 (2%)	49	67
All	All	846/885 (96%)	818 (97%)	28 (3%)	38	55

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	72	ARG
1	A	126	LYS
1	A	174	GLN
1	A	199	ARG
1	A	252	TRP
1	A	286	THR
1	A	289	LEU
1	A	290	THR
1	A	295	LEU
1	A	301	LEU
1	A	349	LEU
1	A	394	GLN
1	A	399	GLU
1	A	448	ARG
1	A	449	GLU
1	A	497	THR
1	A	546	GLU
1	A	551	LEU
2	B	8	VAL
2	B	69	THR
2	B	74	LEU
2	B	175	ASN
2	B	232	TYR
2	B	277	ARG
2	B	287	LYS
2	B	330	GLN
2	B	417	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	197	GLN
1	A	258	GLN
1	A	373	GLN
1	A	394	GLN
1	A	475	GLN
1	A	520	GLN
1	A	539	HIS
2	B	197	GLN
2	B	330	GLN
2	B	334	GLN
2	B	340	GLN
2	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

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	$\# Z > 2$
3	494	A	601	-	29,32,32	1.45	3 (10%)	34,43,43	2.24	7 (20%)

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	494	A	601	-	-	3/13/14/14	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	494	C0Z-N0S	3.76	1.42	1.35
3	A	601	494	C0H-C0G	2.09	1.43	1.39
3	A	601	494	C0D-C0C	2.06	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	494	O0B-C05-C04	7.55	131.32	115.73
3	A	601	494	O0B-C05-C00	-5.82	110.19	123.58
3	A	601	494	C0Y-C0X-N0W	-3.60	115.39	123.31
3	A	601	494	C0O-O0B-C05	3.12	125.32	117.69
3	A	601	494	C04-O0A-C0C	2.78	124.94	118.00
3	A	601	494	C0G-C0F-C0E	2.14	121.62	119.55
3	A	601	494	C0C-C0D-C0E	2.08	120.57	118.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	494	O0B-C0O-C0P-N0S
3	A	601	494	C04-C05-O0B-C0O
3	A	601	494	C00-C05-O0B-C0O

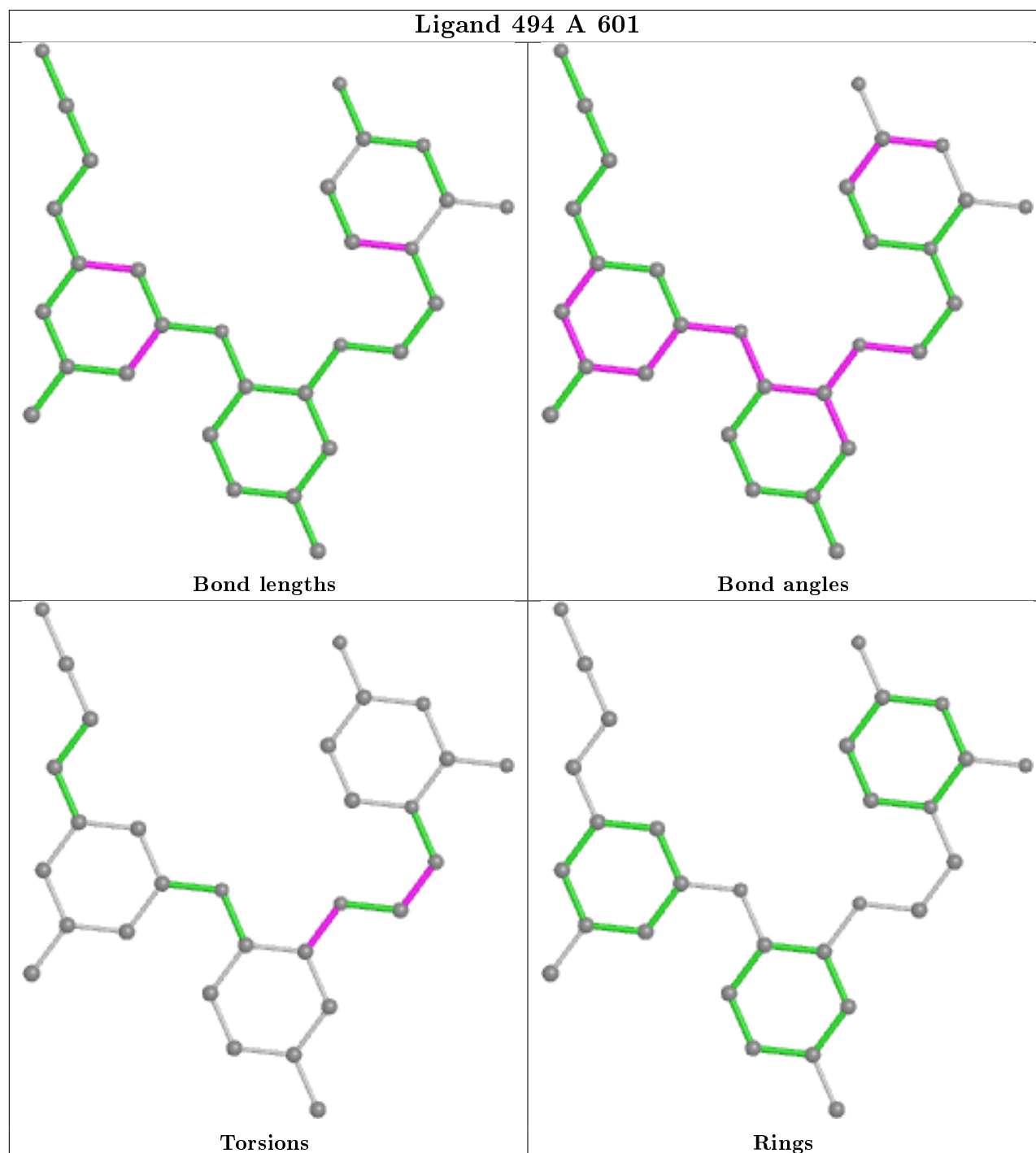
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	494	3	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

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	A	538/557 (96%)	0.62	51 (9%) 8 6	31, 65, 110, 138	0
2	B	405/428 (94%)	0.84	54 (13%) 3 2	35, 63, 120, 132	0
All	All	943/985 (95%)	0.71	105 (11%) 5 3	31, 64, 116, 138	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	VAL	9.7
2	B	90	VAL	9.3
2	B	168	LEU	7.2
2	B	209	LEU	7.2
2	B	191	SER	7.0
2	B	232	TYR	6.5
1	A	287	LYS	6.4
1	A	552	VAL	6.2
2	B	206	ARG	6.1
1	A	26	LEU	6.0
1	A	252	TRP	5.9
1	A	551	LEU	5.8
1	A	294	PRO	5.4
1	A	289	LEU	5.1
1	A	254	VAL	5.1
1	A	24	TRP	5.0
1	A	75	VAL	5.0
1	A	61	PHE	4.9
2	B	356	ARG	4.9
1	A	74	LEU	4.8
2	B	190	GLY	4.8
2	B	178	ILE	4.7
2	B	88	TRP	4.7
2	B	202	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	548	VAL	4.2
1	A	60	VAL	4.1
1	A	14	PRO	3.9
2	B	180	ILE	3.9
2	B	166	LYS	3.9
1	A	286	THR	3.9
1	A	298	GLU	3.8
2	B	241	VAL	3.8
2	B	359	GLY	3.6
1	A	291	GLU	3.6
1	A	549	ASP	3.5
2	B	195	ILE	3.5
2	B	67	ASP	3.5
2	B	237	ASP	3.4
1	A	288	ALA	3.4
1	A	283	LEU	3.3
2	B	116	PHE	3.2
2	B	149	LEU	3.2
2	B	198	HIS	3.2
2	B	107	THR	3.1
2	B	189	VAL	3.1
1	A	124	PHE	3.1
2	B	205	LEU	3.0
2	B	93	GLY	3.0
2	B	85	GLN	3.0
1	A	247	PRO	3.0
2	B	13	LYS	2.9
2	B	239	TRP	2.9
1	A	62	ALA	2.9
1	A	132	ILE	2.9
2	B	204	GLU	2.8
1	A	214	LEU	2.8
1	A	76	ASP	2.8
2	B	94	ILE	2.8
1	A	17	ASP	2.8
1	A	244	ILE	2.7
2	B	234	LEU	2.7
1	A	293	ILE	2.7
2	B	238	LYS	2.7
1	A	246	LEU	2.7
2	B	242	GLN	2.7
2	B	315	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	236	PRO	2.6
1	A	285	GLY	2.6
1	A	301	LEU	2.5
1	A	16	MET	2.5
2	B	165	THR	2.5
1	A	297	GLU	2.5
2	B	89	GLU	2.5
1	A	253	THR	2.5
2	B	208	HIS	2.5
1	A	295	LEU	2.5
1	A	30	LYS	2.4
2	B	118	VAL	2.4
2	B	196	GLY	2.4
2	B	91	GLN	2.4
1	A	303	LEU	2.3
2	B	109	LEU	2.3
2	B	278	GLN	2.3
2	B	69	THR	2.3
1	A	15	GLY	2.3
2	B	150	PRO	2.3
2	B	155	GLY	2.3
2	B	92	LEU	2.3
1	A	255	ASN	2.3
1	A	279	LEU	2.2
1	A	111	VAL	2.2
1	A	544	GLY	2.2
2	B	14	PRO	2.2
1	A	87	PHE	2.2
2	B	65	LYS	2.1
2	B	102	LYS	2.1
2	B	193	LEU	2.1
1	A	19	PRO	2.1
2	B	371	ALA	2.1
2	B	87	PHE	2.1
1	A	10	VAL	2.1
2	B	425	LEU	2.1
1	A	11	LYS	2.0
1	A	534	ALA	2.0
1	A	77	PHE	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](#)

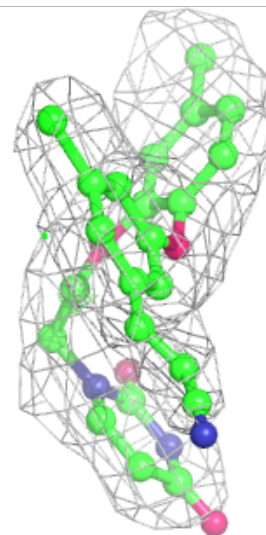
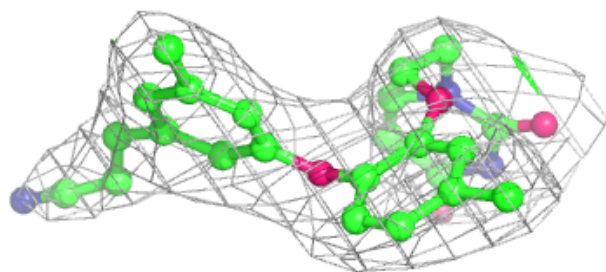
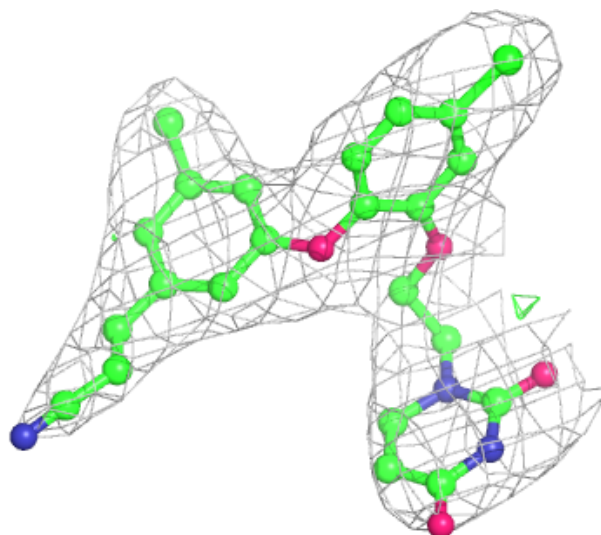
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	494	A	601	30/30	0.90	0.21	45,53,67,71	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 494 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.