



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:25 AM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

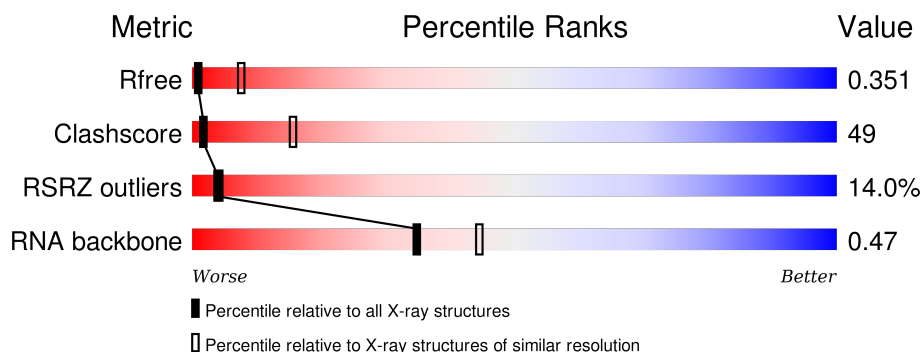
1 Overall quality at a glance

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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. 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			

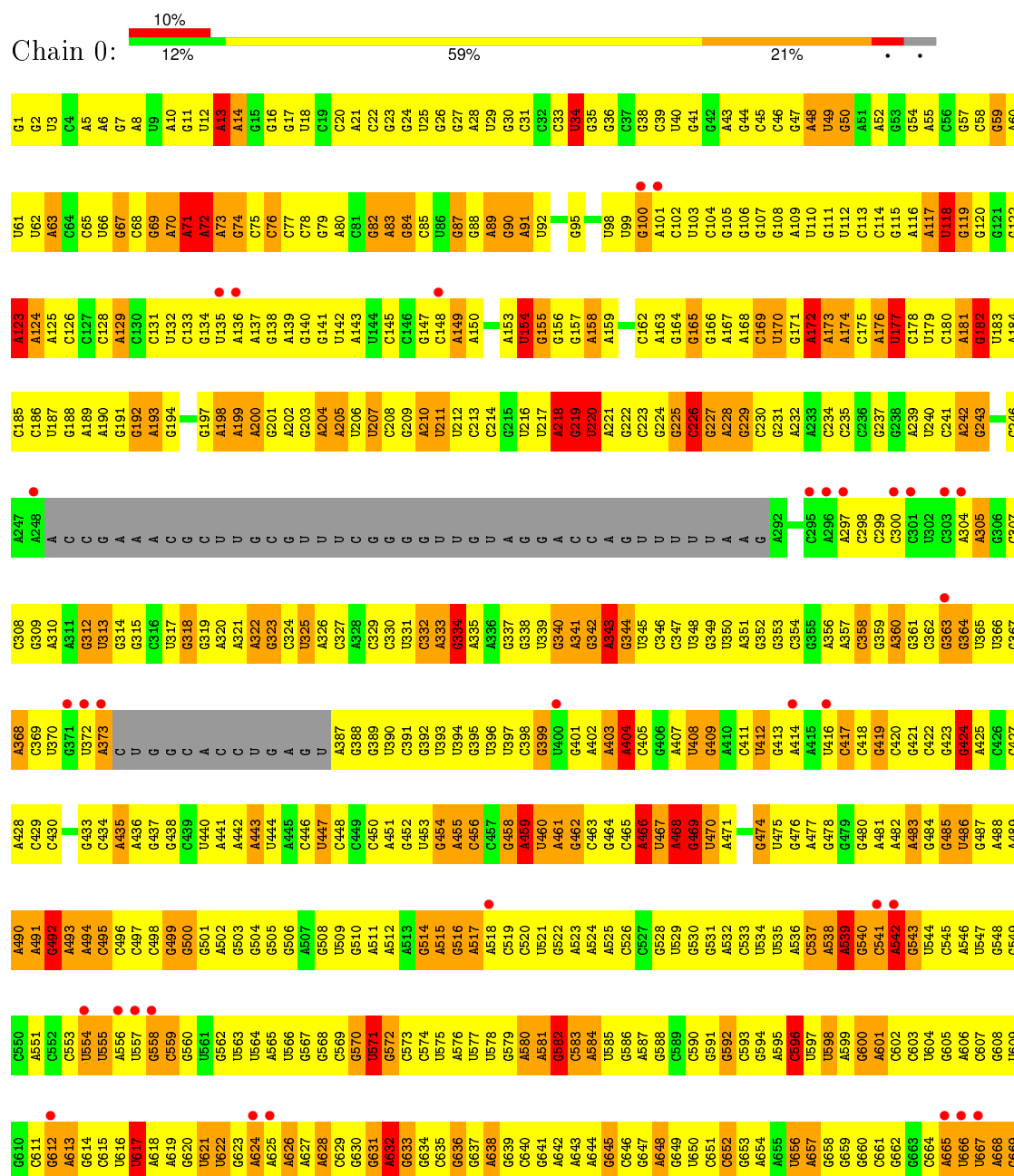
- Molecule 4 is a protein called Trigger Factor.

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

3 Residue-property plots

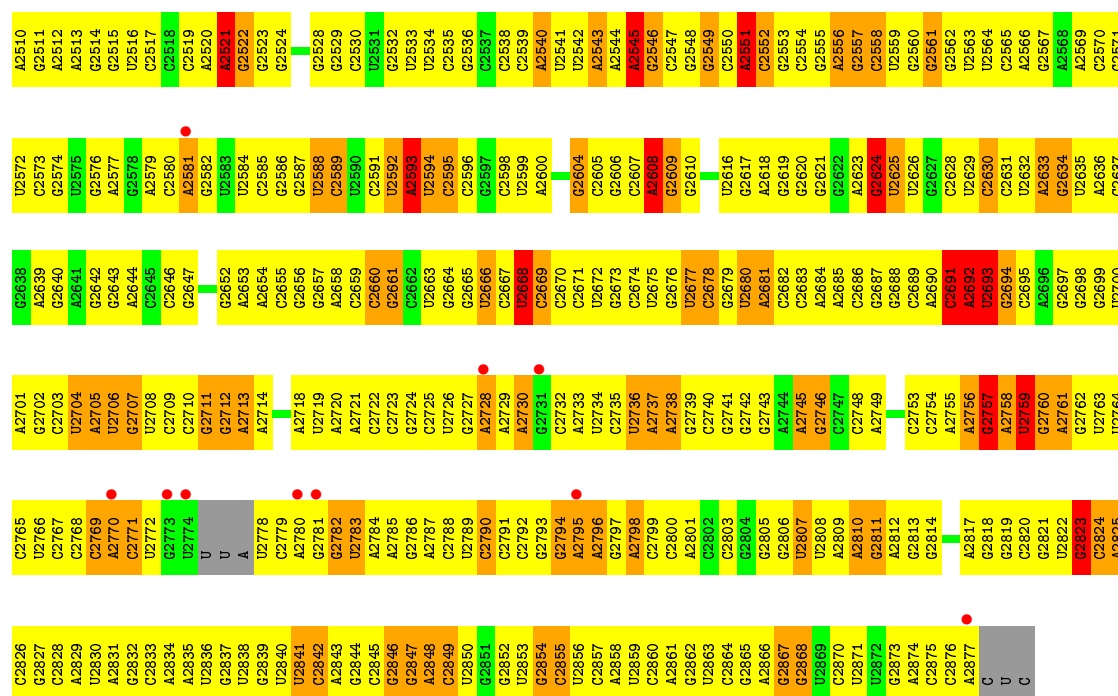
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

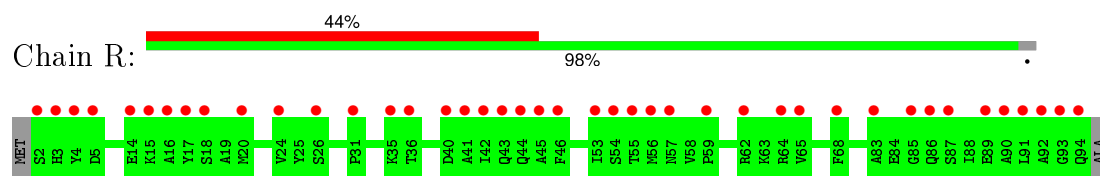


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G1533	C1472	G1350	A1349	A1289	G1228	G1168	A1106	U1046	A984	A924	U860	U800	C738	C672
A1534	U1473	G1351	G1350	A1290	G1229	C1169	A1107	U1047	G985	U925	G861	G739	G673	G617
C1535	A1474	U1413	G1352	A1291	G1230	A1170	U1108	U1048	A986	C926	A862	A740	U674	U674
G1536	G1475	G1353	G1352	A1292	A1231	A1171	U1109	U1049	G987	C927	C863	C803	C741	C675
U1537	G1476	A1354	A1353	A1293	U1232	U1172	G1110	G1050	G988	C928	C864	C804	G742	G676
A1538	C1477	A1355	A1354	A1294	A1233	G1173	C1111	U1051	G989	A929	A865	A805	G743	G677
U1539	A1477	G1356	A1355	U1295	A1234	G1174	U1112	C1052	A990	A930	G869	G806	G744	G678
G1540	G1479	U1357	G1356	G1296	G1235	A1175	G1113	G1053	A991	G931	C807	C808	C745	G678
C1541	G1480	U1357	U1357	A1297	G1236	U1176	A1114	C1054	A992	G932	C809	C809	C746	G678
G1542	U1481	A1358	G1358	G1298	G1237	U1177	C1115	U1055	C993	G933	C870	C809	A747	G678
U1543	G1482	A1359	G1359	A1299	G1238	U1178	U1116	A1056	A994	G934	U871	U810	A748	G678
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C1552	C1491	G1368	G1368	C1308	U1247	A1187	G1125	A1065	C1003	U943	C880	C819	G758	G678
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C1561	G1500	G1377	G1377	G1317	C1256	G1196	C1134	G1074	A1012	A952	A891	C828	G767	G678
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G1566	U1505	A1445	G1382	G1322	G1261	G1201	A1139	G1079	U1020	G957	G	A834	G772	G678
C1567	U1506	A1446	C1383	G1323	U1262	U1202	A1140	A1080	A1021	G958	C	U835	G773	G678
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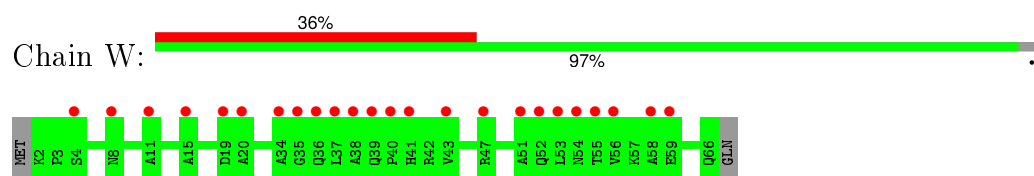
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C2493	G2433	C2372	A2309	A2245	A	C2124	U2064	A2003	G1942	G1882	C1758	A1634
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C2495	G2435	A2374	U2311	A2247	U	U2126	G2066	U2005	C1944	A1884	G1760	C1636
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C2500	C2440	A2381	G2316	A2253	U	G2132	G2071	G2010	U1950	U1889	C1765	C1641
U2501	U2441	C2382	G2317	A2254	U	U2133	C2072	U2011	G1951	G1890	U1766	G1642
G2502	C2442	C2383	G2320	G2255	A	U2134	A2073	A2012	C1822	C1827	A1706	A1643
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G2504	G2444	U2385	G2322	G2257	A	G2136	U2075	A1953	C1824	C1830	U1768	G1645
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G2508	U2448	G2389	A2325	G2261	A	G2140	U2080	C2019	U1959	U1897	A1774	A1649
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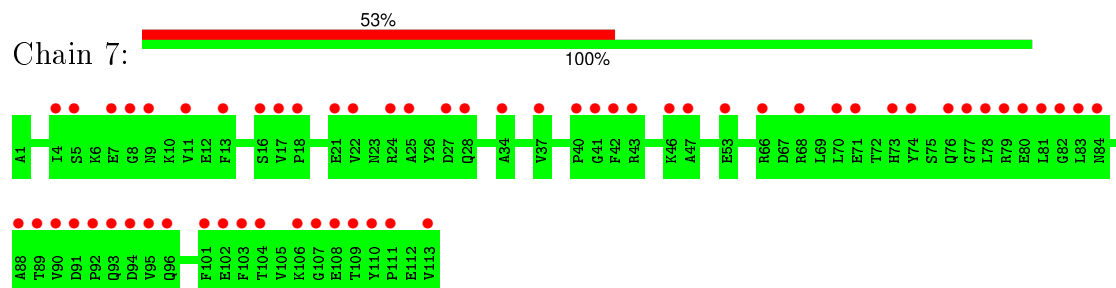
• Molecule 2: 50S ribosomal protein L23



• Molecule 3: 50S ribosomal protein L29



• Molecule 4: Trigger Factor



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	98.5	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 68.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 297349 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	59630	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0	2766/2880 (96%)	0.59	300 (10%) 8 7	21, 75, 199, 205	0
2	R	93/95 (97%)	2.47	42 (45%) 0 0	16, 63, 157, 200	0
3	W	65/67 (97%)	1.98	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%)	0.80	426 (14%) 4 4	16, 76, 200, 205	0

The worst 5 of 426 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	7	84	ASN	17.8
2	R	90	ALA	16.5
4	7	110	TYR	15.2
2	R	93	GLY	13.8
4	7	77	GLY	13.8

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 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.