



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:32 PM UTC

PDB ID : 1IKV / pdb_00001ikv
Title : K103N Mutant HIV-1 Reverse Transcriptase in Complex with Efavirenz
Authors : Lindberg, J.; Unger, T.
Deposited on : 2001-05-07
Resolution : 3.00 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

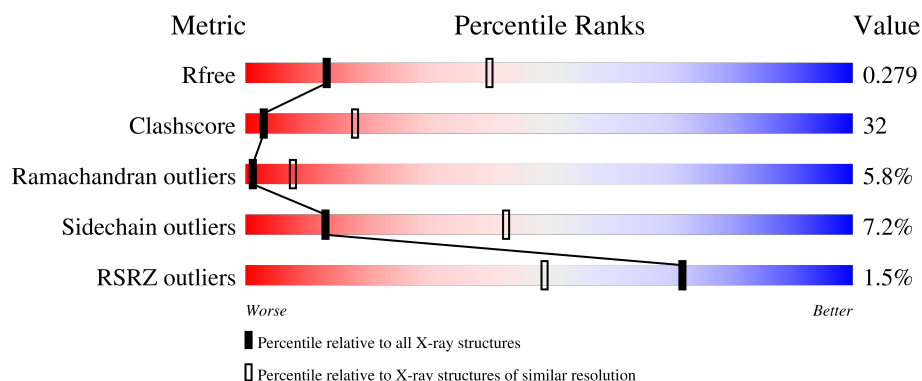
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	560	 43% 48% 7% ..
2	B	427	 41% 45% 8% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7872 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 POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	2	0	0
			4514	2921	752	833	8			

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	478	GLN	GLU	engineered mutation	UNP P03366

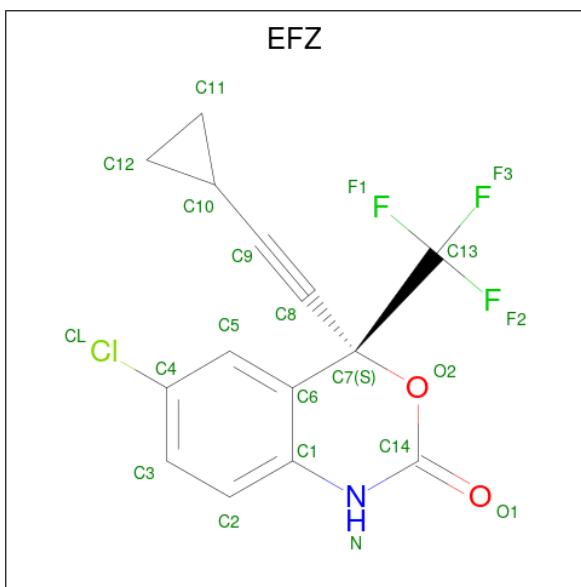
- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	30	0	0
			3337	2174	548	609	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1103	ASN	LYS	engineered mutation	UNP P03366

- Molecule 3 is (-)-6-CHLORO-4-CYCLOPROPYLETHYNYL-4-TRIFLUOROMETHYL-1,4-DIHYDRO-2H-3,1-BENZOXAZIN-2-ONE (CCD ID: EFZ) (formula: C₁₄H₉ClF₃NO₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
3	A	1	21	14	1	3	1	2	0	0

R1083	P1157	V1241	A1304	T1377
T1084	A1158	Q1242	E1305	E1378
Q1085	I1159	P1243	M1306	S1379
D1086	I1167	I1244	R1307	I1380
F1087	L1168	V1245	L1310	V1381
W1088	P1247	L1246	V1314	I1382
F1089	E1169	E1248	V1317	W1383
V1090	P1170	K1249	V1317	P1387
Q1091	N1175	D1250	D1320	K1388
K1102	S1251	S1251	D1320	L1391
ASN	W1252	T1253	K1323	F1392
K1104	V1254	V1254	D1324	I1393
D1110	Y1183	I1257	L1325	Q1394
V1111	M1184	K1258	I1326	K1395
G1112	D1185	Q1259	Q1330	E1396
D1113	L1186	L1260	G1333	T1397
D1114	L1187	V1261	Q1334	W1398
A1114	Y1188	G1262	G1335	W1401
Y1115	V1189	K1263	T1338	W1402
F1116	I1195	L1264	I1341	W1410
S1117	G1196	N1265	Y1342	I1411
V1118	I1197	W1266	E1343	W1414
P1119	H1198	A1267	Q1344	E1415
L1120	I1198	Q1268	F1345	F1416
D1121	K1201	S1268	I1346	N1418
E1122	I1202	Q1269	K1347	T1419
D1123	I1203	Y1270	M1348	P1420
F1124	E1204	Y1271	L1349	F1421
R1125	L1205	I1274	K1350	V1423
K1126	R1206	K1275	T1351	K1424
Y1127	L1209	Q1278	G1352	L1425
F1130	L1214	L1279	K1353	W1426
I1131	T1215	C1280	Y1354	Y1427
P1133	T1216	K1281	A1355	
S1134	P1217	L1282	A1355	
I1135	ASP	L1283	R1356	
N1136	LYS	R1284	NET	
E1138	LYS	G1285	ARG	
N1137	HIS	T1286	GLY	
T1139	GLN	K1287	ALA	
P1140	LYS	A1288	HIS	
G1141	GLU	L1289	T1362	
I1142	PRO	T1290	N1363	
R1143	PRO	E1291	D1364	
Y1144	PHE	V1292	V1365	
Q1145	LEU	T1293	K1366	
Y1146	TRP	P1294		
N1147	NET	L1295		
V1148	G1231	T1296		
L1149	Y1232	E1297		
P1150	P1150	E1298		
Q1151	E1233	A1299		
G1152	L1234	E1300		
W1153	H1235	L1301		
K1154	P1236	E1302		
G1155	D1237	L1303		
S1156				

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.63Å 157.17Å 156.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 3.00 24.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.3 (24.84-3.00) 87.2 (24.84-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.294 0.217 , 0.279	Depositor DCC
R_{free} test set	1524 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7872	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EFZ

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	0.51	0/4631	0.99	13/6291 (0.2%)
2	B	0.51	0/3430	1.00	22/4660 (0.5%)
All	All	0.51	0/8061	0.99	35/10951 (0.3%)

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1293	ILE	N-CA-C	7.29	115.93	107.84
1	A	13	LYS	CA-C-N	6.90	128.47	119.84
1	A	13	LYS	C-N-CA	6.90	128.47	119.84
2	B	1235	HIS	CA-C-N	6.72	126.99	119.32
2	B	1235	HIS	C-N-CA	6.72	126.99	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4514	0	4565	296	0
2	B	3337	0	3365	225	0
3	A	21	0	8	0	0
All	All	7872	0	7938	504	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 32.

The worst 5 of 504 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:223:LYS:HG3	1:A:224:GLU:H	1.05	1.09
2:B:1283:LEU:HD13	2:B:1293:ILE:HB	1.37	1.05
1:A:278:GLN:HE21	1:A:298:GLU:HB2	1.20	1.03
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.48	0.94
2:B:1246:LEU:HD12	2:B:1307:ARG:HB3	1.47	0.93

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	552/560 (99%)	438 (79%)	78 (14%)	36 (6%)	1	5
2	B	396/427 (93%)	333 (84%)	44 (11%)	19 (5%)	2	11
All	All	948/987 (96%)	771 (81%)	122 (13%)	55 (6%)	1	8

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ILE
2	B	1065	LYS
2	B	1252	TRP
2	B	1267	ALA
2	B	1294	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	494/500 (99%)	453 (92%)	41 (8%)	10	37
2	B	368/389 (95%)	347 (94%)	21 (6%)	18	52
All	All	862/889 (97%)	800 (93%)	62 (7%)	13	43

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	MET
2	B	1345	PRO
1	A	432	GLU
2	B	1330	GLN
2	B	1422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1081	ASN
2	B	1182	GLN
2	B	1332	GLN
2	B	1258	GLN
2	B	1161	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 [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	EFZ	A	2000	-	23,23,23	4.36	12 (52%)	36,36,36	1.85	10 (27%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EFZ	A	2000	-	-	4/10/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	EFZ	C4-CL	-16.68	1.35	1.74
3	A	2000	EFZ	C9-C8	5.51	1.35	1.19
3	A	2000	EFZ	C7-C6	5.00	1.58	1.51
3	A	2000	EFZ	C5-C6	4.01	1.45	1.39
3	A	2000	EFZ	C1-C6	3.49	1.44	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	EFZ	C12-C10-C9	-4.10	109.42	119.09
3	A	2000	EFZ	O2-C7-C13	3.59	111.29	104.78
3	A	2000	EFZ	C7-O2-C14	-3.54	115.21	121.48
3	A	2000	EFZ	O2-C14-N	3.25	122.41	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	EFZ	O2-C7-C6	2.97	113.84	111.61

There are no chirality outliers.

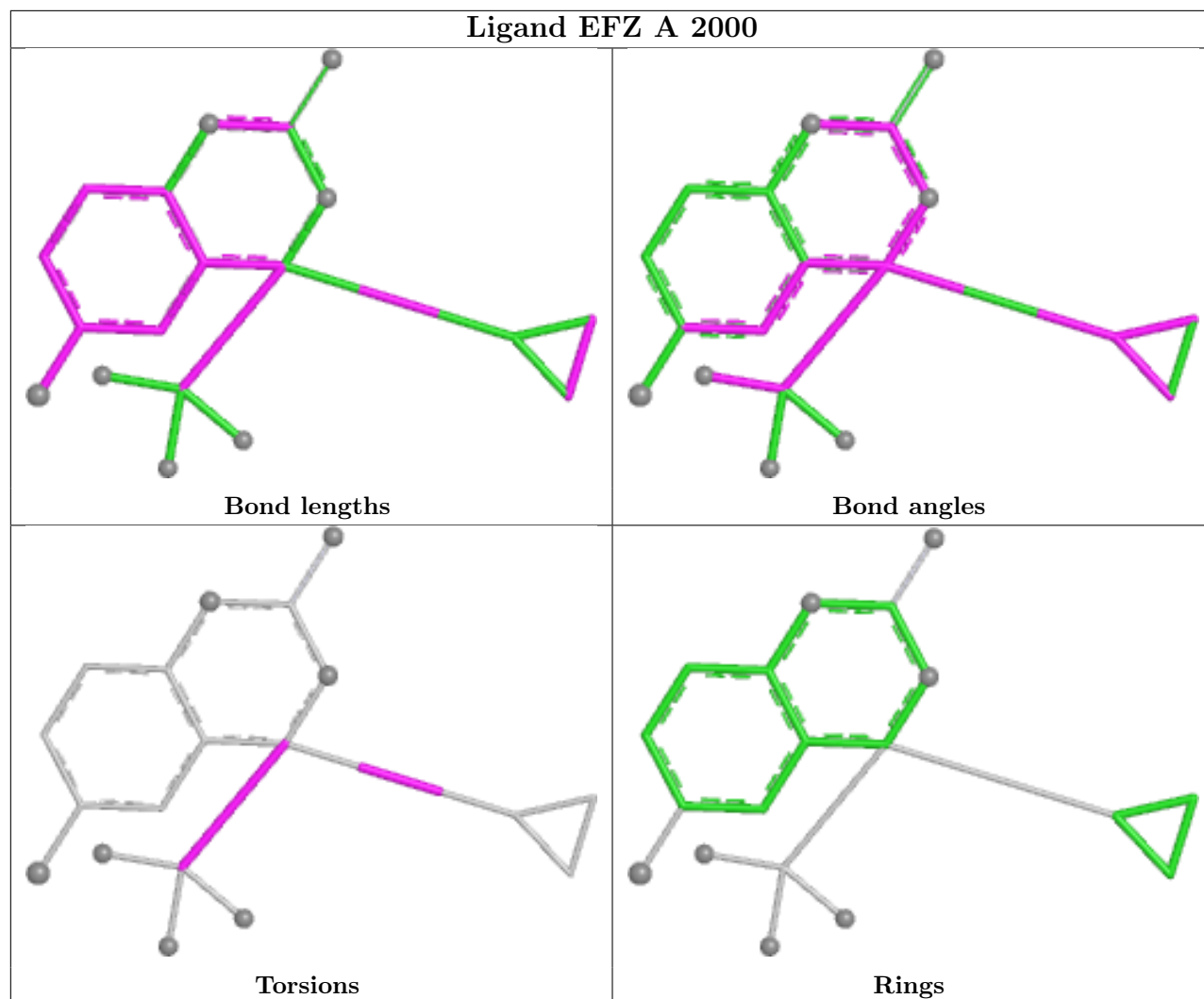
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2000	EFZ	F1-C13-C7-O2
3	A	2000	EFZ	C7-C8-C9-C10
3	A	2000	EFZ	F3-C13-C7-O2
3	A	2000	EFZ	F2-C13-C7-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	556/560 (99%)	-0.20	7 (1%)	75 53	13, 52, 88, 125	2 (0%)
2	B	404/427 (94%)	-0.25	7 (1%)	69 45	14, 43, 106, 122	9 (2%)
All	All	960/987 (97%)	-0.22	14 (1%)	72 49	13, 48, 99, 125	11 (1%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1427	TYR	3.7
1	A	539	HIS	3.6
2	B	1283	LEU	3.4
2	B	1253	THR	3.0
1	A	446	ALA	2.8

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](#)

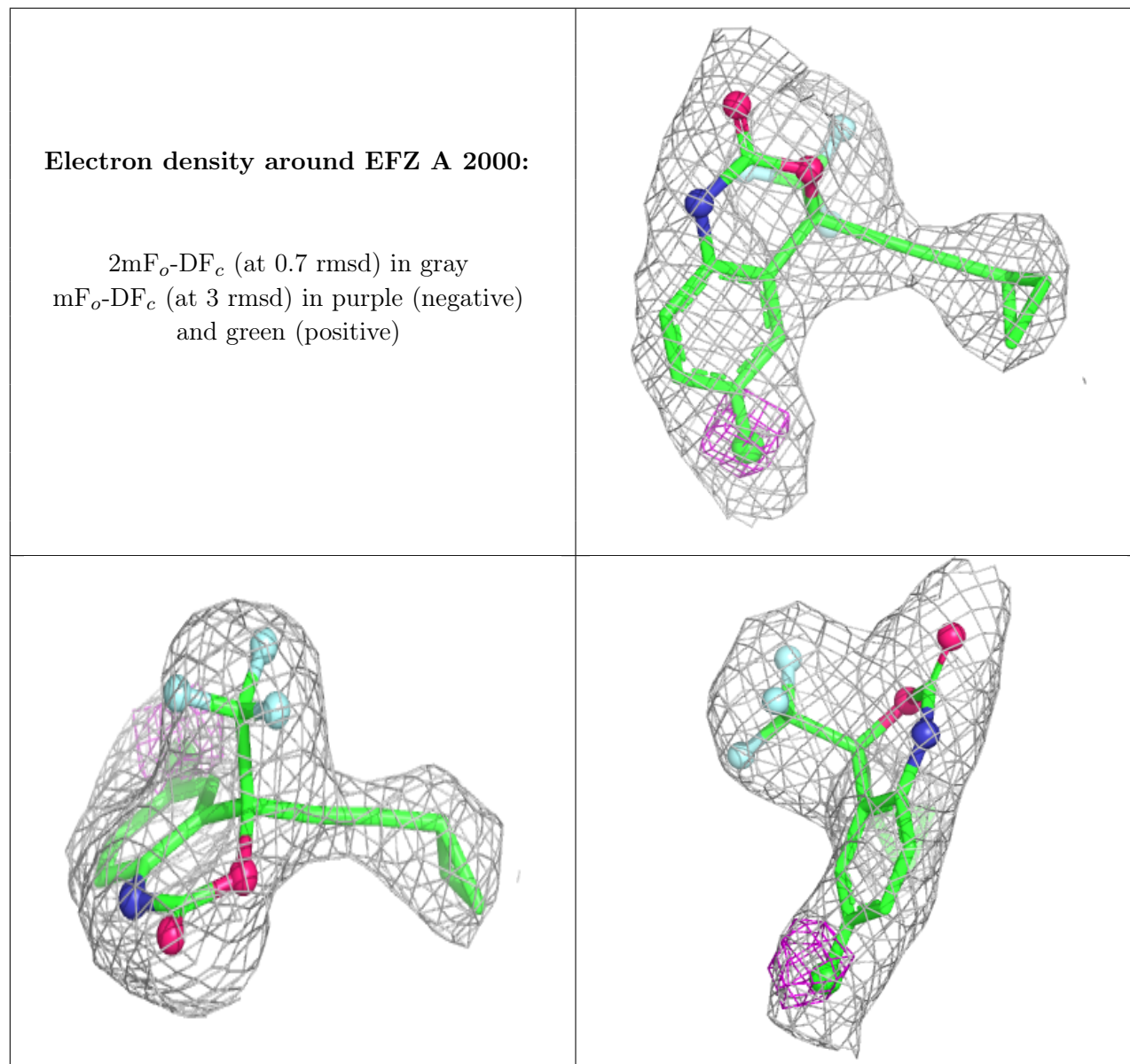
There are no oligosaccharides in this entry.

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	EFZ	A	2000	21/21	0.95	0.08	31,34,36,36	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.