wwPDB X-ray Structure Validation Summary Report (i)

May 7, 2026 – 11:07 AM EDT

PDB ID	:	1SV5 / pdb_00001sv5
Title	:	CRYSTAL STRUCTURE OF K103N MUTANT HIV-1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH JANSSEN-R165335
Authors	:	Das, K.; Arnold, E.
Deposited on	:	2004-03-27
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

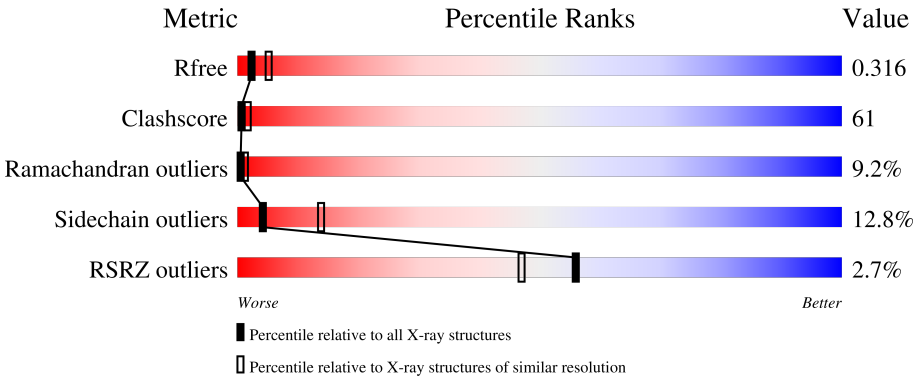
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 <=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	560	2% 23% 57% 16%
2	B	430	3% 28% 48% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	65B	A	600	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7905 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4435	2873	739	816	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

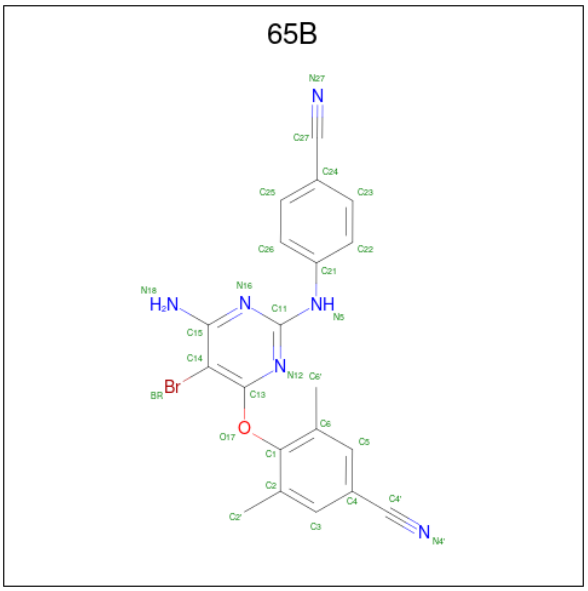
- Molecule 2 is a protein called Reverse Transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3442	2238	570	628	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-({6-AMINO-5-BROMO-2-[(4-CYANOPHENYL)AMINO]PYRIMIDIN-4-YL}OXY)-3,5-DIMETHYLBENZONITRILE (CCD ID: 65B) (formula: $C_{20}H_{15}BrN_6O$).



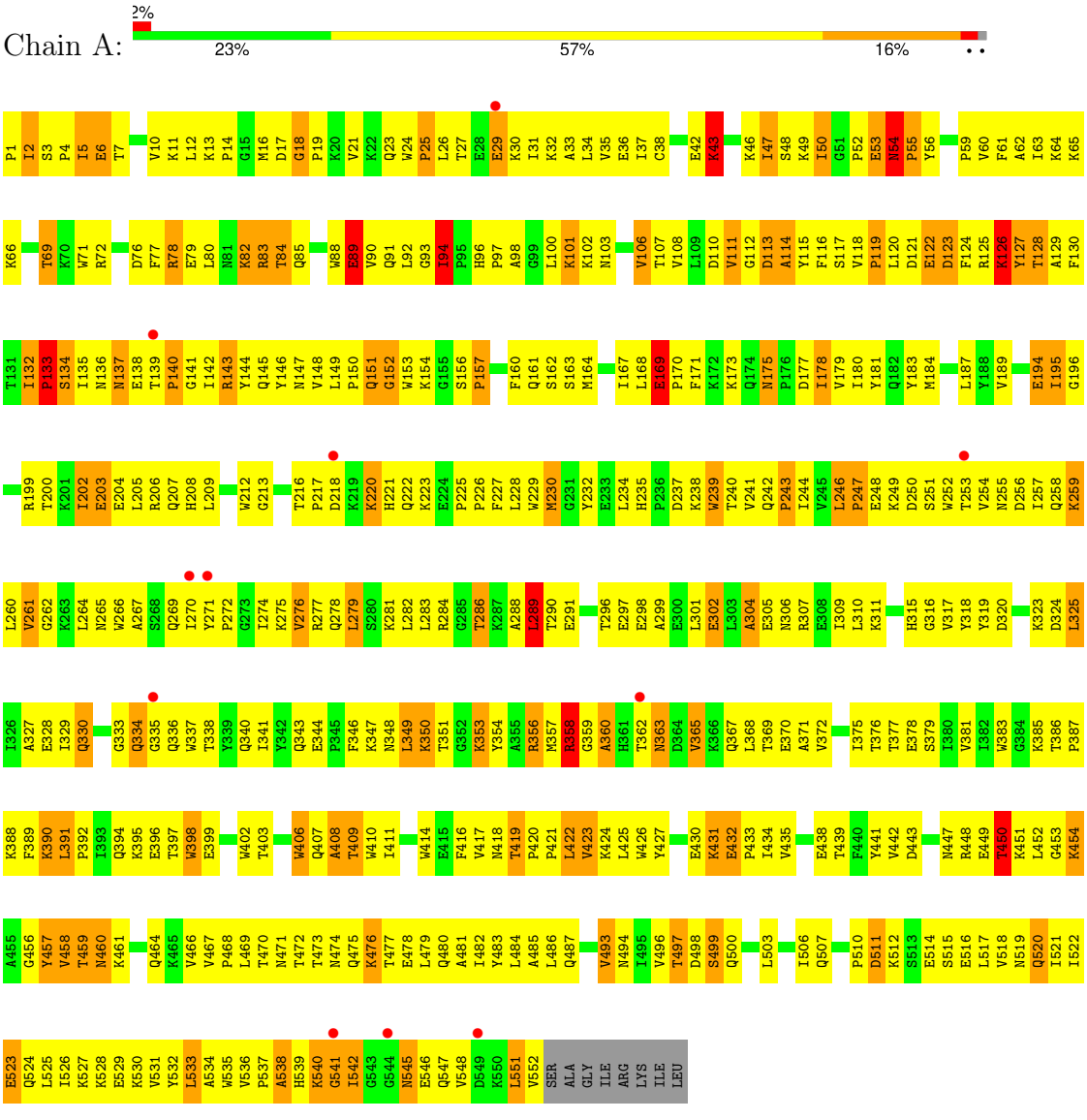
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	A	1	28	1	20	6	1	0	0

3 Residue-property plots (i)

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.

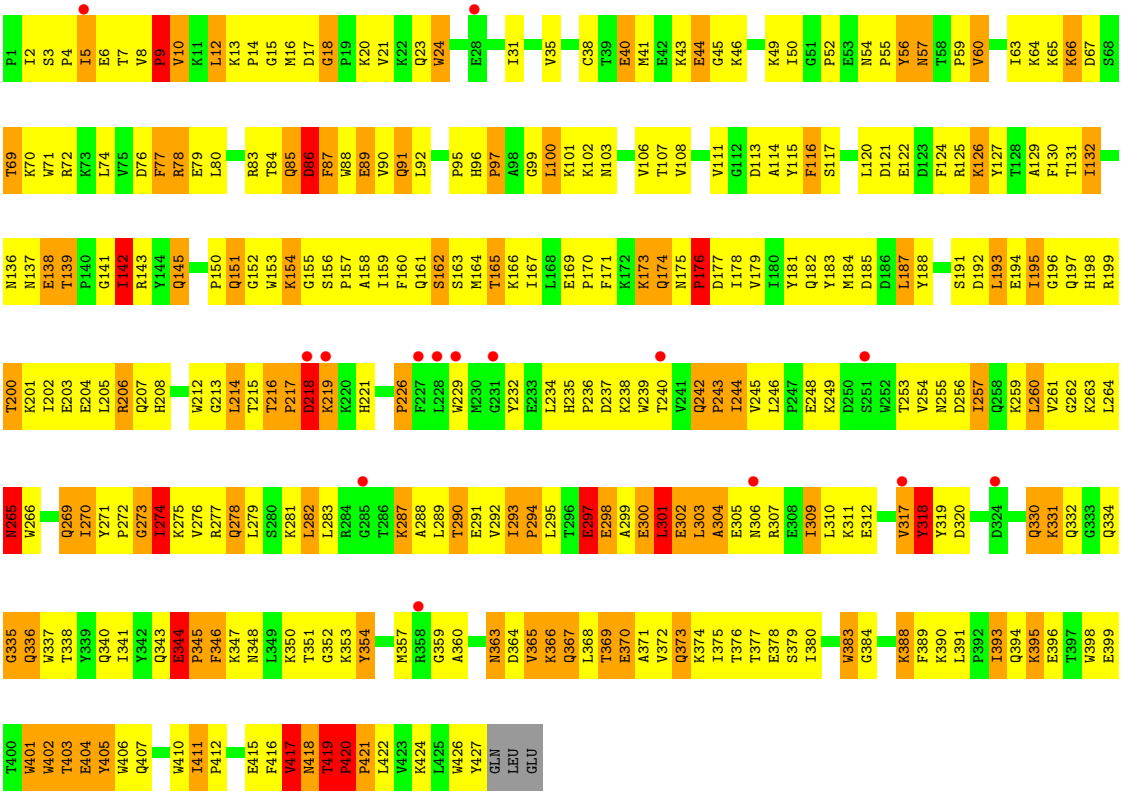
• Molecule 1: Reverse Transcriptase

Chain A:



• Molecule 2: Reverse Transcriptase

Chain B:


P1 I2 S3 P4 I5 E6 T7 V8 P9 V10 K11 L12 K13 P14 G15 M16 D17 G18 P19 K20 V21 K22 Q23 W24 E28 I31 V35 C38 T39 E40 M41 E42 K43 E44 G45 K46 K49 I50 G51 P52 E53 N54 P55 Y56 M57 T58 P59 V60 I63 K64 K65 K66 D67 S68
T69 K70 W71 R72 K73 L74 V75 D76 F77 R78 E79 L80 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 P95 H96 P97 A98 G99 L100 K101 K102 N103 V106 T107 V108 V111 G112 D113 A114 Y115 F116 S117 L120 D121 E122 D123 F124 R125 K126 Y127 T128 A129 F130 T131 I132
N136 N137 E138 T139 P140 G141 I142 R143 Y144 Q145 P150 Q151 G152 W153 K154 G155 S156 P157 A158 I159 F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 K172 K173 Q174 N175 P176 D177 I178 V179 I180 Y181 Q182 Y183 M184 D185 D186 L187 Y188 S191 D192 L193 E194 I195 G196 Q197 H198 R199
T200 K201 I202 E203 E204 L205 R206 Q207 H208 W212 G213 L214 T215 T216 P217 D218 K219 K220 H221 P226 F227 L228 W229 M230 G231 Y232 E233 L234 H235 P236 D237 K238 W239 T240 V241 Q242 P243 I244 V245 L246 P247 E248 K249 D250 S251 W252 T253 V254 N255 D256 I257 Q258 K259 L260 V261 G262 K263 L264
N265 W266 Q269 I270 Y271 P272 G273 Y274 K275 V276 R277 Q278 L279 S280 K281 L282 L283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 A304 E305 N306 R307 E308 I309 L310 K311 E312 V317 Y318 Y319 D320 D324 Q330 K331 Q332 G333 Q334
G335 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 K350 T351 G352 K353 Y354 M357 R358 G359 A360 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380 W383 G384 K388 F389 K390 L391 P392 I393 Q394 K395 E396 T397 W398 E399
T400 W401 W402 T403 E404 Y405 W406 Q407 W410 I411 P412 E415 F416 V417 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 GLN LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	222.51Å 67.74Å 103.29Å 90.00° 107.47° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.95-2.90) 95.0 (19.95-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.326 0.249 , 0.316	Depositor DCC
R_{free} test set	1624 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7905	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 65B

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	0.72	1/4553 (0.0%)	1.25	50/6196 (0.8%)
2	B	0.81	1/3542 (0.0%)	1.48	71/4826 (1.5%)
All	All	0.76	2/8095 (0.0%)	1.36	121/11022 (1.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	ILE	CA-CB	-6.83	1.47	1.54
2	B	60	VAL	CA-CB	-5.64	1.48	1.55

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	219	LYS	N-CA-C	-14.60	93.76	113.18
2	B	218	ASP	N-CA-C	14.43	132.03	108.52
2	B	89	GLU	N-CA-C	-12.69	97.89	113.50
1	A	132	ILE	CA-C-N	11.64	134.39	119.84
1	A	132	ILE	C-N-CA	11.64	134.39	119.84

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	4435	0	4426	581	0
2	B	3442	0	3399	399	0
3	A	28	0	15	9	0
All	All	7905	0	7840	967	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 61.

The worst 5 of 967 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)
2:B:274:ILE:HG12	2:B:306:ASN:HB3	1.21	1.15
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.27	1.09
2:B:13:LYS:HG2	2:B:87:PHE:HB2	1.37	1.06
2:B:85:GLN:HG3	2:B:154:LYS:HG2	1.31	1.06
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.33	1.06

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	550/560 (98%)	410 (74%)	94 (17%)	46 (8%)	0 1
2	B	425/430 (99%)	310 (73%)	71 (17%)	44 (10%)	0 1
All	All	975/990 (98%)	720 (74%)	165 (17%)	90 (9%)	0 1

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	289	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	334	GLN
1	A	360	ALA
1	A	433	PRO

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	475/500 (95%)	422 (89%)	53 (11%)	6 19
2	B	367/392 (94%)	312 (85%)	55 (15%)	3 10
All	All	842/892 (94%)	734 (87%)	108 (13%)	4 14

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	40	GLU
2	B	177	ASP
2	B	369	THR
2	B	49	LYS
2	B	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	ASN
2	B	348	ASN
1	A	509	GLN
2	B	208	HIS
1	A	487	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 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	65B	A	600	-	30,30,30	2.98	16 (53%)	40,42,42	2.39	7 (17%)

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	65B	A	600	-	-	4/12/12/12	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	65B	C22-C21	7.91	1.52	1.39
3	A	600	65B	C1-C2	4.69	1.48	1.40
3	A	600	65B	C13-N12	4.65	1.39	1.32
3	A	600	65B	C1-C6	4.56	1.48	1.40
3	A	600	65B	C23-C22	4.29	1.45	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	65B	C1-O17-C13	-5.88	110.71	116.84
3	A	600	65B	C14-C13-N12	-5.77	117.57	123.78
3	A	600	65B	O17-C13-C14	5.72	121.58	117.89
3	A	600	65B	C11-N16-C15	5.65	121.17	116.59
3	A	600	65B	N16-C11-N12	-5.27	117.63	126.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	65B	C14-C13-O17-C1
3	A	600	65B	C26-C21-N5-C11
3	A	600	65B	C22-C21-N5-C11
3	A	600	65B	N12-C13-O17-C1

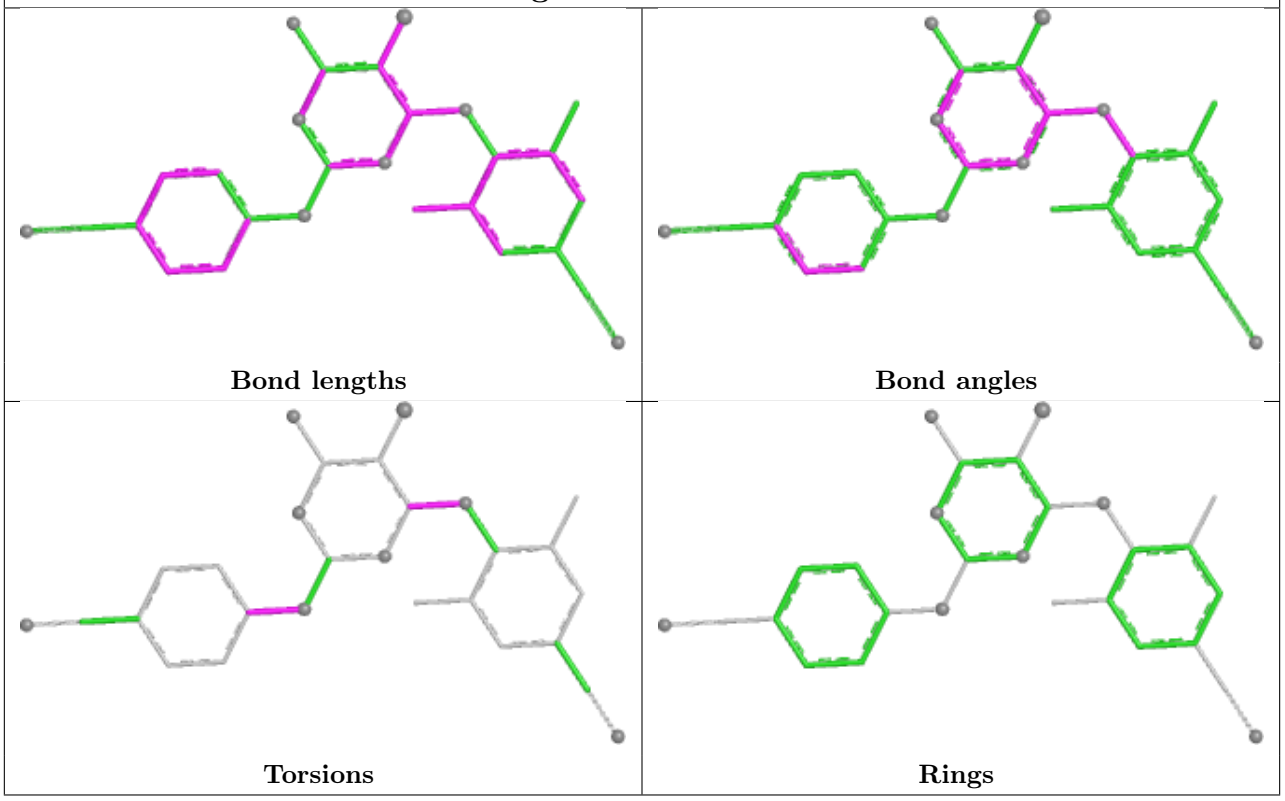
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	65B	9	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 then 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.

Ligand 65B A 600



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^{th} 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	552/560 (98%)	-0.02	11 (1%) 65 56	47, 87, 120, 120	0
2	B	427/430 (99%)	0.03	15 (3%) 47 38	36, 77, 120, 120	0
All	All	979/990 (98%)	0.00	26 (2%) 56 47	36, 83, 120, 120	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	28	GLU	4.0
2	B	228	LEU	4.0
2	B	218	ASP	3.6
2	B	227	PHE	3.4
2	B	358	ARG	3.3

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 oligosaccharides in this entry.

6.4 Ligands

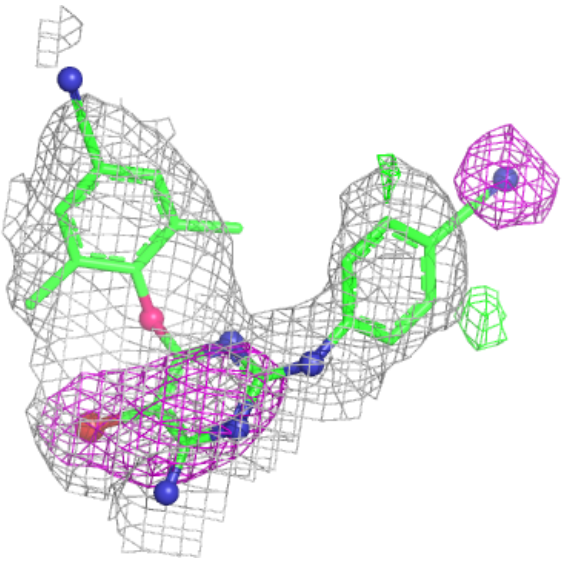
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

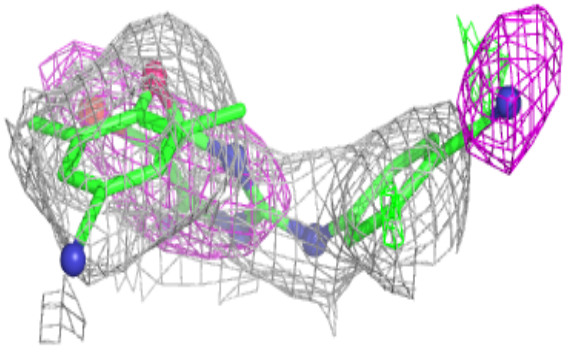
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	65B	A	600	28/28	0.78	0.13	58,72,83,108	0

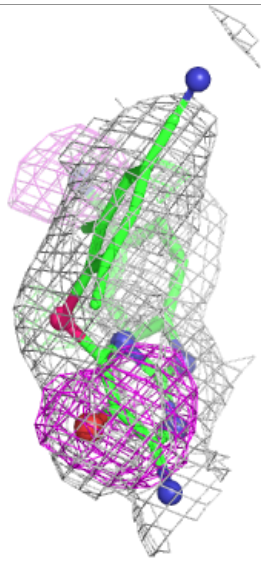
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 65B A 600:

$2mF_o$-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.