



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:03 pm BST

PDB ID : 6DTW
Title : HIV-1 Reverse Transcriptase Y181C Mutant in complex with JLJ 578
Authors : Sasaki, T.; Gannam, Z.T.K.; Anderson, K.S.; Jorgensen, W.L.; Lee, W.
Deposited on : 2018-06-18
Resolution : 2.74 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

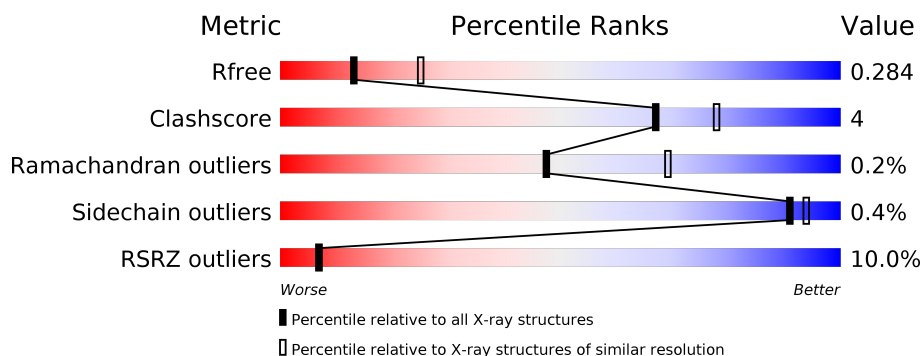
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	
2	B	428	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7815 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	544	Total	C	N	O	S	0	0	0
			4407	2851	730	817	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

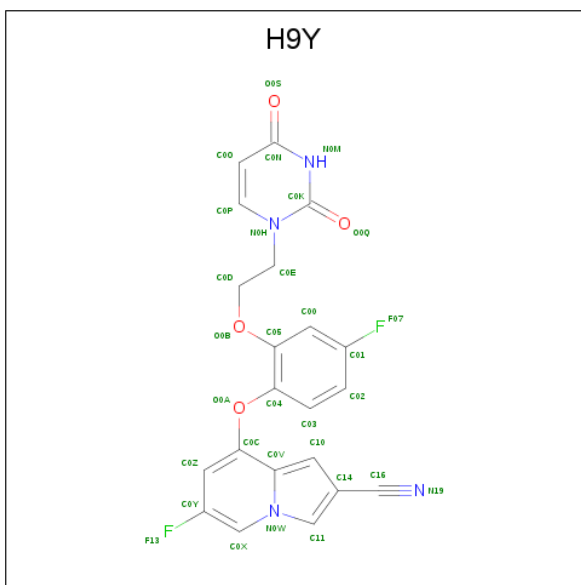
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3342	2174	552	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 8-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]-4-fluorophenoxy}-6-fluoroindolizine-2-carbonitrile (three-letter code: H9Y) (formula: C₂₁H₁₄F₂N₄O₄) (labeled as "Ligand of Interest" by author).

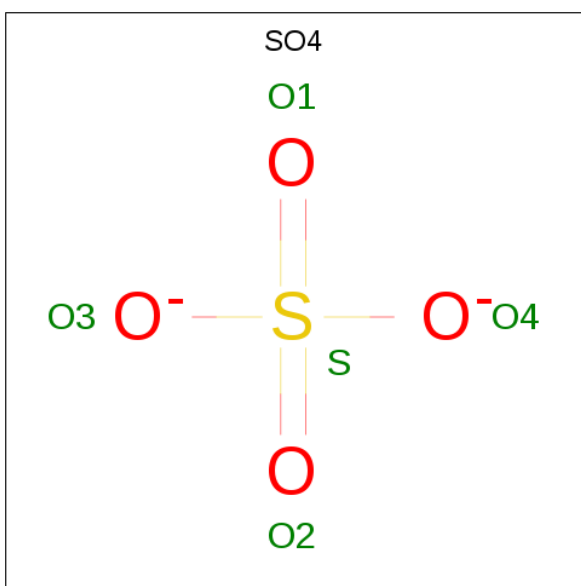


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			31	21	2	4	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

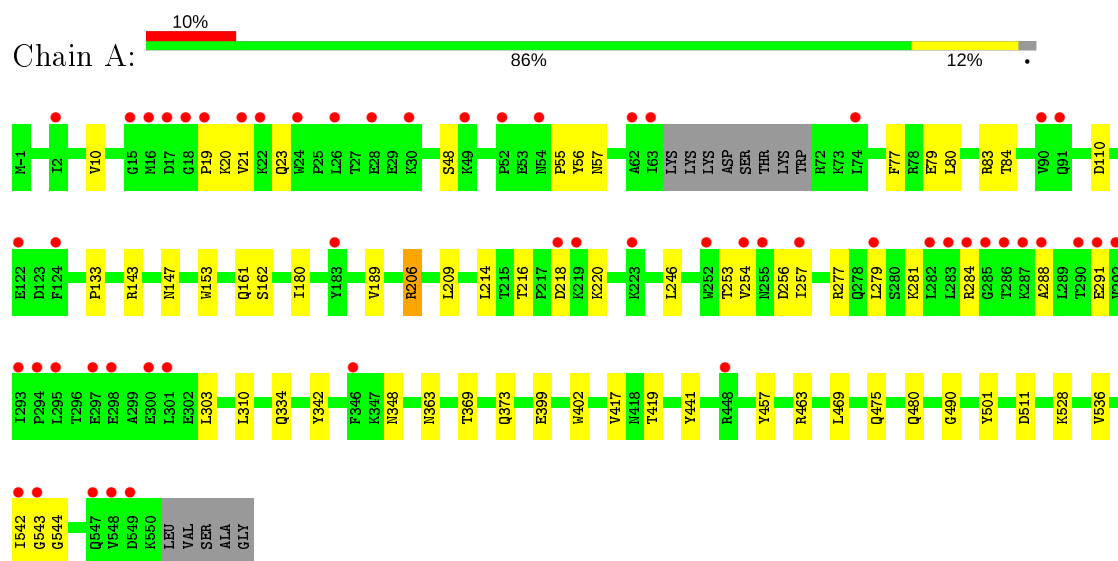
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	10	Total	O	0	0
			10	10		

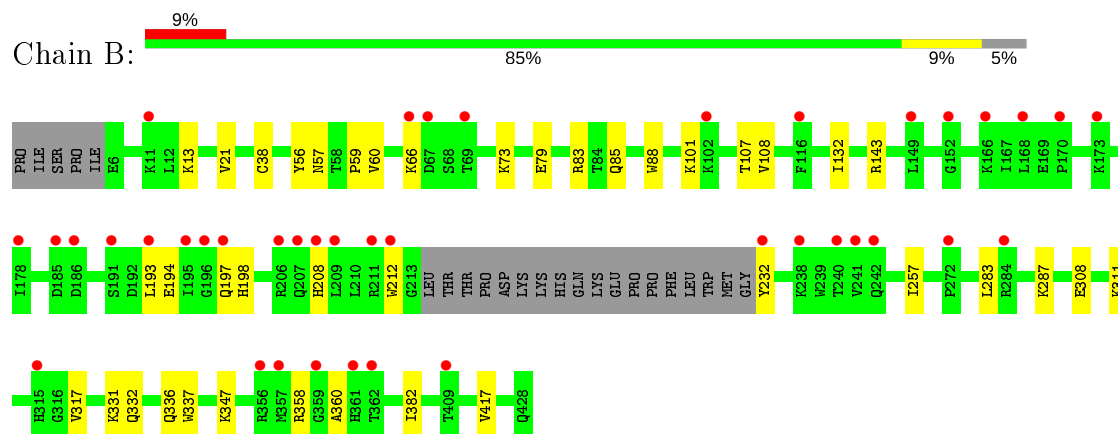
3 Residue-property plots [i](#)

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



- Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.29 Å 73.90 Å 108.25 Å 90.00° 99.50° 90.00°	Depositor
Resolution (Å)	34.90 – 2.74 34.90 – 2.74	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.90-2.74) 98.4 (34.90-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.72 Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.242 , 0.284 0.243 , 0.284	Depositor DCC
R_{free} test set	2000 reflections (6.08%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.0	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	0.91	EDS
Total number of atoms	7815	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: H9Y, MG, 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	0/4521	0.42	0/6147
2	B	0.24	0/3437	0.41	0/4670
All	All	0.24	0/7958	0.41	0/10817

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	4407	0	4448	40	0
2	B	3342	0	3357	22	0
3	A	31	0	0	0	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
6	A	19	0	0	1	0
6	B	10	0	0	0	0
All	All	7815	0	7805	61	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 (61) 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:281:LYS:HG2	1:A:284:ARG:HH11	1.65	0.62
1:A:490:GLY:O	1:A:528:LYS:NZ	2.29	0.61
1:A:369:THR:O	1:A:373:GLN:HG2	2.00	0.61
1:A:55:PRO:HG2	1:A:143:ARG:HH22	1.68	0.59
2:B:66:LYS:HE2	2:B:358:ARG:HH22	1.69	0.56
1:A:536:VAL:HB	1:A:542:ILE:HD13	1.86	0.56
2:B:56:TYR:O	2:B:143:ARG:NH2	2.39	0.54
2:B:308:GLU:HA	2:B:311:LYS:HE2	1.90	0.53
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.39	0.52
1:A:279:LEU:HD11	1:A:303:LEU:HD11	1.93	0.51
1:A:48:SER:HG	1:A:147:ASN:HD21	1.59	0.51
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.93	0.51
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.92	0.50
1:A:79:GLU:OE2	1:A:83:ARG:NH2	2.44	0.50
2:B:317:VAL:HG22	2:B:347:LYS:HD2	1.92	0.49
1:A:543:GLY:HA3	2:B:283:LEU:O	2.13	0.49
1:A:253:THR:HG23	1:A:256:ASP:H	1.79	0.48
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.95	0.48
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.96	0.48
1:A:21:VAL:O	1:A:57:ASN:ND2	2.45	0.48
2:B:332:GLN:HB2	2:B:336:GLN:HB2	1.96	0.48
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.80	0.46
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.51	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.46
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.51	0.46
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.97	0.46
2:B:85:GLN:HG3	2:B:88:TRP:CZ2	2.50	0.46
2:B:60:VAL:HG21	2:B:73:LYS:HE2	1.96	0.46
1:A:23:GLN:HG2	1:A:133:PRO:HG3	1.98	0.46
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.31	0.46
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.16	0.45
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.98	0.45
2:B:21:VAL:O	2:B:57:ASN:ND2	2.43	0.45
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.99	0.45
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.99	0.45
2:B:79:GLU:O	2:B:83:ARG:HG2	2.17	0.44
1:A:281:LYS:HA	1:A:284:ARG:HG3	1.99	0.44
2:B:257:ILE:HB	2:B:283:LEU:HD21	2.00	0.44
1:A:253:THR:O	1:A:257:ILE:HG13	2.18	0.43
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.83	0.43
1:A:110:ASP:N	1:A:110:ASP:OD1	2.48	0.43
1:A:441:TYR:CG	1:A:544:GLY:HA3	2.53	0.43
2:B:108:VAL:HB	2:B:232:TYR:HB2	2.01	0.43
1:A:463:ARG:NH1	6:A:705:HOH:O	2.48	0.43
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.34	0.43
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.53	0.42
1:A:288:ALA:HB3	1:A:291:GLU:HB2	2.01	0.42
1:A:254:VAL:HG23	1:A:291:GLU:HB3	2.01	0.42
2:B:13:LYS:HE3	2:B:85:GLN:H	1.85	0.42
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.50	0.41
1:A:80:LEU:O	1:A:84:THR:OG1	2.28	0.41
1:A:417:VAL:HG22	1:A:419:THR:HG23	2.02	0.41
2:B:194:GLU:HB3	2:B:197:GLN:HG2	2.01	0.41
1:A:20:LYS:HE3	1:A:56:TYR:CE1	2.56	0.41
1:A:55:PRO:HG2	1:A:143:ARG:NH2	2.33	0.40
1:A:206:ARG:NH2	1:A:216:THR:O	2.54	0.40
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.40
2:B:208:HIS:O	2:B:212:TRP:HD1	2.05	0.40
1:A:161:GLN:HG3	1:A:162:SER:N	2.36	0.40
2:B:101:LYS:HD3	2:B:382:ILE:HG23	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	540/557 (97%)	519 (96%)	20 (4%)	1 (0%)	47	69
2	B	401/428 (94%)	387 (96%)	13 (3%)	1 (0%)	47	69
All	All	941/985 (96%)	906 (96%)	33 (4%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	LYS
2	B	360	ALA

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	483/495 (98%)	482 (100%)	1 (0%)	93	96
2	B	366/390 (94%)	364 (100%)	2 (0%)	88	92
All	All	849/885 (96%)	846 (100%)	3 (0%)	91	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
2	B	287	LYS
2	B	417	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
5	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.06	0
3	H9Y	A	601	-	29,34,34	1.60	5 (17%)	30,48,48	1.72	7 (23%)

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	H9Y	A	601	-	-	0/10/12/12	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	H9Y	C0Z-C0Y	4.36	1.45	1.37
3	A	601	H9Y	C0P-N0H	3.86	1.42	1.35
3	A	601	H9Y	C02-C01	2.42	1.41	1.37
3	A	601	H9Y	C00-C05	2.36	1.43	1.38
3	A	601	H9Y	C00-C01	2.32	1.41	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	H9Y	C0X-C0Y-C0Z	-3.95	117.75	122.01
3	A	601	H9Y	C0O-C0N-N0M	-3.87	114.80	123.31
3	A	601	H9Y	C0C-C0V-N0W	-2.79	115.43	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	H9Y	F13-C0Y-C0X	2.71	122.76	118.36
3	A	601	H9Y	C0C-C0Z-C0Y	2.55	121.66	116.48
3	A	601	H9Y	C02-C01-C00	-2.45	120.11	123.29
3	A	601	H9Y	O0B-C0D-C0E	2.07	109.39	107.28

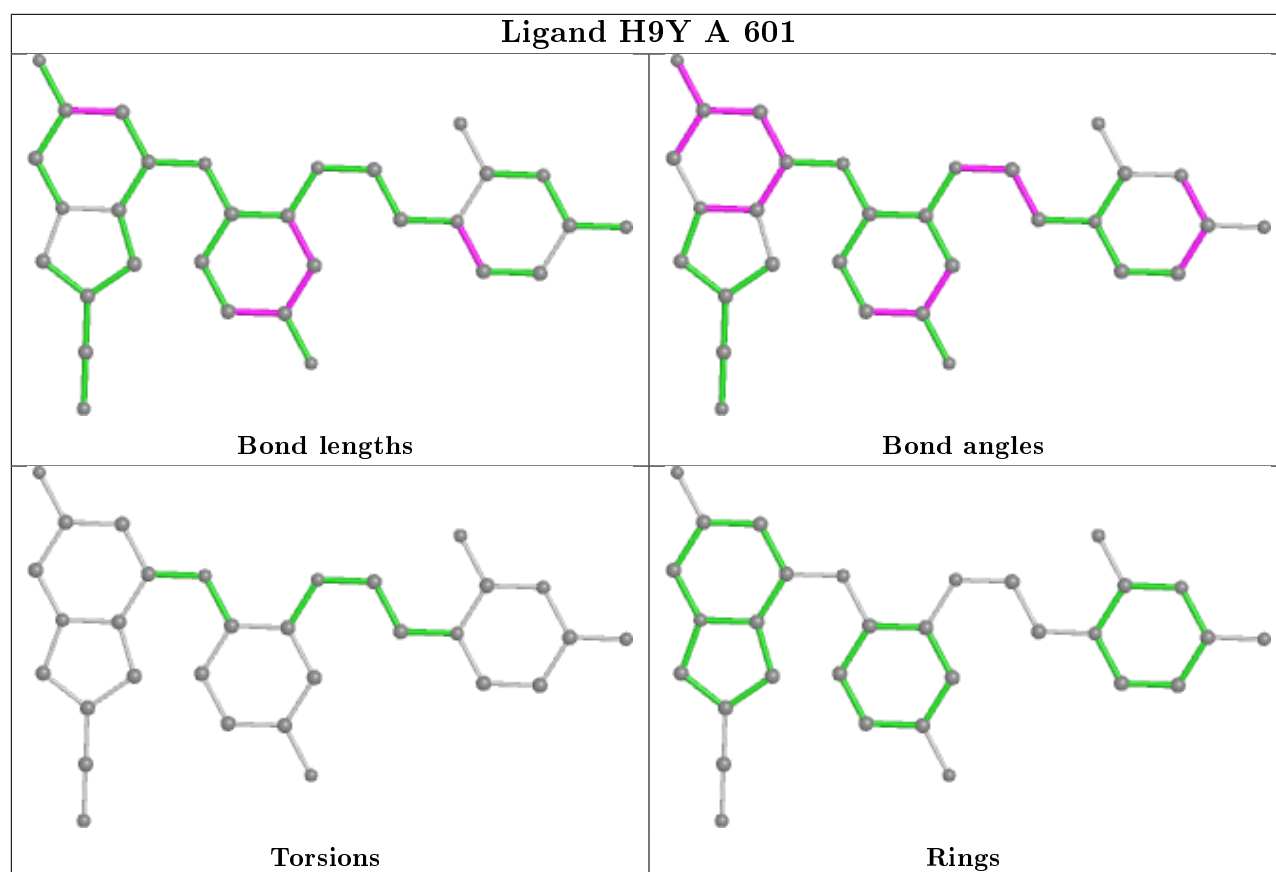
There are no chirality outliers.

There are no torsion outliers.

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, 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	544/557 (97%)	0.51	55 (10%) 7 6	48, 89, 169, 196	0
2	B	405/428 (94%)	0.50	40 (9%) 7 7	52, 87, 153, 182	0
All	All	949/985 (96%)	0.50	95 (10%) 7 7	48, 88, 163, 196	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	17.3
1	A	19	PRO	9.2
2	B	232	TYR	8.0
1	A	218	ASP	7.0
1	A	287	LYS	6.4
1	A	295	LEU	6.2
1	A	301	LEU	5.5
1	A	288	ALA	5.4
1	A	54	ASN	5.1
2	B	191	SER	4.8
1	A	292	VAL	4.7
1	A	252	TRP	4.7
1	A	24	TRP	4.6
1	A	297	GLU	4.6
2	B	149	LEU	4.5
1	A	22	LYS	4.4
1	A	294	PRO	4.4
2	B	356	ARG	4.3
2	B	212	TRP	4.3
1	A	300	GLU	4.2
1	A	286	THR	4.0
2	B	211	ARG	4.0
1	A	298	GLU	4.0
2	B	284	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	219	LYS	3.7
2	B	170	PRO	3.6
1	A	548	VAL	3.6
2	B	195	ILE	3.6
2	B	357	MET	3.5
1	A	254	VAL	3.5
1	A	283	LEU	3.5
1	A	279	LEU	3.4
2	B	409	THR	3.3
1	A	74	LEU	3.3
1	A	257	ILE	3.3
2	B	173	LYS	3.2
1	A	49	LYS	3.2
1	A	62	ALA	3.2
2	B	209	LEU	3.1
1	A	293	ILE	3.1
2	B	186	ASP	3.1
2	B	238	LYS	3.1
1	A	26	LEU	3.0
1	A	542	ILE	3.0
1	A	291	GLU	2.9
1	A	21	VAL	2.9
2	B	206	ARG	2.9
2	B	272	PRO	2.9
2	B	196	GLY	2.9
2	B	152	GLY	2.8
1	A	282	LEU	2.8
2	B	241	VAL	2.8
2	B	185	ASP	2.7
2	B	193	LEU	2.7
1	A	16	MET	2.7
1	A	549	ASP	2.7
1	A	15	GLY	2.7
1	A	63	ILE	2.7
1	A	290	THR	2.6
1	A	543	GLY	2.6
1	A	448	ARG	2.6
1	A	346	PHE	2.6
2	B	178	ILE	2.5
2	B	361	HIS	2.5
2	B	359	GLY	2.5
2	B	11	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	17	ASP	2.5
1	A	91	GLN	2.5
1	A	90	VAL	2.5
1	A	223	LYS	2.5
1	A	122	GLU	2.5
1	A	2	ILE	2.4
2	B	168	LEU	2.4
2	B	362	THR	2.4
2	B	67	ASP	2.4
2	B	69	THR	2.4
2	B	242	GLN	2.3
1	A	124	PHE	2.3
1	A	284	ARG	2.3
1	A	547	GLN	2.2
2	B	166	LYS	2.2
2	B	116	PHE	2.2
2	B	197	GLN	2.2
1	A	285	GLY	2.1
1	A	183	TYR	2.1
1	A	18	GLY	2.1
2	B	208	HIS	2.1
1	A	28	GLU	2.1
2	B	240	THR	2.1
1	A	30	LYS	2.0
1	A	255	ASN	2.0
2	B	102	LYS	2.0
2	B	315	HIS	2.0
2	B	207	GLN	2.0
2	B	66	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

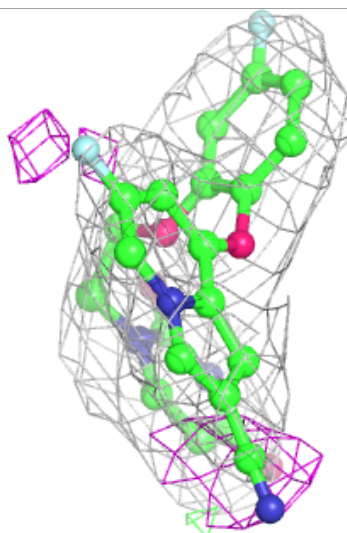
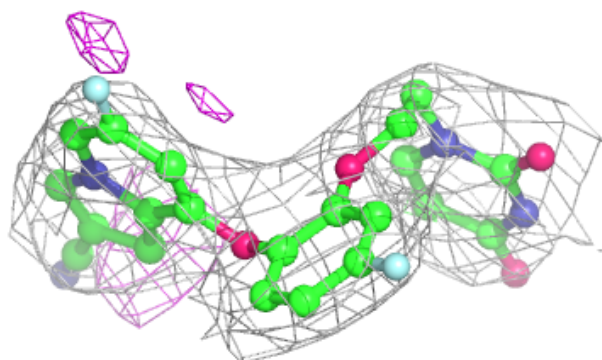
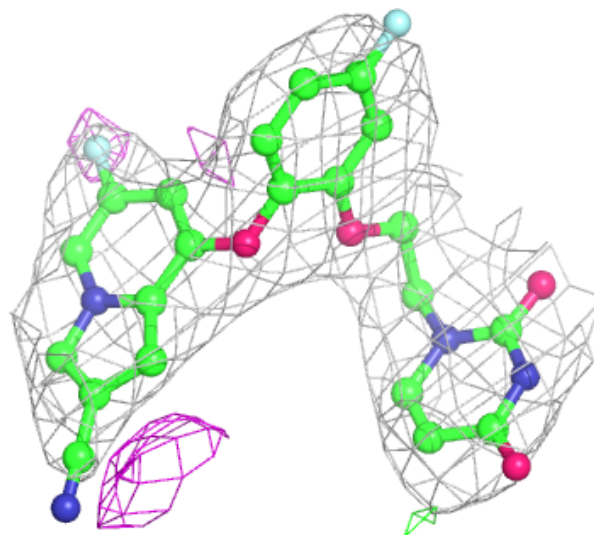
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	603	5/5	0.82	0.19	100,112,130,134	0
4	MG	A	602	1/1	0.82	0.24	85,85,85,85	0
3	H9Y	A	601	31/31	0.92	0.20	56,68,79,97	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 H9Y 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

There are no such residues in this entry.