



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 10:21 PM EST

PDB ID : 4V42
Title : Crystal structure of the ribosome at 5.5 Å resolution.
Authors : Yusupov, M.M.; Yusupova, G.Z.; Baucom, A.; Lieberman, K.; Earnest, T.N.;
Cate, J.H.D.; Noller, H.F.
Deposited on : 2001-03-30
Resolution : 5.50 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 ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

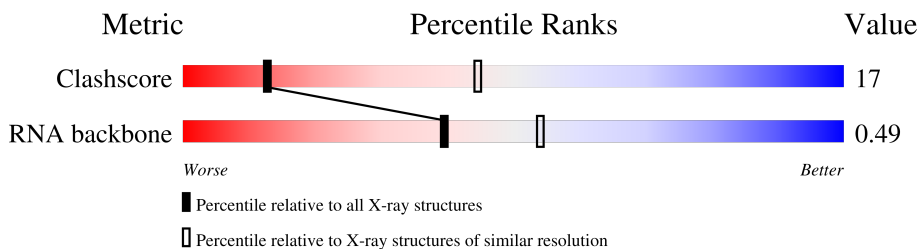
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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	141614	1010 (7.10-3.90)
RNA backbone	3102	1074 (7.80-3.00)

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	AA	1522	
2	AB	76	
2	AC	76	
3	AD	74	
4	A1	6	
5	AE	256	
6	AF	239	
7	AG	209	
8	AH	162	

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Mol	Chain	Length	Quality of chain
9	AI	101	100%
10	AJ	156	98%
11	AK	138	100%
12	AL	128	97%
13	AM	105	90% 7%
14	AN	129	92% 8%
15	AO	135	91% 8%
16	AP	126	98%
17	AQ	61	93% 5%
18	AR	89	99%
19	AS	91	91% 9%
20	AT	105	99%
21	AU	88	83% 17%
22	AV	93	86% 14%
23	AW	106	93% 7%
24	AX	26	92% 8%
25	BA	2916	98%
26	BB	123	98%
27	BC	228	96%
28	BD	178	92% 5%
29	BE	338	54% 43%
30	BF	246	72% 23%
31	BG	176	69% 31%
32	BH	177	93% 7%
33	BI	128	98%

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Mol	Chain	Length	Quality of chain
33	BJ	128	 100%
34	BK	149	 99%
35	BL	141	 94% 6%
36	BM	145	 80% 19%
37	BN	122	 100%
38	BO	164	 50% 49%
39	BP	138	 99%
40	BQ	186	 56% 5% 39%
41	BR	66	 79% 21%
42	BS	113	 97%
43	BT	84	 89% 10%
44	BU	119	 92% 8%
45	BV	94	 95% 5%
46	BW	70	 91% 9%
47	BX	60	 98%

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
2	M2G	AB	26	-	-	X	-
3	5MC	AD	49	-	-	X	-
3	4SU	AD	8	-	-	X	-

2 Entry composition i

There are 47 unique types of molecules in this entry. The entry contains 14656 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 30S 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	AA	1519	Total	P	0	0	1519
			1519	1519			

- Molecule 2 is a RNA chain called TRNA(PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			
2	AC	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	10	2MG	G	modified residue	GB 176479
AB	16	H2U	U	modified residue	GB 176479
AB	17	H2U	U	modified residue	GB 176479
AB	26	M2G	G	modified residue	GB 176479
AB	32	OMC	C	modified residue	GB 176479
AB	34	OMG	G	modified residue	GB 176479
AB	37	YG	G	modified residue	GB 176479
AB	39	PSU	U	modified residue	GB 176479
AB	40	5MC	C	modified residue	GB 176479
AB	46	7MG	G	modified residue	GB 176479
AB	49	5MC	C	modified residue	GB 176479
AB	54	5MU	U	modified residue	GB 176479
AB	55	PSU	U	modified residue	GB 176479
AB	58	1MA	A	modified residue	GB 176479
AC	10	2MG	G	modified residue	GB 176479
AC	16	H2U	U	modified residue	GB 176479
AC	17	H2U	U	modified residue	GB 176479
AC	26	M2G	G	modified residue	GB 176479

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	32	OMC	C	modified residue	GB 176479
AC	34	OMG	G	modified residue	GB 176479
AC	37	YG	G	modified residue	GB 176479
AC	39	PSU	U	modified residue	GB 176479
AC	40	5MC	C	modified residue	GB 176479
AC	46	7MG	G	modified residue	GB 176479
AC	49	5MC	C	modified residue	GB 176479
AC	54	5MU	U	modified residue	GB 176479
AC	55	PSU	U	modified residue	GB 176479
AC	58	1MA	A	modified residue	GB 176479

- Molecule 3 is a RNA chain called TRNA(PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S		
3	AD	74	1570	702	269	524	74	1	0	0

- Molecule 4 is a RNA chain called A- AND P-SITE MESSENGER RNA CODONS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	A1	6	120	54	12	48	6		0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
5	AE	234	234	234	0	0	234

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
6	AF	206	206	206	0	0	206

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
7	AG	208	208	208	0	0	208

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	AH	150	Total C 150 150	0	0	150

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	AI	101	Total C 101 101	0	0	101

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	AJ	155	Total C 155 155	0	0	155

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	AK	138	Total C 138 138	0	0	138

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	AL	127	Total C 127 127	0	0	127

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	AM	98	Total C 98 98	0	0	98

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	AN	119	Total C 119 119	0	0	119

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	AO	124	Total C 124 124	0	0	124

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	AP	125	Total C 125 125	0	0	125

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	AQ	60	Total C 60 60	0	0	60

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	AR	88	Total C 88 88	0	0	88

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	AS	83	Total C 83 83	0	0	83

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	AT	104	Total C 104 104	0	0	104

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	AU	73	Total C 73 73	0	0	73

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	AV	80	Total C 80 80	0	0	80

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	AW	99	Total C 99 99	0	0	99

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	AX	24	Total C 24 24	0	0	24

- Molecule 25 is a RNA chain called 50S 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	BA	2889	Total P 2889 2889	0	0	2889

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	insertion	? 48268

- Molecule 26 is a RNA chain called 50S 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	BB	123	Total P 123 123	0	0	123

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	insertion	GB 176261

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	BC	224	Total C 224 224	0	0	224

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	BD	173	Total C 173 173	0	0	173

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	BE	191	Total C 191 191	0	0	191

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BE	113	SER	ASP	conflict	UNP P20279
BE	114	ASP	VAL	conflict	UNP P20279
BE	115	ARG	PRO	conflict	UNP P20279
BE	116	LEU	GLU	conflict	UNP P20279
BE	119	ALA	ASP	conflict	UNP P20279
BE	120	LEU	PRO	conflict	UNP P20279
BE	122	ILE	ALA	conflict	UNP P20279
BE	123	VAL	ALA	conflict	UNP P20279
BE	125	ASP	GLU	conflict	UNP P20279

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	BF	189	Total C 189 189	0	0	189

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	GLU	GLN	conflict	UNP P12735

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	BG	122	Total C 122 122	0	0	122

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	BH	164	Total C 164 164	0	0	164

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	BI	128	Total C 128 128	0	0	128
33	BJ	128	Total C 128 128	0	0	128

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	BK	148	Total C 148 148	0	0	148

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	BL	133	Total C 133 133	0	0	133

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BM	117	Total C 117 117	0	0	117

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	BN	122	Total C 122 122	0	0	122

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BO	84	Total C 84 84	0	0	84

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	BP	138	Total C 138 138	0	0	138

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	BQ	113	Total C 113 113	0	0	113

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	BR	52	Total C 52 52	0	0	52

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	BS	110	Total C 110 110	0	0	110

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
43	BT	76	Total C 76 76	0	0	76

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	BU	110	Total C 110 110	0	0	110

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	BV	89	Total C 89 89	0	0	89

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	BW	64	Total C 64 64	0	0	64

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	BX	60	Total C 60 60	0	0	60

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.

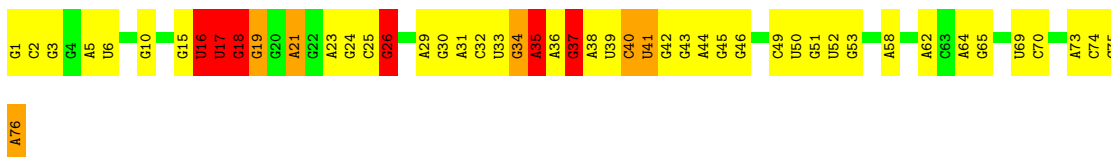
- Molecule 1: 30S 16S RIBOSOMAL RNA

Chain AA:  99%



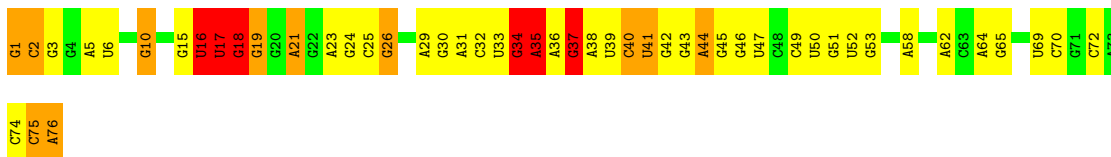
- Molecule 2: TRNA(PHE)

Chain AB:  36% 49% 8% 8%



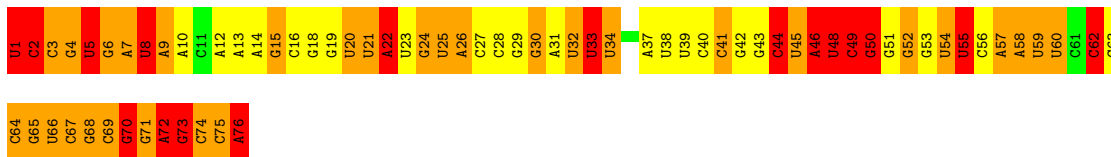
- Molecule 2: TRNA(PHE)

Chain AC:  34% 43% 14% 8%



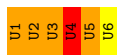
- Molecule 3: TRNA(PHE)

Chain AD:  5% 30% 42% 23%



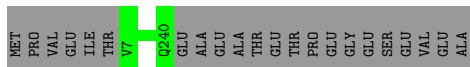
- Molecule 4: A- AND P-SITE MESSENGER RNA CODONS

Chain A1:  17% 67% 17%




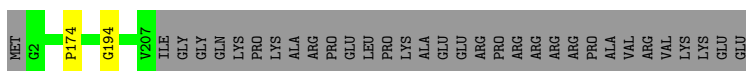
- Molecule 5: 30S RIBOSOMAL PROTEIN S2

Chain AE:  91% 9%



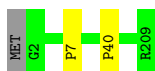
- Molecule 6: 30S RIBOSOMAL PROTEIN S3

Chain AF:  85% 14%



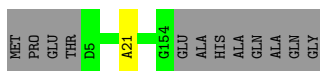
- Molecule 7: 30S RIBOSOMAL PROTEIN S4

Chain AG:  99%



- Molecule 8: 30S RIBOSOMAL PROTEIN S5

Chain AH:  92% 7%



- Molecule 9: 30S RIBOSOMAL PROTEIN S6

Chain AI:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 30S RIBOSOMAL PROTEIN S7

Chain AJ:  98%



- Molecule 11: 30S RIBOSOMAL PROTEIN S8

Chain AK:  100%

There are no outlier residues recorded for this chain.

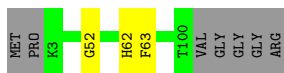
- Molecule 12: 30S RIBOSOMAL PROTEIN S9

Chain AL:  97% ..



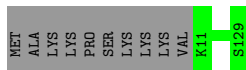
- Molecule 13: 30S RIBOSOMAL PROTEIN S10

Chain AM:  90% • 7%



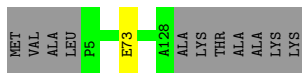
- Molecule 14: 30S RIBOSOMAL PROTEIN S11

Chain AN:  92% 8%



- Molecule 15: 30S RIBOSOMAL PROTEIN S12

Chain AO:  91% • 8%



- Molecule 16: 30S RIBOSOMAL PROTEIN S13

Chain AP:  98% ..



- Molecule 17: 30S RIBOSOMAL PROTEIN S14

Chain AQ:  93% • 5%



- Molecule 18: 30S RIBOSOMAL PROTEIN S15

Chain AR:  99% •



- Molecule 19: 30S RIBOSOMAL PROTEIN S16

Chain AS:  91% 9%



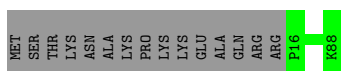
- Molecule 20: 30S RIBOSOMAL PROTEIN S17

Chain AT: 99%



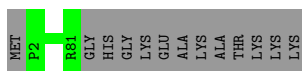
- Molecule 21: 30S RIBOSOMAL PROTEIN S18

Chain AU: 83% 17%



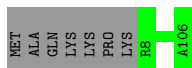
- Molecule 22: 30S RIBOSOMAL PROTEIN S19

Chain AV: 86% 14%



- Molecule 23: 30S RIBOSOMAL PROTEIN S20

Chain AW: 93% 7%



- Molecule 24: 30S RIBOSOMAL PROTEIN THX

Chain AX: 92% 8%



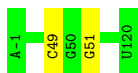
- Molecule 25: 50S 23S RIBOSOMAL RNA

Chain BA: 98%



- Molecule 26: 50S 5S RIBOSOMAL RNA

Chain BB:  98%



- Molecule 27: 50S RIBOSOMAL PROTEIN L1

Chain BC:  96%



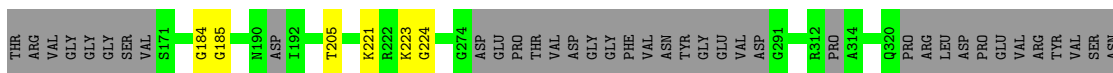
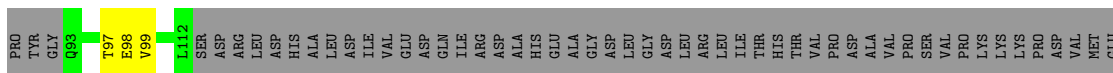
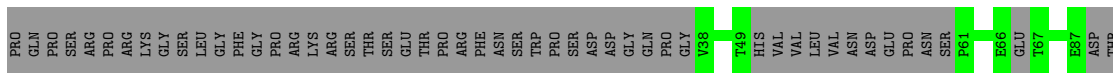
- Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain BD:  92%



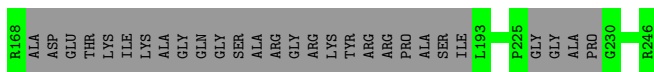
- Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain BE:  54%



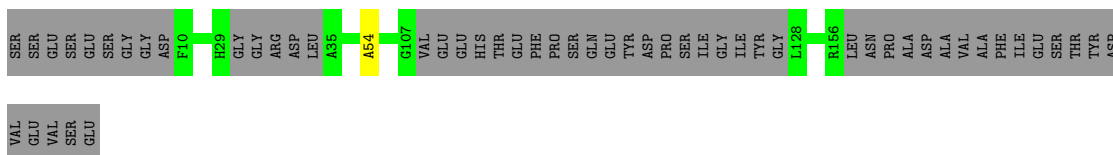
- Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain BF:  72%



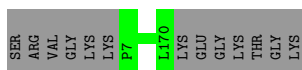
- Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain BG:  69%



- Molecule 32: 50S RIBOSOMAL PROTEIN L6

Chain BH: 93% 7%



- Molecule 33: 50S RIBOSOMAL PROTEIN L7/L12

Chain BI: 98%



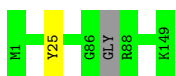
- Molecule 33: 50S RIBOSOMAL PROTEIN L7/L12

Chain BJ: 100%

There are no outlier residues recorded for this chain.

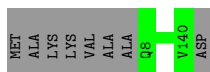
- Molecule 34: 50S RIBOSOMAL PROTEIN L9

Chain BK: 99%



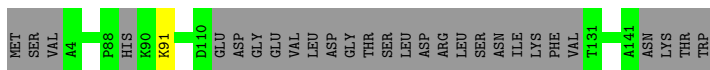
- Molecule 35: 50S RIBOSOMAL PROTEIN L11

Chain BL: 94% 6%



- Molecule 36: 50S RIBOSOMAL PROTEIN L13

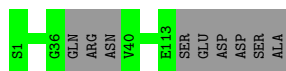
Chain BM: 80% 19%



- Molecule 37: 50S RIBOSOMAL PROTEIN L14

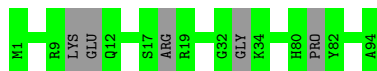
Chain BN: 100%

There are no outlier residues recorded for this chain.



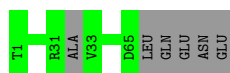
- Molecule 45: 50S RIBOSOMAL PROTEIN L25

Chain BV: 95% 5%



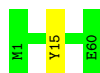
- Molecule 46: 50S RIBOSOMAL PROTEIN L29

Chain BW: 91% 9%



- Molecule 47: 50S RIBOSOMAL PROTEIN L30

Chain BX: 98% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	507.20Å 507.20Å 803.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	250.00 – 5.50	Depositor
% Data completeness (in resolution range)	95.3 (250.00-5.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14656	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, YG, M2G, OMG, 2MG, 4SU, H2U, OMC, PSU, 5MU, 5MC, 7MG

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
2	AB	1.21	4/1486 (0.3%)	1.43	13/2311 (0.6%)
2	AC	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
3	AD	1.95	17/1616 (1.1%)	2.85	154/2512 (6.1%)
4	A1	2.35	5/131 (3.8%)	2.46	3/200 (1.5%)
All	All	1.60	33/4720 (0.7%)	2.07	192/7338 (2.6%)

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
2	AB	0	3
2	AC	0	3
All	All	0	6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AD	33	U	O3'-P	31.20	1.98	1.61
2	AC	74	C	O3'-P	-27.00	1.28	1.61
2	AB	75	C	O3'-P	-26.77	1.29	1.61
2	AC	75	C	O3'-P	-25.61	1.30	1.61
3	AD	15	G	O3'-P	24.09	1.90	1.61
3	AD	26	A	O3'-P	-22.70	1.33	1.61
2	AB	34	OMG	O3'-P	19.78	1.84	1.61
3	AD	24	G	O3'-P	18.93	1.83	1.61
3	AD	56	C	O3'-P	17.60	1.82	1.61
3	AD	25	U	O3'-P	16.97	1.81	1.61
2	AC	44	A	O3'-P	-16.93	1.40	1.61
2	AC	72	C	O3'-P	-15.82	1.42	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AD	21	H2U	O3'-P	-13.66	1.44	1.61
3	AD	46	A	O3'-P	12.75	1.76	1.61
4	A1	4	U	O3'-P	-12.24	1.46	1.61
4	A1	1	U	O3'-P	-12.22	1.46	1.61
4	A1	5	U	O3'-P	-12.18	1.46	1.61
4	A1	2	U	O3'-P	-12.14	1.46	1.61
3	AD	76	A	C6-N6	-11.63	1.24	1.33
3	AD	22	A	N9-C4	-10.71	1.31	1.37
3	AD	72	A	O3'-P	10.28	1.73	1.61
3	AD	45	U	O3'-P	-10.16	1.49	1.61
3	AD	8	4SU	O3'-P	-9.14	1.50	1.61
4	A1	3	U	O3'-P	-8.92	1.50	1.61
3	AD	75	C	O3'-P	-8.38	1.51	1.61
2	AC	35	A	O3'-P	8.14	1.71	1.61
3	AD	73	G	O3'-P	-7.55	1.52	1.61
2	AC	1	G	OP3-P	-7.29	1.52	1.61
2	AB	1	G	OP3-P	-7.17	1.52	1.61
3	AD	55	PSU	O3'-P	7.13	1.69	1.61
2	AC	76	A	C2'-O2'	6.54	1.50	1.41
2	AB	73	A	O3'-P	6.25	1.68	1.61
3	AD	5	U	C4-O4	5.04	1.27	1.23

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	35	A	P-O3'-C3'	41.11	169.03	119.70
3	AD	25	U	P-O3'-C3'	31.41	157.40	119.70
3	AD	75	C	P-O3'-C3'	-29.51	84.29	119.70
4	A1	3	U	P-O3'-C3'	27.61	152.83	119.70
3	AD	8	4SU	O3'-P-O5'	-27.11	52.48	104.00
2	AC	35	A	P-O3'-C3'	27.09	152.21	119.70
3	AD	24	G	P-O3'-C3'	-24.71	90.05	119.70
2	AC	74	C	O3'-P-O5'	24.46	150.48	104.00
3	AD	15	G	P-O3'-C3'	24.38	148.95	119.70
3	AD	31	A	OP2-P-O3'	22.97	155.72	105.20
3	AD	40	C	OP2-P-O3'	21.31	152.09	105.20
3	AD	15	G	O3'-P-O5'	21.08	144.06	104.00
2	AB	34	OMG	O3'-P-O5'	19.74	141.50	104.00
3	AD	31	A	O3'-P-O5'	-19.29	67.36	104.00
3	AD	40	C	O3'-P-O5'	-17.73	70.32	104.00
3	AD	44	C	O3'-P-O5'	17.45	137.16	104.00
3	AD	72	A	P-O3'-C3'	16.50	139.50	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	8	4SU	OP1-P-O3'	15.84	140.04	105.20
3	AD	16	C	P-O3'-C3'	15.77	138.62	119.70
2	AC	35	A	OP1-P-O3'	14.55	137.21	105.20
2	AC	72	C	O3'-P-O5'	13.96	130.53	104.00
3	AD	29	G	OP1-P-O3'	-13.71	75.03	105.20
2	AB	75	C	P-O3'-C3'	13.47	135.87	119.70
4	A1	3	U	O3'-P-O5'	13.43	129.52	104.00
3	AD	32	U	OP1-P-O3'	-13.32	75.90	105.20
3	AD	33	U	P-O3'-C3'	13.07	135.38	119.70
3	AD	8	4SU	P-O3'-C3'	-12.81	104.33	119.70
2	AC	75	C	P-O3'-C3'	12.71	134.96	119.70
2	AC	76	A	O5'-P-OP2	-12.60	94.36	105.70
2	AB	73	A	P-O3'-C3'	-12.54	104.65	119.70
3	AD	1	U	P-O3'-C3'	11.82	133.89	119.70
3	AD	75	C	O3'-P-O5'	11.78	126.38	104.00
2	AB	35	A	OP1-P-O3'	11.50	130.50	105.20
3	AD	5	U	C2-N3-C4	-11.49	120.11	127.00
2	AB	75	C	OP2-P-O3'	11.40	130.27	105.20
2	AC	1	G	P-O3'-C3'	11.12	133.05	119.70
3	AD	44	C	P-O3'-C3'	-11.08	106.41	119.70
3	AD	46	A	OP1-P-O3'	10.98	129.36	105.20
3	AD	31	A	OP1-P-O3'	-10.76	81.54	105.20
3	AD	56	C	P-O3'-C3'	-10.66	106.90	119.70
3	AD	32	U	O4'-C1'-N1	10.49	116.59	108.20
2	AC	74	C	OP2-P-O3'	-10.18	82.80	105.20
2	AB	34	OMG	OP2-P-O3'	-10.14	82.88	105.20
3	AD	33	U	OP1-P-O3'	9.86	126.90	105.20
3	AD	40	C	OP1-P-O3'	-9.75	83.74	105.20
2	AC	35	A	OP2-P-O3'	-9.65	83.97	105.20
2	AC	34	OMG	O3'-P-O5'	9.62	122.28	104.00
3	AD	29	G	O3'-P-O5'	9.56	122.16	104.00
3	AD	21	H2U	P-O3'-C3'	9.55	131.17	119.70
2	AC	44	A	OP2-P-O3'	9.54	126.19	105.20
3	AD	75	C	OP1-P-O3'	-9.44	84.43	105.20
2	AC	34	OMG	OP2-P-O3'	-9.29	84.77	105.20
3	AD	42	G	OP1-P-O3'	-9.29	84.77	105.20
3	AD	5	U	N3-C4-C5	9.02	120.01	114.60
2	AC	72	C	OP1-P-O3'	-8.99	85.42	105.20
3	AD	48	U	C2-N3-C4	-8.90	121.66	127.00
2	AB	35	A	O3'-P-O5'	-8.88	87.12	104.00
3	AD	27	C	OP1-P-O3'	-8.86	85.72	105.20
2	AB	76	A	P-O5'-C5'	-8.79	106.84	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	32	U	O3'-P-O5'	8.77	120.67	104.00
3	AD	1	U	C2-N3-C4	-8.76	121.75	127.00
3	AD	59	U	C2-N3-C4	-8.57	121.86	127.00
3	AD	74	C	P-O3'-C3'	-8.55	109.44	119.70
3	AD	1	U	N3-C4-C5	8.46	119.68	114.60
2	AC	18	G	C5'-C4'-O4'	-8.43	98.99	109.10
2	AB	18	G	C5'-C4'-O4'	-8.38	99.04	109.10
3	AD	46	A	OP2-P-O3'	-8.28	86.98	105.20
3	AD	46	A	P-O3'-C3'	-8.24	109.81	119.70
3	AD	48	U	N3-C4-C5	8.22	119.53	114.60
3	AD	28	C	OP1-P-O3'	-8.22	87.12	105.20
3	AD	30	G	O4'-C1'-N9	8.18	114.75	108.20
2	AC	74	C	P-O3'-C3'	-8.14	109.93	119.70
3	AD	59	U	N3-C4-C5	8.11	119.47	114.60
3	AD	5	U	N1-C2-N3	8.05	119.73	114.90
3	AD	66	U	N3-C4-C5	7.95	119.37	114.60
3	AD	15	G	OP1-P-O3'	-7.94	87.74	105.20
3	AD	75	C	P-O5'-C5'	-7.92	108.22	120.90
3	AD	27	C	OP2-P-O3'	7.92	122.62	105.20
3	AD	62	C	O4'-C1'-N1	7.91	114.53	108.20
3	AD	15	G	OP2-P-O3'	-7.90	87.82	105.20
3	AD	60	U	C2-N3-C4	-7.89	122.26	127.00
2	AC	72	C	P-O3'-C3'	-7.86	110.27	119.70
3	AD	29	G	OP2-P-O3'	7.83	122.43	105.20
2	AC	44	A	O3'-P-O5'	-7.83	89.13	104.00
3	AD	44	C	OP1-P-O3'	-7.80	88.04	105.20
3	AD	33	U	OP2-P-O3'	-7.71	88.24	105.20
2	AC	75	C	O3'-P-O5'	7.59	118.42	104.00
3	AD	64	C	O4'-C1'-N1	7.52	114.22	108.20
3	AD	21	H2U	O3'-P-O5'	7.37	118.01	104.00
2	AC	75	C	O5'-P-OP1	-7.31	99.12	105.70
3	AD	60	U	N3-C4-C5	7.30	118.98	114.60
3	AD	57	A	P-O3'-C3'	7.29	128.45	119.70
3	AD	42	G	O4'-C1'-N9	7.25	114.00	108.20
3	AD	41	C	O4'-C1'-N1	7.17	113.94	108.20
3	AD	25	U	OP1-P-O3'	7.15	120.93	105.20
3	AD	62	C	N1-C1'-C2'	-7.13	104.16	112.00
3	AD	40	C	O4'-C1'-N1	6.97	113.78	108.20
3	AD	58	A	N1-C2-N3	-6.96	125.82	129.30
3	AD	5	U	P-O3'-C3'	6.94	128.03	119.70
3	AD	75	C	O4'-C1'-N1	6.94	113.75	108.20
3	AD	22	A	C8-N9-C4	6.85	108.54	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	76	A	N1-C2-N3	-6.84	125.88	129.30
3	AD	30	G	C1'-O4'-C4'	-6.78	104.48	109.90
3	AD	72	A	N1-C2-N3	-6.76	125.92	129.30
3	AD	32	U	N1-C1'-C2'	-6.73	104.60	112.00
3	AD	66	U	C2-N3-C4	-6.65	123.01	127.00
3	AD	60	U	P-O3'-C3'	-6.61	111.76	119.70
3	AD	39	U	OP2-P-O3'	6.58	119.68	105.20
3	AD	41	C	OP2-P-O3'	6.49	119.49	105.20
3	AD	26	A	O3'-P-O5'	6.45	116.26	104.00
3	AD	7	A	O4'-C1'-N9	6.42	113.33	108.20
3	AD	2	C	O4'-C1'-N1	6.33	113.27	108.20
3	AD	42	G	O3'-P-O5'	6.31	115.99	104.00
3	AD	76	A	C5-C6-N1	-6.31	114.55	117.70
3	AD	64	C	P-O3'-C3'	-6.25	112.20	119.70
3	AD	66	U	OP1-P-OP2	-6.22	110.26	119.60
3	AD	75	C	N3-C4-C5	-6.20	119.42	121.90
3	AD	2	C	N3-C4-C5	-6.19	119.42	121.90
3	AD	69	C	O4'-C1'-N1	6.19	113.15	108.20
3	AD	70	G	C5-C6-N1	6.17	114.59	111.50
3	AD	7	A	N1-C2-N3	-6.17	126.22	129.30
3	AD	48	U	OP1-P-OP2	-6.12	110.41	119.60
3	AD	25	U	O3'-P-O5'	-6.12	92.37	104.00
3	AD	57	A	N1-C2-N3	-6.06	126.27	129.30
3	AD	4	G	C5-C6-N1	6.03	114.51	111.50
3	AD	32	U	C5'-C4'-O4'	6.00	116.29	109.10
3	AD	62	C	N3-C4-C5	-5.99	119.50	121.90
2	AB	76	A	O5'-P-OP2	-5.97	100.33	105.70
3	AD	28	C	O3'-P-O5'	5.96	115.33	104.00
3	AD	50	G	C5-C6-N1	5.95	114.48	111.50
2	AB	15	G	N9-C1'-C2'	-5.94	105.47	112.00
3	AD	4	G	O4'-C1'-N9	5.93	112.95	108.20
2	AC	15	G	N9-C1'-C2'	-5.93	105.48	112.00
4	A1	3	U	OP2-P-O3'	-5.92	92.17	105.20
3	AD	62	C	OP1-P-OP2	-5.92	110.73	119.60
3	AD	73	G	O4'-C1'-N9	5.90	112.92	108.20
3	AD	65	G	C5-C6-N1	5.87	114.44	111.50
3	AD	29	G	C5'-C4'-C3'	-5.86	106.62	116.00
3	AD	64	C	N1-C1'-C2'	-5.85	105.56	112.00
3	AD	74	C	N3-C4-C5	-5.85	119.56	121.90
3	AD	63	C	OP1-P-OP2	-5.84	110.83	119.60
3	AD	2	C	OP1-P-OP2	-5.84	110.84	119.60
3	AD	51	G	C5-C6-N1	5.83	114.41	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	5	U	O4'-C1'-N1	5.82	112.86	108.20
3	AD	73	G	C5-C6-N1	5.81	114.41	111.50
3	AD	44	C	N1-C2-O2	5.77	122.36	118.90
3	AD	74	C	O5'-P-OP1	5.75	117.60	110.70
3	AD	60	U	O4'-C1'-N1	5.72	112.77	108.20
3	AD	1	U	N1-C2-N3	5.69	118.31	114.90
3	AD	6	G	C5-C6-N1	5.67	114.33	111.50
2	AC	74	C	N1-C1'-C2'	5.66	121.36	114.00
3	AD	64	C	OP1-P-OP2	-5.62	111.16	119.60
3	AD	3	C	N3-C4-C5	-5.62	119.65	121.90
3	AD	68	G	OP1-P-OP2	-5.60	111.19	119.60
3	AD	57	A	OP1-P-OP2	-5.58	111.24	119.60
3	AD	30	G	N9-C1'-C2'	-5.56	105.88	112.00
3	AD	42	G	C1'-O4'-C4'	-5.54	105.47	109.90
3	AD	6	G	P-O3'-C3'	-5.50	113.10	119.70
3	AD	71	G	C5-C6-N1	5.48	114.24	111.50
3	AD	66	U	C5-C4-O4	-5.45	122.63	125.90
3	AD	32	U	OP2-P-O3'	5.45	117.19	105.20
3	AD	70	G	O4'-C1'-N9	5.45	112.56	108.20
3	AD	57	A	C5-C6-N1	-5.42	114.99	117.70
3	AD	76	A	C6-N1-C2	5.42	121.85	118.60
3	AD	48	U	N1-C2-N3	5.41	118.15	114.90
3	AD	41	C	P-O5'-C5'	5.40	129.54	120.90
3	AD	67	C	N3-C4-C5	-5.40	119.74	121.90
3	AD	59	U	OP1-P-OP2	-5.40	111.51	119.60
3	AD	33	U	O4'-C1'-N1	5.39	112.51	108.20
3	AD	26	A	O4'-C1'-N9	5.37	112.49	108.20
3	AD	1	U	C5-C4-O4	-5.36	122.68	125.90
3	AD	64	C	N3-C4-C5	-5.34	119.76	121.90
3	AD	58	A	C6-N1-C2	5.28	121.77	118.60
3	AD	31	A	O4'-C1'-N9	5.26	112.41	108.20
3	AD	69	C	N3-C4-C5	-5.26	119.80	121.90
3	AD	6	G	OP1-P-OP2	-5.21	111.78	119.60
3	AD	7	A	C6-N1-C2	5.21	121.73	118.60
3	AD	72	A	OP2-P-O3'	-5.19	93.78	105.20
3	AD	21	H2U	OP1-P-O3'	-5.18	93.81	105.20
3	AD	74	C	OP1-P-OP2	-5.11	111.94	119.60
3	AD	57	A	C6-N1-C2	5.10	121.66	118.60
3	AD	59	U	N1-C2-N3	5.10	117.96	114.90
3	AD	63	C	O5'-P-OP2	5.09	116.80	110.70
3	AD	52	G	C5-C6-N1	5.08	114.04	111.50
3	AD	42	G	OP2-P-O3'	5.08	116.37	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	60	U	N1-C2-N3	5.08	117.95	114.90
3	AD	70	G	OP1-P-OP2	-5.07	111.99	119.60
2	AC	21	A	C5'-C4'-C3'	5.04	124.06	116.00
2	AB	21	A	C5'-C4'-C3'	5.03	124.05	116.00
3	AD	72	A	OP1-P-OP2	-5.03	112.05	119.60
3	AD	7	A	C5-C6-N1	-5.00	115.20	117.70
3	AD	28	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	18	G	Sidechain
2	AB	19	G	Sidechain
2	AB	62	A	Sidechain
2	AC	18	G	Sidechain
2	AC	19	G	Sidechain
2	AC	62	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	AA	1519	0	0	16	0
2	AB	1652	0	862	56	0
2	AC	1652	0	862	53	0
3	AD	1570	0	801	105	0
4	A1	120	0	61	5	0
5	AE	234	0	0	0	0
6	AF	206	0	0	2	0
7	AG	208	0	0	2	0
8	AH	150	0	0	1	0
9	AI	101	0	0	0	0
10	AJ	155	0	0	4	0
11	AK	138	0	0	0	0
12	AL	127	0	0	3	0
13	AM	98	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AN	119	0	0	0	0
15	AO	124	0	0	1	0
16	AP	125	0	0	2	0
17	AQ	60	0	0	4	0
18	AR	88	0	0	0	0
19	AS	83	0	0	0	0
20	AT	104	0	0	0	0
21	AU	73	0	0	0	0
22	AV	80	0	0	0	0
23	AW	99	0	0	0	0
24	AX	24	0	0	0	0
25	BA	2889	0	0	33	0
26	BB	123	0	0	2	0
27	BC	224	0	0	4	0
28	BD	173	0	0	6	0
29	BE	191	0	0	7	0
30	BF	189	0	0	9	0
31	BG	122	0	0	1	0
32	BH	164	0	0	0	0
33	BI	128	0	0	3	0
33	BJ	128	0	0	0	0
34	BK	148	0	0	1	0
35	BL	133	0	0	0	0
36	BM	117	0	0	1	0
37	BN	122	0	0	0	0
38	BO	84	0	0	2	0
39	BP	138	0	0	2	0
40	BQ	113	0	0	6	0
41	BR	52	0	0	0	0
42	BS	110	0	0	0	0
43	BT	76	0	0	1	0
44	BU	110	0	0	0	0
45	BV	89	0	0	0	0
46	BW	64	0	0	0	0
47	BX	60	0	0	1	0
All	All	14656	0	2586	285	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 17.

All (285) 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)
30:BF:100:LEU:CA	30:BF:101:ASP:CA	1.80	1.54
2:AC:1:G:N2	2:AC:2:C:H41	1.22	1.34
1:AA:430:A:P	7:AG:7:PRO:CA	2.16	1.32
28:BD:196:ASN:CA	28:BD:197:GLY:CA	2.06	1.31
3:AD:75:C:C2'	3:AD:76:A:H5'	1.59	1.30
2:AC:1:G:N2	2:AC:2:C:N4	1.77	1.29
40:BQ:59:ALA:CA	40:BQ:60:SER:CA	2.12	1.27
3:AD:75:C:H2'	3:AD:76:A:C5'	1.62	1.27
1:AA:923:A:P	8:AH:21:ALA:CA	2.26	1.23
25:BA:955:C:P	39:BP:10:ILE:CA	2.26	1.23
3:AD:33:U:O3'	3:AD:34:U:P	1.98	1.21
3:AD:48:U:O3'	3:AD:49:5MC:P	1.99	1.20
25:BA:636:G:P	38:BO:126:SER:CA	2.32	1.18
2:AB:33:U:C2	2:AB:35:A:H5'	1.77	1.17
13:AM:63:PHE:CA	17:AQ:58:LYS:CA	2.24	1.14
2:AB:25:C:C2'	2:AB:26:M2G:H5'	1.72	1.12
2:AC:25:C:O3'	2:AC:26:M2G:P	2.12	1.08
25:BA:2060:A:P	30:BF:66:GLY:CA	2.45	1.05
25:BA:451:C:P	30:BF:48:SER:CA	2.45	1.04
3:AD:73:G:O2'	3:AD:74:C:H5'	1.58	1.04
28:BD:113:MET:CA	28:BD:114:GLU:CA	2.35	1.03
2:AB:25:C:C2'	2:AB:26:M2G:C5'	2.34	1.02
3:AD:8:4SU:C4'	3:AD:49:5MC:H5'	1.91	0.99
2:AB:25:C:H2'	2:AB:26:M2G:C5'	1.91	0.98
2:AB:33:U:O2	2:AB:35:A:H5'	1.64	0.98
13:AM:62:HIS:CA	17:AQ:59:ALA:CA	2.41	0.97
26:BB:51:G:P	40:BQ:72:GLU:CA	2.53	0.96
1:AA:948:C:P	16:AP:109:THR:CA	2.55	0.95
3:AD:8:4SU:C5'	3:AD:49:5MC:H5'	1.98	0.94
25:BA:452:G:P	30:BF:52:ALA:CA	0.84	0.93
29:BE:184:GLY:CA	29:BE:185:GLY:CA	2.46	0.93
25:BA:2093:G:P	34:BK:25:TYR:CA	2.56	0.93
25:BA:380:U:P	25:BA:2233:U:P	2.66	0.93
2:AC:41:U:H5'	2:AC:41:U:H6	1.34	0.93
3:AD:37:A:O3'	3:AD:38:U:P	2.28	0.92
3:AD:33:U:H5'	10:AJ:77:SER:CA	2.00	0.92
25:BA:607:U:P	30:BF:105:LYS:CA	2.58	0.91
3:AD:8:4SU:O2'	3:AD:46:A:H1'	1.71	0.91
2:AB:41:U:H5'	2:AB:41:U:H6	1.35	0.90
2:AC:33:U:C2	2:AC:35:A:H5'	2.06	0.90
2:AB:25:C:H2'	2:AB:26:M2G:O4'	1.71	0.90
2:AC:1:G:H22	2:AC:2:C:N4	1.65	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AD:8:4SU:H5''	3:AD:49:5MC:H5'	1.55	0.88
3:AD:66:U:H2'	3:AD:67:C:C6	2.08	0.88
25:BA:1820:U:P	28:BD:158:GLY:CA	2.61	0.87
25:BA:2785:C:P	29:BE:99:VAL:CA	2.63	0.87
25:BA:1997:G:P	29:BE:221:LYS:CA	2.62	0.86
3:AD:19:G:H4'	3:AD:20:H2U:OP1	1.73	0.86
25:BA:1994:C:P	29:BE:224:GLY:CA	2.63	0.86
25:BA:469:G:P	30:BF:56:THR:CA	2.64	0.86
3:AD:73:G:C2'	3:AD:74:C:H5'	2.05	0.86
2:AC:10:2MG:C5	2:AC:26:M2G:HM12	2.12	0.84
3:AD:14:A:H2'	3:AD:15:G:C8	2.12	0.84
3:AD:69:C:H2'	3:AD:70:G:C8	2.11	0.84
3:AD:1:U:H2'	3:AD:2:C:H6	1.42	0.83
3:AD:8:4SU:H4'	3:AD:49:5MC:H5'	1.60	0.83
2:AB:25:C:H2'	2:AB:26:M2G:C4'	2.09	0.83
2:AC:33:U:O2	2:AC:35:A:H3'	1.80	0.82
3:AD:52:G:H1	3:AD:62:C:H42	1.24	0.82
2:AC:25:C:H2'	2:AC:26:M2G:O4'	1.80	0.81
25:BA:1826:G:P	28:BD:227:VAL:CA	2.70	0.80
25:BA:2123:G:P	27:BC:129:ARG:CA	2.70	0.80
1:AA:521:G:P	15:AO:73:GLU:CA	2.69	0.80
3:AD:69:C:H2'	3:AD:70:G:H8	1.44	0.80
3:AD:3:C:O2'	3:AD:4:G:H5'	1.83	0.79
3:AD:1:U:H2'	3:AD:2:C:C6	2.17	0.78
3:AD:66:U:H2'	3:AD:67:C:H6	1.44	0.78
3:AD:24:G:C6	3:AD:25:U:C4	2.73	0.77
2:AB:33:U:C2	2:AB:35:A:C5'	2.65	0.77
2:AC:1:G:H21	2:AC:2:C:N4	1.80	0.77
3:AD:8:4SU:H5''	3:AD:49:5MC:C5'	2.17	0.74
2:AB:25:C:O2'	2:AB:26:M2G:H5'	1.85	0.74
2:AC:34:OMG:H8	2:AC:34:OMG:OP1	1.71	0.74
2:AB:34:OMG:OP1	2:AB:34:OMG:H8	1.71	0.73
2:AC:10:2MG:C4	2:AC:26:M2G:HM12	2.22	0.73
2:AB:37:YG:C1'	2:AB:37:YG:H31	2.19	0.73
2:AC:10:2MG:C5	2:AC:26:M2G:CM1	2.71	0.73
1:AA:1060:C:P	13:AM:52:GLY:CA	2.77	0.73
3:AD:68:G:O2'	3:AD:69:C:H5'	1.88	0.73
2:AB:37:YG:H31	2:AB:37:YG:C2'	2.20	0.72
2:AC:37:YG:C1'	2:AC:37:YG:H31	2.19	0.72
2:AC:37:YG:H31	2:AC:37:YG:C2'	2.20	0.72
3:AD:67:C:H2'	3:AD:68:G:H8	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BB:49:C:P	40:BQ:110:THR:CA	2.77	0.72
25:BA:558:G:P	36:BM:91:LYS:CA	2.77	0.72
3:AD:22:A:H5'	3:AD:22:A:H8	1.54	0.72
2:AB:44:A:O3'	2:AB:45:G:P	2.49	0.71
25:BA:1995:U:P	29:BE:223:LYS:CA	2.79	0.71
2:AC:37:YG:N20	2:AC:37:YG:H101	2.06	0.70
2:AB:37:YG:N20	2:AB:37:YG:H101	2.06	0.70
3:AD:24:G:C5	3:AD:25:U:C5	2.80	0.70
2:AB:37:YG:H31	2:AB:37:YG:H1'	1.74	0.69
3:AD:25:U:H2'	3:AD:26:A:C8	2.27	0.69
3:AD:37:A:C3'	3:AD:38:U:P	2.81	0.69
2:AC:37:YG:H31	2:AC:37:YG:H1'	1.74	0.68
2:AC:1:G:N2	2:AC:2:C:C4	2.61	0.68
2:AC:34:OMG:HN1	4:A1:3:U:H3	1.40	0.68
3:AD:22:A:H2'	3:AD:23:U:H5'	1.74	0.68
3:AD:37:A:H3'	3:AD:38:U:P	2.35	0.67
25:BA:1084:A:P	33:BI:37:VAL:CA	2.82	0.67
2:AC:1:G:H22	2:AC:2:C:H41	1.25	0.66
2:AC:44:A:C2'	2:AC:45:G:H5'	2.25	0.66
3:AD:54:5MU:C2'	3:AD:55:PSU:H5''	2.26	0.66
40:BQ:53:ASN:CA	40:BQ:54:GLY:CA	2.74	0.66
29:BE:97:THR:CA	29:BE:98:GLU:CA	2.74	0.66
2:AB:26:M2G:HM22	2:AB:44:A:C2	2.32	0.65
40:BQ:60:SER:CA	40:BQ:61:ALA:CA	2.75	0.64
2:AC:26:M2G:HM22	2:AC:44:A:C2	2.32	0.64
3:AD:52:G:H1	3:AD:62:C:N4	1.93	0.64
3:AD:73:G:N2	3:AD:74:C:H1'	2.13	0.64
30:BF:81:PRO:CA	30:BF:89:ALA:CA	2.76	0.63
3:AD:37:A:H61	10:AJ:84:ASN:CA	2.12	0.63
3:AD:67:C:H2'	3:AD:68:G:C8	2.35	0.62
2:AC:37:YG:H101	2:AC:37:YG:C21	2.30	0.62
13:AM:62:HIS:CA	17:AQ:58:LYS:CA	2.78	0.62
3:AD:73:G:H2'	3:AD:74:C:H5'	1.82	0.61
2:AB:40:5MC:H2'	2:AB:41:U:H5'	1.82	0.61
2:AB:37:YG:H101	2:AB:37:YG:C21	2.30	0.61
25:BA:636:G:P	38:BO:128:GLY:CA	2.88	0.61
2:AC:44:A:O2'	2:AC:45:G:H5'	1.99	0.61
2:AB:44:A:H3'	2:AB:45:G:P	2.41	0.61
2:AC:40:5MC:H2'	2:AC:41:U:H5'	1.82	0.61
3:AD:33:U:C5'	10:AJ:77:SER:CA	2.78	0.61
25:BA:2680:C:P	29:BE:205:THR:CA	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:41:U:H5'	2:AB:41:U:C6	2.27	0.60
3:AD:73:G:N2	3:AD:74:C:C1'	2.64	0.60
3:AD:22:A:C2'	3:AD:23:U:H5'	2.31	0.60
3:AD:1:U:O2'	3:AD:2:C:H5'	2.01	0.60
2:AC:41:U:H2'	2:AC:42:G:O4'	2.03	0.59
3:AD:8:4SU:HO2'	3:AD:46:A:H1'	1.65	0.59
3:AD:55:PSU:H2'	3:AD:57:A:OP2	2.02	0.59
25:BA:2125:G:P	27:BC:104:LEU:CA	2.91	0.59
25:BA:270(Y):G:P	25:BA:273:G:P	3.01	0.59
3:AD:73:G:C2'	3:AD:74:C:C5'	2.80	0.58
2:AC:41:U:H6	2:AC:41:U:C5'	2.13	0.58
2:AB:41:U:H2'	2:AB:42:G:O4'	2.03	0.58
3:AD:25:U:O4	3:AD:26:A:N6	2.37	0.57
2:AB:64:A:H2'	2:AB:65:G:O4'	2.04	0.57
25:BA:1084:A:P	33:BI:34:ALA:CA	2.92	0.57
2:AB:41:U:H6	2:AB:41:U:C5'	2.13	0.57
2:AC:64:A:H2'	2:AC:65:G:O4'	2.04	0.57
2:AC:41:U:H5'	2:AC:41:U:C6	2.27	0.57
2:AC:44:A:H2'	2:AC:45:G:O4'	2.04	0.57
3:AD:10:A:C6	3:AD:26:A:C2	2.93	0.57
3:AD:62:C:H2'	3:AD:62:C:O2	2.03	0.57
1:AA:427:U:P	7:AG:40:PRO:CA	2.93	0.56
2:AB:16:H2U:O2'	2:AB:17:H2U:OP2	2.21	0.56
1:AA:1109:C:P	1:AA:1191:A:P	3.03	0.56
3:AD:14:A:N6	3:AD:46:A:C2	2.74	0.56
25:BA:970:C:P	47:BX:15:TYR:CA	2.93	0.56
2:AB:29:A:O2'	2:AB:30:G:H5'	2.06	0.56
2:AB:25:C:C4	2:AB:26:M2G:C8	2.94	0.55
3:AD:70:G:H2'	3:AD:71:G:H8	1.70	0.55
2:AB:44:A:C3'	2:AB:45:G:P	2.95	0.55
3:AD:22:A:H2'	3:AD:23:U:C5'	2.36	0.55
1:AA:1367:C:P	12:AL:114:TYR:CA	2.95	0.55
27:BC:156:ILE:CA	27:BC:157:LYS:CA	2.85	0.55
1:AA:1236:A:P	1:AA:1305:G:P	3.04	0.55
2:AC:29:A:O2'	2:AC:30:G:H5'	2.06	0.55
3:AD:19:G:C4'	3:AD:20:H2U:OP1	2.40	0.55
3:AD:53:G:H2'	3:AD:53:G:N3	2.22	0.55
2:AB:25:C:C5	2:AB:26:M2G:C8	2.95	0.54
3:AD:8:4SU:O2'	3:AD:46:A:C1'	2.49	0.54
2:AB:33:U:O2	2:AB:35:A:H3'	2.07	0.54
3:AD:69:C:C2	3:AD:70:G:N7	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:607:U:P	30:BF:104:ASP:CA	2.95	0.54
2:AB:16:H2U:H1'	2:AB:17:H2U:OP2	2.08	0.54
25:BA:2312:U:P	31:BG:54:ALA:CA	2.96	0.54
3:AD:75:C:C2	3:AD:76:A:H4'	2.42	0.54
3:AD:50:G:O6	3:AD:65:G:C6	2.61	0.54
3:AD:25:U:H2'	3:AD:26:A:H8	1.71	0.54
3:AD:65:G:O2'	3:AD:66:U:H5'	2.08	0.54
2:AC:16:H2U:H1'	2:AC:17:H2U:OP2	2.08	0.53
3:AD:25:U:N3	3:AD:26:A:C5	2.78	0.52
3:AD:75:C:H2'	3:AD:76:A:H5'	0.70	0.52
3:AD:22:A:H5'	3:AD:22:A:C8	2.41	0.52
2:AC:16:H2U:O2'	2:AC:17:H2U:OP2	2.21	0.52
25:BA:1107:G:P	33:BI:27:ASP:CA	2.98	0.52
3:AD:69:C:N3	3:AD:70:G:N7	2.57	0.52
2:AB:40:5MC:H2'	2:AB:41:U:C5'	2.40	0.51
3:AD:25:U:C2	3:AD:26:A:C8	2.98	0.51
2:AB:33:U:O2'	2:AB:35:A:N7	2.36	0.51
2:AC:40:5MC:H2'	2:AC:41:U:C5'	2.40	0.51
3:AD:7:A:C8	3:AD:49:5MC:HM52	2.45	0.51
2:AC:69:U:H2'	2:AC:70:C:C6	2.46	0.51
3:AD:53:G:C2	3:AD:62:C:C2	2.99	0.51
2:AB:16:H2U:H52	2:AC:47:U:O4	2.11	0.50
2:AB:30:G:O2'	2:AB:31:A:H5'	2.12	0.50
2:AB:69:U:H2'	2:AB:70:C:C6	2.46	0.50
1:AA:785:G:P	25:BA:1837:C:P	3.10	0.50
2:AB:25:C:N4	2:AB:26:M2G:C5	2.80	0.50
2:AC:23:A:O2'	2:AC:24:G:H5'	2.12	0.50
2:AB:23:A:O2'	2:AB:24:G:H5'	2.12	0.49
2:AC:30:G:O2'	2:AC:31:A:H5'	2.12	0.49
3:AD:50:G:C6	3:AD:65:G:N1	2.80	0.49
2:AB:25:C:C5	2:AB:26:M2G:N7	2.80	0.49
3:AD:69:C:C2	3:AD:70:G:C8	3.00	0.49
25:BA:1342:A:P	43:BT:54:THR:CA	3.00	0.49
3:AD:73:G:H2'	3:AD:74:C:C5'	2.42	0.49
28:BD:116:MET:CA	28:BD:117:SER:CA	2.90	0.49
2:AB:25:C:H2'	2:AB:26:M2G:H5'	1.58	0.49
13:AM:63:PHE:CA	17:AQ:57:ARG:CA	2.91	0.49
3:AD:59:U:C5	3:AD:60:U:C4	3.01	0.49
3:AD:71:G:H2'	3:AD:72:A:H8	1.78	0.49
3:AD:73:G:H2'	3:AD:73:G:N3	2.28	0.48
3:AD:50:G:C6	3:AD:65:G:C6	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1250:A:P	12:AL:68:GLY:CA	3.02	0.48
28:BD:76:ARG:CA	28:BD:113:MET:CA	2.91	0.47
3:AD:24:G:C6	3:AD:25:U:C5	3.03	0.47
3:AD:73:G:O2'	3:AD:74:C:C5'	2.48	0.47
1:AA:1108:G:P	6:AF:174:PRO:CA	3.03	0.47
1:AA:1229:A:P	16:AP:116:THR:CA	3.02	0.47
2:AB:25:C:C4	2:AB:26:M2G:N7	2.83	0.47
2:AB:33:U:O2'	2:AB:35:A:C8	2.63	0.47
2:AC:37:YG:H31	2:AC:37:YG:O2'	2.15	0.47
3:AD:4:G:C2'	3:AD:5:U:O5'	2.64	0.46
3:AD:12:A:O2'	3:AD:13:A:H5'	2.16	0.46
1:AA:1206:G:P	6:AF:194:GLY:CA	3.04	0.46
3:AD:7:A:N7	3:AD:49:5MC:HM52	2.31	0.46
2:AC:33:U:O2	2:AC:35:A:H5'	2.13	0.45
2:AB:37:YG:H31	2:AB:37:YG:O2'	2.15	0.45
3:AD:1:U:O2'	3:AD:2:C:C5'	2.63	0.45
25:BA:2486:G:P	39:BP:144:THR:CA	3.05	0.45
40:BQ:111:PRO:CA	40:BQ:114:LYS:CA	2.95	0.45
3:AD:70:G:H2'	3:AD:71:G:C8	2.50	0.45
3:AD:22:A:H2'	3:AD:23:U:O4'	2.17	0.45
3:AD:54:5MU:H2'	3:AD:55:PSU:H5''	1.98	0.45
2:AB:43:G:H2'	2:AB:44:A:C8	2.52	0.45
2:AB:50:U:O2'	2:AB:51:G:H5'	2.17	0.45
2:AC:16:H2U:C2'	2:AC:17:H2U:OP2	2.65	0.45
3:AD:43:G:H2'	3:AD:44:C:O4'	2.16	0.45
2:AC:50:U:O2'	2:AC:51:G:H5'	2.17	0.44
3:AD:50:G:C6	3:AD:65:G:C2	3.05	0.44
2:AC:23:A:H2'	2:AC:24:G:C8	2.52	0.44
2:AC:43:G:H2'	2:AC:44:A:C8	2.53	0.44
3:AD:46:A:H2'	3:AD:48:U:C4'	2.47	0.44
4:A1:2:U:H2'	4:A1:3:U:C6	2.52	0.44
2:AB:50:U:C2'	2:AB:51:G:H5'	2.48	0.44
4:A1:1:U:H2'	4:A1:2:U:C6	2.52	0.44
2:AB:23:A:H2'	2:AB:24:G:C8	2.52	0.44
3:AD:24:G:C4	3:AD:25:U:C5	3.06	0.44
1:AA:783:C:P	1:AA:1516:G:P	3.16	0.44
2:AB:16:H2U:C2'	2:AB:17:H2U:OP2	2.65	0.44
2:AC:34:OMG:H3'	2:AC:35:A:H5''	2.00	0.44
4:A1:4:U:H2'	4:A1:5:U:C6	2.52	0.44
4:A1:5:U:H2'	4:A1:6:U:C6	2.52	0.43
2:AB:32:OMC:O5'	2:AB:32:OMC:H6	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AD:73:G:N2	3:AD:74:C:O4'	2.52	0.43
2:AC:44:A:C2'	2:AC:45:G:C5'	2.96	0.43
3:AD:9:A:N6	3:AD:46:A:C2	2.86	0.43
2:AC:50:U:C2'	2:AC:51:G:H5'	2.48	0.43
3:AD:33:U:O2'	10:AJ:84:ASN:CA	2.67	0.43
3:AD:24:G:C4	3:AD:25:U:C6	3.07	0.43
2:AC:32:OMC:H6	2:AC:32:OMC:O5'	2.01	0.43
27:BC:159:GLY:CA	27:BC:160:ARG:CA	2.97	0.43
25:BA:39:C:P	30:BF:94:THR:CA	3.08	0.42
3:AD:65:G:H2'	3:AD:66:U:C6	2.54	0.42
3:AD:66:U:C4	3:AD:67:C:N4	2.88	0.42
3:AD:74:C:H2'	3:AD:75:C:O4'	2.19	0.42
2:AB:37:YG:H32	2:AB:38:A:O4'	2.20	0.42
3:AD:4:G:H2'	3:AD:5:U:O5'	2.21	0.41
3:AD:50:G:C5	3:AD:65:G:C2	3.09	0.41
25:BA:1442:G:P	25:BA:1630:G:P	3.18	0.41
2:AB:25:C:C4	2:AB:26:M2G:C5	3.09	0.41
3:AD:69:C:C4	3:AD:70:G:N7	2.88	0.41
2:AC:37:YG:H32	2:AC:38:A:O4'	2.20	0.41
3:AD:8:4SU:H6	3:AD:8:4SU:O5'	2.19	0.41
2:AC:39:PSU:N1	2:AC:40:5MC:HM52	2.36	0.41
1:AA:1368:G:P	12:AL:113:LYS:CA	3.08	0.41
2:AC:52:U:O2'	2:AC:53:G:H5'	2.20	0.41
3:AD:25:U:C4	3:AD:26:A:C5	3.09	0.41
2:AB:5:A:H2'	2:AB:6:U:O4'	2.21	0.41
2:AC:5:A:H2'	2:AC:6:U:O4'	2.21	0.41
3:AD:25:U:O4	3:AD:26:A:C6	2.74	0.41
3:AD:46:A:H2'	3:AD:48:U:O5'	2.21	0.41
3:AD:57:A:H2'	3:AD:58:A:H5'	2.03	0.41
3:AD:75:C:C2	3:AD:76:A:H5'	2.56	0.41
25:BA:2393:A:P	25:BA:2429:G:P	3.18	0.41
2:AB:39:PSU:N1	2:AB:40:5MC:HM52	2.36	0.40
2:AB:52:U:O2'	2:AB:53:G:H5'	2.20	0.40
2:AB:16:H2U:C1'	2:AB:17:H2U:OP2	2.69	0.40
2:AC:16:H2U:C1'	2:AC:17:H2U:OP2	2.69	0.40
2:AB:34:OMG:OP1	2:AB:34:OMG:C8	2.64	0.40
3:AD:62:C:O2	3:AD:62:C:C2'	2.62	0.40
3:AD:75:C:C2'	3:AD:76:A:C5'	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	0/1522	-	-
2	AB	74/76 (97%)	13 (17%)	3 (4%)
2	AC	75/76 (98%)	13 (17%)	3 (4%)
25	BA	0/2916	-	-
26	BB	0/123	-	-
3	AD	73/74 (98%)	26 (35%)	2 (2%)
4	A1	5/6 (83%)	1 (20%)	0
All	All	227/4793 (4%)	53 (23%)	8 (3%)

All (53) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	AB	2	C
2	AB	3	G
2	AB	17	H2U
2	AB	18	G
2	AB	19	G
2	AB	21	A
2	AB	26	M2G
2	AB	35	A
2	AB	36	A
2	AB	37	YG
2	AB	41	U
2	AB	74	C
2	AB	76	A
2	AC	2	C
2	AC	3	G
2	AC	17	H2U
2	AC	18	G
2	AC	19	G

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Mol	Chain	Res	Type
2	AC	21	A
2	AC	34	OMG
2	AC	35	A
2	AC	36	A
2	AC	37	YG
2	AC	41	U
2	AC	75	C
2	AC	76	A
3	AD	2	C
3	AD	5	U
3	AD	6	G
3	AD	8	4SU
3	AD	9	A
3	AD	18	G
3	AD	20	H2U
3	AD	21	H2U
3	AD	22	A
3	AD	30	G
3	AD	32	U
3	AD	34	U
3	AD	41	C
3	AD	44	C
3	AD	45	U
3	AD	46	A
3	AD	48	U
3	AD	49	5MC
3	AD	50	G
3	AD	55	PSU
3	AD	62	C
3	AD	64	C
3	AD	70	G
3	AD	72	A
3	AD	73	G
3	AD	76	A
4	A1	4	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	H2U
2	AB	18	G
2	AB	35	A

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Mol	Chain	Res	Type
2	AC	16	H2U
2	AC	18	G
2	AC	35	A
3	AD	1	U
3	AD	33	U

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

34 non-standard protein/DNA/RNA residues are 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
2	OMG	AB	34	4,2	18,26,27	1.05	2 (11%)	19,38,41	0.87	1 (5%)
2	2MG	AC	10	2	18,26,27	1.10	1 (5%)	16,38,41	0.75	0
2	1MA	AB	58	2	16,25,26	2.83	4 (25%)	18,37,40	2.21	5 (27%)
2	OMC	AC	32	2	19,22,23	0.47	0	26,31,34	0.57	0
2	YG	AB	37	2	31,42,43	0.93	1 (3%)	33,62,65	2.59	10 (30%)
2	H2U	AB	17	2	18,21,22	0.65	0	21,30,33	0.98	1 (4%)
2	5MU	AC	54	2	19,22,23	0.51	0	28,32,35	0.65	0
3	5MU	AD	54	3	19,22,23	0.75	0	28,32,35	1.29	2 (7%)
2	5MC	AB	40	2	18,22,23	0.45	0	26,32,35	0.70	1 (3%)
2	H2U	AC	17	2	18,21,22	0.68	1 (5%)	21,30,33	0.99	2 (9%)
2	5MC	AB	49	2	18,22,23	0.75	0	26,32,35	0.73	1 (3%)
2	OMC	AB	32	2	19,22,23	0.47	0	26,31,34	0.57	0
3	4SU	AD	8	3	18,21,22	0.36	0	26,30,33	0.33	0
2	5MU	AB	54	2	19,22,23	0.53	0	28,32,35	0.65	0
2	2MG	AB	10	2	18,26,27	1.08	2 (11%)	16,38,41	0.74	0
2	PSU	AC	55	2	18,21,22	0.72	0	22,30,33	0.85	0
2	H2U	AC	16	2	18,21,22	0.74	1 (5%)	21,30,33	1.14	2 (9%)
2	YG	AC	37	2	31,42,43	0.92	1 (3%)	33,62,65	2.60	10 (30%)
3	PSU	AD	55	3	18,21,22	0.62	0	22,30,33	0.83	1 (4%)
2	OMG	AC	34	4,2	18,26,27	1.04	2 (11%)	19,38,41	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	M2G	AC	26	2	20,27,28	1.21	2 (10%)	22,40,43	0.78	0
2	7MG	AC	46	2	22,26,27	1.07	2 (9%)	29,39,42	1.20	3 (10%)
3	5MC	AD	49	3	18,22,23	0.58	0	26,32,35	0.94	2 (7%)
2	PSU	AB	39	2	18,21,22	0.70	0	22,30,33	0.68	0
2	H2U	AB	16	2	18,21,22	0.74	1 (5%)	21,30,33	1.14	2 (9%)
3	H2U	AD	20	3	18,21,22	0.31	0	21,30,33	0.69	0
3	H2U	AD	21	3	18,21,22	0.44	0	21,30,33	0.65	0
2	PSU	AC	39	2	18,21,22	0.70	0	22,30,33	0.68	0
2	5MC	AC	40	2	18,22,23	0.45	0	26,32,35	0.70	1 (3%)
2	M2G	AB	26	2	20,27,28	1.20	2 (10%)	22,40,43	0.78	0
2	1MA	AC	58	2	16,25,26	2.84	4 (25%)	18,37,40	2.21	5 (27%)
2	PSU	AB	55	2	18,21,22	0.73	0	22,30,33	0.85	0
2	7MG	AB	46	2	22,26,27	1.10	2 (9%)	29,39,42	1.21	3 (10%)
2	5MC	AC	49	2	18,22,23	0.75	0	26,32,35	0.72	1 (3%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	AB	34	4,2	-	1/5/27/28	0/3/3/3
2	2MG	AC	10	2	-	0/5/27/28	0/3/3/3
2	1MA	AB	58	2	-	0/3/25/26	0/3/3/3
2	OMC	AC	32	2	-	0/9/27/28	0/2/2/2
2	YG	AB	37	2	-	8/20/42/43	0/3/4/4
2	H2U	AB	17	2	-	1/7/38/39	0/2/2/2
2	5MU	AC	54	2	-	0/7/25/26	0/2/2/2
3	5MU	AD	54	3	-	2/7/25/26	0/2/2/2
2	5MC	AB	40	2	-	1/7/25/26	0/2/2/2
2	H2U	AC	17	2	-	0/7/38/39	0/2/2/2
2	5MC	AB	49	2	-	0/7/25/26	0/2/2/2
2	OMC	AB	32	2	-	0/9/27/28	0/2/2/2
3	4SU	AD	8	3	-	0/7/25/26	0/2/2/2
2	5MU	AB	54	2	-	0/7/25/26	0/2/2/2
2	2MG	AB	10	2	-	0/5/27/28	0/3/3/3
2	PSU	AC	55	2	-	0/7/25/26	0/2/2/2
2	H2U	AC	16	2	-	4/7/38/39	0/2/2/2
2	YG	AC	37	2	-	7/20/42/43	0/3/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	AD	55	3	-	4/7/25/26	0/2/2/2
2	OMG	AC	34	4,2	-	1/5/27/28	0/3/3/3
2	M2G	AC	26	2	-	0/7/29/30	0/3/3/3
2	7MG	AC	46	2	-	2/7/37/38	0/3/3/3
3	5MC	AD	49	3	-	2/7/25/26	0/2/2/2
2	PSU	AB	39	2	-	0/7/25/26	0/2/2/2
2	H2U	AB	16	2	-	4/7/38/39	0/2/2/2
3	H2U	AD	20	3	-	2/7/38/39	0/2/2/2
3	H2U	AD	21	3	-	2/7/38/39	0/2/2/2
2	PSU	AC	39	2	-	0/7/25/26	0/2/2/2
2	5MC	AC	40	2	-	1/7/25/26	0/2/2/2
2	M2G	AB	26	2	-	0/7/29/30	0/3/3/3
2	1MA	AC	58	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	55	2	-	0/7/25/26	0/2/2/2
2	7MG	AB	46	2	-	2/7/37/38	0/3/3/3
2	5MC	AC	49	2	-	0/7/25/26	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AC	58	1MA	C6-N6	8.07	1.48	1.27
2	AB	58	1MA	C6-N6	8.02	1.48	1.27
2	AC	58	1MA	C2-N3	6.91	1.37	1.29
2	AB	58	1MA	C2-N3	6.90	1.37	1.29
2	AC	26	M2G	C5-C6	-3.12	1.41	1.47
2	AC	10	2MG	C5-C6	-3.08	1.41	1.47
2	AB	26	M2G	C5-C6	-3.07	1.41	1.47
2	AB	46	7MG	C4-N9	3.07	1.41	1.37
2	AB	10	2MG	C5-C6	-3.00	1.41	1.47
2	AC	46	7MG	C4-N9	2.95	1.41	1.37
2	AB	46	7MG	C5-N7	2.82	1.38	1.35
2	AC	46	7MG	C5-N7	2.67	1.38	1.35
2	AC	16	H2U	C2-N1	2.59	1.39	1.35
2	AB	26	M2G	C8-N7	-2.59	1.30	1.35
2	AC	26	M2G	C8-N7	-2.59	1.30	1.35
2	AB	16	H2U	C2-N1	2.58	1.39	1.35
2	AB	58	1MA	C8-N7	-2.36	1.31	1.35
2	AC	58	1MA	C8-N7	-2.30	1.31	1.35
2	AC	34	OMG	C8-N7	-2.29	1.31	1.35
2	AB	34	OMG	C8-N7	-2.28	1.31	1.35
2	AB	58	1MA	C5-C4	-2.23	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AC	58	1MA	C5-C4	-2.18	1.37	1.43
2	AC	37	YG	C8-N7	-2.16	1.31	1.35
2	AB	37	YG	C8-N7	-2.15	1.31	1.35
2	AB	10	2MG	C8-N7	-2.06	1.31	1.35
2	AC	17	H2U	C2-N1	2.03	1.38	1.35
2	AB	34	OMG	C5-C6	-2.03	1.43	1.47
2	AC	34	OMG	C5-C6	-2.00	1.43	1.47

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	37	YG	C11-C12-N1	8.57	111.36	106.53
2	AB	37	YG	C11-C12-N1	8.54	111.35	106.53
2	AC	37	YG	C24-O23-C21	6.29	123.08	115.66
2	AB	37	YG	C24-O23-C21	6.26	123.05	115.66
2	AC	58	1MA	CM1-N1-C6	-5.20	112.39	120.27
2	AB	58	1MA	CM1-N1-C6	-5.20	112.40	120.27
2	AC	37	YG	C3-N3-C4	5.00	125.58	116.71
2	AB	37	YG	C3-N3-C4	4.98	125.55	116.71
2	AC	58	1MA	CM1-N1-C2	4.56	130.15	120.55
2	AB	58	1MA	CM1-N1-C2	4.55	130.13	120.55
2	AC	37	YG	O23-C21-N20	4.40	118.53	110.80
2	AB	37	YG	O23-C21-N20	4.39	118.51	110.80
2	AB	58	1MA	N1-C2-N3	4.29	131.03	126.02
2	AC	58	1MA	N1-C2-N3	4.28	131.02	126.02
2	AB	46	7MG	C4-C5-N7	4.02	111.11	105.53
2	AC	46	7MG	C4-C5-N7	4.01	111.10	105.53
3	AD	54	5MU	C5-C4-N3	3.49	118.29	115.31
2	AC	37	YG	C4-N3-C2	-3.40	111.85	122.15
2	AB	37	YG	C4-N3-C2	-3.38	111.89	122.15
2	AC	37	YG	O23-C21-O22	-3.35	119.65	124.58
2	AB	37	YG	O23-C21-O22	-3.33	119.69	124.58
3	AD	54	5MU	C4-N3-C2	-2.97	123.50	127.35
2	AC	37	YG	C19-O18-C16	2.90	122.49	115.94
2	AB	37	YG	C19-O18-C16	2.89	122.47	115.94
2	AB	16	H2U	C4-N3-C2	2.86	128.16	125.79
2	AC	16	H2U	C4-N3-C2	2.84	128.15	125.79
2	AB	46	7MG	N9-C8-N7	2.80	107.38	103.38
2	AC	46	7MG	N9-C8-N7	2.75	107.31	103.38
2	AB	46	7MG	CM7-N7-C5	2.75	133.49	126.40
2	AC	46	7MG	CM7-N7-C5	2.75	133.49	126.40
2	AC	58	1MA	N1-C6-N6	2.67	126.55	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	58	1MA	N1-C6-N6	2.65	126.51	119.77
2	AC	37	YG	C3-N3-C2	2.60	122.57	120.13
2	AB	37	YG	C3-N3-C2	2.60	122.56	120.13
2	AB	49	5MC	C5-C6-N1	-2.57	120.69	123.34
2	AC	49	5MC	C5-C6-N1	-2.57	120.70	123.34
2	AB	40	5MC	C5-C6-N1	-2.55	120.71	123.34
2	AC	40	5MC	C5-C6-N1	-2.52	120.75	123.34
2	AC	37	YG	O6-C6-C5	2.47	128.55	124.17
2	AB	37	YG	O6-C6-C5	2.44	128.50	124.17
2	AC	17	H2U	C4-N3-C2	2.41	127.79	125.79
2	AB	16	H2U	O3'-C3'-C2'	2.39	119.56	111.82
2	AC	16	H2U	O3'-C3'-C2'	2.38	119.51	111.82
2	AC	37	YG	O18-C16-C15	2.37	117.57	111.52
2	AB	37	YG	O18-C16-C15	2.36	117.56	111.52
3	AD	55	PSU	O4'-C1'-C2'	2.32	108.42	105.14
2	AB	17	H2U	C4-N3-C2	2.31	127.71	125.79
2	AB	34	OMG	O6-C6-C5	2.26	128.79	124.37
2	AC	34	OMG	O6-C6-C5	2.23	128.72	124.37
3	AD	49	5MC	C5-C4-N3	-2.21	119.29	121.67
2	AB	58	1MA	O4'-C1'-C2'	-2.20	103.71	106.93
2	AC	58	1MA	O4'-C1'-C2'	-2.18	103.74	106.93
2	AC	17	H2U	C5-C4-N3	-2.03	114.37	116.65
3	AD	49	5MC	C2'-C1'-N1	-2.01	107.52	113.22

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AB	16	H2U	O4'-C1'-N1-C2
2	AB	16	H2U	O4'-C1'-N1-C6
2	AB	16	H2U	C2'-C1'-N1-C6
2	AB	37	YG	C12-C13-C14-C15
2	AB	37	YG	C15-C16-O18-C19
2	AB	46	7MG	C2'-C1'-N9-C8
2	AC	16	H2U	O4'-C1'-N1-C2
2	AC	16	H2U	O4'-C1'-N1-C6
2	AC	16	H2U	C2'-C1'-N1-C6
2	AC	37	YG	C12-C13-C14-C15
2	AC	37	YG	C15-C16-O18-C19
2	AC	46	7MG	C2'-C1'-N9-C8
2	AB	37	YG	O17-C16-O18-C19
2	AC	37	YG	O17-C16-O18-C19

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Mol	Chain	Res	Type	Atoms
3	AD	21	H2U	O4'-C4'-C5'-O5'
3	AD	49	5MC	O4'-C4'-C5'-O5'
3	AD	49	5MC	C3'-C4'-C5'-O5'
3	AD	55	PSU	C3'-C4'-C5'-O5'
3	AD	55	PSU	O4'-C4'-C5'-O5'
2	AB	16	H2U	C2'-C1'-N1-C2
2	AC	16	H2U	C2'-C1'-N1-C2
2	AB	37	YG	C13-C14-C15-C16
2	AC	37	YG	C13-C14-C15-C16
3	AD	21	H2U	C4'-C5'-O5'-P
2	AB	34	OMG	C4'-C5'-O5'-P
2	AC	34	OMG	C4'-C5'-O5'-P
3	AD	55	PSU	O4'-C1'-C5-C4
2	AB	46	7MG	C2'-C1'-N9-C4
2	AC	46	7MG	C2'-C1'-N9-C4
2	AB	37	YG	C3'-C4'-C5'-O5'
2	AB	40	5MC	O4'-C4'-C5'-O5'
2	AC	40	5MC	O4'-C4'-C5'-O5'
3	AD	20	H2U	C2'-C1'-N1-C6
2	AB	37	YG	C14-C15-C16-O18
2	AC	37	YG	C14-C15-C16-O18
2	AB	37	YG	C13-C14-C15-N20
2	AC	37	YG	C13-C14-C15-N20
3	AD	54	5MU	C3'-C4'-C5'-O5'
3	AD	54	5MU	O4'-C4'-C5'-O5'
3	AD	55	PSU	O4'-C1'-C5-C6
3	AD	20	H2U	O4'-C4'-C5'-O5'
2	AB	37	YG	C14-C15-C16-O17
2	AC	37	YG	C14-C15-C16-O17
2	AB	17	H2U	C2'-C1'-N1-C6

There are no ring outliers.

22 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AB	34	OMG	2	0
2	AC	10	2MG	3	0
2	AC	32	OMC	1	0
2	AB	37	YG	7	0
2	AB	17	H2U	4	0
3	AD	54	5MU	2	0
2	AB	40	5MC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AC	17	H2U	4	0
2	AB	32	OMC	1	0
3	AD	8	4SU	9	0
2	AC	16	H2U	4	0
2	AC	37	YG	7	0
3	AD	55	PSU	3	0
2	AC	34	OMG	3	0
2	AC	26	M2G	6	0
3	AD	49	5MC	8	0
2	AB	39	PSU	1	0
2	AB	16	H2U	5	0
3	AD	20	H2U	2	0
2	AC	39	PSU	1	0
2	AC	40	5MC	3	0
2	AB	26	M2G	14	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	AD	10
2	AB	4
2	AC	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AB	44:A	O3'	45:G	P	2.49
1	AD	37:A	O3'	38:U	P	2.28
1	AC	25:C	O3'	26:M2G	P	2.12
1	AD	48:U	O3'	49:5MC	P	1.99
1	AD	33:U	O3'	34:U	P	1.98
1	AD	7:A	O3'	8:4SU	P	1.92
1	AD	15:G	O3'	16:C	P	1.90
1	AB	34:OMG	O3'	35:A	P	1.84
1	AD	24:G	O3'	25:U	P	1.83
1	AD	56:C	O3'	57:A	P	1.82
1	AD	25:U	O3'	26:A	P	1.81
1	AD	46:A	O3'	48:U	P	1.76
1	AD	26:A	O3'	27:C	P	1.33
1	AB	33:U	O3'	34:OMG	P	1.32
1	AC	75:C	O3'	76:A	P	1.30
1	AB	75:C	O3'	76:A	P	1.29
1	AC	74:C	O3'	75:C	P	1.28
1	AC	36:A	O3'	37:YG	P	1.18

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.