



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2018 – 03:05 AM EST

PDB ID : 2AAR  
Title : Structure of trigger factor binding domain in biologically homologous complex with eubacterial ribosome.  
Authors : Baram, D.; Pyetan, E.; Sittner, A.; Auerbach-Nevo, T.; Bashan, A.; Yonath, A.  
Deposited on : 2005-07-14  
Resolution : 3.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

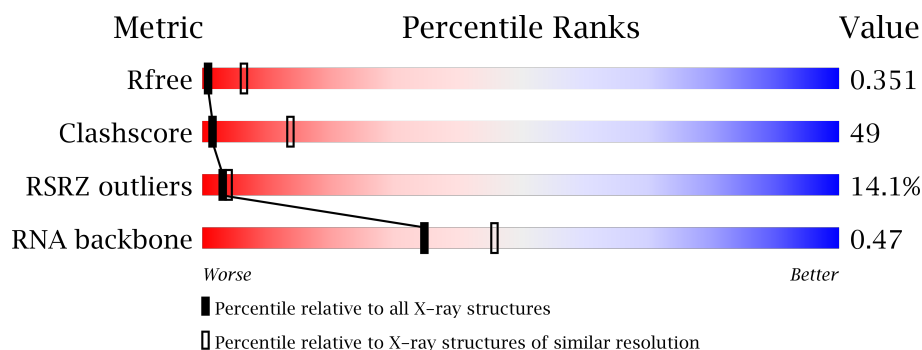
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	0	2880	
2	R	95	
3	W	67	
4	7	113	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 59630 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

- Molecule 2 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	R	93	Total	C	0	0	93
			93	93			

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	W	65	Total	C	0	0	65
			65	65			

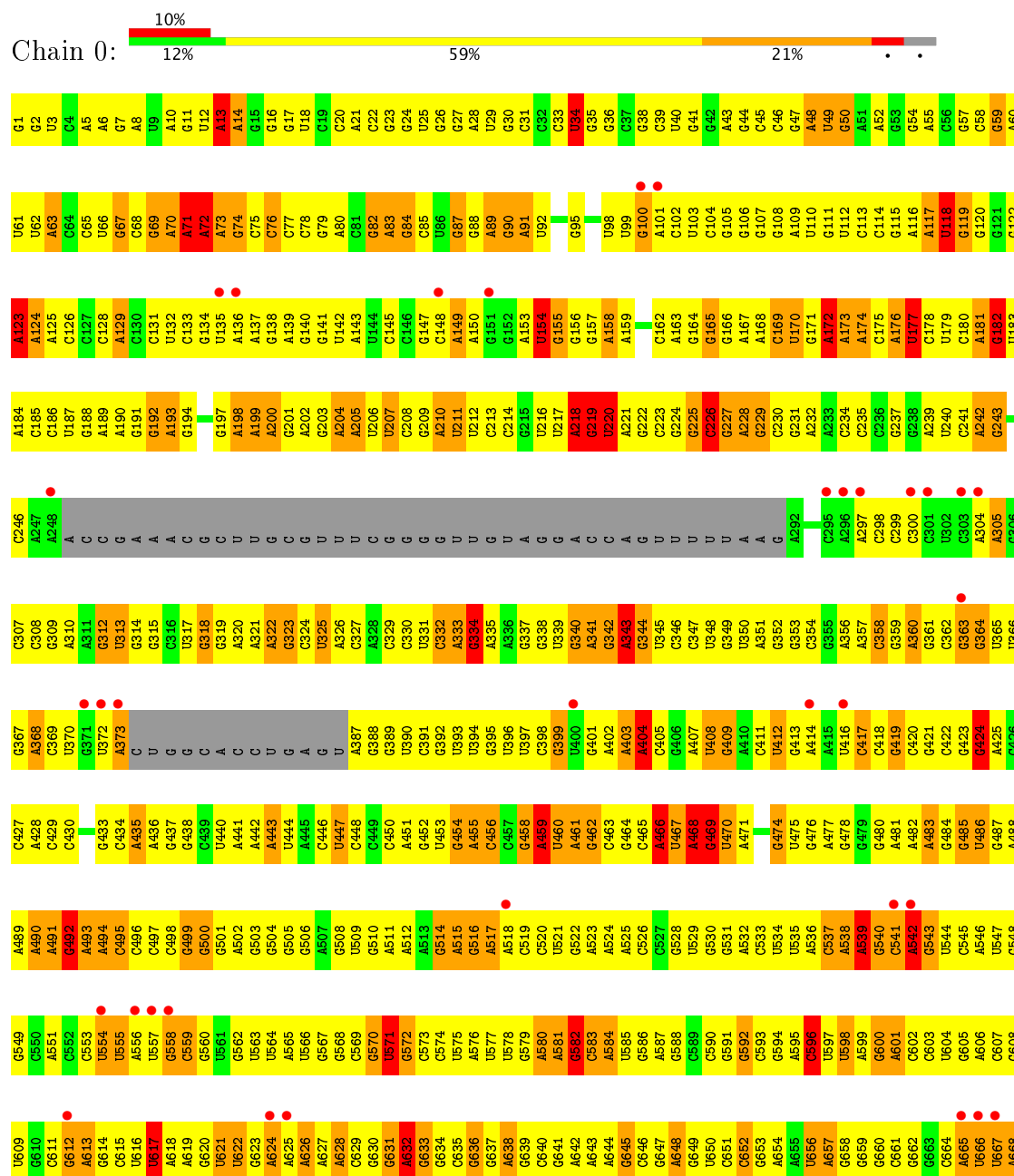
- Molecule 4 is a protein called Trigger Factor.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	7	113	Total	C	0	0	113
			113	113			

### 3 Residue-property plots

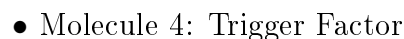
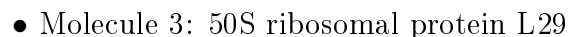
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 23S ribosomal RNA



U1530	C1531	U1469	C1346	U1286	G1225	G1165	C1103	A1043	C981	A921	U857	A797	G735	G669
G1470	U1409	G1470	C1347	A1287	A1226	A1166	G1104	U1044	C982	A922	G858	G798	G736	U670
C1471	U1410	U1410	A1288	A1289	A1227	A1167	U1105	U1045	G983	A923	U859	C799	C737	A671
C1472	G1411	A1288	A1289	A1290	G1229	G1168	A1106	U1046	A984	C924	U860	U800	G738	C672
A1473	U1412	G1290	G1350	A1291	C1230	C1169	A1107	U1047	G985	U925	G861	A801	G739	U674
A1474	U1413	G1351	G1352	A1292	C1231	U1170	U1108	U1048	A986	C926	A862	A802	G740	U673
U1475	G1414	G1352	G1353	A1293	A1231	A1171	A1109	C1049	G987	C927	C863	C803	G741	C675
G1476	C1415	A1293	A1353	A1294	A1232	U1172	G1110	G1050	G988	G928	C864	C804	G742	G676
C1477	A1416	G1294	A1354	G1294	A1233	U1173	C1111	U1051	G989	A929	A865	A806	A743	G677
U1478	C1417	U1295	A1355	U1295	C1234	G1174	U1112	G1052	A990	A930	G744	A807	G745	G678
C1540	G1418	G1356	G1356	G1296	C1235	A1175	C1113	G1053	A991	A931	C870	C808	G746	A681
G1419	G1419	U1357	U1357	A1297	G1236	U1176	A1114	G1054	A992	G932	C871	C809	G747	A682
G1480	G1480	G1358	G1358	G1298	G1237	U1177	C1115	A1055	C993	G933	C870	C809	G748	A683
U1481	A1420	C1358	C1358	A1298	G1238	U1178	U1116	U1056	A994	G934	C871	C809	A747	A684
U1482	U1421	G1359	G1359	A1299	A1238	C1178	U1116	U1056	A995	G935	C872	U810	A748	U685
G1483	U1422	G1360	G1360	A1299	A1239	A1179	G1117	A1057	A996	C936	U873	U811	G751	U686
A1486	G1425	G1361	G1361	U1301	G1240	A1180	G1118	A1058	C997	A936	U874	A813	G752	C686
U1487	U1426	A1362	A1362	C1302	G1241	C1181	U1119	A1059	C997	C937	G875	G814	U753	G687
G1488	G1427	C1363	C1363	U1303	A1242	U1182	C1120	C1060	C998	G938	G876	A815	G754	A688
C1489	G1428	G1364	G1364	U1304	G1243	C1183	G1121	A1061	A999	C939	A876	U816	C755	A689
U1490	A1429	U1365	U1365	C1305	U1244	G1184	A1122	G1062	G1000	G940	C877	A817	C756	C691
C1491	G1430	A1366	A1366	C1306	G1245	C1185	G1123	C1063	C1001	U941	C878	C818	U757	G692
U1492	U1431	A1367	A1367	U1307	G1246	G1186	U1124	A1064	C1002	U942	A879	C819	G758	A693
A1493	G1432	G1368	G1368	C1308	U1247	A1187	G1125	A1065	C1003	U943	C880	C820	C759	G694
G1494	G1433	G1369	G1369	G1309	G1248	A1188	A1126	G1066	A1004	A944	C881	U820	C760	G695
U1495	U1434	U1370	U1370	C1310	G1249	C1189	C1127	G1067	U1005	G945	C882	A821	U760	U696
G1496	G1435	G1371	G1371	C1311	A1250	C1190	G1128	A1068	C1006	U946	A883	G822	G761	U697
C1497	G1436	A1372	A1372	G1312	G1251	G1191	A1129	G1069	A1007	C947	C887	U823	A762	G699
G1498	U1437	G1373	G1373	U1313	C1252	A1192	U1130	G1070	C1008	C948	G888	U824	A763	A698
U1499	A1438	G1374	G1374	A1314	G1253	G1193	C1131	U1071	C1009	G949	C889	C825	A764	C700
C1500	G1439	C1375	C1375	A1315	G1254	U1194	G1132	U1072	U1010	G950	C890	U826	G765	U701
A1501	U1440	G1376	G1376	A1316	A1255	U1195	G1133	G1073	A1011	G951	U890	C827	A766	G702
G1502	G1441	C1377	C1377	G1317	C1256	G1196	C1134	G1074	A1012	A952	A891	C828	G767	A703
U1503	A1442	A1318	A1318	U1318	U1257	U1197	G1135	U1075	C1016	G953	G	C829	U768	G704
G1504	G1443	C1319	C1319	G1319	G1258	C1198	G1136	U1076	C1017	U954	G	C830	C769	C705
C1505	U1444	A1320	A1320	A1320	A1259	U1199	U1137	U1077	A956	G955	G	G831	G770	U707
A1445	A1445	A1321	A1321	G1321	A1260	G1200	A1138	A1078	U1019	G957	G	A832	C771	A706
U1446	U1446	G1322	G1322	U1262	G1261	G1201	A1139	G1079	C	G958	C	A833	G772	G708
G1508	U1447	C1323	C1323	U1263	U1262	U1202	A1140	A1080	A1020	C959	C	A834	G773	A709
A1509	A1448	G1324	G1324	G1263	G1263	A1203	U1141	A1081	A1021	U960	C	U835	U774	C710
C1510	G1449	U1325	U1325	C1264	G1264	G1204	G1142	C1082	A1022	G961	A	U837	G775	C711
U1511	U1450	G1326	G1326	G1265	G1265	G1205	A1143	A1083	U1023	C962	C	A838	G776	A712
C1512	G1451	C1327	C1327	G1266	G1266	G1206	U1144	C1084	G1024	G963	C	U839	G777	G713
U1513	U1452	U1328	U1328	A1267	A1267	G1207	G1145	G1085	A1025	A964	A	U840	G778	A718
C1514	A1453	U1329	U1329	U1268	U1268	A1208	U1146	C1086	U1026	G965	G	G841	G781	A719
U1515	U1454	G1330	G1330	G1269	G1269	G1209	G1147	C1087	C1027	U966	C	A846	U784	C725
G1516	C1455	G1331	G1331	C1270	C1270	G1210	G1148	A1088	G1028	G967	U	C847	G785	C726
C1517	U1456	G1332	G1332	C1271	C1271	G1211	G1149	C1089	C1029	G968	C	A848	G786	U727
U1518	G1457	G1333	G1333	G1272	G1272	U1212	C1150	C1090	U1030	U969	A	C849	G789	G728
C1519	A1458	A1334	A1334	G1273	G1273	U1213	U1151	G1091	C1031	U970	C	C851	G791	A729
U1520	U1459	A1335	A1335	C1274	C1274	C1214	C1152	U1092	A1032	A971	C	U852	U792	C730
C1521	G1460	G1336	G1336	A1275	A1275	A1215	U1153	U1093	G1033	G972	A911	C853	G793	A731
U1522	U1461	G1337	G1337	A1278	A1278	G1216	A1154	C1094	U1034	C973	A912	A848	G794	G732
A1523	C1462	G1338	G1338	G1279	G1279	U1217	G1155	A1095	G1035	U973	A913	C854	A795	G733
C1524	A1463	U1339	U1339	C1280	C1280	C1218	U1159	A1096	G1036	U974	C914	C855	G796	A796
U1525	U1464	C1340	C1340	A1281	A1281	G1219	C1160	G1097	U1037	G975	C915	U856	U797	G734
A1526	A1465	G1341	G1341	A1282	A1282	G1220	U1161	G1098	U1038	G977	C916	C857	G798	
U1527	G1466	U1342	U1342	A1283	A1283	C1221	U1162	A1099	A1039	G978	A918	C858	A799	
C1528	U1467	C1343	C1343	G1284	G1284	G1222	C1163	U1100	A1040	U979	U919	G859	A799	
U1529	C1529	G1344	G1344	A1285	A1285	G1223	U1101	U1101	G1042	G980	G920	A856	A796	





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.39Å 407.06Å 692.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 19.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-3.50) 100.0 (19.99-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.52Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.251 , 0.320 0.293 , 0.351	Depositor DCC
$R_{free}$ test set	13460 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	98.5	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 68.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	59630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0	0.65	7/66467 (0.0%)	0.84	119/103673 (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	0	0	128

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	700	C	N1-C2	10.10	1.50	1.40
1	0	538	A	C5-C6	-5.66	1.35	1.41
1	0	788	G	N9-C4	5.49	1.42	1.38
1	0	2593	A	C5-C6	-5.46	1.36	1.41
1	0	774	A	C5-C6	-5.29	1.36	1.41

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1279	G	N9-C1'-C2'	10.85	128.10	114.00
1	0	1266	G	N9-C1'-C2'	10.62	127.81	114.00
1	0	765	C	O4'-C1'-N1	9.33	115.66	108.20
1	0	2237	C	N1-C1'-C2'	9.28	126.06	114.00
1	0	985	G	N9-C1'-C2'	9.24	126.01	114.00

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	123	A	Sidechain
1	0	154	U	Sidechain
1	0	67	G	Sidechain
1	0	71	A	Sidechain

## 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	0	59359	0	29917	4315	0
2	R	93	0	0	0	0
3	W	65	0	0	0	0
4	7	113	0	0	0	0
All	All	59630	0	29917	4315	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 49.

The worst 5 of 4315 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)
1:0:541:C:O2'	1:0:2018:G:N2	1.63	1.29
1:0:788:G:H22	1:0:801:A:P	1.58	1.26
1:0:1066:G:H3'	1:0:1067:G:H4'	1.23	1.20
1:0:2170:C:H2'	1:0:2171:U:H5'	1.23	1.17
1:0:1314:A:O2'	1:0:1315:A:H3'	1.42	1.15

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	657 (23%)	223 (8%)

5 of 657 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	14	A
1	0	34	U
1	0	45	C
1	0	48	A

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1263	G
1	0	1469	U
1	0	2608	A
1	0	1278	A
1	0	1333	G

## 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](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2766/2880 (96%)	0.56	301 (10%) 6 7	21, 75, 199, 205	0
2	R	93/95 (97%)	2.46	42 (45%) 0 0	16, 63, 157, 200	0
3	W	65/67 (97%)	1.96	24 (36%) 0 0	21, 86, 159, 200	0
4	7	113/113 (100%)	3.78	60 (53%) 0 0	16, 120, 200, 200	0
All	All	3037/3155 (96%)	0.77	427 (14%) 3 4	16, 76, 200, 205	0

The worst 5 of 427 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	7	84	ASN	17.7
2	R	90	ALA	16.5
4	7	110	TYR	15.3
2	R	93	GLY	14.0
4	7	77	GLY	14.0

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.