



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:02 PM UTC

PDB ID : 2VG6 / pdb_00002vg6
Title : Crystal structures of HIV-1 reverse transcriptase complexes with thiocarba-
mate non-nucleoside inhibitors
Authors : Spallarossa, A.; Cesarini, S.; Ranise, A.; Ponassi, M.; Unge, T.; Bolognesi, M.
Deposited on : 2007-11-08
Resolution : 3.01 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 ⓘ 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

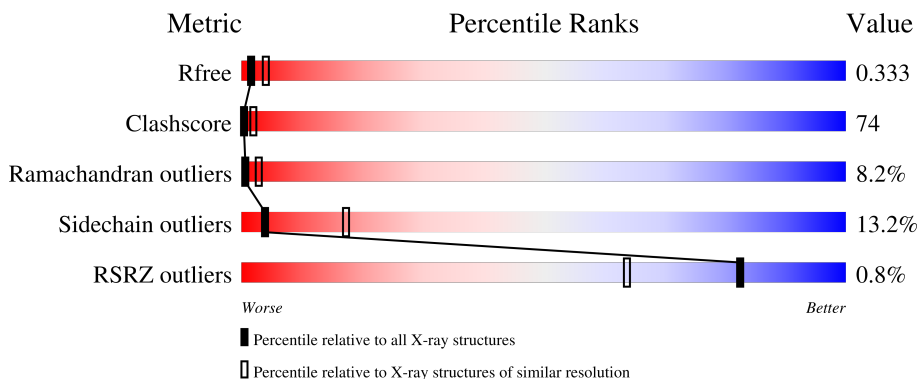
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	27% 53% 18% ..
2	B	428	24% 55% 13% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7856 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.

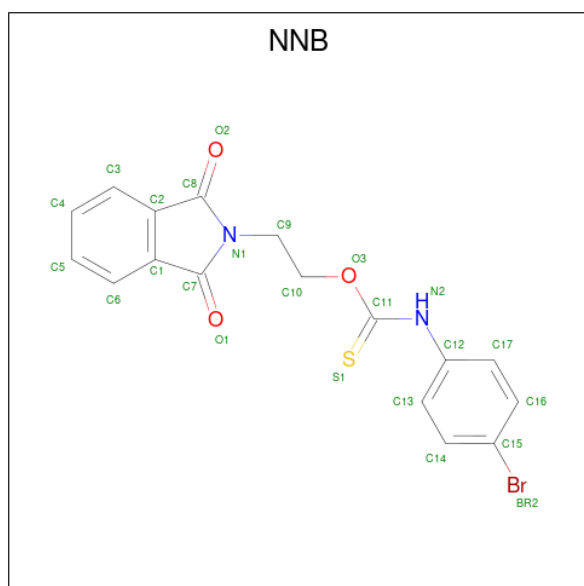
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	1
			4468	2893	745	822	8			

- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3318	2163	543	605	7			

- Molecule 3 is O-[2-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)ethyl] (4-bromophenyl)thiocarbamate (CCD ID: NNB) (formula: C₁₇H₁₃BrN₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O S	0	0
			24	1	17	2	3 1		

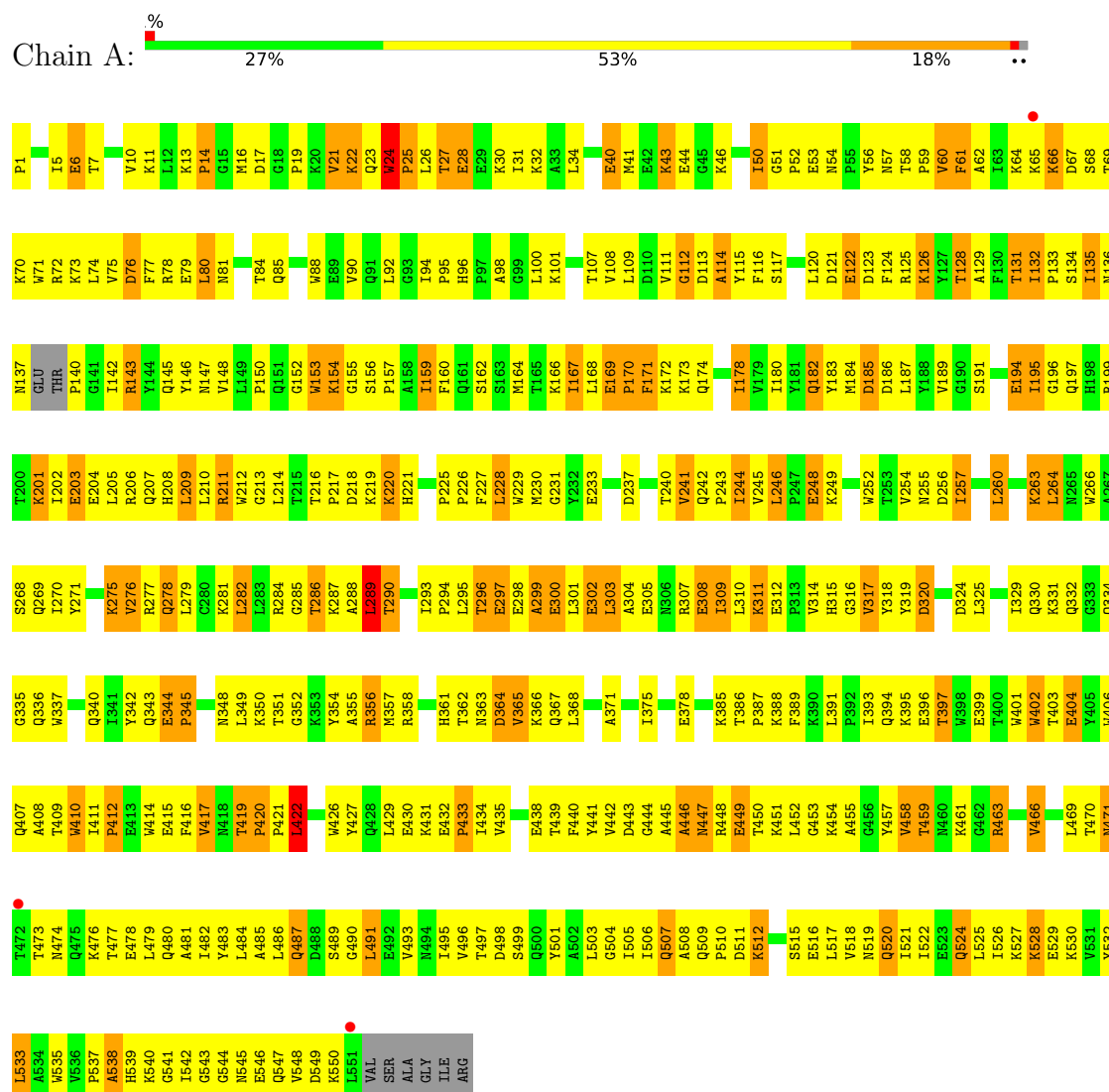
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	24	Total 24	O 24	0	0

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: REVERSE TRANSCRIPTASE/RIBONUCLEASE H



• Molecule 2: P51 RT



I1393	Q1394	K1395	W1398	E1399	T1400	W1401	W1402	T1403	E1404	Y1405	W1406	Q1407	W1410	W1414	E1415	F1416	V1417	N1418	T1419	P1420	P1421	L1422	V1423	K1424	L1425	W1426	Y1427	Q1428																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
I1329	Q1330	K1331	Q1332	G1333	Q1334	G1335	Q1336	W1337	T1338	Y1339	Q1340	I1341	Y1342	Q1343	E1344	P1345	F1346	K1347	N1348	L1349	K1350	T1351	G1352	K1353	Y1354	A1355	ARG	MET	ARG	GLY	ALA	H1361	T1362	N1363	D1364	V1365	K1366	Q1367	E1370	K1374	T1375	T1376	T1377	E1378	S1379	I1380	V1381	I1382	W1383	G1384	K1385	K1388	F1389	K1390	L1391	P1392																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
W1266	E1204	L1205	R1206	L1209	L1210	R1211	W1212	G1213	L1214	THR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU	PRO	PHE	LEU	TRP	M1230	G1231	Y1232	E1233	L1234	H1235	P1236	W1239	T1240	V1241	L1242	Q1243	P1243	T1244	V1245	M1246	R1247	E1248	K1249	L1250	P1251	S1251	T1252	T1253	V1254	N1255	D1256	Q1257	Q1258	P1321	S1322	K1323	G1262	K1263	L1325	I1326																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
I1143	R1067	D1067	S1068	Y1146	N1147	W1148	L1149	P1150	Q1151	G1152	W1153	L1154	G1155	S1156	P1157	L1158	G1159	F1160	Q1161	S1162	S1163	M1164	I1167	L1168	E1169	P1170	K1171	K1172	G1173	L1174	Q1175	N1176	P1176	D1177	I1178	V1179	Q1182	Y1183	M1184	D1185	D1186	L1187	Y1188	V1189	G1190	S1191	D1192	L1193	E1194	I1195	G1196	Q1197	H1198	R1199	T1200	K1201	L1202	E1203																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
PRO	ILE	SER	PRO	R1072	K1073	L1074	V1075	D1076	F1077	R1078	E1079	L1080	N1081	G1082	R1083	T1084	Q1085	D1086	F1087	W1088	E1089	V1090	Q1091	L1092	G1093	I1094	P1097	I1031	A1098	K1032	A1033	L1034	V1035	E1036	K1037	C1038	K1104	S1105	V1111	G1112	D1113	A1114	Y1115	F1116	S1117	V1118	P1119	L1120	D1121	E1122	D1123	F1124	R1125	K1126	F1130	I1135	N1136																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.59Å 157.18Å 154.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.01 20.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	83.8 (20.00-3.01) 83.4 (20.00-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.244 , 0.335 0.237 , 0.333	Depositor DCC
R_{free} test set	1236 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7856	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: NNB

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	0.33	1/4585 (0.0%)	0.72	5/6226 (0.1%)
2	B	0.30	0/3411	0.68	3/4632 (0.1%)
All	All	0.32	1/7996 (0.0%)	0.71	8/10858 (0.1%)

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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	550	LYS	C-N	-6.97	1.23	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	TRP	CA-C-N	5.95	127.28	119.84
1	A	24	TRP	C-N-CA	5.95	127.28	119.84
1	A	420	PRO	N-CA-C	5.95	117.96	110.70
1	A	320	ASP	CA-C-N	5.72	125.85	119.32
1	A	320	ASP	C-N-CA	5.72	125.85	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	4468	0	4527	663	1
2	B	3318	0	3341	527	0
3	A	24	0	13	2	0
4	A	22	0	0	10	1
4	B	24	0	0	10	0
All	All	7856	0	7881	1166	1

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 74.

The worst 5 of 1166 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:1266:TRP:CH2	2:B:1346:PHE:HZ	1.25	1.49
2:B:1266:TRP:CH2	2:B:1346:PHE:CZ	1.99	1.48
1:A:450:THR:CG2	1:A:452:LEU:HD22	1.51	1.40
1:A:344:GLU:HB3	1:A:345:PRO:CD	1.49	1.36
2:B:1282:LEU:O	2:B:1287:LYS:NZ	1.67	1.26

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:CD2	4:A:2013:HOH:O[3_555]	2.06	0.14

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	545/557 (98%)	390 (72%)	110 (20%)	45 (8%)	0	3
2	B	393/428 (92%)	293 (75%)	68 (17%)	32 (8%)	1	3
All	All	938/985 (95%)	683 (73%)	178 (19%)	77 (8%)	0	3

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	28	GLU
1	A	114	ALA
1	A	135	ILE
1	A	153	TRP

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	490/497 (99%)	424 (86%)	66 (14%)	4	16
2	B	366/390 (94%)	319 (87%)	47 (13%)	4	18
All	All	856/887 (96%)	743 (87%)	113 (13%)	4	17

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1415	GLU
2	B	1046	LYS
2	B	1403	THR
2	B	1330	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1330	GLN
2	B	1418	ASN
2	B	1332	GLN
2	B	1348	ASN
1	A	367	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	NNB	A	1551	-	26,26,26	2.50	6 (23%)	36,36,36	3.13	12 (33%)

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	NNB	A	1551	-	-	0/10/26/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1551	NNB	C1-C7	-6.19	1.38	1.48
3	A	1551	NNB	C2-C8	-5.82	1.39	1.48
3	A	1551	NNB	C7-N1	-5.54	1.33	1.39
3	A	1551	NNB	C8-N1	-5.41	1.33	1.39
3	A	1551	NNB	C12-N2	-4.14	1.33	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1551	NNB	C10-O3-C11	-12.75	109.05	119.04
3	A	1551	NNB	O3-C11-S1	-6.59	119.76	125.07
3	A	1551	NNB	C12-N2-C11	-5.42	120.71	130.07
3	A	1551	NNB	C1-C7-N1	4.86	109.48	105.88
3	A	1551	NNB	O3-C11-N2	4.31	120.63	112.20

There are no chirality outliers.

There are no torsion outliers.

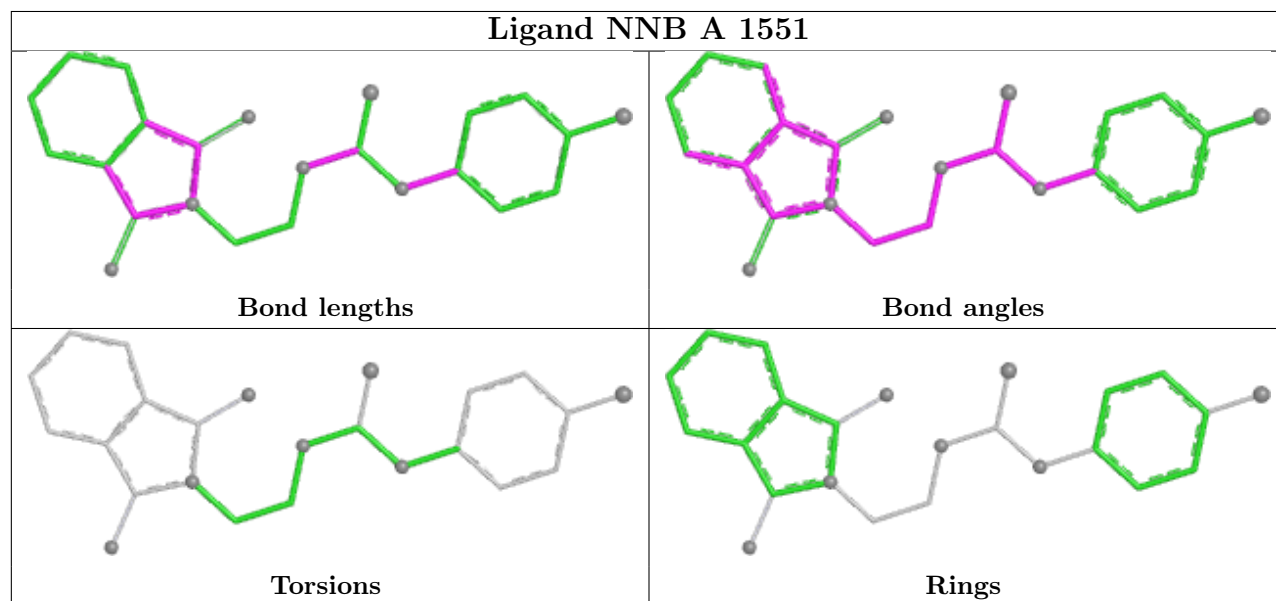
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1551	NNB	2	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	549/557 (98%)	-0.06	3 (0%)	87 72	16, 41, 62, 79	0
2	B	401/428 (93%)	-0.12	5 (1%)	76 55	18, 36, 74, 85	0
All	All	950/985 (96%)	-0.09	8 (0%)	82 64	16, 40, 67, 85	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	THR	3.6
1	A	551	LEU	2.7
2	B	1230	MET	2.4
2	B	1276	VAL	2.2
2	B	1399	GLU	2.1

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](#)

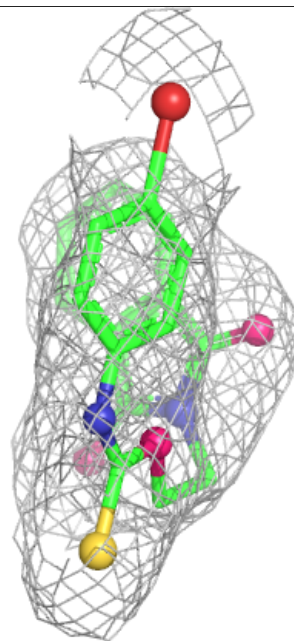
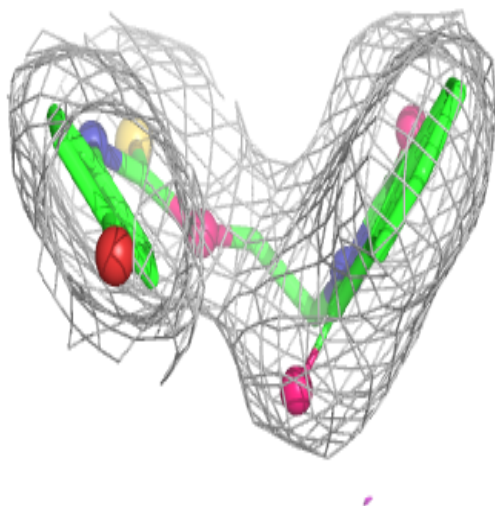
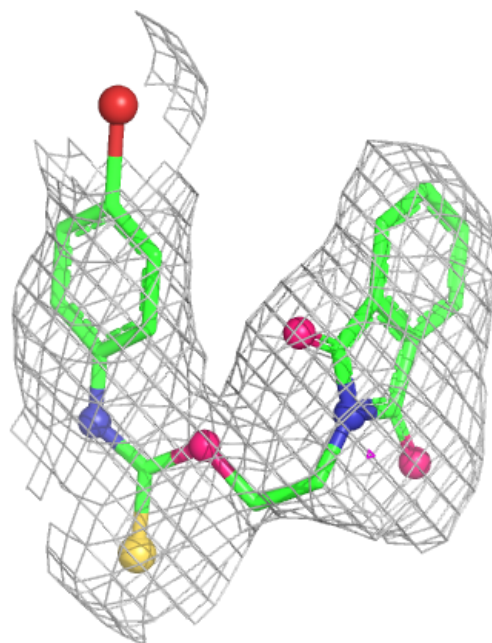
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NNB	A	1551	24/24	0.98	0.07	23,27,40,44	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 NNB A 1551:

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.