



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:58 am BST

PDB ID : 1JBR  
Title : Crystal Structure of the Ribotoxin Restrictocin and a 31-mer SRD RNA Inhibitor  
Authors : Yang, X.; Gerczei, T.; Glover, L.; Correll, C.C.  
Deposited on : 2001-06-06  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

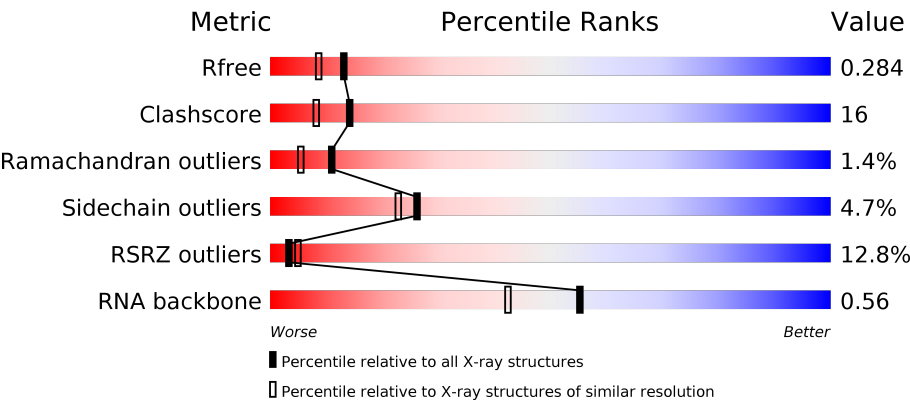
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)
RNA backbone	3102	1060 (2.60-1.72)

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 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	C	18	<div><div></div><div>61%22%17%</div></div>
2	F	13	<div><div></div><div>46%46%8%</div></div>
3	D	31	<div><div>3%</div><div>65%29%. .</div></div>
4	A	149	<div><div>12%</div><div>81%18%. .</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	B	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	A23	C	17	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3883 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 5'-R(\*GP\*CP\*GP\*CP\*UP\*CP\*CP\*UP\*CP\*AP\*GP\*UP\*AP\*CP\*GP\*AP\*GP\*(A23))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	18	Total	C	N	O	P	0	0	0
			383	171	69	125	18			

- Molecule 2 is a RNA chain called 5'-R(\*GP\*GP\*AP\*AP\*CP\*CP\*GP\*GP\*AP\*GP\*CP\*GP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	13	Total	C	N	O	P	0	0	0
			281	126	57	86	12			

- Molecule 3 is a RNA chain called 31-mer SRD RNA analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	31	Total	C	N	O	P	0	0	0
			664	297	126	211	30			

- Molecule 4 is a protein called Restrictocin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	149	Total	C	N	O	S	0	0	0
			1191	748	217	221	5			
4	B	149	Total	C	N	O	S	0	0	0
			1191	748	217	221	5			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total	K	0	0
			3	3		
5	C	1	Total	K	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total K 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	20	Total O 20 20	0	0
6	F	21	Total O 21 21	0	0
6	D	39	Total O 39 39	0	0
6	A	54	Total O 54 54	0	0
6	B	34	Total O 34 34	0	0



● Molecule 1: 5'-R(\*GP\*CP\*GP\*CP\*UP\*CP\*CP\*UP\*CP\*AP\*GP\*UP\*AP\*CP\*GP\*AP\*GP\*(A23))-3'

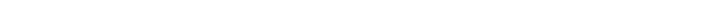
G0	G10	U11	A12	C13	G14	A15	G16	A17
----	-----	-----	-----	-----	-----	-----	-----	-----

Chain F:  46% 46% 8%

Diagram of a 1D chain with 10 sites. Sites 1, 3, 5, 7, and 9 are yellow and labeled G18, A21, C22, C23, G24, G25, A26, and C30 respectively. Sites 2, 4, 6, 8, and 10 are orange and unlabeled. Horizontal lines connect sites 1-2, 2-3, 3-4, 4-5, 5-6, 6-7, 7-8, 8-9, and 9-10.

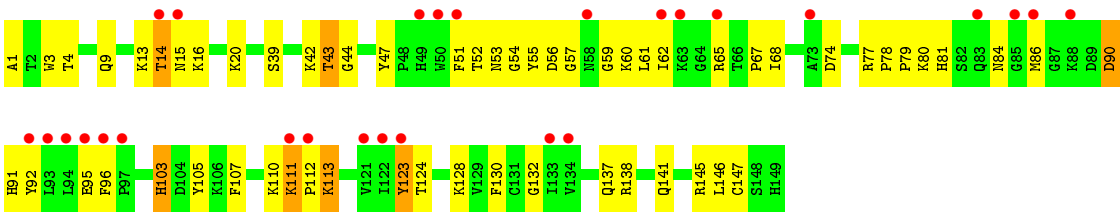
Chain D:  3% 65% 29%

A horizontal bar chart showing the distribution of 32 categories. The categories are G0, U7, C8, A9, G10, U11, A12, C13, G16, A17, G18, G27, C28, G29, and C30. The bars are colored in a repeating pattern of green, yellow, and orange. A red dot is placed above the G16 bar.

Chain A:  12% 81% 18%

Category	Count
A1	1
T2	1
W3	1
T4	1
N11	1
N15	1
F51	1
T52	1
K60	1
L61	1
I62	1
K63	1
G64	1
R65	1
K69	1
K72	1
A73	1
D74	1
K80	1
Q83	1
N84	1
G85	1
M86	1
G87	1
K88	1
D89	1
D90	1
H91	1
Y92	1
L93	1
L94	1
T98	1
F99	1
P100	1
K110	1
K111	1
P112	1
A119	1
R120	1
V121	1
I122	1
P126	1
F130	1
G131	1
G132	1
I133	1
V134	1
D143	1
L144	1
C147	1
S148	1
H149	1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.40 Å   109.70 Å   40.00 Å 90.00°   97.80°   90.00°	Depositor
Resolution (Å)	19.96 – 2.15 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	88.4 (19.96-2.15) 88.5 (19.95-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.15 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.232   ,   0.290 0.222   ,   0.284	Depositor DCC
$R_{free}$ test set	2437 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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

Bond lengths and bond angles in the following residue types are not validated in this section: K, A23

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	C	0.45	0/399	0.83	0/620
2	F	0.39	0/315	0.69	0/491
3	D	0.49	1/743 (0.1%)	0.80	2/1158 (0.2%)
4	A	0.39	0/1229	0.64	0/1660
4	B	0.37	0/1229	0.64	0/1660
All	All	0.41	1/3915 (0.0%)	0.70	2/5589 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	17	A	O3'-P	-5.13	1.54	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	17	A	O4'-C1'-C2'	5.71	112.74	107.60
3	D	17	A	C4'-C3'-C2'	5.18	107.78	102.60

There are no chirality outliers.

There are no planarity outliers.

### 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	C	383	0	195	20	0
2	F	281	0	145	7	0
3	D	664	0	340	4	0
4	A	1191	0	1133	29	0
4	B	1191	0	1133	56	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
5	F	1	0	0	0	0
6	A	54	0	0	5	0
6	B	34	0	0	4	0
6	C	20	0	0	2	0
6	D	39	0	0	0	0
6	F	21	0	0	1	0
All	All	3883	0	2946	104	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 16.

All (104) 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:C:15:A:H4'	1:C:16:G:H5'	1.05	1.05
4:B:62:ILE:HG23	4:B:65:ARG:HG3	1.47	0.97
1:C:17:A23:H2	4:A:52:THR:H	1.40	0.87
1:C:15:A:C4'	1:C:16:G:H5'	1.99	0.84
1:C:16:G:N7	4:A:65:ARG:CZ	2.46	0.78
4:B:54:GLY:O	4:B:62:ILE:HG22	1.84	0.77
4:B:14:THR:HG21	4:B:16:LYS:HE3	1.65	0.76
4:B:80:LYS:HB3	4:B:91:HIS:H	1.52	0.74
1:C:17:A23:C2	4:A:52:THR:H	2.03	0.71
4:A:60:LYS:NZ	4:A:60:LYS:HB2	2.05	0.71
1:C:17:A23:PC	2:F:18:G:H5''	2.32	0.70
4:B:14:THR:O	4:B:16:LYS:N	2.22	0.70
4:A:84:ASN:HD22	4:A:86:MET:CE	2.05	0.69
4:B:39:SER:HB2	4:B:42:LYS:HE2	1.74	0.68
4:B:1:ALA:HB3	6:B:175:HOH:O	1.93	0.68
1:C:10:G:OP2	4:A:110:LYS:HE2	1.96	0.66
4:B:113:LYS:HB3	4:B:113:LYS:HZ2	1.61	0.66
4:B:14:THR:HG22	4:B:16:LYS:HG2	1.79	0.65
4:B:14:THR:CG2	4:B:16:LYS:HG2	2.27	0.65
4:B:113:LYS:HB3	4:B:113:LYS:NZ	2.13	0.64
4:B:137:GLN:HE21	4:B:145:ARG:NH1	1.95	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:72:LYS:HB2	4:A:72:LYS:NZ	2.13	0.63
1:C:16:G:H4'	1:C:17:A23:OP1	2.00	0.61
4:B:62:ILE:HG23	4:B:65:ARG:CG	2.25	0.59
4:B:61:LEU:HD13	4:B:62:ILE:N	2.17	0.59
4:B:55:TYR:HD2	4:B:59:GLY:O	1.85	0.59
1:C:16:G:H3'	6:C:219:HOH:O	2.03	0.59
4:B:56:ASP:OD2	4:B:60:LYS:HB3	2.02	0.59
4:A:84:ASN:HD22	4:A:86:MET:HE2	1.68	0.58
4:B:137:GLN:HG3	4:B:145:ARG:CZ	2.33	0.58
1:C:17:A23:H2	4:A:52:THR:HG23	1.87	0.57
4:B:61:LEU:HD21	4:B:67:PRO:CG	2.35	0.57
4:B:14:THR:CG2	4:B:16:LYS:HE3	2.34	0.56
4:A:4:THR:O	4:A:147:CYS:HB3	2.05	0.56
4:B:62:ILE:CG2	4:B:65:ARG:HG3	2.31	0.56
4:B:1:ALA:HB1	6:B:154:HOH:O	2.06	0.55
4:B:80:LYS:HB2	4:B:91:HIS:NE2	2.22	0.55
4:B:80:LYS:HB2	4:B:91:HIS:CE1	2.42	0.55
4:A:62:ILE:O	4:A:63:LYS:HB2	2.08	0.54
1:C:17:A23:HN61	4:A:65:ARG:HH22	1.53	0.54
4:A:60:LYS:HZ3	4:A:60:LYS:HB2	1.72	0.53
4:A:61:LEU:HG	4:A:63:LYS:H	1.72	0.53
1:C:17:A23:H8	6:A:191:HOH:O	2.08	0.53
4:B:74:ASP:HA	4:B:77:ARG:HH21	1.73	0.53
3:D:12:A:H2'	3:D:13:C:O4'	2.08	0.53
2:F:23:C:H2'	2:F:24:G:H5'	1.91	0.52
4:B:51:PHE:HB2	4:B:95:GLU:HB3	1.92	0.51
4:A:80:LYS:HB3	4:A:91:HIS:CD2	2.46	0.50
1:C:17:A23:O2C	2:F:18:G:H5''	2.11	0.50
4:B:96:PHE:CZ	4:B:105:TYR:HB3	2.45	0.50
4:B:79:PRO:HG3	6:B:183:HOH:O	2.11	0.49
4:B:14:THR:C	4:B:16:LYS:H	2.13	0.49
4:B:61:LEU:HD21	4:B:67:PRO:HG3	1.95	0.49
4:A:84:ASN:HD22	4:A:86:MET:HE3	1.78	0.49
4:B:74:ASP:OD2	4:B:124:THR:HG21	2.13	0.48
4:B:68:ILE:HD11	4:B:146:LEU:HB2	1.95	0.48
4:B:57:GLY:HA2	4:B:81:HIS:HB3	1.94	0.48
4:A:11:ASN:O	4:A:15:ASN:HA	2.14	0.48
4:B:65:ARG:NH1	6:B:181:HOH:O	2.46	0.48
4:A:3:TRP:HA	4:A:148:SER:O	2.14	0.47
4:A:143:ASP:HB3	6:A:203:HOH:O	2.13	0.47
4:B:47:TYR:O	4:B:107:PHE:HB2	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:C:C2'	2:F:24:G:H5'	2.44	0.47
4:B:111:LYS:HA	4:B:112:PRO:HA	1.73	0.47
4:A:60:LYS:HZ2	4:A:60:LYS:HB2	1.78	0.47
1:C:17:A23:O3'	2:F:18:G:H5''	2.15	0.47
4:B:53:ASN:OD1	4:B:68:ILE:HG22	2.15	0.46
4:B:80:LYS:HB2	4:B:91:HIS:CD2	2.51	0.46
1:C:12:A:H2'	1:C:13:C:O4'	2.16	0.46
3:D:7:U:H2'	3:D:8:C:O4'	2.16	0.46
4:B:78:PRO:HA	4:B:79:PRO:HD3	1.68	0.45
2:F:25:G:P	6:F:204:HOH:O	2.74	0.45
4:A:100:PRO:HD2	6:A:152:HOH:O	2.16	0.45
4:B:84:ASN:ND2	4:B:86:MET:HB2	2.32	0.45
4:B:4:THR:O	4:B:147:CYS:HB3	2.17	0.45
4:B:43:THR:HB	4:B:107:PHE:O	2.17	0.44
4:A:134:VAL:HG23	4:A:144:LEU:HD22	2.00	0.44
3:D:10:G:H5'	4:B:44:GLY:HA2	1.98	0.43
4:B:130:PHE:CZ	4:B:132:GLY:HA2	2.54	0.43
4:B:13:LYS:O	4:B:14:THR:CB	2.65	0.43
1:C:14:G:H2'	1:C:15:A:C8	2.53	0.43
3:D:17:A:H5''	3:D:17:A:N3	2.34	0.43
1:C:17:A23:C2	4:A:52:THR:HG23	2.48	0.42
1:C:17:A23:C3'	6:C:221:HOH:O	2.67	0.42
4:B:3:TRP:HE3	4:B:147:CYS:HB2	1.84	0.42
1:C:17:A23:H2'	6:A:191:HOH:O	2.17	0.42
4:A:3:TRP:CD2	4:A:149:HIS:HB3	2.55	0.42
1:C:17:A23:C2	4:A:52:THR:N	2.78	0.42
4:A:130:PHE:CZ	4:A:132:GLY:HA2	2.55	0.41
4:B:124:THR:O	4:B:128:LYS:HA	2.19	0.41
4:B:80:LYS:O	4:B:90:ASP:HB3	2.19	0.41
4:A:72:LYS:HB2	4:A:72:LYS:HZ2	1.82	0.41
4:B:39:SER:CB	4:B:42:LYS:HE2	2.47	0.41
4:A:62:ILE:HG22	4:A:65:ARG:HB2	2.01	0.41
4:B:14:THR:C	4:B:16:LYS:N	2.74	0.41
2:F:21:A:H2'	2:F:22:C:C6	2.55	0.41
4:A:80:LYS:HE3	6:A:177:HOH:O	2.21	0.41
4:B:123:TYR:CD1	4:B:123:TYR:N	2.89	0.41
4:B:137:GLN:HG3	4:B:145:ARG:NH2	2.36	0.41
4:B:9:GLN:NE2	4:B:20:LYS:HG3	2.36	0.41
4:B:103:HIS:ND1	4:B:103:HIS:C	2.75	0.40
4:B:52:THR:O	4:B:53:ASN:HB3	2.22	0.40
4:B:110:LYS:O	4:B:111:LYS:C	2.60	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:81:HIS:HD2	4:B:92:TYR:CE2	2.40	0.40

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	
4	A	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
4	B	147/149 (99%)	136 (92%)	7 (5%)	4 (3%)	5	1
All	All	294/298 (99%)	275 (94%)	15 (5%)	4 (1%)	11	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	15	ASN
4	B	43	THR
4	B	14	THR
4	B	111	LYS

### 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	
4	A	128/128 (100%)	122 (95%)	6 (5%)	26	23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	128/128 (100%)	122 (95%)	6 (5%)	26	23
All	All	256/256 (100%)	244 (95%)	12 (5%)	26	23

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	60	LYS
4	A	74	ASP
4	A	83	GLN
4	A	110	LYS
4	A	112	PRO
4	A	126	PRO
4	B	90	ASP
4	B	103	HIS
4	B	113	LYS
4	B	123	TYR
4	B	138	ARG
4	B	141	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	9	GLN
4	A	83	GLN
4	A	84	ASN
4	A	127	ASN
4	A	137	GLN
4	A	140	ASN
4	A	141	GLN
4	B	9	GLN
4	B	84	ASN
4	B	137	GLN
4	B	140	ASN
4	B	141	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	17/18 (94%)	3 (17%)	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	12/13 (92%)	2 (16%)	0
3	D	30/31 (96%)	7 (23%)	1 (3%)
All	All	59/62 (95%)	12 (20%)	1 (1%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	10	G
1	C	16	G
1	C	17	A23
2	F	21	A
2	F	26	A
3	D	9	A
3	D	10	G
3	D	16	G
3	D	17	A
3	D	18	G
3	D	27	G
3	D	29	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	17	A

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	A23	C	17	1	19,28,29	0.80	0	19,43,46	1.53	4 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A23	C	17	1	-	2/3/35/36	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	A23	O2'-C2'-C3'	3.37	111.27	105.08
1	C	17	A23	C5-C6-N6	2.26	123.78	120.35
1	C	17	A23	C1'-N9-C4	-2.21	122.76	126.64
1	C	17	A23	C5'-C4'-C3'	2.04	121.17	114.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	17	A23	O4'-C4'-C5'-O5'
1	C	17	A23	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	17	A23	13	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	C	17/18 (94%)	-0.43	0 <span>100</span> <span>100</span>	30, 44, 74, 106	0
2	F	13/13 (100%)	-0.63	0 <span>100</span> <span>100</span>	40, 46, 57, 57	0
3	D	31/31 (100%)	-0.56	1 (3%) 47 56	40, 50, 63, 91	0
4	A	149/149 (100%)	0.63	18 (12%) <span>4</span> <span>6</span>	23, 43, 69, 73	0
4	B	149/149 (100%)	1.00	27 (18%) <span>1</span> <span>1</span>	28, 50, 79, 86	0
All	All	359/360 (99%)	0.59	46 (12%) <span>3</span> <span>5</span>	23, 47, 74, 106	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	93	LEU	5.0
4	B	122	ILE	5.0
4	B	111	LYS	4.8
4	A	122	ILE	4.6
4	A	133	ILE	4.2
4	B	121	VAL	3.8
4	A	93	LEU	3.8
4	B	88	LYS	3.8
4	B	94	LEU	3.8
4	B	86	MET	3.7
4	A	121	VAL	3.6
4	B	73	ALA	3.6
4	B	92	TYR	3.3
4	B	134	VAL	3.2
4	B	15	ASN	3.1
4	B	112	PRO	3.0
4	A	86	MET	3.0
4	B	63	LYS	3.0
4	B	58	ASN	3.0
4	B	51	PHE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	A	83	GLN	2.9
4	B	97	PRO	2.9
4	B	62	ILE	2.8
4	A	134	VAL	2.7
4	A	132	GLY	2.7
4	A	94	LEU	2.7
4	B	50	TRP	2.6
4	B	14	THR	2.6
4	A	120	ARG	2.6
4	B	96	PHE	2.5
4	A	98	THR	2.5
4	B	83	GLN	2.5
4	A	119	ALA	2.5
4	B	123	TYR	2.5
4	B	133	ILE	2.4
4	A	51	PHE	2.4
4	A	92	TYR	2.3
4	B	85	GLY	2.3
4	B	65	ARG	2.3
4	B	95	GLU	2.2
3	D	16	G	2.1
4	A	89	ASP	2.1
4	B	49	HIS	2.1
4	A	69	LYS	2.1
4	A	63	LYS	2.1
4	A	88	LYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	A23	C	17	25/26	0.76	0.26	98,102,107,108	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	K	D	205	1/1	0.93	0.14	65,65,65,65	0
5	K	D	204	1/1	0.94	0.09	53,53,53,53	0
5	K	D	201	1/1	0.98	0.08	50,50,50,50	0
5	K	F	203	1/1	0.98	0.07	44,44,44,44	0
5	K	C	202	1/1	0.99	0.07	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.