



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:57 AM UTC

PDB ID : 5C42 / pdb_00005c42
Title : Crystal Structure of HIV-1 Reverse Transcriptase (K101P) Variant in Complex with 8-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)indoline-2-carbonitrile (JLJ555), a non-nucleoside inhibitor
Authors : Frey, K.M.; Gray, W.T.; Anderson, K.S.
Deposited on : 2015-06-17
Resolution : 3.50 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

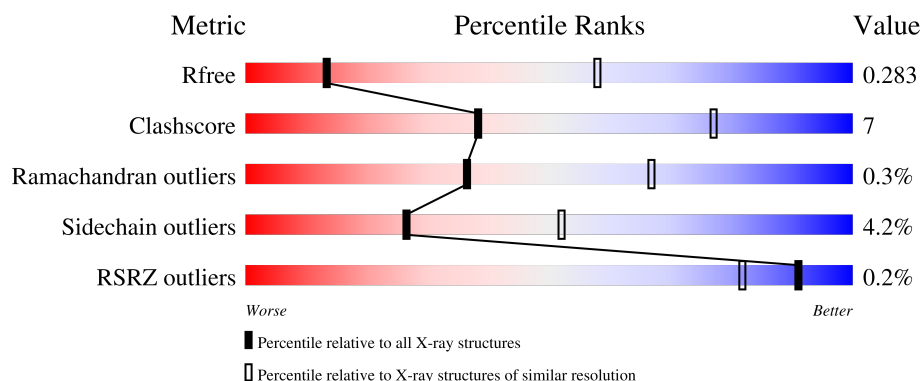
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 ≥ 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	 73% 22% ..
2	B	428	 82% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7923 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 HIV-1 Reverse Transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4391	2842	727	815	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	101	PRO	LYS	engineered mutation	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

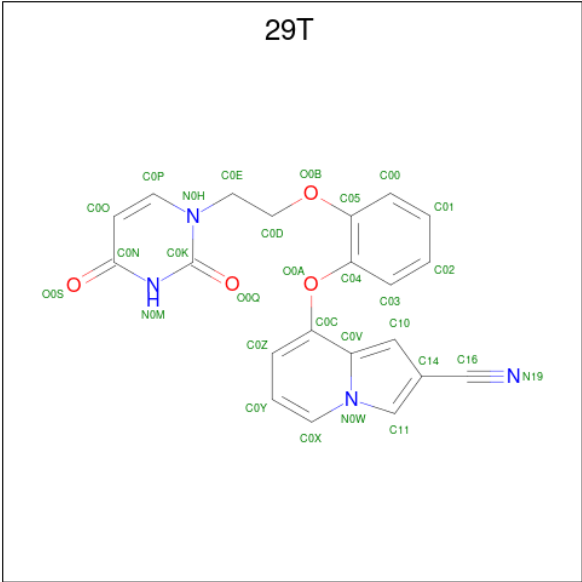
- Molecule 2 is a protein called HIV-1 Reverse Transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3503	2281	582	633	7			

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]phenoxy}indolizine-2-carbonitrile (CCD ID: 29T) (formula: C₂₁H₁₆N₄O₄).

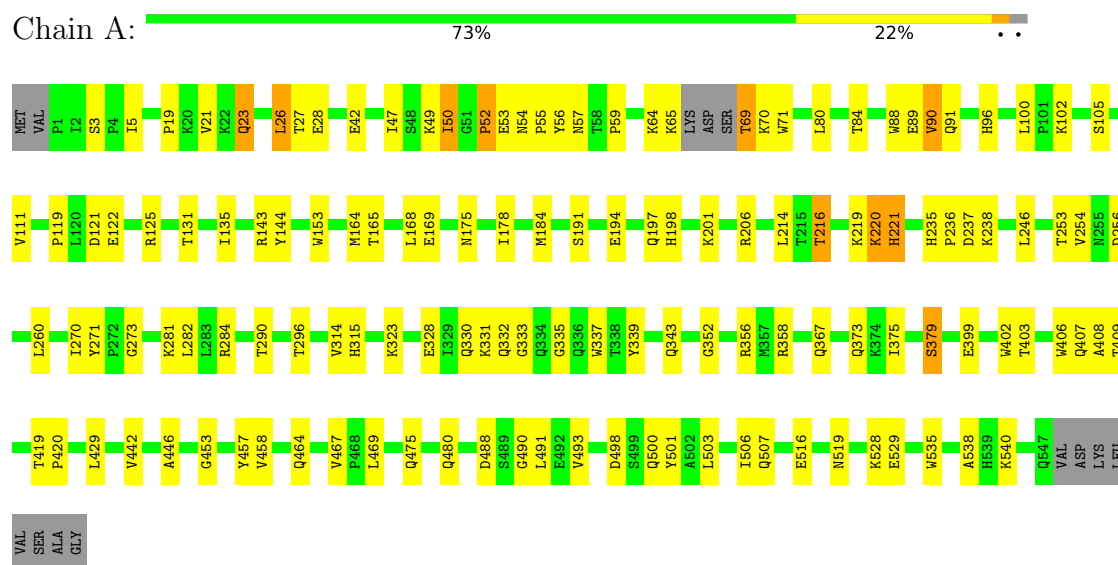


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	21	4	4		

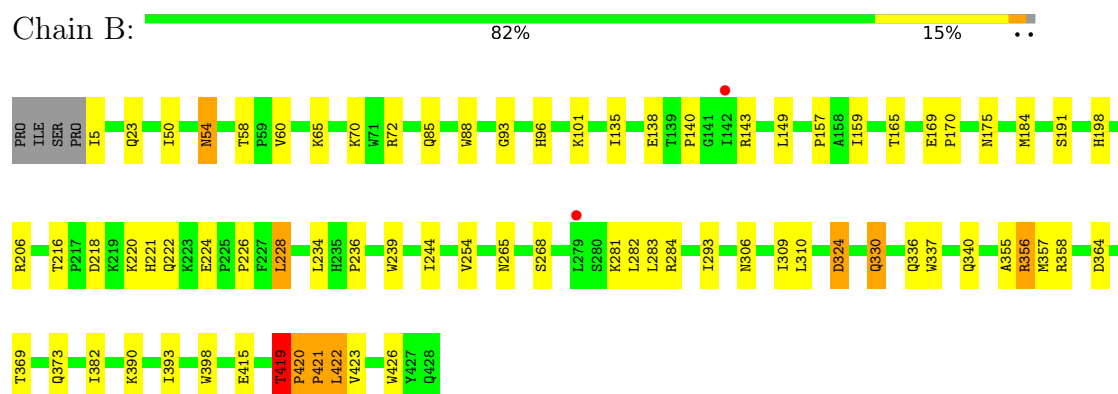
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: HIV-1 Reverse Transcriptase, p66 subunit



- Molecule 2: HIV-1 Reverse Transcriptase, 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	224.20Å 69.01Å 104.28Å 90.00° 106.49° 90.00°	Depositor
Resolution (Å)	38.22 – 3.50 38.22 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.22-3.50) 93.8 (38.22-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.282 0.242 , 0.283	Depositor DCC
R_{free} test set	2000 reflections (8.38%)	wwPDB-VP
Wilson B-factor (Å ²)	127.8	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: 29T

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	0.31	0/4507	0.83	11/6134 (0.2%)
2	B	0.31	0/3606	0.83	8/4901 (0.2%)
All	All	0.31	0/8113	0.83	19/11035 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASN	CA-C-N	14.61	135.06	119.87
1	A	54	ASN	C-N-CA	14.61	135.06	119.87
2	B	420	PRO	CA-C-N	12.83	135.88	119.84
2	B	420	PRO	C-N-CA	12.83	135.88	119.84
1	A	169	GLU	CA-C-N	-8.34	113.22	121.65
1	A	169	GLU	C-N-CA	-8.34	113.22	121.65
1	A	184	MET	CB-CA-C	-6.04	109.60	116.54
2	B	420	PRO	N-CA-C	6.03	118.06	110.70
1	A	335	GLY	N-CA-C	-5.57	106.97	115.00
1	A	52	PRO	CA-C-O	-5.37	115.03	121.48
2	B	54	ASN	CA-C-N	5.34	124.95	119.56
2	B	54	ASN	C-N-CA	5.34	124.95	119.56
1	A	467	VAL	CA-C-N	5.13	124.89	119.76
1	A	467	VAL	C-N-CA	5.13	124.89	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	419	THR	N-CA-C	5.08	121.05	109.81
1	A	96	HIS	CA-C-N	5.04	125.32	119.47
1	A	96	HIS	C-N-CA	5.04	125.32	119.47
2	B	224	GLU	CA-C-N	5.02	125.55	120.38
2	B	224	GLU	C-N-CA	5.02	125.55	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	419	THR	Peptide

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	4391	0	4402	71	0
2	B	3503	0	3530	43	0
3	A	29	0	16	1	0
All	All	7923	0	7948	110	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 7.

All (110) 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:HE	1.49	0.76
1:A:56:TYR:O	1:A:143:ARG:NH2	2.20	0.74
1:A:23:GLN:NE2	1:A:131:THR:O	2.22	0.72
2:B:157:PRO:HG3	2:B:184:MET:HA	1.75	0.69
2:B:221:HIS:HE1	2:B:228:LEU:HD13	1.58	0.68
1:A:26:LEU:HG	1:A:27:THR:HG23	1.76	0.67
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.60	0.66
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:ARG:HE	2:B:357:MET:H	1.46	0.63
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.81	0.63
1:A:100:LEU:HB3	3:A:601:29T:H11	1.81	0.62
2:B:330:GLN:OE1	2:B:340:GLN:NE2	2.33	0.61
2:B:54:ASN:O	2:B:143:ARG:NH2	2.36	0.59
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.85	0.59
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.35	0.59
2:B:191:SER:OG	2:B:198:HIS:ND1	2.28	0.58
2:B:206:ARG:HD2	2:B:218:ASP:HB3	1.86	0.57
2:B:206:ARG:NH1	2:B:216:THR:OG1	2.37	0.57
1:A:64:LYS:HZ1	1:A:71:TRP:CD1	2.23	0.57
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.86	0.56
2:B:282:LEU:HG	2:B:293:ILE:HD11	1.87	0.56
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.71	0.55
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.87	0.54
1:A:282:LEU:HD21	1:A:296:THR:HG23	1.88	0.54
1:A:52:PRO:HA	1:A:53:GLU:C	2.32	0.54
1:A:50:ILE:O	1:A:143:ARG:HB2	2.07	0.54
1:A:281:LYS:HA	1:A:284:ARG:HG3	1.88	0.54
2:B:423:VAL:HG12	2:B:426:TRP:CE3	2.42	0.54
1:A:3:SER:HB2	1:A:119:PRO:HD3	1.89	0.53
1:A:490:GLY:O	1:A:528:LYS:NZ	2.32	0.53
1:A:102:LYS:NZ	1:A:236:PRO:O	2.28	0.53
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.45	0.52
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.91	0.52
2:B:149:LEU:HD21	2:B:159:ILE:HD12	1.91	0.52
2:B:65:LYS:HA	2:B:72:ARG:HD2	1.92	0.51
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.92	0.51
1:A:42:GLU:OE1	1:A:49:LYS:NZ	2.42	0.51
1:A:356:ARG:NE	1:A:358:ARG:O	2.44	0.51
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.25	0.51
2:B:220:LYS:C	2:B:222:GLN:H	2.17	0.51
2:B:324:ASP:N	2:B:324:ASP:OD1	2.45	0.50
1:A:253:THR:HG23	1:A:256:ASP:H	1.77	0.49
1:A:328:GLU:HG2	1:A:330:GLN:HE22	1.77	0.49
1:A:337:TRP:HE1	1:A:367:GLN:NE2	2.10	0.49
1:A:69:THR:HG23	1:A:70:LYS:HG3	1.95	0.48
1:A:28:GLU:HG3	1:A:135:ILE:HD13	1.96	0.48
1:A:88:TRP:CH2	2:B:140:PRO:HB2	2.49	0.48
2:B:423:VAL:HG12	2:B:426:TRP:HE3	1.77	0.47
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CH2	2:B:420:PRO:HD2	2.49	0.47
2:B:281:LYS:O	2:B:284:ARG:HB2	2.15	0.47
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	0.46
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.97	0.46
2:B:50:ILE:HG12	2:B:143:ARG:HB3	1.98	0.46
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.98	0.46
2:B:96:HIS:NE2	2:B:382:ILE:O	2.41	0.46
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.51	0.45
1:A:446:ALA:HA	1:A:453:GLY:HA3	1.97	0.45
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.98	0.45
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.52	0.45
1:A:191:SER:OG	1:A:198:HIS:ND1	2.49	0.45
2:B:244:ILE:HD12	2:B:310:LEU:HD11	1.98	0.45
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.99	0.45
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.64	0.45
1:A:122:GLU:OE1	1:A:125:ARG:NH1	2.50	0.44
1:A:194:GLU:HB3	1:A:197:GLN:HG3	1.99	0.44
2:B:88:TRP:O	2:B:93:GLY:HA2	2.18	0.44
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.52	0.44
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.99	0.44
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.53	0.44
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.25	0.44
1:A:253:THR:OG1	1:A:254:VAL:N	2.50	0.44
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.33	0.43
1:A:164:MET:HE1	1:A:214:LEU:HD13	2.00	0.43
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.83	0.43
2:B:422:LEU:O	2:B:422:LEU:HD23	2.17	0.43
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.86	0.43
1:A:90:VAL:HG23	1:A:91:GLN:H	1.82	0.43
1:A:246:LEU:HD22	1:A:260:LEU:HD12	2.00	0.43
1:A:323:LYS:HB2	1:A:343:GLN:NE2	2.34	0.43
2:B:265:ASN:O	2:B:268:SER:OG	2.27	0.43
2:B:336:GLN:HE21	2:B:358:ARG:NH2	2.17	0.43
1:A:220:LYS:HB3	1:A:221:HIS:H	1.68	0.42
1:A:271:TYR:CD2	1:A:314:VAL:HG12	2.54	0.42
1:A:375:ILE:O	1:A:379:SER:HB2	2.20	0.42
1:A:270:ILE:HG23	1:A:271:TYR:H	1.83	0.42
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.83	0.42
1:A:57:ASN:OD1	1:A:131:THR:OG1	2.25	0.42
2:B:169:GLU:HB3	2:B:170:PRO:HD3	2.00	0.42
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:OG	1:A:198:HIS:ND1	2.52	0.42
2:B:220:LYS:HB3	2:B:221:HIS:H	1.73	0.42
1:A:131:THR:HG23	1:A:143:ARG:HD2	2.01	0.41
1:A:235:HIS:HB2	1:A:238:LYS:O	2.20	0.41
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.62	0.41
1:A:19:PRO:O	1:A:56:TYR:HB3	2.21	0.41
1:A:206:ARG:HE	1:A:216:THR:HB	1.85	0.41
1:A:491:LEU:HB3	1:A:529:GLU:HG3	2.02	0.41
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.86	0.41
2:B:101:LYS:HD3	2:B:382:ILE:HG23	2.03	0.41
2:B:135:ILE:O	2:B:138:GLU:HG3	2.19	0.41
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.56	0.41
1:A:238:LYS:HD2	1:A:315:HIS:NE2	2.36	0.41
1:A:191:SER:HG	1:A:198:HIS:CE1	2.39	0.41
1:A:273:GLY:HA2	1:A:332:GLN:NE2	2.36	0.41
2:B:421:PRO:C	2:B:423:VAL:H	2.29	0.41
1:A:419:THR:HA	1:A:420:PRO:HD3	1.84	0.41
2:B:23:GLN:HE22	2:B:60:VAL:H	1.68	0.41
2:B:336:GLN:HG2	2:B:355:ALA:HB2	2.03	0.40
2:B:356:ARG:HA	2:B:356:ARG:HD2	1.82	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%)	513 (95%)	27 (5%)	0	100	100
2	B	422/428 (99%)	394 (93%)	25 (6%)	3 (1%)	18	51
All	All	962/985 (98%)	907 (94%)	52 (5%)	3 (0%)	36	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	422	LEU
2	B	226	PRO
2	B	421	PRO

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%)	452 (95%)	25 (5%)	21	47
2	B	384/390 (98%)	373 (97%)	11 (3%)	37	60
All	All	861/885 (97%)	825 (96%)	36 (4%)	26	52

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	26	LEU
1	A	50	ILE
1	A	65	LYS
1	A	69	THR
1	A	89	GLU
1	A	90	VAL
1	A	111	VAL
1	A	165	THR
1	A	168	LEU
1	A	175	ASN
1	A	178	ILE
1	A	216	THR
1	A	219	LYS
1	A	220	LYS
1	A	221	HIS
1	A	237	ASP
1	A	290	THR
1	A	373	GLN
1	A	379	SER
1	A	403	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	409	THR
1	A	493	VAL
1	A	500	GLN
1	A	507	GLN
2	B	5	ILE
2	B	58	THR
2	B	70	LYS
2	B	165	THR
2	B	175	ASN
2	B	228	LEU
2	B	234	LEU
2	B	324	ASP
2	B	330	GLN
2	B	356	ARG
2	B	419	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	367	GLN
1	A	394	GLN
1	A	428	GLN
1	A	474	ASN
1	A	507	GLN
1	A	519	ASN
2	B	23	GLN
2	B	175	ASN
2	B	278	GLN
2	B	330	GLN
2	B	332	GLN
2	B	340	GLN
2	B	373	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	29T	A	601	-	32,32,32	1.29	2 (6%)	38,44,44	1.85	8 (21%)

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	29T	A	601	-	-	0/10/12/12	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	29T	C0P-N0H	4.03	1.42	1.37
3	A	601	29T	C0Z-C0C	2.03	1.43	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	29T	C0E-N0H-C0K	7.11	125.55	118.48
3	A	601	29T	C0E-N0H-C0P	-3.84	114.31	119.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	29T	C0X-N0W-C0V	2.75	125.73	121.77
3	A	601	29T	C0X-N0W-C11	-2.70	125.50	130.31
3	A	601	29T	C11-C14-C16	2.34	129.53	125.22
3	A	601	29T	C10-C14-C16	-2.28	121.87	125.61
3	A	601	29T	C0D-C0E-N0H	2.19	115.91	111.70
3	A	601	29T	O0Q-C0K-N0H	2.08	124.63	122.87

There are no chirality outliers.

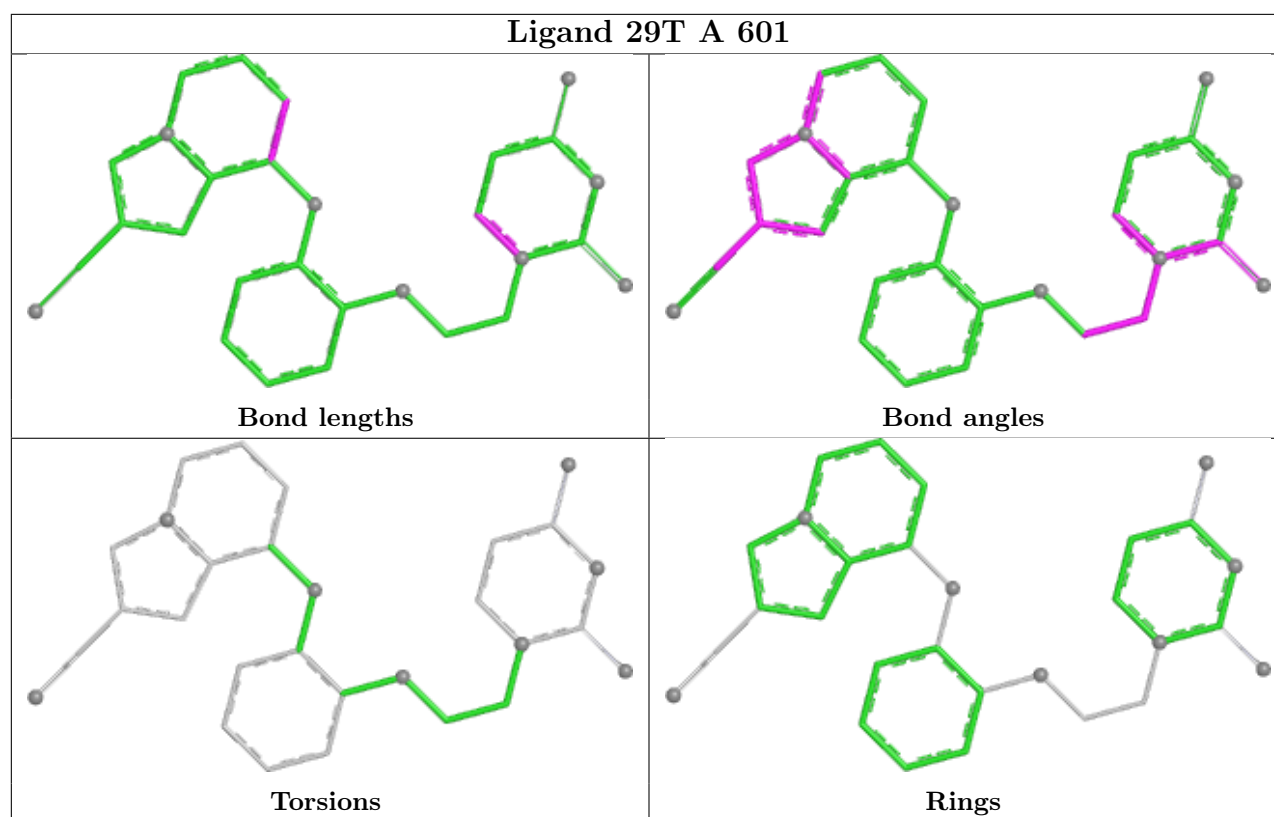
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	29T	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, 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%)	-0.41	0	100 100	98, 143, 187, 263	1 (0%)
2	B	424/428 (99%)	-0.42	2 (0%)	87 68	91, 132, 216, 290	0
All	All	968/985 (98%)	-0.42	2 (0%)	91 82	91, 139, 208, 290	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	279	LEU	2.9
2	B	142	ILE	2.3

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 oligosaccharides 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.

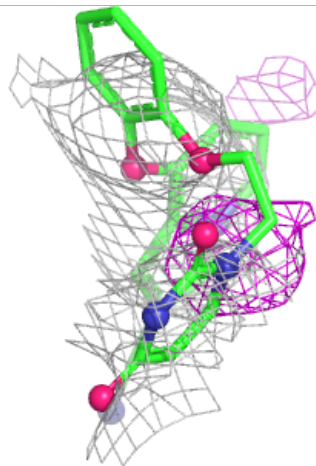
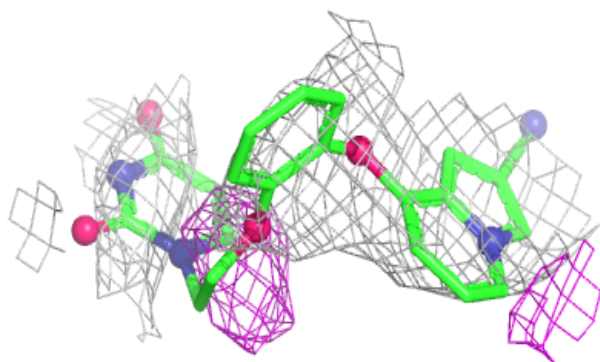
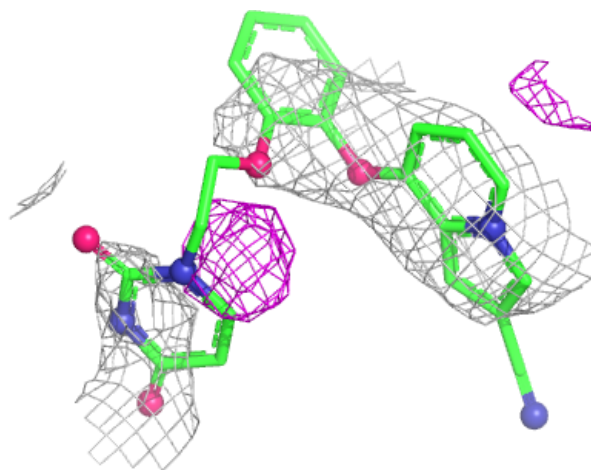
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	29T	A	601	29/29	0.92	0.11	112,132,151,153	0

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 29T 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.