wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2020 – 01:15 am BST

PDB ID	:	2VG6
Title	:	Crystal structures of HIV-1 reverse transcriptase complexes with thiocarbamate 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

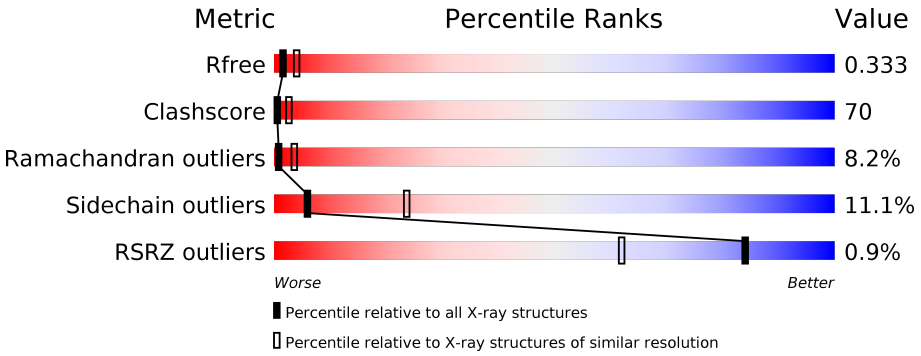
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (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 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 <=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	% 31% 53% 15% •
2	B	428	% 27% 55% 11% • 6%

2 Entry composition

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.

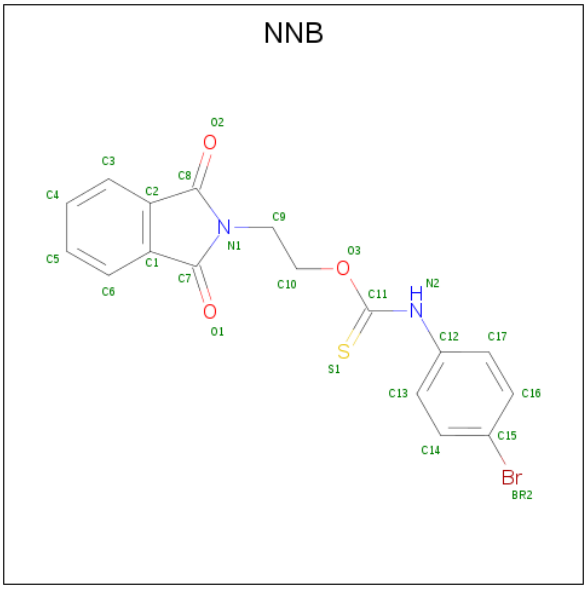
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

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

- Molecule 2 is a protein called P51 RT.

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

- Molecule 3 is O-[2-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)ethyl] (4-bromophenyl)thiocarbamate (three-letter code: NNB) (formula: $C_{17}H_{13}BrN_2O_3S$).



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

- Molecule 4 is water.

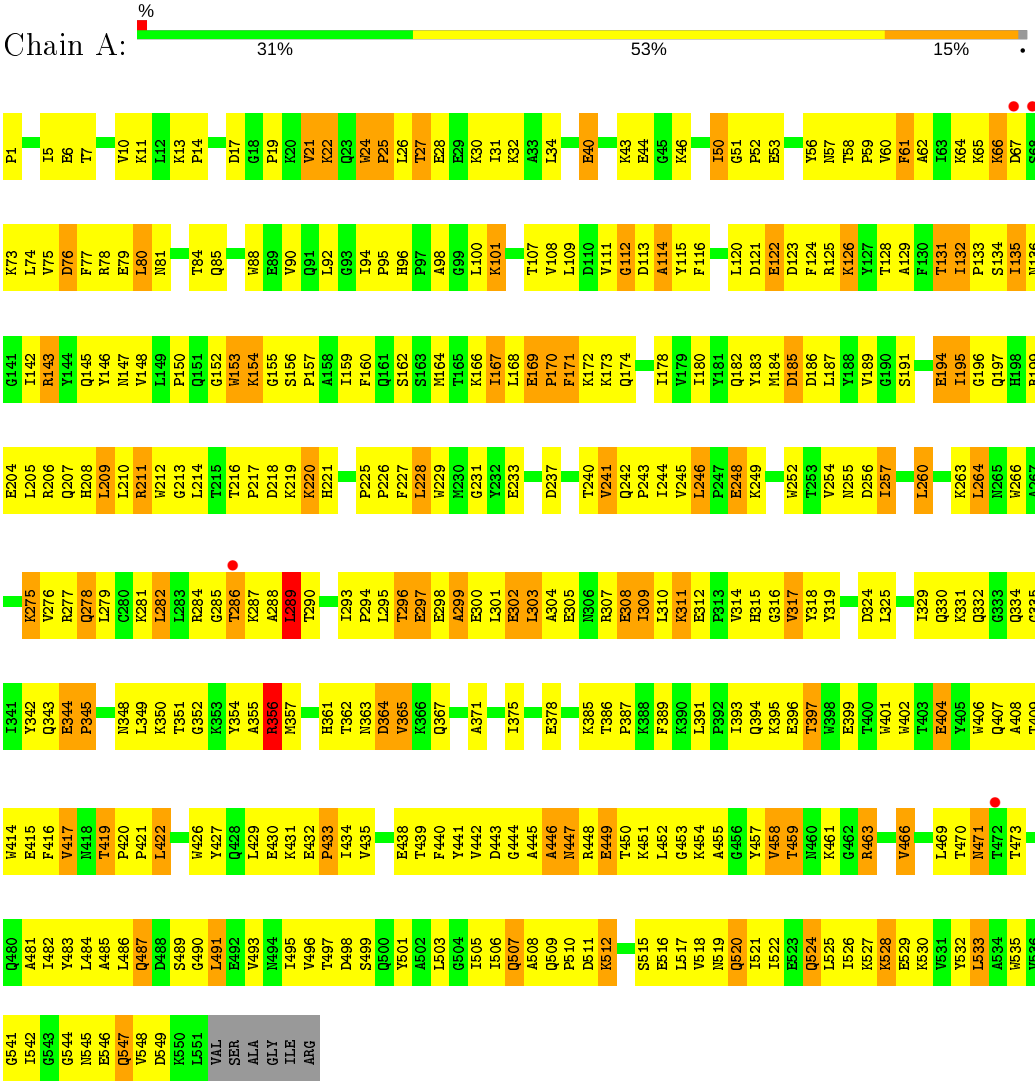
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	22	Total O 22 22	0	0
4	B	24	Total O 24 24	0	0

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.

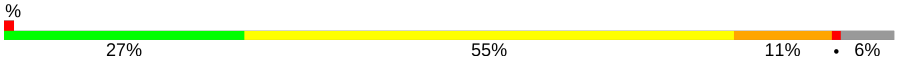
- Molecule 1: REVERSE TRANSCRIPTASE/RIBONUCLEASE H

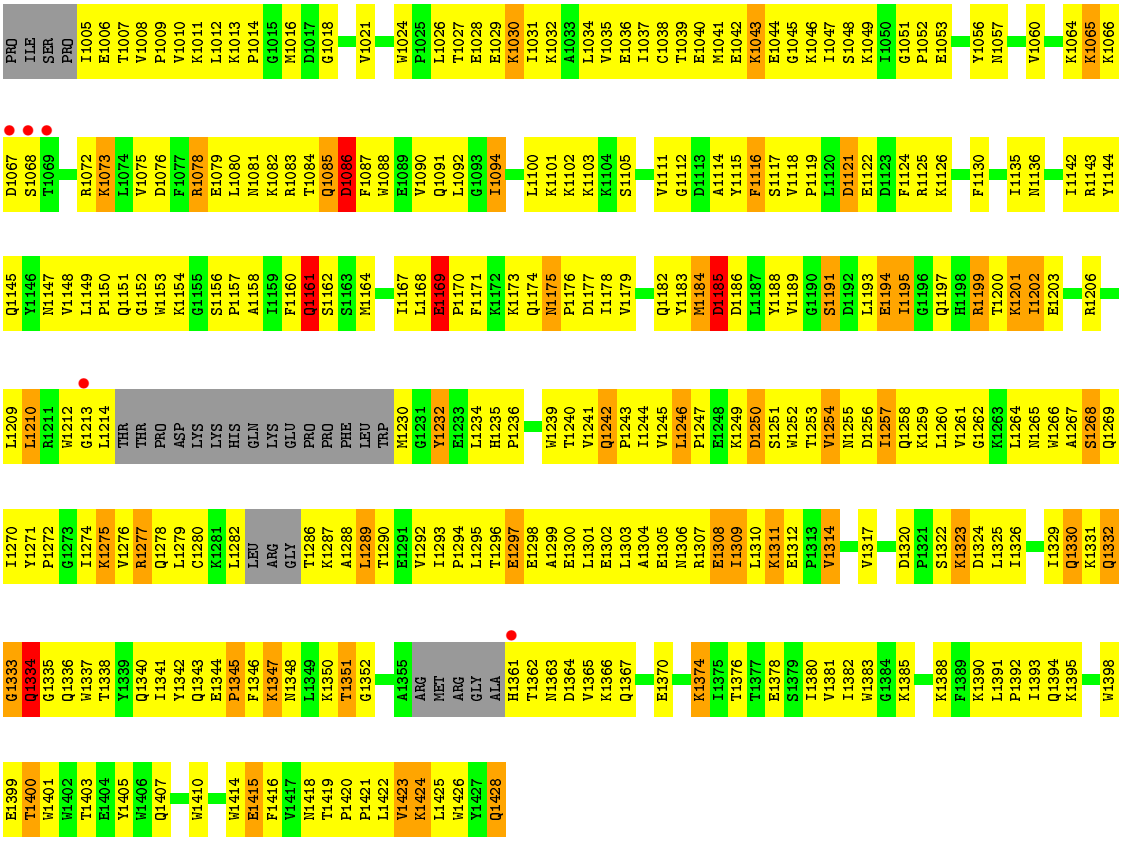
Chain A:



- Molecule 2: P51 RT

Chain B:




PRO I1005 E1006 T1007 V1008 P1009 V1010 K1011 L1012 K1013 P1014 G1015 M1016 D1017 G1018 V1021 W1024 P1025 L1026 T1027 E1028 E1029 K1030 I1031 K1032 A1033 L1034 V1035 E1036 I1037 C1038 T1039 E1040 M1041 E1042 K1043 E1044 G1045 K1046 I1047 S1048 K1049 I1050 G1051 P1052 E1053 Y1056 N1057 V1060 K1064 K1066
ILE
SER
PRO
D1067 S1068 T1069 R1072 K1073 L1074 V1075 D1076 F1077 R1078 E1079 L1080 N1081 K1082 R1083 T1084 Q1085 D1086 F1087 W1088 E1089 V1090 Q1091 L1092 G1093 I1094 L1100 K1101 K1102 K1103 K1104 S1105 V1111 G1112 D1113 A1114 Y1115 F1116 S1117 V1118 P1119 L1120 D1121 E1122 D1123 F1124 R1125 K1126 F1130 I1135 N1136 I1142 R1143 Y1144
Q1145 Y1146 N1147 V1148 L1149 P1150 Q1151 G1152 W1153 K1154 G1155 S1156 P1157 A1158 I1159 F1160 Q1161 S1162 S1163 M1164 I1167 L1168 E1169 P1170 F1171 K1172 K1173 Q1174 M1175 P1176 D1177 I1178 V1179 Q1182 Y1183 M1184 D1185 D1186 L1187 Y1188 V1189 G1190 S1191 D1192 L1193 E1194 I1195 G1196 Q1197 H1198 R1199 T1200 K1201 I1202 E1203 R1206
L1209 L1210 R1211 W1212 G1213 L1214 THR THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP M1230 G1231 Y1232 E1233 L1234 H1235 P1236 W1239 T1240 V1241 Q1242 P1243 I1244 V1245 L1246 P1247 E1248 K1249 D1250 S1251 W1252 T1253 V1254 N1255 D1256 I1257 Q1258 K1259 L1260 V1261 G1262 K1263 L1264 N1265 W1266 A1267 S1268 Q1269
I1270 Y1271 P1272 G1273 I1274 K1275 V1276 R1277 Q1278 L1279 C1280 K1281 L1282 LEU ARG GLY T1286 K1287 A1288 L1289 T1290 E1291 V1292 I1293 P1294 L1295 T1296 E1297 E1298 A1299 E1300 L1301 E1302 L1303 A1304 E1305 N1306 R1307 E1308 I1309 L1310 K1311 E1312 P1313 V1314 V1317 D1320 P1321 S1322 K1323 D1324 L1325 I1326 I1329 Q1330 K1331 Q1332
G1333 Q1334 G1335 Q1336 W1337 T1338 Y1339 Q1340 I1341 Y1342 Q1343 E1344 P1345 F1346 K1347 N1348 L1349 K1350 T1351 G1352 A1355 ARG MET ARG GLY ALA H1361 T1362 N1363 D1364 V1365 K1366 Q1367 E1370 K1374 I1375 T1376 T1377 E1378 S1379 I1380 V1381 I1382 W1383 G1384 K1385 K1388 F1389 K1390 L1391 P1392 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

4 Data and refinement statistics (i)

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 19.93 – 3.01	Depositor EDS
% Data completeness (in resolution range)	83.8 (20.00-3.01) 83.8 (19.93-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.32 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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: 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	0.28	1/4585 (0.0%)	0.43	0/6226
2	B	0.24	0/3411	0.41	0/4632
All	All	0.26	1/7996 (0.0%)	0.42	0/10858

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	478	GLU	CD-OE2	7.34	1.33	1.25

There are no bond angle outliers.

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	624	1
2	B	3318	0	3341	499	0
3	A	24	0	13	2	0
4	A	22	0	0	9	1
4	B	24	0	0	10	0
All	All	7856	0	7881	1099	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 70.

The worst 5 of 1099 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 (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	545/557 (98%)	390 (72%)	110 (20%)	45 (8%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	393/428 (92%)	293 (75%)	68 (17%)	32 (8%)	1 4
All	All	938/985 (95%)	683 (73%)	178 (19%)	77 (8%)	1 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 (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	490/497 (99%)	434 (89%)	56 (11%)	5 22
2	B	366/390 (94%)	327 (89%)	39 (11%)	6 25
All	All	856/887 (96%)	761 (89%)	95 (11%)	6 23

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	THR
1	A	524	GLN
2	B	1351	THR
1	A	404	GLU
1	A	449	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	500	GLN
2	B	1096	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1407	GLN
1	A	545	ASN
2	B	1136	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 (i)

There are no carbohydrates 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	NNB	A	1551	-	26,26,26	2.49	6 (23%)	36,36,36	3.17	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	-6.11	1.38	1.48
3	A	1551	NNB	C2-C8	-5.75	1.39	1.48
3	A	1551	NNB	C7-N1	-5.55	1.33	1.39
3	A	1551	NNB	C8-N1	-5.42	1.33	1.39
3	A	1551	NNB	C12-N2	-4.12	1.33	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1551	NNB	C10-O3-C11	-12.38	109.05	119.11
3	A	1551	NNB	O3-C11-S1	-7.81	119.76	125.10
3	A	1551	NNB	C12-N2-C11	-5.20	120.71	130.00
3	A	1551	NNB	C1-C7-N1	5.06	109.48	105.88
3	A	1551	NNB	C2-C8-N1	4.44	109.03	105.88

There are no chirality outliers.

There are no torsion outliers.

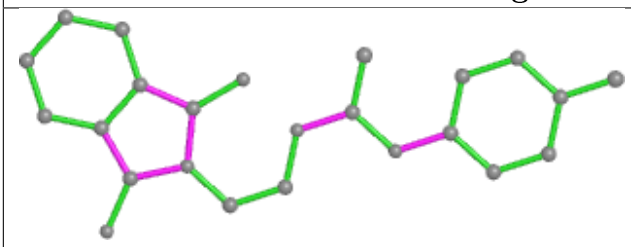
There are no ring outliers.

1 monomer is involved in 2 short contacts:

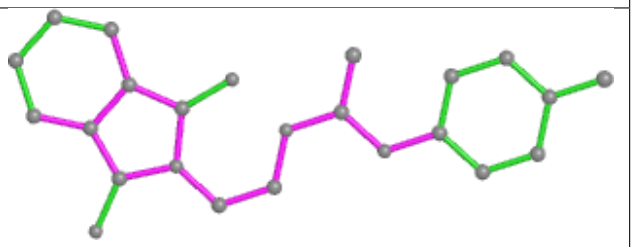
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1551	NNB	2	0

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 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.

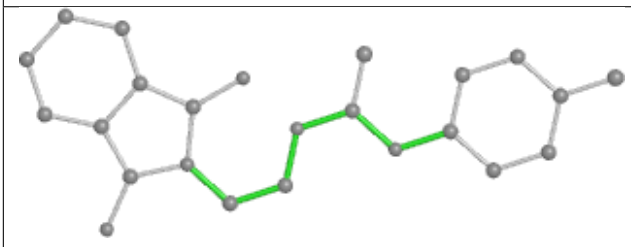
Ligand NNB A 1551



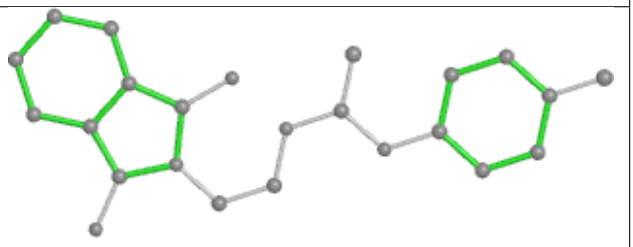
Bond lengths



Bond angles



Torsions



Rings

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	549/557 (98%)	-0.42	4 (0%)	87	68	16, 41, 62, 79	0
2	B	401/428 (93%)	-0.45	5 (1%)	79	53	18, 37, 74, 85	0
All	All	950/985 (96%)	-0.43	9 (0%)	84	62	16, 40, 67, 85	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	3.5
2	B	1361	HIS	3.0
2	B	1069	THR	2.5
2	B	1068	SER	2.4
1	A	472	THR	2.4

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

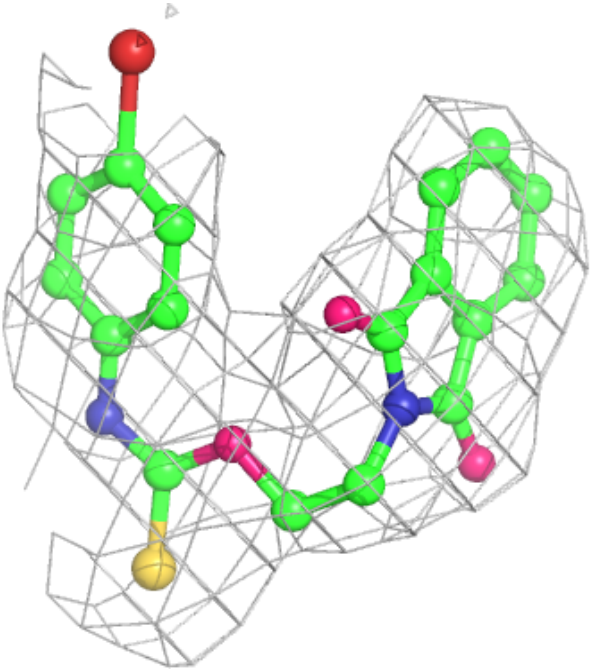
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

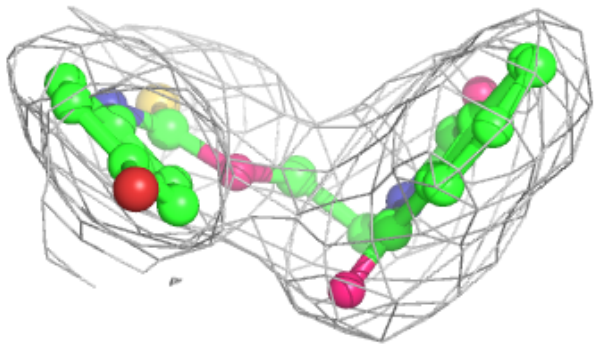
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NNB	A	1551	24/24	0.98	0.14	23,27,40,44	0

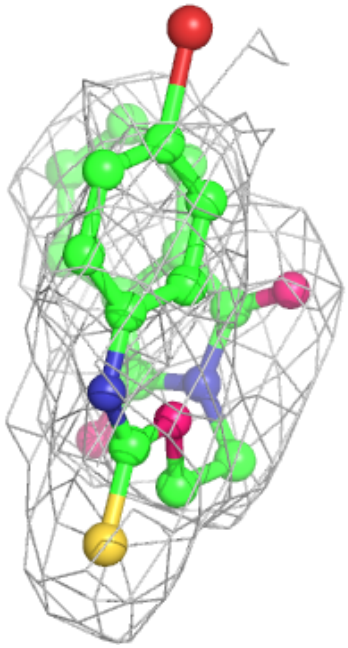
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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