



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:46 PM UTC

PDB ID : 2D3O / pdb_00002d3o
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)

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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

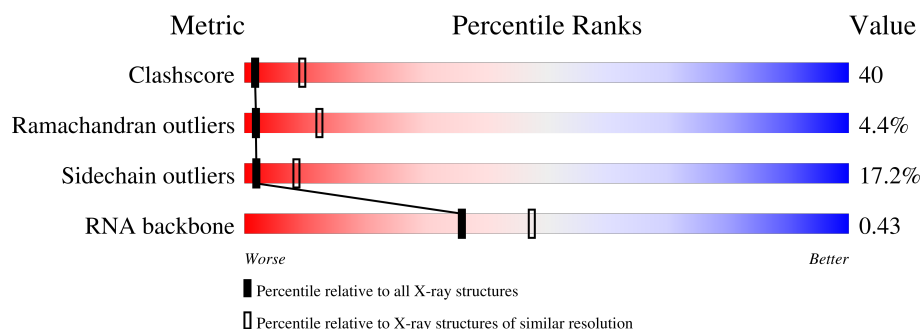
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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 $\leq 5\%$.

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.

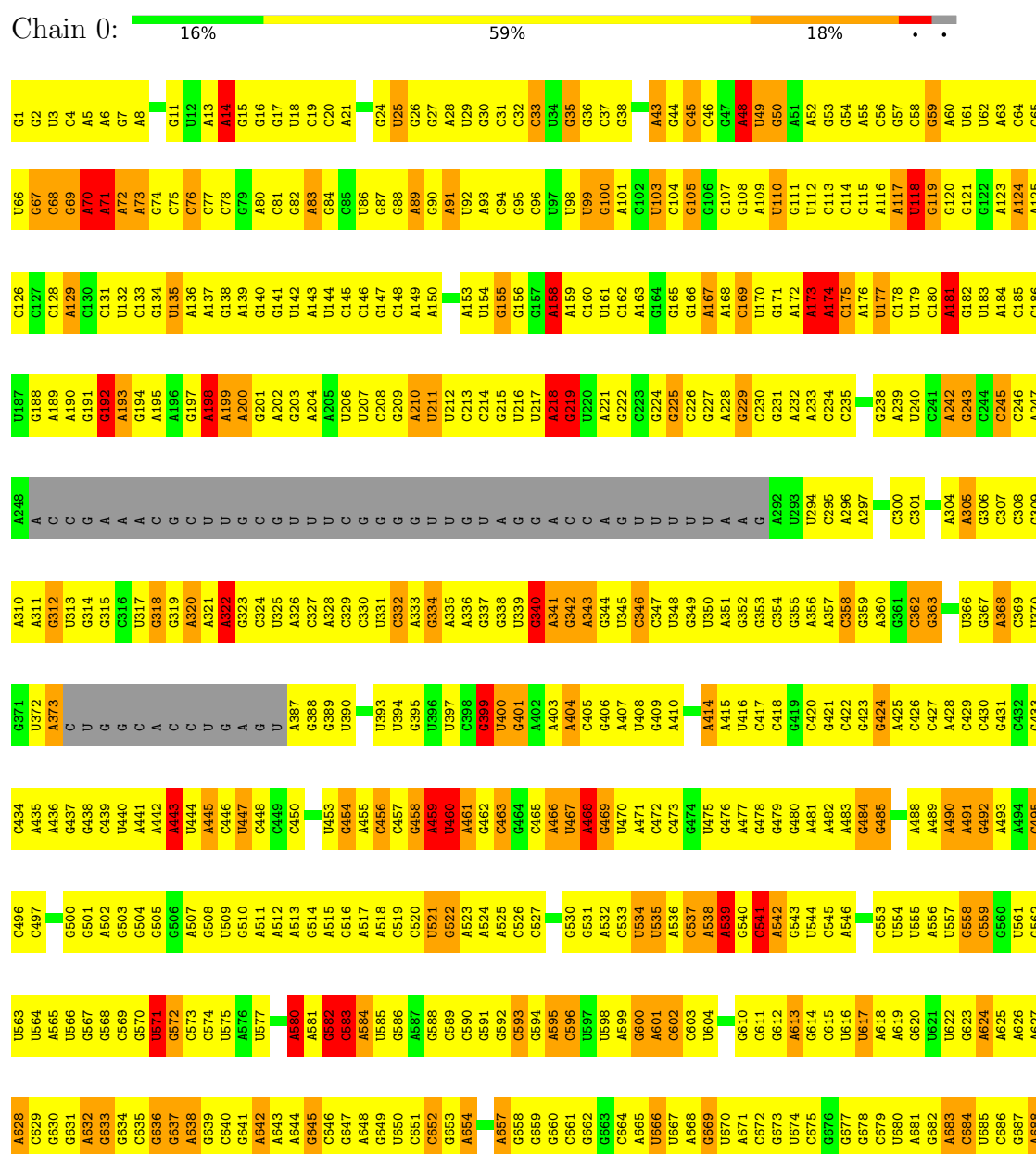
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	1	100	Total	C	N	O	0	0	0
			788	494	146	148			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

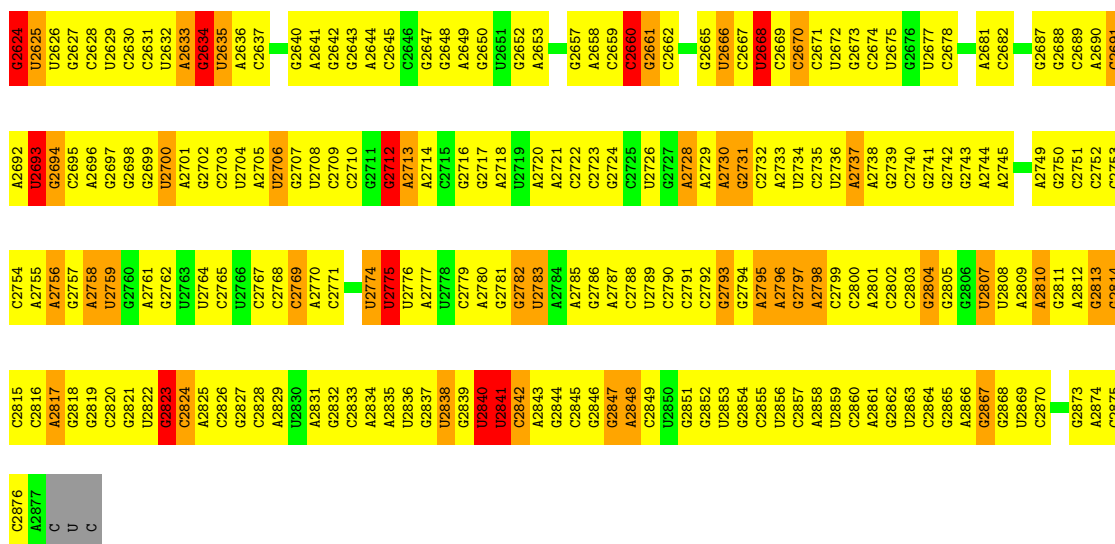
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



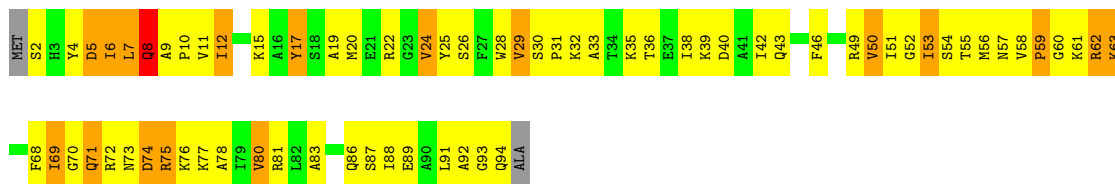
C1580	C1581	A1582	A1583	G1584	A1585	A1586	A1587	A1588	A1589	C1590	U1591	U1592	C1593	U1594	A1595	A1596	A1597	A1598	A1599	U1600	G1601	A1602	A1603	A1604	A1605	A1606	A1607	U1608	A1609	G1610	A1611	U1612	C1613	C1614	C1615	A1619	C1620	G1621	G1622	C1623	A1624	A1625	A1626	C1627	C1628	G1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	U1637	G1642		U1647				
C1514	U1515	A1516	C1517	C1518	G1519	G1520	U1521	C1522	A1523	C1524	C1528	C1529	U1530	A1531	A1532	A1533	A1534	A1535	C1536	U1537	A1538	A1539	C1540	G1541	G1542	G1543	A1544	G1545	C1546	C1549	C1550	U1551	C1552	G1553	G1557	C1558	G1559	A1560	A1561	G1562	U1563	U1564	A1567	A1568	A1569	C1570	C1572	G1573	A1574	C1575	C1576	U1577	A1512								
A1453	U1454	C1455	C1456	A1457	A1458	U1459	C1460	C1461	C1462	A1463	A1464	C1465	C1466	U1467	A1468	U1469	U1470	G1471	C1472	U1473	G1474	U1475	C1476	U1477	U1478	G1479	G1480	U1481	U1482	U1483	U1484	U1485	C1486	C1487	G1488	C1489	U1490	C1491	A1492	A1493	G1494	A1495	G1496	C1497	C1498	A1499	U1500	C1501	G1502	G1503	U1504	U1505	G1508	A1509	U1510	A1511	A1512	U1513			
U1392	G1393	G1394	A1395	C1396	G1397	A1398	C1399	A1400	G1401	G1402	U1403	A1404	A1405	A1406	G1407	A1408	U1409	U1410	C1411	C1412	U1413	G1414	C1415	C1416	C1417	G1418	A1419	A1420	U1421	C1422	A1423	U1424	G1425	U1426	G1427	G1428	A1429		A1433	U1434	G1435	G1436	A1437	G1438	G1439	G1440	A1441	C1442	C1443	C1444	A1445	U1446	U1447	A1448	C1449	G1450	U1451	U1452			
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C1514	U1515	A1516	C1517	C1518	G1519	G1520	U1521	C1522	A1523	C1524	C1528	C1529	U1530	A1531	A1532	A1533	A1534	A1535	C1536	U1537	A1538	A1539	C1540	G1541	G1542	G1543	A1544	G1545	C1546	C1549	C1550	U1551	C1552	G1553	G1557	C1558	G1559	A1560	A1561	G1562	U1563	U1564	A1567	A1568	A1569	C1570	C1572	G1573	A1574	C1575	C1576	U1577	A1512								
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G752	U753	G754	C755	C756	U757	G758	C759	U760	G761	A762	U763	A764	C765	A766	G767		U770	C771	C772	G773	C774	U775	G776	A777	G778	U779	U780	G781	A782	C783	U784	U785	C786	G787	G788	A789	U790	U791	U792	G793	A794	A795	A796	U797	G798	C799	U800	A801	G802	C803	A804	G805	A806	G807	C808	C809	U810	G811	C812	G812	
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C935	A936	C937	G938	C939	G940	U941	U942	U943	A944																																																				





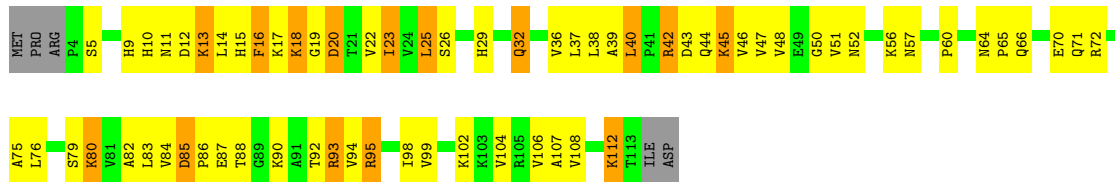
• Molecule 2: 50S RIBOSOMAL PROTEIN L23

Chain R: 25% 54% 18% ..



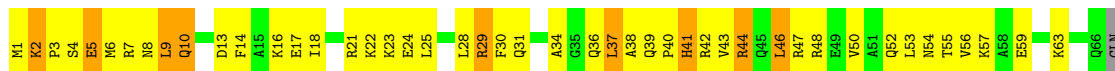
• Molecule 3: 50S RIBOSOMAL PROTEIN L24

Chain S: 37% 45% 13% .



• Molecule 4: 50S RIBOSOMAL PROTEIN L29

Chain W: 30% 55% 13% .



• Molecule 5: Trigger Factor

Chain 1: 40% 40% 9% 11%



H74	Y75	S76	Q77		R80	E81		V87	D88	A89	T90	V91		V96	Q97	S98	G99	Q100	A101	F102	E103	F104	T105	V106	K107	G108	E109	THR	TYR	PRO
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4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.50Å 410.50Å 695.20Å 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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	2/67338 (0.0%)	0.86	165/105044 (0.2%)
2	R	0.53	0/737	1.15	7/988 (0.7%)
3	S	0.48	0/835	1.00	4/1121 (0.4%)
4	W	0.45	0/537	0.81	0/714
5	1	0.50	0/802	0.94	2/1084 (0.2%)
All	All	0.47	2/70249 (0.0%)	0.86	178/108951 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2776	U	C1'-N1	6.58	1.58	1.48
1	0	2775	U	C1'-N1	6.41	1.58	1.48

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1975	G	C2'-C3'-O3'	10.66	125.50	109.50
2	R	71	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	0	1141	U	C2'-C3'-O3'	10.07	124.61	109.50
5	1	65	GLN	OE1-CD-NE2	-9.81	112.79	122.60
3	S	44	GLN	OE1-CD-NE2	-9.78	112.82	122.60

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 [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	60132	0	30298	3516	0
2	R	726	0	753	130	0
3	S	825	0	881	119	0
4	W	533	0	558	81	0
5	1	788	0	784	75	0
All	All	63004	0	33274	3852	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 3852 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
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
1:0:918:A:H2'	1:0:919:U:H5''	1.29	1.15

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	1	9
3	S	108/115 (94%)	79 (73%)	24 (22%)	5 (5%)	2	11
4	W	64/67 (96%)	54 (84%)	8 (12%)	2 (3%)	3	17
5	1	98/112 (88%)	81 (83%)	13 (13%)	4 (4%)	2	14
All	All	361/389 (93%)	284 (79%)	61 (17%)	16 (4%)	2	12

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 ⓘ

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%)	1	6
3	S	91/96 (95%)	74 (81%)	17 (19%)	1	6
4	W	54/55 (98%)	44 (82%)	10 (18%)	1	7
5	1	83/93 (89%)	72 (87%)	11 (13%)	4	15
All	All	303/320 (95%)	251 (83%)	52 (17%)	2	8

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	95	ARG
4	W	37	LEU
5	1	100	GLN
3	S	104	VAL
4	W	6	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
4	W	54	ASN
5	1	24	ASN
5	1	100	GLN
5	1	55	ASN
3	S	57	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2798/2880 (97%)	582 (20%)	88 (3%)

5 of 582 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	1777	A
1	0	2237	C
1	0	1811	A
1	0	2016	A
1	0	2409	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 oligosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.