Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 06:06 PM EDT

PDB ID	:	1P6V
Title	:	Crystal structure of the tRNA domain of transfer-messenger RNA in complex with SmpB
Authors	:	Gutmann, S.; Haebel, P.W.; Metzinger, L.; Sutter, M.; Felden, B.; Ban, N.
Deposited on	:	2003-04-30
Resolution	:	3.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

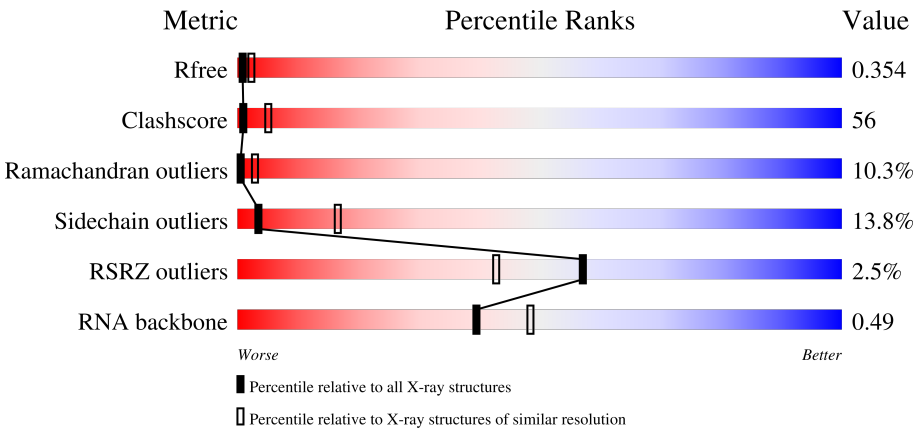
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 <=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	B	68	3%; 16%, 31%, 13%, 6%, 34%
1	D	68	6%, 15%, 13%, •, 65%
2	A	156	3%; 22%, 42%, 15%, •, 20%
2	C	156	%; 18%, 47%, 15%, •, 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3519 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 45-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	45	955	426	167	318	44	0	0	0
1	D	24	510	228	91	168	23	0	0	0

- Molecule 2 is a protein called SsrA-binding protein.

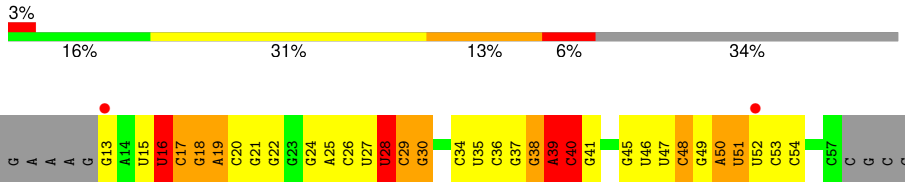
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	125	1027	671	179	176	1	0	0	0
2	C	125	1027	671	179	176	1	0	0	0

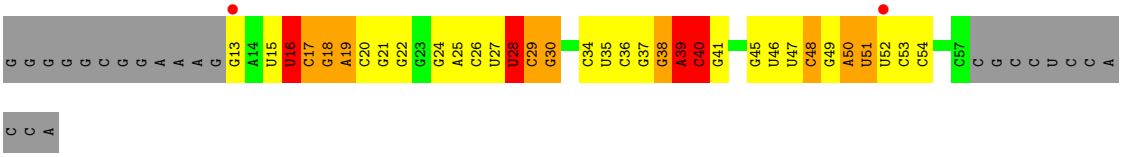
3 Residue-property plots (i)

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: 45-MER

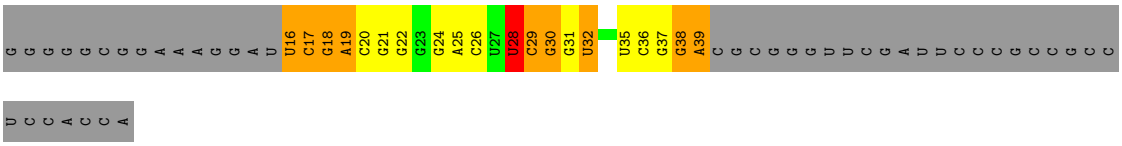
Chain B:





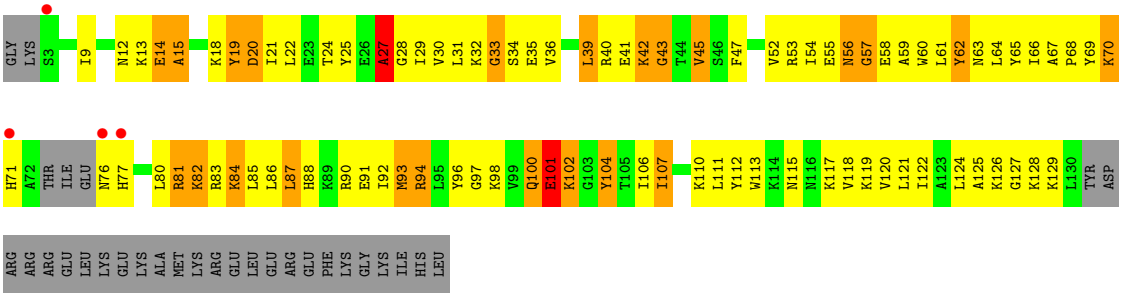
- Molecule 1: 45-MER

Chain D:



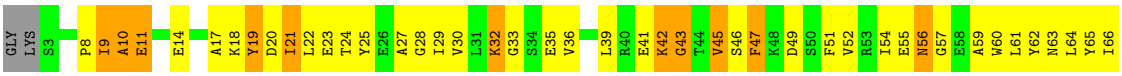
- Molecule 2: SsrA-binding protein

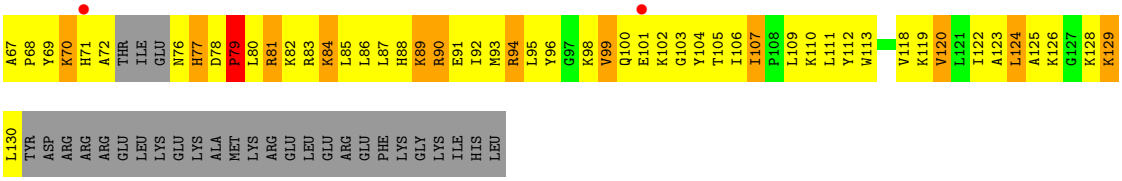
Chain A:



- Molecule 2: SsrA-binding protein

Chain C:




A67
P68
Y69
K70
H71
A72
THR
ILE
GLU
N76
H77
D78
P79
L80
R81
K82
R83
K84
L85
L86
L87
H88
K89
R90
E91
I92
M93
R94
L95
Y96
G97
K98
V99
Q100
E101
K102
G103
Y104
T105
I106
I107
P108
L109
K110
L111
Y112
W113
V118
K119
V120
L121
I122
A123
L124
A125
K126
G127
K128
K129
L130
TYR
ASP
ARG
ARG
ARG
GLU
LEU
LYS
GLU
LYS
ALA
MET
LYS
ARG
GLU
LEU
GLU
ARG
GLU
PHE
LYS
GLY
LYS
ILE
HIS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.68Å 99.68Å 207.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.20 45.94 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.94-3.20) 94.0 (45.94-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.302 , 0.360 0.296 , 0.354	Depositor DCC
R_{free} test set	1647 reflections (7.79%)	wwPDB-VP
Wilson B-factor (Å^2)	119.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 95.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	3519	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	B	0.53	0/1065	0.88	5/1659 (0.3%)
1	D	0.63	0/569	0.85	0/886
2	A	0.44	0/1046	0.81	4/1400 (0.3%)
2	C	0.36	0/1046	0.65	0/1400
All	All	0.48	0/3726	0.80	9/5345 (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	B	0	3
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	40	C	N1-C1'-C2'	6.63	122.62	114.00
1	B	16	U	N1-C1'-C2'	6.52	122.48	114.00
2	A	62	TYR	N-CA-C	6.31	128.04	111.00
1	B	18	G	C2'-C3'-O3'	6.12	123.49	113.70
2	A	19	TYR	N-CA-C	5.86	126.83	111.00
2	A	27	ALA	N-CA-C	5.82	126.71	111.00
1	B	18	G	N9-C1'-C2'	5.49	121.13	114.00
1	B	39	A	O4'-C1'-N9	5.41	112.53	108.20
2	A	82	LYS	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	16	U	Sidechain
1	B	28	U	Sidechain
1	B	40	C	Sidechain
1	D	28	U	Sidechain
1	D	32	U	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	B	955	0	487	56	0
1	D	510	0	261	57	0
2	A	1027	0	1098	124	0
2	C	1027	0	1098	159	0
All	All	3519	0	2944	365	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 56.

All (365) 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:A:84:LYS:H	2:A:84:LYS:HD3	1.16	1.08
2:C:84:LYS:H	2:C:84:LYS:HE2	0.95	1.07
2:C:107:ILE:HD13	2:C:107:ILE:H	1.23	1.00
2:A:27:ALA:HB2	2:A:120:VAL:N	1.78	0.99
2:A:27:ALA:CB	2:A:120:VAL:H	1.76	0.98
2:A:27:ALA:HB2	2:A:120:VAL:H	1.28	0.97
1:D:39:A:H1'	2:C:36:VAL:HG21	1.44	0.97
2:A:12:ASN:HB2	2:A:47:PHE:HD1	1.30	0.95
2:C:86:LEU:O	2:C:87:LEU:HD12	1.66	0.95
2:C:84:LYS:HE2	2:C:84:LYS:N	1.80	0.95
2:C:88:HIS:HB2	2:C:91:GLU:HG3	1.49	0.95
1:D:28:U:H2'	1:D:30:G:H22	1.33	0.94
2:C:84:LYS:H	2:C:84:LYS:CE	1.81	0.92
2:A:84:LYS:HD3	2:A:84:LYS:N	1.86	0.91
2:C:95:LEU:HB3	2:C:106:ILE:HD11	1.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47:PHE:HB3	2:C:64:LEU:HD12	1.56	0.88
1:B:28:U:H2'	1:B:30:G:H22	1.41	0.85
2:C:47:PHE:H	2:C:47:PHE:HD2	1.23	0.85
2:A:9:ILE:HD13	2:A:39:LEU:HD22	1.56	0.85
1:B:39:A:N1	2:A:118:VAL:HG23	1.93	0.84
2:A:94:ARG:HG2	2:A:94:ARG:HH11	1.43	0.83
1:D:28:U:H2'	1:D:30:G:N2	1.92	0.82
2:C:68:PRO:HD3	2:C:79:PRO:HG3	1.61	0.82
2:C:66:ILE:CG2	2:C:83:ARG:HH21	1.93	0.82
2:C:64:LEU:HB3	2:C:83:ARG:NH1	1.96	0.81
2:A:12:ASN:HB2	2:A:47:PHE:CD1	2.16	0.80
2:C:22:LEU:O	2:C:23:GLU:HG3	1.82	0.79
2:A:102:LYS:HB3	2:A:102:LYS:HZ3	1.44	0.79
1:B:28:U:H2'	1:B:30:G:N2	1.98	0.79
1:B:47:U:H2'	1:B:48:C:H5"	1.64	0.78
2:A:14:GLU:HB3	2:A:18:LYS:NZ	1.98	0.78
1:D:19:A:N7	2:C:86:LEU:HD23	1.99	0.77
2:C:29:ILE:HG22	2:C:85:LEU:HD22	1.66	0.77
2:C:27:ALA:HA	2:C:87:LEU:HD11	1.66	0.77
2:A:87:LEU:O	2:A:88:HIS:HB2	1.85	0.77
1:B:19:A:H61	1:B:38:G:N2	1.83	0.76
2:A:70:LYS:HE2	2:A:70:LYS:HA	1.66	0.76
2:C:99:VAL:O	2:C:103:GLY:HA2	1.85	0.76
1:D:39:A:N1	2:C:118:VAL:HG23	2.02	0.75
2:C:66:ILE:HG22	2:C:83:ARG:HH21	1.52	0.75
2:C:102:LYS:HB2	2:C:104:TYR:CE2	2.22	0.74
2:C:64:LEU:HB3	2:C:83:ARG:HH12	1.52	0.73
2:A:84:LYS:H	2:A:84:LYS:CD	1.94	0.73
1:D:19:A:N6	1:D:38:G:N2	2.37	0.73
2:A:62:TYR:CE2	2:A:82:LYS:HG2	2.24	0.73
2:C:8:PRO:HA	2:C:112:TYR:HB3	1.69	0.72
2:A:41:GLU:O	2:A:42:LYS:HB2	1.89	0.72
2:C:107:ILE:H	2:C:107:ILE:CD1	1.99	0.71
1:B:19:A:N6	1:B:38:G:N2	2.38	0.71
2:A:102:LYS:HB3	2:A:102:LYS:NZ	2.05	0.71
2:C:39:LEU:HD23	2:C:45:VAL:HG21	1.72	0.71
1:B:45:G:O2'	1:B:46:U:H5'	1.91	0.71
2:A:27:ALA:HB3	2:A:119:LYS:HB3	1.73	0.70
2:A:35:GLU:OE1	2:A:81:ARG:NH1	2.24	0.70
1:B:19:A:OP1	2:A:88:HIS:HA	1.92	0.70
1:B:37:G:N1	1:B:38:G:N2	2.39	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:ARG:HG2	2:C:94:ARG:HH11	1.56	0.69
2:A:24:THR:C	2:A:25:TYR:HD2	1.96	0.69
2:A:81:ARG:NH1	2:A:83:ARG:HE	1.91	0.69
1:D:30:G:H1	2:A:96:TYR:HH	1.40	0.69
2:C:66:ILE:HG23	2:C:77:HIS:NE2	2.07	0.69
1:B:28:U:H4'	1:B:29:C:OP1	1.93	0.69
2:A:100:GLN:O	2:A:102:LYS:N	2.26	0.69
2:C:46:SER:O	2:C:65:TYR:HB3	1.93	0.68
1:B:25:A:H2'	1:B:26:C:H6	1.59	0.68
1:B:35:U:H2'	1:B:36:C:C6	2.29	0.68
1:D:18:G:HO2'	2:C:88:HIS:HA	1.58	0.68
2:C:66:ILE:HG22	2:C:83:ARG:NH2	2.09	0.68
2:C:27:ALA:HB2	2:C:122:ILE:HD13	1.75	0.68
2:A:30:VAL:HB	2:A:84:LYS:HE2	1.74	0.68
1:D:16:U:H4'	1:D:17:C:OP2	1.93	0.67
2:C:41:GLU:O	2:C:42:LYS:HB2	1.93	0.67
1:D:28:U:H4'	1:D:29:C:OP1	1.94	0.67
1:D:30:G:N1	2:A:96:TYR:OH	2.27	0.67
2:A:20:ASP:OD2	2:A:128:LYS:HG2	1.95	0.67
1:D:25:A:H2'	1:D:26:C:H6	1.59	0.66
1:B:39:A:C2	2:A:118:VAL:HG23	2.31	0.66
1:D:35:U:H2'	1:D:36:C:C6	2.31	0.66
2:C:124:LEU:O	2:C:124:LEU:HG	1.95	0.65
1:B:47:U:C2'	1:B:48:C:H5"	2.27	0.65
1:D:19:A:H5'	2:C:87:LEU:O	1.97	0.65
2:A:27:ALA:CB	2:A:120:VAL:N	2.47	0.65
2:C:76:ASN:O	2:C:77:HIS:HB3	1.97	0.65
2:A:27:ALA:HB1	2:A:120:VAL:H	1.60	0.64
2:A:29:ILE:HG22	2:A:85:LEU:CD2	2.26	0.64
2:C:30:VAL:HB	2:C:84:LYS:HE3	1.79	0.64
1:B:39:A:H1'	2:A:36:VAL:HG21	1.78	0.64
2:C:10:ALA:HB1	2:C:47:PHE:CE2	2.33	0.64
2:A:56:ASN:O	2:A:58:GLU:HG3	1.98	0.64
2:A:81:ARG:HH21	2:A:84:LYS:NZ	1.96	0.64
2:C:83:ARG:HG3	2:C:83:ARG:HH11	1.61	0.64
1:D:16:U:H5'	1:D:17:C:OP2	1.97	0.63
2:C:19:TYR:HB3	2:C:126:LYS:O	1.97	0.63
2:A:42:LYS:O	2:A:43:GLY:O	2.16	0.63
2:C:106:ILE:HG22	2:C:106:ILE:O	1.98	0.63
1:D:37:G:C6	1:D:38:G:C2	2.87	0.62
2:A:69:TYR:HB3	2:A:71:HIS:NE2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:ILE:HD13	2:C:107:ILE:N	2.07	0.62
2:C:27:ALA:HB3	2:C:120:VAL:HG13	1.82	0.62
1:D:19:A:C2	1:D:20:C:C2	2.88	0.62
2:C:120:VAL:HG22	2:C:122:ILE:CD1	2.30	0.62
2:C:39:LEU:CD2	2:C:45:VAL:HG21	2.30	0.62
2:A:24:THR:HB	2:A:121:LEU:HD21	1.81	0.62
2:C:29:ILE:CG2	2:C:85:LEU:HD22	2.31	0.61
1:D:26:C:H1'	2:A:101:GLU:HA	1.81	0.61
2:C:10:ALA:HB3	2:C:111:LEU:H	1.64	0.61
2:A:14:GLU:HB3	2:A:18:LYS:HZ1	1.65	0.61
1:B:30:G:N1	2:C:96:TYR:OH	2.33	0.61
2:A:29:ILE:HD12	2:A:31:LEU:HD21	1.80	0.61
2:C:32:LYS:HD3	2:C:81:ARG:NH1	2.16	0.61
2:A:14:GLU:HB3	2:A:18:LYS:HZ2	1.64	0.61
2:C:45:VAL:HG22	2:C:66:ILE:HD12	1.82	0.61
2:C:10:ALA:O	2:C:11:GLU:HB2	1.99	0.61
2:C:35:GLU:OE2	2:C:81:ARG:NH1	2.34	0.60
2:C:66:ILE:HG21	2:C:83:ARG:HH21	1.65	0.60
2:C:94:ARG:HH11	2:C:94:ARG:CG	2.12	0.60
2:C:8:PRO:HA	2:C:112:TYR:CB	2.32	0.60
2:C:23:GLU:HB3	2:C:25:TYR:HE2	1.66	0.60
1:D:19:A:N6	1:D:38:G:H21	1.99	0.60
2:A:94:ARG:HH11	2:A:94:ARG:CG	2.13	0.60
2:A:27:ALA:CB	2:A:119:LYS:HB3	2.32	0.59
2:A:54:ILE:HD13	2:A:59:ALA:HA	1.84	0.59
2:C:120:VAL:HG22	2:C:122:ILE:HD12	1.82	0.59
1:B:37:G:C6	1:B:38:G:C2	2.90	0.59
2:C:35:GLU:HB3	2:C:66:ILE:HG12	1.83	0.59
1:B:25:A:H2'	1:B:26:C:C6	2.37	0.59
2:A:121:LEU:HD23	2:A:122:ILE:N	2.17	0.59
2:A:126:LYS:HG2	2:A:127:GLY:H	1.67	0.59
2:C:86:LEU:HD12	2:C:86:LEU:H	1.68	0.59
1:D:16:U:C4'	1:D:17:C:OP2	2.51	0.59
2:C:47:PHE:N	2:C:47:PHE:CD2	2.66	0.59
1:D:18:G:O2'	2:C:88:HIS:HA	2.03	0.58
1:D:18:G:O2'	1:D:19:A:OP1	2.19	0.58
2:A:28:GLY:O	2:A:85:LEU:HA	2.04	0.58
2:A:19:TYR:HB3	2:A:125:ALA:HB1	1.84	0.58
1:D:25:A:H2'	1:D:26:C:C6	2.37	0.58
1:B:39:A:H5'	1:B:40:C:OP1	2.03	0.58
2:A:80:LEU:O	2:A:81:ARG:O	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:GLU:O	2:C:94:ARG:HB3	2.04	0.58
2:C:19:TYR:CE1	2:C:107:ILE:HG21	2.38	0.57
2:C:19:TYR:CZ	2:C:107:ILE:HG21	2.38	0.57
1:D:20:C:H2'	1:D:21:G:H8	1.68	0.57
2:C:96:TYR:O	2:C:100:GLN:HG2	2.03	0.57
2:A:69:TYR:HB3	2:A:71:HIS:CD2	2.39	0.57
1:B:16:U:O4	2:A:30:VAL:HG13	2.03	0.57
2:C:29:ILE:HG22	2:C:85:LEU:CD2	2.33	0.56
2:C:41:GLU:O	2:C:42:LYS:CB	2.53	0.56
2:A:47:PHE:CE2	2:A:64:LEU:HD11	2.41	0.56
1:D:37:G:C6	1:D:38:G:N2	2.73	0.56
1:D:39:A:H1'	2:C:36:VAL:CG2	2.28	0.56
1:B:24:G:O2'	1:B:25:A:H5'	2.04	0.56
2:A:29:ILE:HG13	2:A:29:ILE:O	2.04	0.56
2:A:39:LEU:HG	2:A:66:ILE:HD11	1.88	0.56
1:B:40:C:C2	1:B:51:U:O2	2.59	0.56
2:A:107:ILE:HD13	2:A:107:ILE:H	1.71	0.56
2:C:109:LEU:HG	2:C:123:ALA:HB2	1.86	0.56
1:D:18:G:O2'	1:D:19:A:P	2.63	0.56
1:D:20:C:H2'	1:D:21:G:C8	2.40	0.56
2:A:83:ARG:HG3	2:A:83:ARG:HH11	1.71	0.56
1:D:32:U:O2	2:A:101:GLU:HG3	2.05	0.56
1:D:18:G:O2'	2:C:87:LEU:O	2.24	0.56
2:A:40:ARG:C	2:A:42:LYS:H	2.09	0.55
2:C:32:LYS:HB2	2:C:35:GLU:OE2	2.07	0.55
2:C:66:ILE:HG23	2:C:66:ILE:O	2.07	0.55
2:C:70:LYS:HA	2:C:70:LYS:HE2	1.88	0.55
1:D:21:G:C2	1:D:37:G:C2	2.94	0.55
2:A:24:THR:O	2:A:25:TYR:HD2	1.88	0.55
2:C:51:PHE:CZ	2:C:62:TYR:CB	2.89	0.55
1:B:50:A:O2'	1:B:51:U:P	2.65	0.55
1:D:24:G:O2'	1:D:25:A:H5'	2.06	0.55
2:A:30:VAL:HG23	2:A:86:LEU:HD11	1.89	0.55
2:A:81:ARG:HH21	2:A:84:LYS:HZ3	1.53	0.55
2:A:128:LYS:O	2:A:129:LYS:HB2	2.07	0.54
2:C:110:LYS:O	2:C:120:VAL:HA	2.07	0.54
1:D:18:G:O2'	2:C:87:LEU:C	2.45	0.54
2:C:21:ILE:HA	2:C:125:ALA:HB2	1.89	0.54
2:C:27:ALA:CB	2:C:120:VAL:HG13	2.37	0.54
2:C:83:ARG:NH1	2:C:83:ARG:HG3	2.20	0.54
2:A:30:VAL:HB	2:A:84:LYS:CE	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:G:O6	1:B:53:C:N4	2.41	0.54
1:D:39:A:C2	2:C:118:VAL:HG23	2.43	0.54
2:C:32:LYS:HD3	2:C:81:ARG:HH12	1.72	0.53
1:B:35:U:H2'	1:B:36:C:H6	1.73	0.53
2:C:10:ALA:O	2:C:11:GLU:CB	2.57	0.53
2:C:9:ILE:HD11	2:C:113:TRP:CD1	2.43	0.53
2:A:21:ILE:N	2:A:21:ILE:HD12	2.24	0.53
1:D:28:U:H5	2:A:100:GLN:HE22	1.56	0.53
2:A:86:LEU:N	2:A:86:LEU:CD1	2.71	0.53
2:C:65:TYR:HE1	2:C:67:ALA:HB2	1.74	0.53
2:C:22:LEU:HB2	2:C:124:LEU:O	2.09	0.52
2:C:77:HIS:C	2:C:77:HIS:CD2	2.82	0.52
1:B:37:G:C6	1:B:38:G:N2	2.77	0.52
2:C:66:ILE:CG2	2:C:83:ARG:NH2	2.68	0.51
2:A:106:ILE:HG12	2:A:124:LEU:HD12	1.91	0.51
2:C:61:LEU:HB2	2:C:85:LEU:HD21	1.92	0.51
2:A:45:VAL:HA	2:A:65:TYR:O	2.11	0.51
2:A:62:TYR:OH	2:A:82:LYS:HE3	2.10	0.51
2:C:60:TRP:CH2	2:C:84:LYS:HD3	2.46	0.51
2:C:32:LYS:O	2:C:35:GLU:N	2.43	0.51
2:C:32:LYS:O	2:C:33:GLY:C	2.49	0.51
1:B:17:C:P	2:A:117:LYS:HE3	2.51	0.51
2:A:29:ILE:HG13	2:A:31:LEU:HG	1.93	0.51
1:B:20:C:H2'	1:B:21:G:C8	2.46	0.51
1:B:21:G:C2	1:B:37:G:C2	2.98	0.50
2:A:113:TRP:CZ3	2:A:118:VAL:HG22	2.46	0.50
1:D:39:A:N1	2:C:118:VAL:N	2.50	0.50
1:B:17:C:OP1	2:A:117:LYS:HE3	2.10	0.50
2:A:13:LYS:O	2:A:15:ALA:N	2.39	0.50
2:A:41:GLU:O	2:A:42:LYS:CB	2.59	0.50
2:A:66:ILE:O	2:A:66:ILE:CG2	2.58	0.50
1:D:21:G:C6	1:D:37:G:N1	2.80	0.49
2:A:29:ILE:HG22	2:A:85:LEU:HD23	1.92	0.49
2:C:9:ILE:HG13	2:C:112:TYR:HA	1.95	0.49
2:A:102:LYS:HB2	2:A:104:TYR:CE2	2.47	0.49
2:C:62:TYR:CE2	2:C:82:LYS:HD2	2.48	0.49
2:C:109:LEU:HG	2:C:123:ALA:CB	2.43	0.49
2:A:55:GLU:O	2:A:57:GLY:N	2.46	0.49
2:A:63:ASN:OD1	2:A:80:LEU:HD13	2.13	0.49
2:A:29:ILE:HD11	2:A:31:LEU:HD11	1.95	0.48
1:B:20:C:H2'	1:B:21:G:H8	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:C:H1'	2:C:101:GLU:HA	1.94	0.48
2:C:45:VAL:HG12	2:C:45:VAL:O	2.13	0.48
2:C:95:LEU:HB3	2:C:106:ILE:CD1	2.37	0.48
2:A:30:VAL:CG2	2:A:86:LEU:HD11	2.42	0.48
2:A:94:ARG:CG	2:A:94:ARG:NH1	2.74	0.48
2:C:109:LEU:CD1	2:C:123:ALA:HB2	2.43	0.48
2:A:69:TYR:HD2	2:A:71:HIS:CE1	2.31	0.48
2:A:70:LYS:HA	2:A:70:LYS:CE	2.41	0.48
1:D:37:G:O2'	1:D:38:G:H5'	2.14	0.48
2:A:100:GLN:O	2:A:101:GLU:C	2.51	0.48
1:B:45:G:H1	1:B:53:C:N4	2.11	0.48
1:B:37:G:C6	1:B:38:G:N1	2.81	0.48
1:B:50:A:O2'	1:B:51:U:OP1	2.32	0.48
2:A:29:ILE:HG22	2:A:85:LEU:HD22	1.93	0.47
2:A:98:LYS:HB3	2:A:124:LEU:HD21	1.96	0.47
2:A:87:LEU:O	2:A:91:GLU:HB2	2.15	0.47
2:C:21:ILE:O	2:C:22:LEU:HD23	2.15	0.47
1:D:35:U:H2'	1:D:36:C:H6	1.76	0.47
2:A:19:TYR:O	2:A:20:ASP:O	2.32	0.47
2:C:51:PHE:CZ	2:C:62:TYR:HB3	2.49	0.47
1:D:16:U:C5'	1:D:17:C:OP2	2.63	0.47
2:C:14:GLU:O	2:C:18:LYS:HB2	2.14	0.47
2:C:27:ALA:O	2:C:86:LEU:O	2.33	0.47
1:D:31:G:C5	1:D:32:U:C5	3.03	0.47
2:A:111:LEU:HD23	2:A:120:VAL:HB	1.97	0.47
2:C:9:ILE:HB	2:C:111:LEU:O	2.14	0.47
1:D:37:G:N1	1:D:38:G:N2	2.63	0.47
2:C:47:PHE:HB3	2:C:64:LEU:CD1	2.38	0.47
1:D:19:A:H2'	1:D:20:C:C6	2.51	0.46
2:C:28:GLY:O	2:C:86:LEU:HD12	2.16	0.46
1:B:16:U:O2'	2:A:119:LYS:NZ	2.48	0.46
1:B:16:U:C5	2:A:86:LEU:HD21	2.51	0.46
2:A:115:ASN:HB2	2:A:117:LYS:NZ	2.30	0.46
1:D:18:G:HO2'	1:D:19:A:P	2.34	0.46
1:D:37:G:H2'	1:D:38:G:O4'	2.15	0.46
2:C:17:ALA:O	2:C:128:LYS:HD2	2.15	0.46
2:A:102:LYS:HB2	2:A:104:TYR:CD2	2.50	0.46
2:C:23:GLU:OE1	2:C:25:TYR:OH	2.20	0.46
2:C:64:LEU:O	2:C:79:PRO:O	2.34	0.46
2:C:66:ILE:O	2:C:77:HIS:NE2	2.49	0.46
2:C:77:HIS:O	2:C:79:PRO:HD3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:19:TYR:O	2:A:20:ASP:HB2	2.15	0.46
2:C:39:LEU:HG	2:C:66:ILE:HD11	1.97	0.46
2:C:57:GLY:O	2:C:92:ILE:HD13	2.16	0.46
2:C:35:GLU:HG2	2:C:77:HIS:CE1	2.51	0.45
2:C:36:VAL:O	2:C:39:LEU:HB2	2.16	0.45
2:C:62:TYR:CZ	2:C:82:LYS:HD2	2.51	0.45
2:C:69:TYR:HD2	2:C:71:HIS:NE2	2.13	0.45
1:D:21:G:O2'	1:D:22:G:H5'	2.16	0.45
2:C:54:ILE:HD13	2:C:59:ALA:CB	2.47	0.45
1:B:16:U:H5'	1:B:17:C:OP2	2.16	0.45
1:B:45:G:H1	1:B:53:C:H42	1.64	0.45
1:B:40:C:O2	2:A:40:ARG:NE	2.41	0.45
2:C:20:ASP:OD1	2:C:128:LYS:HG2	2.16	0.45
2:C:41:GLU:OE2	2:C:41:GLU:HA	2.16	0.45
2:A:28:GLY:HA3	2:A:86:LEU:HB2	1.98	0.45
2:A:84:LYS:N	2:A:84:LYS:CD	2.62	0.45
1:D:21:G:C6	1:D:37:G:C6	3.05	0.45
2:C:98:LYS:HD3	2:C:98:LYS:HA	1.80	0.45
1:B:39:A:O2'	1:B:40:C:C6	2.55	0.45
2:C:20:ASP:O	2:C:125:ALA:HB1	2.16	0.45
1:B:27:U:N3	1:B:29:C:N3	2.65	0.45
2:C:120:VAL:CG2	2:C:122:ILE:HD12	2.47	0.44
1:B:21:G:C6	1:B:37:G:N1	2.85	0.44
2:C:94:ARG:CG	2:C:94:ARG:NH1	2.73	0.44
2:A:61:LEU:HD21	2:A:64:LEU:HD13	1.99	0.44
2:C:24:THR:C	2:C:25:TYR:CD2	2.91	0.44
1:B:50:A:C2	1:B:53:C:N4	2.86	0.44
2:C:100:GLN:O	2:C:101:GLU:C	2.56	0.44
1:D:19:A:OP1	2:C:88:HIS:HA	2.17	0.44
2:A:66:ILE:O	2:A:66:ILE:HG23	2.18	0.44
1:B:50:A:N1	1:B:53:C:N3	2.66	0.44
2:C:27:ALA:O	2:C:87:LEU:HD12	2.18	0.43
1:B:21:G:O2'	1:B:22:G:H5'	2.18	0.43
2:A:96:TYR:C	2:A:96:TYR:CD2	2.91	0.43
2:C:69:TYR:O	2:C:71:HIS:N	2.51	0.43
1:B:21:G:C6	1:B:37:G:C6	3.06	0.43
1:D:19:A:C2	1:D:20:C:N1	2.87	0.43
2:A:33:GLY:O	2:A:34:SER:C	2.57	0.43
1:D:29:C:C2'	1:D:30:G:OP2	2.66	0.43
2:A:110:LYS:O	2:A:120:VAL:HA	2.18	0.43
2:A:53:ARG:HD3	2:A:62:TYR:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:GLU:HB3	2:C:56:ASN:H	1.71	0.43
2:A:111:LEU:CD2	2:A:120:VAL:HB	2.47	0.43
2:C:85:LEU:HD13	2:C:122:ILE:CD1	2.48	0.43
1:B:53:C:O2'	1:B:54:C:H5'	2.19	0.43
2:A:87:LEU:O	2:A:91:GLU:OE2	2.37	0.43
2:A:96:TYR:O	2:A:97:GLY:C	2.56	0.43
2:A:22:LEU:HB2	2:A:124:LEU:O	2.18	0.43
1:B:13:G:H22	1:B:49:G:H21	1.66	0.43
2:C:21:ILE:HD12	2:C:21:ILE:H	1.84	0.43
2:C:42:LYS:O	2:C:43:GLY:O	2.37	0.43
1:D:30:G:H8	1:D:30:G:H3'	1.84	0.42
2:A:81:ARG:NH1	2:A:83:ARG:NE	2.64	0.42
2:C:20:ASP:O	2:C:21:ILE:C	2.57	0.42
2:C:109:LEU:CG	2:C:123:ALA:HB2	2.49	0.42
2:A:40:ARG:C	2:A:42:LYS:N	2.69	0.42
2:A:69:TYR:O	2:A:71:HIS:N	2.52	0.42
2:C:54:ILE:CD1	2:C:59:ALA:HB2	2.49	0.42
2:C:78:ASP:O	2:C:80:LEU:N	2.52	0.42
2:C:95:LEU:HD13	2:C:106:ILE:HD13	2.01	0.42
1:B:30:G:H3'	1:B:30:G:H8	1.85	0.42
2:C:100:GLN:OE1	2:C:100:GLN:HA	2.20	0.42
2:C:19:TYR:O	2:C:128:LYS:HE3	2.20	0.42
2:C:95:LEU:O	2:C:96:TYR:C	2.58	0.42
1:D:36:C:O2'	1:D:37:G:H5'	2.19	0.42
2:A:52:VAL:HG13	2:A:60:TRP:O	2.19	0.42
2:A:86:LEU:N	2:A:86:LEU:HD12	2.35	0.42
2:C:88:HIS:O	2:C:89:LYS:C	2.57	0.42
1:B:29:C:C2'	1:B:30:G:OP2	2.67	0.42
1:D:16:U:O2'	2:C:119:LYS:NZ	2.53	0.41
2:C:52:VAL:HG13	2:C:60:TRP:O	2.20	0.41
1:B:28:U:H5	2:C:100:GLN:HE22	1.66	0.41
2:A:76:ASN:O	2:A:77:HIS:HB3	2.20	0.41
2:C:86:LEU:HD12	2:C:86:LEU:N	2.34	0.41
2:A:27:ALA:HB1	2:A:28:GLY:H	1.44	0.41
2:A:30:VAL:HB	2:A:84:LYS:HG2	2.02	0.41
2:A:33:GLY:O	2:A:36:VAL:N	2.52	0.41
2:C:22:LEU:O	2:C:23:GLU:CG	2.63	0.41
2:C:23:GLU:HB3	2:C:25:TYR:CE2	2.50	0.41
1:B:13:G:N2	1:B:49:G:H21	2.19	0.41
2:A:67:ALA:HA	2:A:68:PRO:HD2	1.84	0.41
1:B:25:A:C4	1:B:26:C:C5	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:GLY:O	2:C:92:ILE:HG21	2.20	0.41
2:C:106:ILE:HG23	2:C:122:ILE:HG23	2.03	0.41
1:D:19:A:C2	1:D:20:C:H1'	2.56	0.41
2:A:30:VAL:O	2:A:84:LYS:HE2	2.21	0.41
2:C:90:ARG:HB3	2:C:90:ARG:CZ	2.50	0.41
1:B:45:G:H2'	1:B:46:U:C6	2.56	0.41
1:D:19:A:H2'	1:D:20:C:O4'	2.21	0.41
2:C:9:ILE:HD11	2:C:113:TRP:NE1	2.35	0.41
1:D:29:C:O2'	1:D:30:G:H5"	2.20	0.41
2:A:21:ILE:N	2:A:21:ILE:CD1	2.84	0.41
2:C:52:VAL:HG21	2:C:122:ILE:HG13	2.02	0.41
2:A:128:LYS:O	2:A:129:LYS:CB	2.67	0.40
2:C:28:GLY:O	2:C:86:LEU:N	2.44	0.40
2:C:71:HIS:O	2:C:72:ALA:C	2.59	0.40
2:C:24:THR:O	2:C:25:TYR:CD2	2.74	0.40
2:C:51:PHE:CE2	2:C:62:TYR:HB3	2.56	0.40
2:C:85:LEU:CD1	2:C:122:ILE:HG12	2.52	0.40
2:C:129:LYS:O	2:C:130:LEU:HB2	2.20	0.40
1:B:34:C:H2'	1:B:35:U:O4'	2.22	0.40
1:D:19:A:H2'	1:D:20:C:H6	1.84	0.40
2:A:92:ILE:O	2:A:93:MET:C	2.60	0.40
2:C:35:GLU:O	2:C:39:LEU:HG	2.22	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
2	A	121/156 (78%)	87 (72%)	20 (16%)	14 (12%)	0 2
2	C	121/156 (78%)	88 (73%)	22 (18%)	11 (9%)	1 3
All	All	242/312 (78%)	175 (72%)	42 (17%)	25 (10%)	0 3

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	27	ALA
2	A	42	LYS
2	A	43	GLY
2	A	70	LYS
2	A	81	ARG
2	A	100	GLN
2	A	101	GLU
2	C	43	GLY
2	C	70	LYS
2	C	79	PRO
2	C	129	LYS
2	A	104	TYR
2	C	11	GLU
2	C	42	LYS
2	A	14	GLU
2	A	15	ALA
2	A	20	ASP
2	A	56	ASN
2	C	9	ILE
2	C	81	ARG
2	C	10	ALA
2	C	45	VAL
2	A	33	GLY
2	C	21	ILE
2	A	57	GLY

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	109/137 (80%)	97 (89%)	12 (11%)	6 26
2	C	109/137 (80%)	91 (84%)	18 (16%)	2 10
All	All	218/274 (80%)	188 (86%)	30 (14%)	3 16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	32	LYS
2	A	39	LEU
2	A	45	VAL
2	A	84	LYS
2	A	87	LEU
2	A	90	ARG
2	A	93	MET
2	A	94	ARG
2	A	101	GLU
2	A	102	LYS
2	A	107	ILE
2	A	112	TYR
2	C	19	TYR
2	C	32	LYS
2	C	47	PHE
2	C	49	ASP
2	C	56	ASN
2	C	63	ASN
2	C	77	HIS
2	C	79	PRO
2	C	84	LYS
2	C	89	LYS
2	C	90	ARG
2	C	93	MET
2	C	94	ARG
2	C	99	VAL
2	C	105	THR
2	C	107	ILE
2	C	120	VAL
2	C	124	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	115	ASN
2	C	12	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	44/68 (64%)	13 (29%)	7 (15%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	24/68 (35%)	6 (25%)	4 (16%)
All	All	68/136 (50%)	19 (27%)	11 (16%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	15	U
1	B	16	U
1	B	17	C
1	B	19	A
1	B	29	C
1	B	30	G
1	B	39	A
1	B	40	C
1	B	41	G
1	B	48	C
1	B	50	A
1	B	51	U
1	B	52	U
1	D	17	C
1	D	19	A
1	D	29	C
1	D	30	G
1	D	38	G
1	D	39	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	16	U
1	B	18	G
1	B	28	U
1	B	38	G
1	B	39	A
1	B	40	C
1	B	50	A
1	D	16	U
1	D	18	G
1	D	28	U
1	D	38	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 monosaccharides 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	B	45/68 (66%)	0.64	2 (4%)	34	21	63, 112, 183, 221	0
1	D	24/68 (35%)	0.29	0	100	100	62, 92, 115, 167	0
2	A	125/156 (80%)	0.19	4 (3%)	47	31	48, 80, 170, 204	0
2	C	125/156 (80%)	0.16	2 (1%)	72	59	51, 110, 197, 221	0
All	All	319/448 (71%)	0.25	8 (2%)	57	43	48, 99, 185, 221	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	U	4.4
2	A	3	SER	4.1
1	B	13	G	3.2
2	A	76	ASN	3.1
2	C	71	HIS	2.6
2	A	71	HIS	2.5
2	A	77	HIS	2.3
2	C	101	GLU	2.1

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 monosaccharides 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.