wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 08:02 AM EDT

PDB ID	:	3M8P / pdb_00003m8p
Title	:	HIV-1 RT with NNRTI TMC-125
Authors	:	Harris, S.F.; Villasenor, A.
Deposited on	:	2010-03-18
Resolution	:	2.67 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:

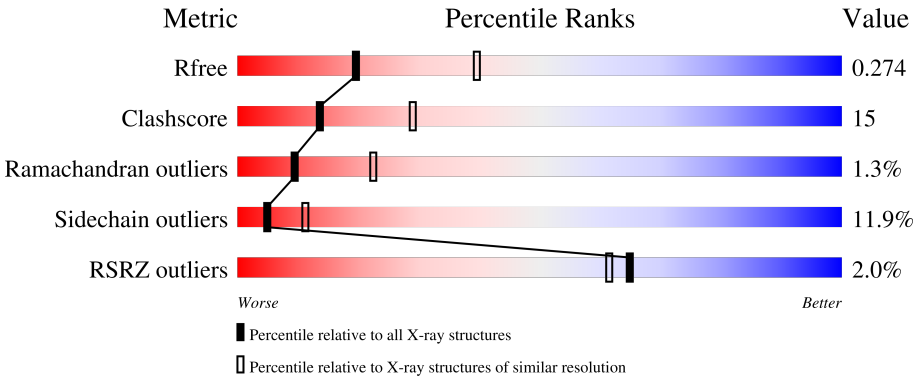
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	561	2% 56% 35% 7%
2	B	440	2% 57% 26% 7% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8138 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.

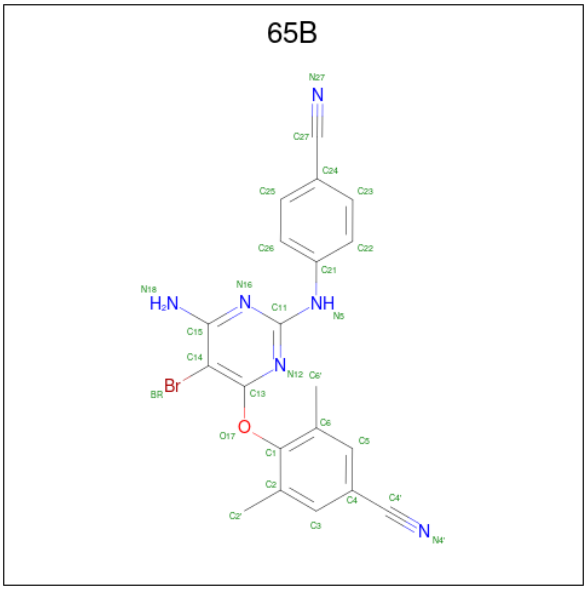
- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	551	4485	2900	748	829	8	0	0	0

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	401	3320	2166	545	602	7	0	0	0

- Molecule 3 is Etravirine (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

- Molecule 4 is water.

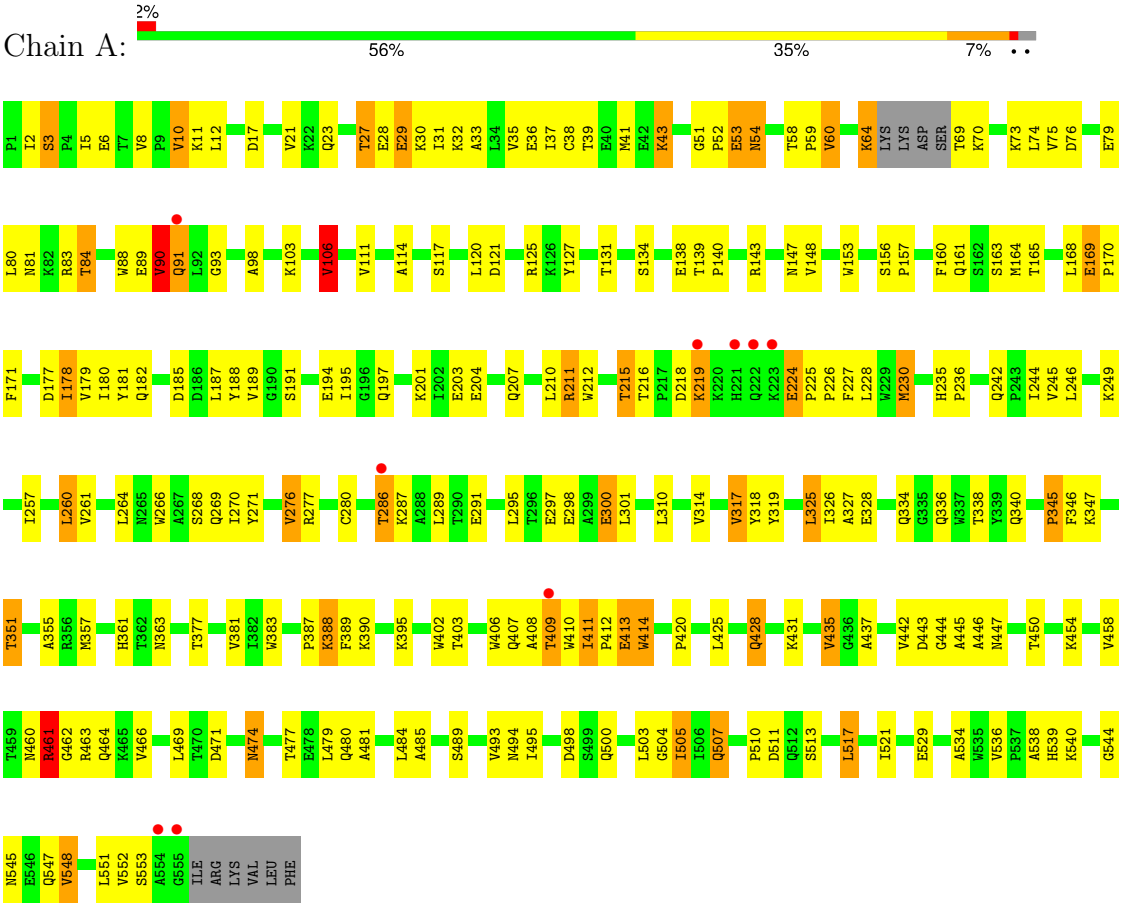
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	169	Total O 169 169	0	0
4	B	136	Total O 136 136	0	0

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.

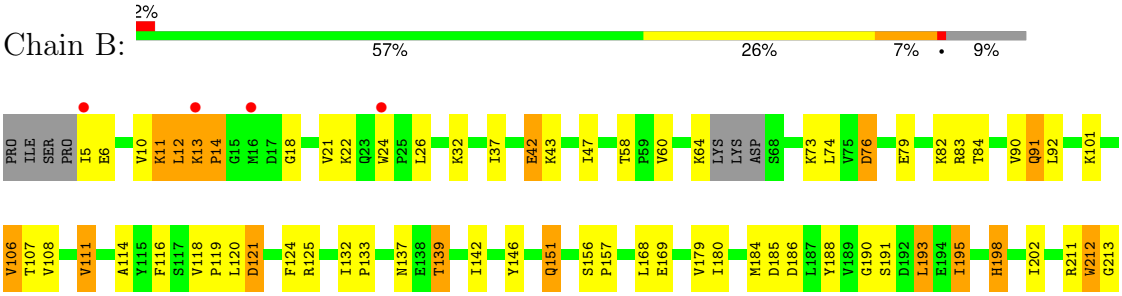
• Molecule 1: Reverse transcriptase/ribonuclease H

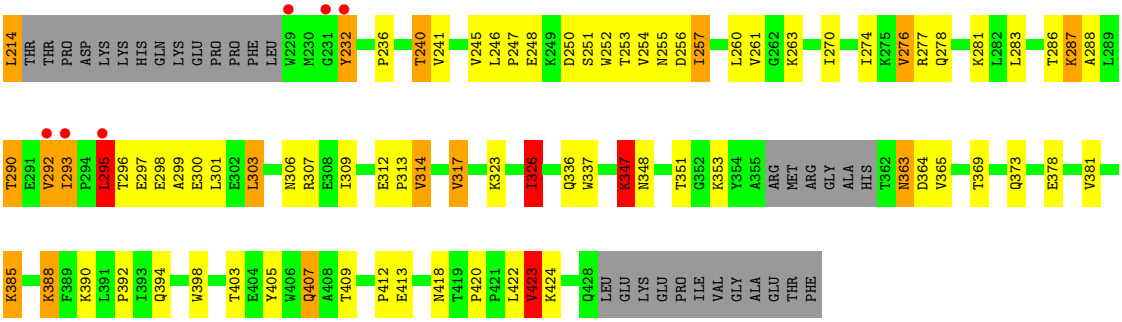
Chain A:



• Molecule 2: p51 RT

Chain B:




L214 THR THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU W229 M230 G231 Y232 P236 T240 V241 V245 L246 P247 E248 K249 D250 S251 W252 T253 V254 N255 D256 I257 L260 V261 G262 K263 I270 I274 K275 V276 R277 Q278 K281 L282 L283 T286 K287 A288 L289
T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 N306 R307 E308 I309 E312 P313 V314 V317 K323 I326 Q336 W337 K347 N348 T351 G352 K353 Y354 A355 ARG MET ARG GLY ALA HIS T362 N363 D364 V365 T369 Q373 E378 V381
K385 K388 P389 K390 L391 P392 I393 Q394 W398 T403 E404 Y405 W406 Q407 A408 T409 P412 E413 N418 T419 P420 P421 L422 V423 K424 Q428 LEU GLU LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.44Å 153.53Å 154.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.01 – 2.67 47.01 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.01-2.67) 99.7 (47.01-2.67)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.209 , 0.283 0.208 , 0.274	Depositor DCC
R_{free} test set	2042 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8138	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	1.56	31/4601 (0.7%)	1.37	34/6252 (0.5%)
2	B	1.56	25/3414 (0.7%)	1.34	25/4640 (0.5%)
All	All	1.56	56/8015 (0.7%)	1.36	59/10892 (0.5%)

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	232	TYR	CA-C	13.47	1.58	1.52
1	A	420	PRO	CA-C	-10.05	1.45	1.52
1	A	409	THR	CA-CB	9.78	1.73	1.53
1	A	224	GLU	CA-C	7.53	1.59	1.52
2	B	412	PRO	N-CA	-7.14	1.39	1.47

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	345	PRO	CA-C-N	8.78	136.31	122.61
1	A	345	PRO	C-N-CA	8.78	136.31	122.61
1	A	420	PRO	O-C-N	8.30	125.05	121.15
2	B	348	ASN	N-CA-C	7.39	120.95	110.23
1	A	38	CYS	N-CA-C	6.94	118.84	111.28

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	4485	0	4530	138	0
2	B	3320	0	3341	98	0
3	A	28	0	15	3	0
4	A	169	0	0	19	0
4	B	136	0	0	10	0
All	All	8138	0	7886	230	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 15.

The worst 5 of 230 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:80:LEU:O	1:A:84:THR:HG22	1.39	1.18
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.33	1.09
1:A:409:THR:HG21	4:A:695:HOH:O	1.63	0.98
1:A:428:GLN:NE2	1:A:431:LYS:HZ1	1.61	0.98
1:A:27:THR:HG21	4:A:722:HOH:O	1.64	0.96

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	547/561 (98%)	509 (93%)	34 (6%)	4 (1%)	18 37
2	B	393/440 (89%)	364 (93%)	21 (5%)	8 (2%)	6 14
All	All	940/1001 (94%)	873 (93%)	55 (6%)	12 (1%)	9 22

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
2	B	13	LYS
1	A	471	ASP
2	B	14	PRO
2	B	22	LYS

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	491/501 (98%)	426 (87%)	65 (13%)	4 8
2	B	365/400 (91%)	328 (90%)	37 (10%)	7 16
All	All	856/901 (95%)	754 (88%)	102 (12%)	5 11

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	ASN
2	B	90	VAL
2	B	409	THR
1	A	517	LEU
2	B	6	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	208	HIS
2	B	394	GLN
2	B	407	GLN
2	B	367	GLN
1	A	480	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	562	-	30,30,30	1.49	5 (16%)	40,42,42	2.96	20 (50%)

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	562	-	-	0/12/12/12	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	562	65B	C13-C14	-3.79	1.33	1.38
3	A	562	65B	C15-N16	-2.93	1.31	1.35
3	A	562	65B	C3-C2	-2.84	1.35	1.39
3	A	562	65B	C3-C4	2.09	1.43	1.39
3	A	562	65B	C11-N5	2.07	1.40	1.36

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	562	65B	C11-N16-C15	7.17	122.41	116.59
3	A	562	65B	O17-C13-C14	-6.19	113.90	117.89
3	A	562	65B	BR-C14-C13	-4.86	114.74	121.55
3	A	562	65B	C14-C13-N12	-4.82	118.60	123.78
3	A	562	65B	O17-C13-N12	4.70	127.49	119.61

There are no chirality outliers.

There are no torsion outliers.

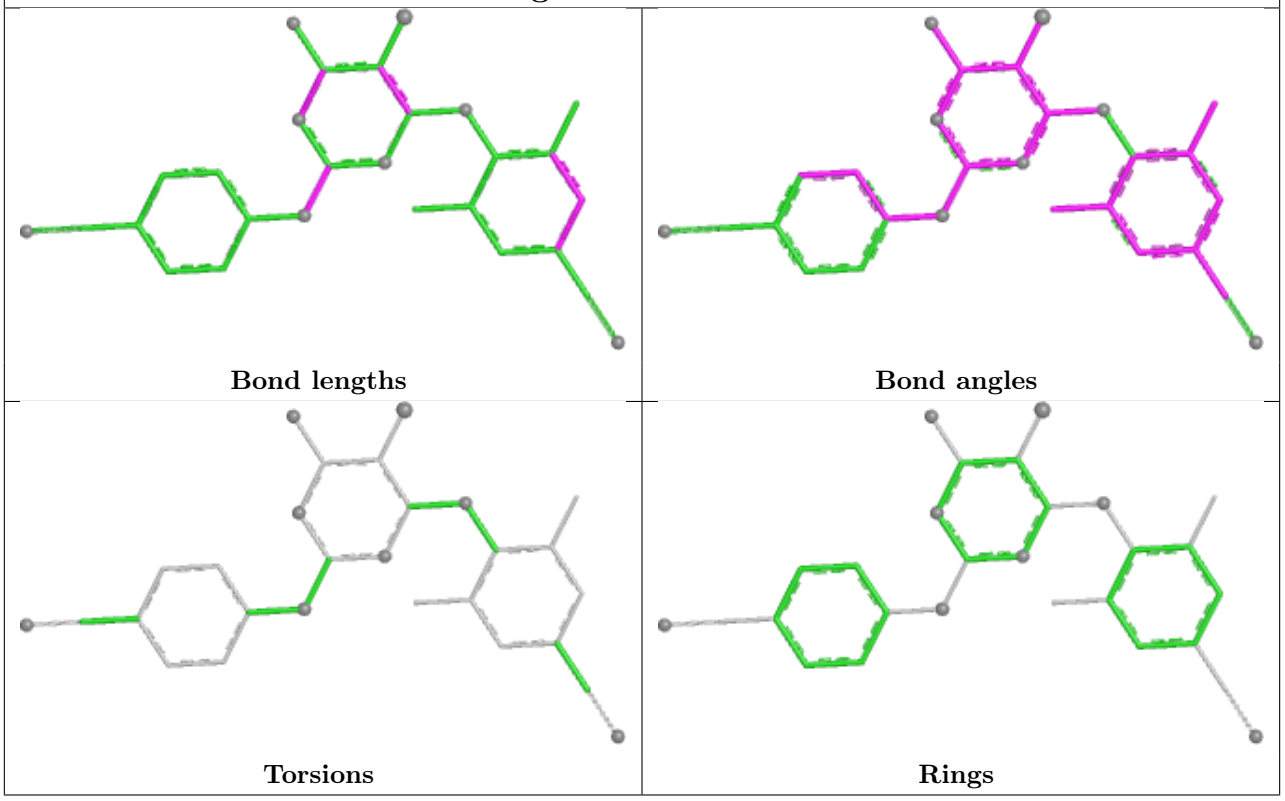
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	562	65B	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 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 562



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, 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	551/561 (98%)	-0.06	9 (1%)	70	68	25, 49, 75, 103	0
2	B	401/440 (91%)	-0.07	10 (2%)	58	54	26, 46, 82, 95	0
All	All	952/1001 (95%)	-0.06	19 (1%)	65	61	25, 48, 79, 103	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	LYS	3.8
1	A	555	GLY	3.1
1	A	222	GLN	3.1
2	B	232	TYR	3.0
2	B	229	TRP	2.8

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

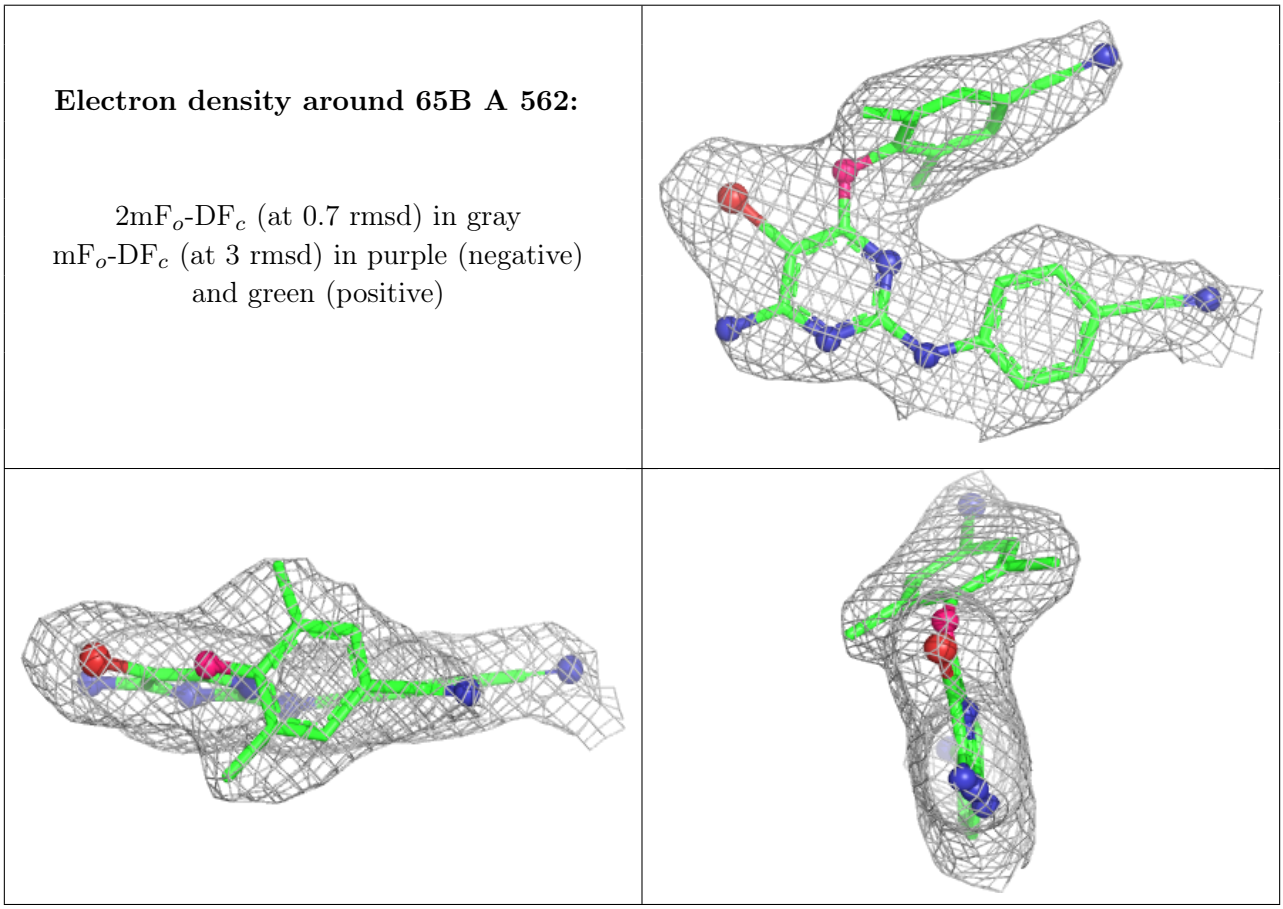
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	562	28/28	0.97	0.06	24,33,40,45	1

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 562:

$2mF_o$-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.