



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:28 AM GMT

PDB ID : 2D3O
Title : Structure of Ribosome Binding Domain of the Trigger Factor on the 50S ribosomal subunit from *D. radiodurans*
Authors : Schlutzen, F.; Wilson, D.N.; Hansen, H.A.; Tian, P.; Harms, J.M.; McInnes, S.J.; Albrecht, R.; Buerger, J.; Wilbanks, S.M.; Fucini, P.
Deposited on : 2005-09-30
Resolution : 3.35 Å(reported)

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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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

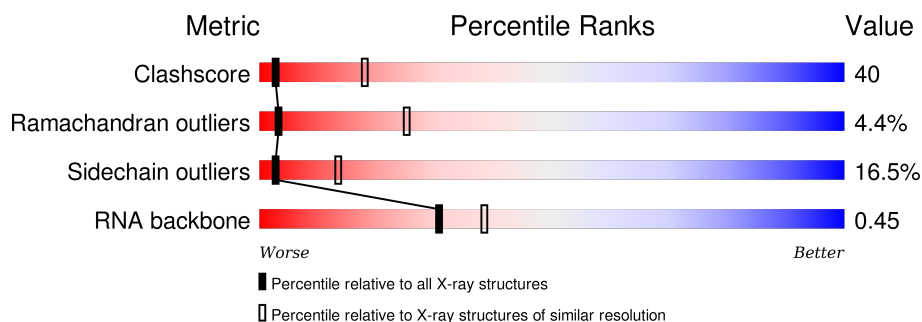
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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))
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RNA backbone	2183	1016 (3.92-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	R	95	
3	S	115	
4	W	67	
5	1	112	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 63004 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	2802	Total	C	N	O	P	0	0	0
			60132	26824	11089	19418	2801			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	W	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 5 is a protein called Trigger Factor.

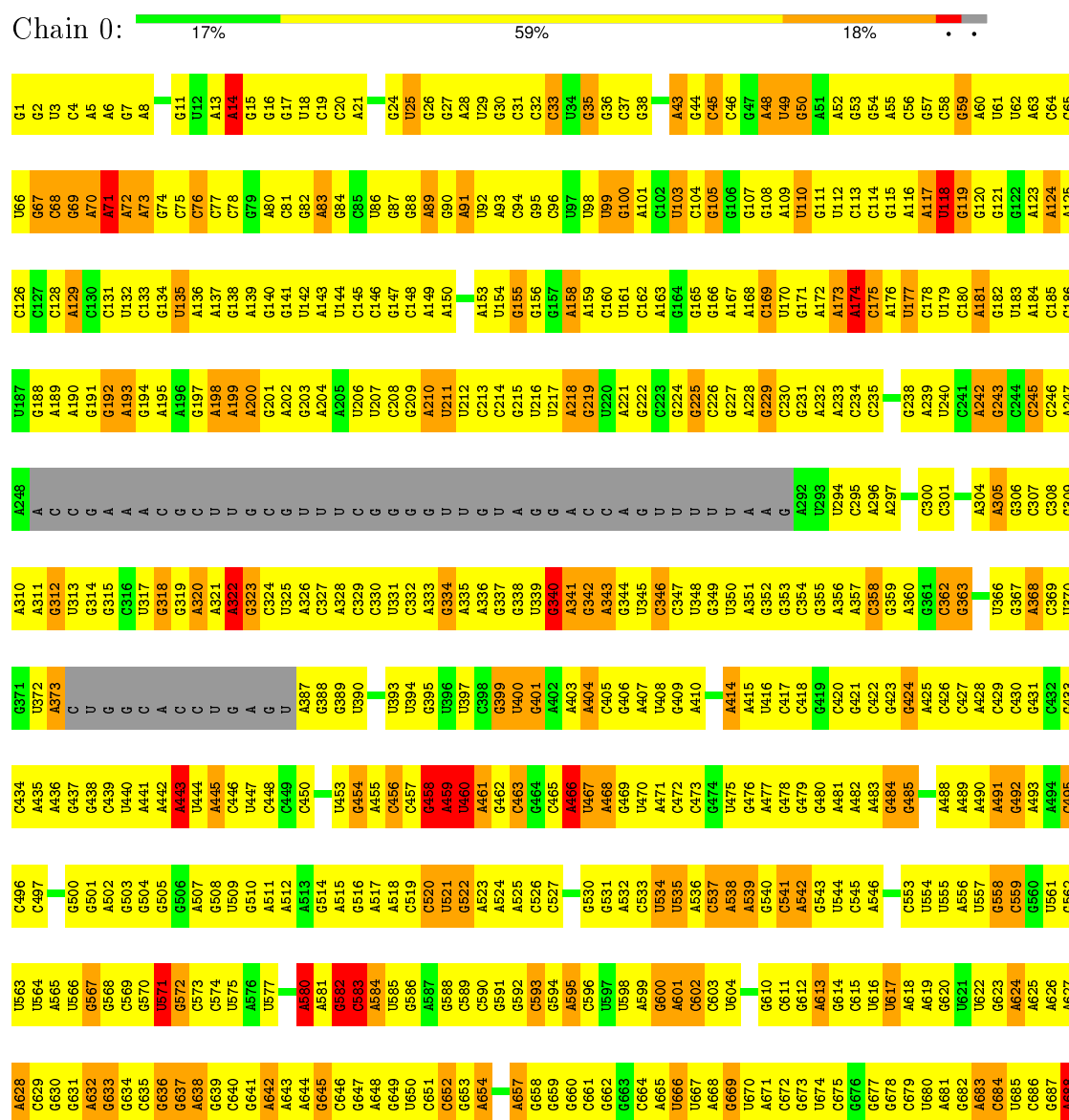
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	1	100	Total	C	N	O	0	0	0
			788	494	146	148			

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 ($RSRZ > 2$). 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.

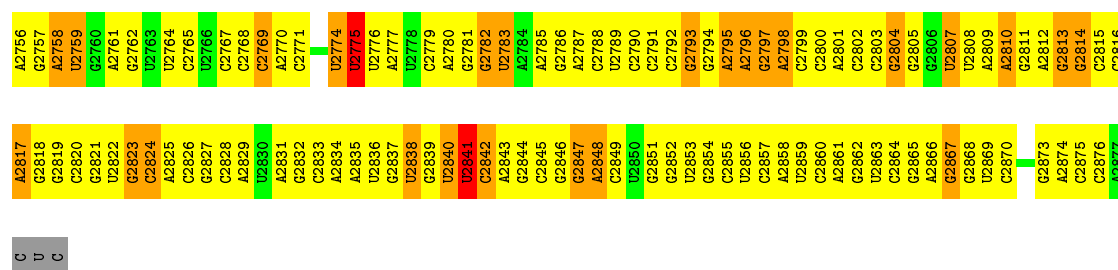
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA

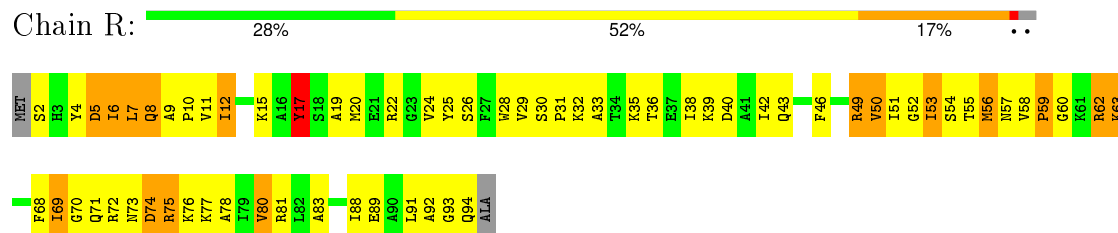


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A1582	A1516	G1394	C1455	G1390	U1197	U1197	C1135	C1002	C937	G875	A815	U754	C691
A1583	C1517	A1395	C1456	A1259	C1198	U1198	G1136	C1003	G938	A876	U816	C755	C692
C1653	C1518	G1332	A1457	G1332	A1260	U1199	A1137	U1072	C939	G877	A817	C756	A693
A1654	G1519	C1333	A1458	A1261	G1200	U1199	A1138	U1005	G940	C878	A818	U757	A694
A1586	G1520	G1338	U1459	A1334	G1201	U1201	A1139	C1006	U941	A879	C819	C758	C695
A1587	U1521	C1339	A1460	A1335	G1202	U1202	A1140	C1007	U942	C880	U820	C759	C696
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C1590	G1402	G1338	A1463	G1338	G1265	G1205	A1143	A1078	A945	A883	U823	A762	C699
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A1595	G1407	G1344	A1469	G1344	U1211	G1149	G1149	C1086	U951		U829		
A1596	A1408	C1345	U1470	C1345	U1212	G1150	C1150	C1087	A952		U830	U770	C705
A1597	A1409	U1346	G1471	U1346	U1215	U1151	C1151	C1088	G953		C831	C771	A706
C1598	U1410	C1347	C1472	C1347	C1217	C1152	C1152	C1089	U954	A891	A832	C772	U707
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U1600	G1412	U1349	A1474	A1349	G1223	U1217	A1154	C1091	A956	G	A834	A774	C710
A1601	U1413	G1350	U1475	G1350	C1218	C1218	G1155	U1092	G957	G	U835	U775	C711
G1602	G1414	U1351	G1476	G1351	G1219	G1219		U1093	C958	G	U836	C776	A712
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A1604	A1416	G1352	U1478	G1352	C1221	U1159	A1158	A1095	G961	C	A838	C778	G714
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C1606	G1418	A1354	G1479	A1354	G1223	C1223	C1160	C1097		A	U840	U779	U715
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G1608	G1543	G1356	U1481	G1356	A1285	U1217	A1154	C1098	G969	C	A842	U781	G717
A1689	A1544	U1357	U1482	U1357	G1291	C1224	A1162	G1098	C969	C	U843	U782	A718
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A1610	C1546	C1422	G1483	C1358	A1293	A1226	C1164	G1100	A970	A	G843	U784	A720
C1687	U1611	A1423	U1484	G1359	G1294	U1227	G1165	U1101	A971	G	G844	U785	C721
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U1690	C1612	C1363	A1486	C1363	G1296	C1229	A1167	G1033	C973	U	A846	U787	C723
A1691	G1613	U1364	C1487	C1364	A1297	C1230	C1168	U1034	U973	U	U847	U788	C724
C1692	U1551	U1365	G1427	U1365	G1298	A1231	C1169	U1035	C975	A	A848	C789	C725
G1553	G1552	A1366	G1428	A1366	A1299	U1232	U1170	A1106	C976	C	G849	C788	C726
		U1367	U1429	A1367	A1300	U1233	A1171	A1107	G977	C	C850	A790	U727
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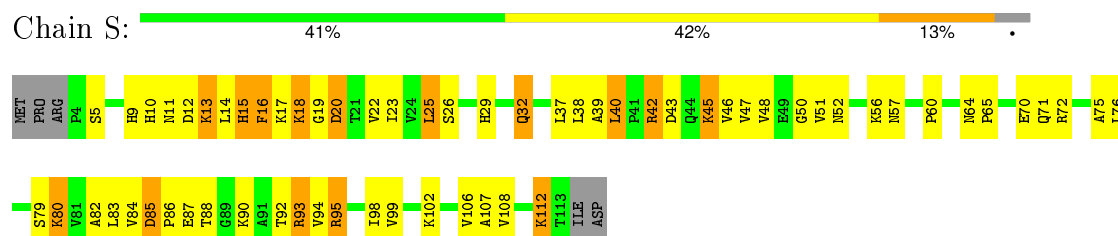
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G2724	C2532	C2657	C2595	G2532	U2472	G2408	C2347	A2281	U2218	G2148	U2069	U2009	U1948	U1881	G1749	G1749
G2725	U2533	G2658	U2596	U2533	G2473	A2409	A2348	C2281	U2219	G2149	G2070	G2010	G1947	U1882	A1750	A1750
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G2739	C2547	U2675	A2611	C2547	G2487	G2423	G2364	C2298	G2234	G2173	G2086	C2026	G1963	C1903	C1765	C1765
C2740	U2548	G2676	G2612	G2548	G2488	G2424	C2365	U2299	G2235	G2174	U2087	G2027	A1964	G1904	U1766	U1766
G2741	G2549	C2677	A2613	G2549	C2489	G2425	U2366	A2300	C2236	A2175	U2087	C2028	U1965	G1905	G1767	G1767
G2742	C2550	U2678	G2614	C2550	U2490	G2426	G2367	G2301	C2237	U2176	G2088	G2029	U1966	G1831	U1768	U1768
G2743	A2551	C2679	U2615	A2551	C2491	A2427	A2367	A2301	G2238	U2177	G2089	G2030	C1967	U1906	U1769	U1769
A2744	C2552	A2681	U2616	C2552	U2492	U2428	G2368	G2302	G2239	U2178	G2090	U2031	C1968	C1907	U1770	U1770
A2745	G2553	C2682	G2617	G2553	C2493	A2429	U2369	G2306	C2240	U2179	U2096	A2032	G1969	A1908	A1771	A1771
G2749	U2554	G2683	A2618	C2554	A2494	A2430	G2370	A2307	C2241	U2180	U2097	G2032	U1909	U1909	C1835	C1835
G2750	G2555	C2684	G2619	G2555	C2495	C2431	A2371	A2308	U2242	U2181	A2097	G2033	G1970	A1910	C1836	C1836
C2751	A2556	U2685	G2620	A2556	U2496	A2432	C2372	A2309	C2242	A2182	G2099	A2034	C1971	A1911	G1837	G1837
G2752	C2557	G2686	G2621	G2557	U2497	G2433	C2373	G2309	A2245	C2183	A2100	G2035	C1972	A1912	G1838	G1838
C2753	U2558	C2687	U2622	C2558	U2498	G2434	C2374	G2310	A2246	C2184	U2105	G2036	C1973	G1913	A1839	A1839
G2754	G2559	A2688	G2623	G2559	C2499	C2435	G2375	U2311	A2247	U2185	U2106	A2037	U1974	U1914	A1777	A1777
A2755	C2560	U2689	U2624	C2560	G2500	U2436	G2376	A2312	A2248	C2186	G2106	C2038	G1975	A1915	G1841	U1778



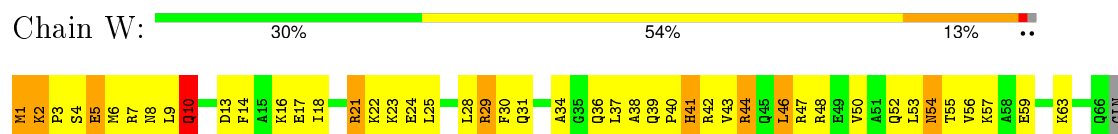
- Molecule 2: 50S RIBOSOMAL PROTEIN L23



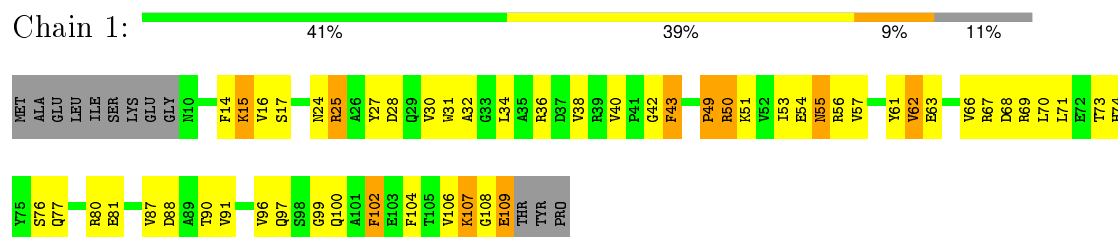
- Molecule 3: 50S RIBOSOMAL PROTEIN L24



- Molecule 4: 50S RIBOSOMAL PROTEIN L29



- Molecule 5: Trigger Factor



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.50 Å 410.50 Å 695.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.35	Depositor
% Data completeness (in resolution range)	(Not available) (29.84-3.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.299 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	63004	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

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	0.67	3/67338 (0.0%)	0.82	72/105044 (0.1%)
2	R	0.48	0/737	0.80	0/988
3	S	0.42	0/835	0.73	1/1121 (0.1%)
4	W	0.44	0/537	0.58	0/714
5	1	0.48	0/802	0.68	0/1084
All	All	0.66	3/70249 (0.0%)	0.82	73/108951 (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	169
2	R	0	1
All	All	0	170

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2776	U	C1'-N1	6.38	1.58	1.48
1	0	2775	U	C1'-N1	6.21	1.58	1.48
1	0	567	G	C5-C6	-5.13	1.37	1.42

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2034	A	N9-C1'-C2'	10.22	127.28	114.00
1	0	1342	U	N1-C1'-C2'	9.78	126.71	114.00
1	0	1467	U	N1-C1'-C2'	8.63	125.23	114.00
1	0	2775	U	C2-N1-C1'	-8.26	107.78	117.70
1	0	1631	C	N1-C1'-C2'	8.21	124.68	114.00

There are no chirality outliers.

5 of 170 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	14	A	Sidechain
1	0	25	U	Sidechain
1	0	43	A	Sidechain
1	0	71	A	Sidechain

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	0	60132	0	30298	3519	0
2	R	726	0	753	126	0
3	S	825	0	881	117	0
4	W	533	0	558	81	0
5	1	788	0	784	74	0
All	All	63004	0	33274	3848	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 40.

The worst 5 of 3848 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:R:69:ILE:CG2	2:R:70:GLY:H	1.26	1.38
1:0:1325:U:H1'	1:0:1619:A:N1	1.50	1.25
2:R:69:ILE:HG22	2:R:70:GLY:N	1.30	1.19
3:S:92:THR:HB	3:S:95:ARG:HH22	1.05	1.18
1:0:67:G:H21	1:0:72:A:H2'	1.09	1.16

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	
2	R	91/95 (96%)	70 (77%)	16 (18%)	5 (6%)	2	18
3	S	108/115 (94%)	79 (73%)	24 (22%)	5 (5%)	3	23
4	W	64/67 (96%)	54 (84%)	8 (12%)	2 (3%)	5	35
5	1	98/112 (88%)	81 (83%)	13 (13%)	4 (4%)	3	27
All	All	361/389 (93%)	284 (79%)	61 (17%)	16 (4%)	3	25

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	42	ARG
3	S	65	PRO
4	W	2	LYS
5	1	49	PRO
2	R	69	ILE

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	
2	R	75/76 (99%)	61 (81%)	14 (19%)	2	8
3	S	91/96 (95%)	77 (85%)	14 (15%)	3	16
4	W	54/55 (98%)	43 (80%)	11 (20%)	1	6
5	1	83/93 (89%)	72 (87%)	11 (13%)	5	21
All	All	303/320 (95%)	253 (84%)	50 (16%)	3	13

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	40	LEU
3	S	112	LYS
5	1	88	ASP
3	S	43	ASP
3	S	80	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	S	64	ASN
3	S	71	GLN
5	1	55	ASN
3	S	57	ASN
5	1	24	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2798/2880 (97%)	580 (20%)	88 (3%)

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	14	A
1	0	25	U
1	0	33	C
1	0	35	G
1	0	45	C

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1342	U
1	0	1664	G
1	0	2660	C
1	0	1355	A
1	0	1626	A

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.