



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:52 AM UTC

PDB ID : 2NR0 / pdb_00002nr0
Title : Crystal structure of pseudouridine synthase TruA in complex with leucyl tRNA
Authors : Hur, S.; Stroud, R.M.
Deposited on : 2006-11-01
Resolution : 3.90 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)	:	2.0
EDS	:	3.0
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

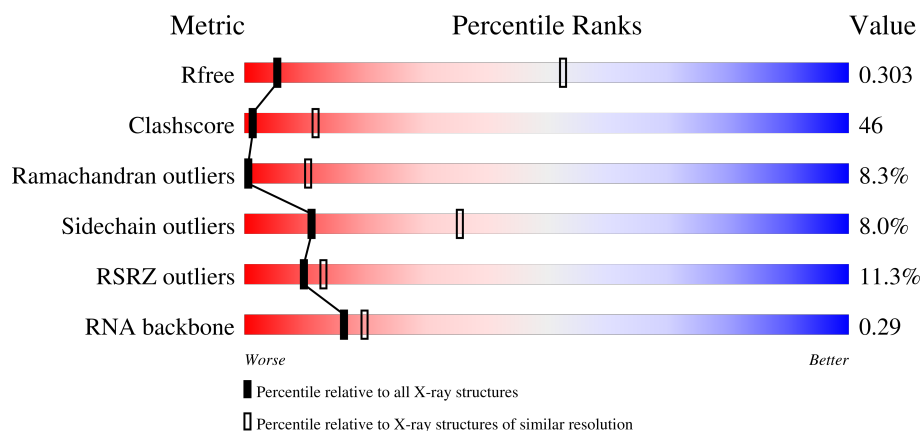
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

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	E	87	32% 16% 53% 21% 7%
1	F	87	36% 7% 41% 23% 11% 17%
1	G	87	18% 14% 30% 29% 5% 23%
1	H	87	28% 21% 30% 20% 5% 25%

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Mol	Chain	Length	Quality of chain			
2	A	270	4% 27% 57% 12%	..		
2	B	270	4% 28% 58% 11%	..		
2	C	270	5% 26% 59% 10%	..		
2	D	270	6% 27% 59% 11%	..		

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14269 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 leucyl tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	81	Total	C	N	O	P	0	0	0
			1682	748	292	562	80			
1	F	72	Total	C	N	O	P	0	2	0
			1544	687	266	518	73			
1	G	67	Total	C	N	O	P	0	0	0
			1422	634	251	471	66			
1	H	65	Total	C	N	O	P	0	0	0
			1343	595	236	448	64			

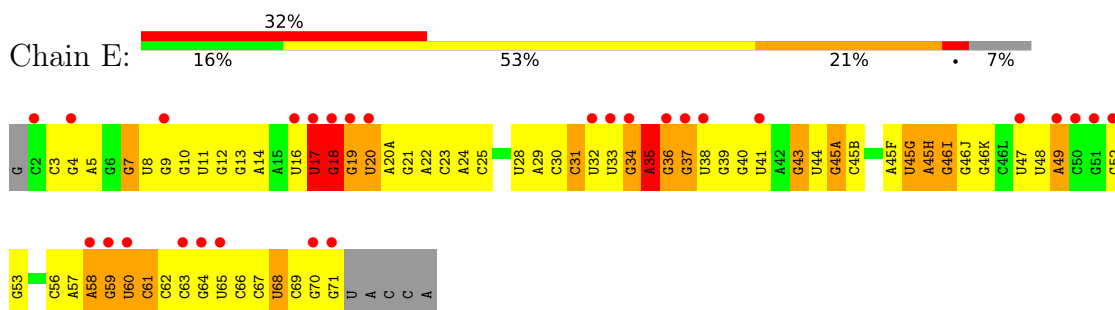
- Molecule 2 is a protein called tRNA pseudouridine synthase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	264	Total	C	N	O	S	0	0	0
			2071	1316	378	369	8			
2	B	264	Total	C	N	O	S	0	0	0
			2082	1323	378	373	8			
2	C	264	Total	C	N	O	S	0	0	0
			2056	1308	371	369	8			
2	D	264	Total	C	N	O	S	0	0	0
			2069	1317	373	371	8			

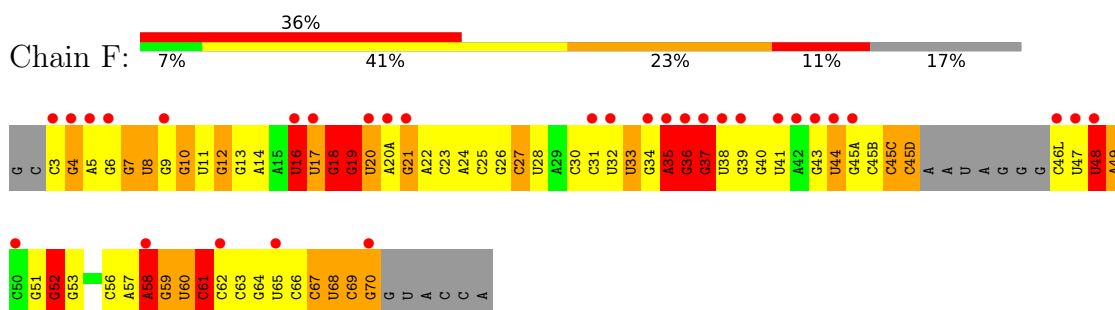
3 Residue-property plots [i](#)

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 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.

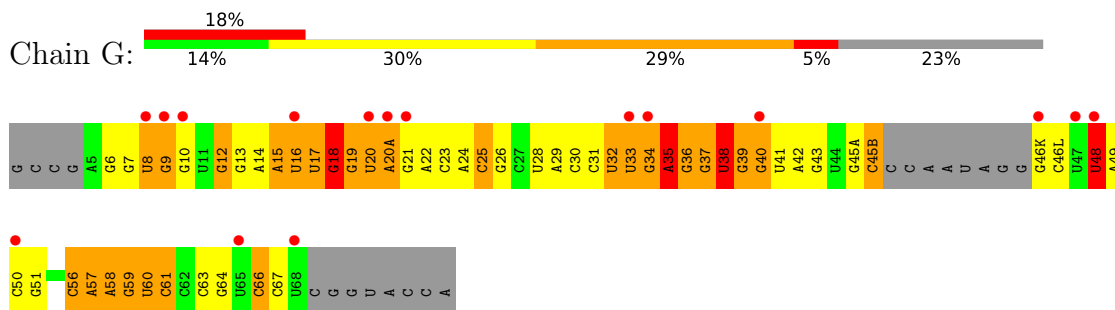
• Molecule 1: leucyl tRNA



• Molecule 1: leucyl tRNA

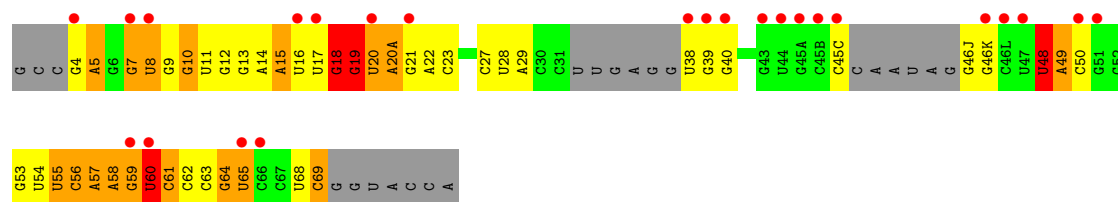


• Molecule 1: leucyl tRNA

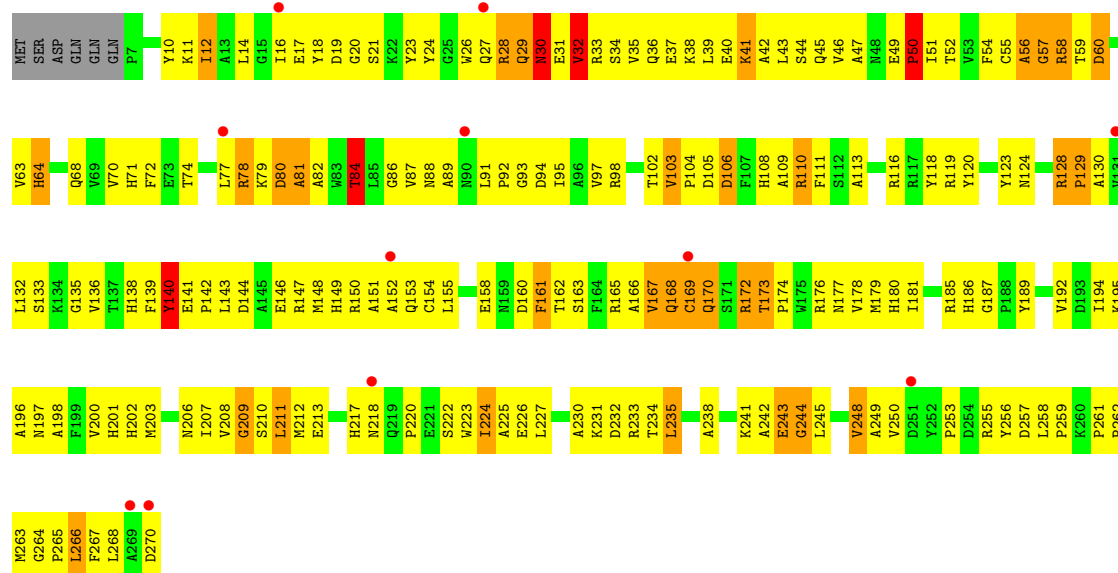


• Molecule 1: leucyl tRNA

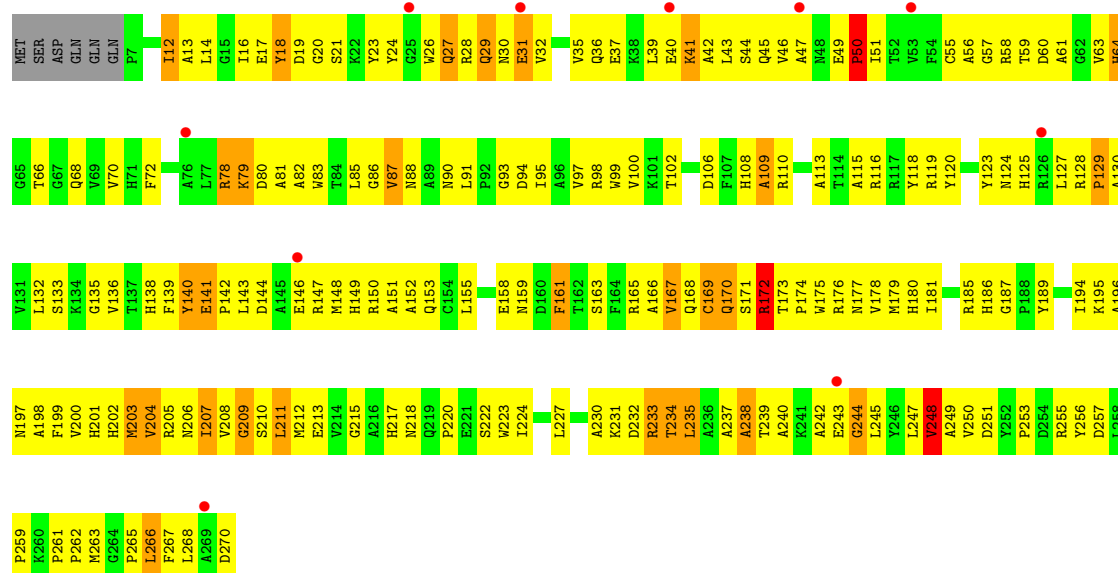




• Molecule 2: tRNA pseudouridine synthase A



• Molecule 2: tRNA pseudouridine synthase A



Chain C:

5% 26% 59% 10%

MET SER ASP GLN GLN P7 P8 T12 T13 T14 T15 T16 T17 T18 T19 T20 T21 T22 T23 T24 T25 T26 T27 T28 T29 T30 T31 T32 T33 T34 T35 T36 T37 T38 T39 T40 T41 T42 T43 T44 T45 T46 T47 T48 T49 T50 T51 T52 T53 T54 T55 T56 T57 T58 T59 T60 T61 T62 T63 T64 T65 T66 T67 T68 T69 T70 T71 T72 T73 T74 T75 T76 T77 T78 T79 T80 T81 T82 T83 T84 T85 T86 T87 T88 T89 T90 T91 T92 T93 T94 T95 T96 T97 T98 T99 T100 T101 T102 T103 T104 T105 T106 T107 T108 T109 T110 T111 T112 T113 T114 T115 T116 T117 T118 T119 T120 T121 T122 T123 T124 T125 T126 T127 T128 T129 T130 T131 T132 T133 T134 T135 T136 T137 T138 T139 T140 T141 T142 T143 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T195 T196 T197 T198 T199 T200 T201 T202 T203 T204 T205 T206 T207 T208 T209 T210 T211 T212 T213 T214 T215 T216 T217 T218 T219 T220 T221 T222 T223 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T824 T825 T826 T827 T828 T829 T830 T831 T832 T833 T834 T835 T836 T837 T838 T839 T840 T841 T842 T843 T844 T845 T846 T847 T848 T849 T850 T851 T852 T853 T854 T855 T856 T857 T858 T859 T860 T861 T862 T863 T864 T865 T866 T867 T868 T869 T870 T871 T872 T873 T874 T875 T876 T877 T878 T879 T880 T881 T882 T883 T884 T885 T886 T887 T888 T889 T890 T891 T892 T893 T894 T895 T896 T897 T898 T899 T900 T901 T902 T903 T904 T905 T906 T907 T908 T909 T910 T911 T912 T913 T914 T915 T916 T917 T918 T919 T920 T921 T922 T923 T924 T925 T926 T927 T928 T929 T930 T931 T932 T933 T934 T935 T936 T937 T938 T939 T940 T941 T942 T943 T944 T945 T946 T947 T948 T949 T950 T951 T952 T953 T954 T955 T956 T957 T958 T959 T960 T961 T962 T963 T964 T965 T966 T967 T968 T969 T970 T971 T972 T973 T974 T975 T976 T977 T978 T979 T980 T981 T982 T983 T984 T985 T986 T987 T988 T989 T990 T991 T992 T993 T994 T995 T996 T997 T998 T999 T1000 T1001 T1002 T1003 T1004 T1005 T1006 T1007 T1008 T1009 T1010 T1011 T1012 T1013 T1014 T1015 T1016 T1017 T1018 T1019 T1020 T1021 T1022 T1023 T1024 T1025 T1026 T1027 T

Chain D:

6% 27% 59% 11%

MET SER ASP GLN GLN P7 Y10 K11 I12 A13 L14 G15 I16 E17 Y18 D19 G20 S21 Z22 Y23 Y24 G25 W26 Q27 R28 Q29 N30 E31 V32 R33 V34 V35 Q36 E37 K38 L39 E40 E41 K42 L43 S44 Q45 V46 A47 A48 E49 P50 I51 T52 T53 C55 A56 G57 D60 A61 G62 W63 H64 Q68 V69 V70 H71 F72 A76 L77 R78 K79 D80 A81 A82 W83 E84 T84 L85 G86 V87 N88 K89 N90 L91 P92 G93 D94 I95 A96 V97 R98 W99 S100 K101 T102 V103 P104 D105 E106 C109 Q170 S171 R172 T173 P174 W175 R176 N177 V178 M179 H180 I181 R185 H186 G187 P188 Y189 R192 V193 H194 T195 K196 L197 A198 F199 V200 H201 H202 M203 V204 R205 R206 A211 M212 M213 H217 N218 Q219 P220 E221 S222 W223 I224 A225 E226 L227 A230 K231 D232 R233 T234 L235 C236 A237 A238 T239 A240 K241 E243 G244 L245 V248 A249 V250 D251 R255 V256 D257 L258 P259 K260 P261 P262 M263 G264 P265 L266 F267 L268 A269 D270

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.03Å 149.29Å 291.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 50.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-3.90) 89.3 (50.00-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.298 , 0.350 0.260 , 0.303	Depositor DCC
R_{free} test set	1361 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	14269	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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

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	E	0.50	1/1877 (0.1%)	0.90	7/2922 (0.2%)
1	F	0.49	0/1723	0.96	10/2683 (0.4%)
1	G	0.47	0/1588	0.92	8/2473 (0.3%)
1	H	0.44	0/1495	0.89	5/2323 (0.2%)
2	A	0.79	0/2127	1.04	11/2899 (0.4%)
2	B	0.78	0/2138	1.06	9/2913 (0.3%)
2	C	0.79	0/2111	1.09	16/2879 (0.6%)
2	D	0.78	0/2125	1.03	13/2897 (0.4%)
All	All	0.67	1/15184 (0.0%)	0.99	79/21989 (0.4%)

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	F	0	4
1	G	0	1
1	H	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	35	A	O3'-P	-6.35	1.51	1.61

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	35	A	P-O3'-C3'	9.25	134.08	120.20
2	B	141	GLU	CA-C-N	8.50	128.52	119.76
2	B	141	GLU	C-N-CA	8.50	128.52	119.76
1	E	17	U	C4'-C3'-O3'	-7.10	102.35	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	G	C4'-C3'-O3'	-7.00	102.50	113.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	19	G	Sidechain
1	F	36	G	Sidechain
1	F	37	G	Sidechain
1	F	52	G	Sidechain
1	G	38	U	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	E	1682	0	846	91	0
1	F	1544	0	779	98	0
1	G	1422	0	718	91	0
1	H	1343	0	678	52	0
2	A	2071	0	2012	215	0
2	B	2082	0	2029	219	0
2	C	2056	0	1988	222	0
2	D	2069	0	2012	222	0
All	All	14269	0	11062	1153	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 46.

The worst 5 of 1153 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:E:34:G:H4'	1:E:35:A:OP1	1.48	1.13
1:H:58:A:H4'	1:H:59:G:OP1	1.45	1.10
2:B:88:ASN:HA	2:B:91:LEU:HD12	1.38	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:ARG:HG2	2:C:29:GLN:H	1.20	1.03
1:H:15:A:H61	1:H:48:U:H3	1.02	0.99

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	A	262/270 (97%)	195 (74%)	46 (18%)	21 (8%)	1	11
2	B	262/270 (97%)	192 (73%)	50 (19%)	20 (8%)	1	12
2	C	262/270 (97%)	193 (74%)	44 (17%)	25 (10%)	0	8
2	D	262/270 (97%)	196 (75%)	45 (17%)	21 (8%)	1	11
All	All	1048/1080 (97%)	776 (74%)	185 (18%)	87 (8%)	0	10

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	58	ARG
2	A	80	ASP
2	A	109	ALA
2	A	167	VAL
2	A	243	GLU

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	A	210/223 (94%)	189 (90%)	21 (10%)	7	27
2	B	213/223 (96%)	194 (91%)	19 (9%)	9	32
2	C	207/223 (93%)	195 (94%)	12 (6%)	18	44
2	D	211/223 (95%)	196 (93%)	15 (7%)	13	40
All	All	841/892 (94%)	774 (92%)	67 (8%)	11	35

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	50	PRO
2	D	78	ARG
2	D	234	THR
2	B	31	GLU
2	B	29	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	45	GLN
2	D	202	HIS
2	D	124	ASN
2	D	182	ASN
2	B	138	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	79/87 (90%)	26 (32%)	5 (6%)
1	F	68/87 (78%)	35 (51%)	9 (13%)
1	G	65/87 (74%)	27 (41%)	5 (7%)
1	H	59/87 (67%)	21 (35%)	5 (8%)
All	All	271/348 (77%)	109 (40%)	24 (8%)

5 of 109 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	3	C
1	E	8	U
1	E	10	G

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Mol	Chain	Res	Type
1	E	17	U
1	E	18	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	G	18	G
1	G	58	A
1	G	37	G
1	G	60	U
1	F	16	U

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	38:U	O3'	39[B]:G	P	10.17

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	E	81/87 (93%)	1.93	28 (34%) 1 2	14, 61, 98, 105	4 (4%)
1	F	72/87 (82%)	2.48	31 (43%) 0 1	6, 41, 111, 131	10 (13%)
1	G	67/87 (77%)	1.44	16 (23%) 2 4	14, 51, 105, 121	2 (2%)
1	H	65/87 (74%)	1.66	24 (36%) 1 2	5, 52, 121, 138	2 (3%)
2	A	264/270 (97%)	0.47	11 (4%) 40 30	1, 12, 32, 50	0
2	B	264/270 (97%)	0.49	10 (3%) 44 32	1, 12, 33, 50	0
2	C	264/270 (97%)	0.46	14 (5%) 32 25	1, 13, 34, 50	0
2	D	264/270 (97%)	0.54	17 (6%) 25 22	1, 11, 34, 51	0
All	All	1341/1428 (93%)	0.79	151 (11%) 10 13	1, 16, 78, 138	18 (1%)

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	36	G	15.5
1	F	39[A]	G	14.3
1	F	37	G	13.2
1	E	17	U	12.0
1	F	38	U	11.9

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.