wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2022 – 01:33 PM EST

PDB ID	:	1JGP
Title	:	The Path of Messenger RNA Through the Ribosome. THIS FILE, 1JGP, CONTAINS THE 30S RIBOSOME SUBUNIT, THREE TRNA, AND MRNA MOLECULES. 50S RIBOSOME SUBUNIT IS IN THE FILE 1GIY
Authors	:	Yusupova, G.Z.; Yusupov, M.M.; Cate, J.H.D.; Noller, H.F.
Deposited on	:	2001-06-26
Resolution	:	7.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

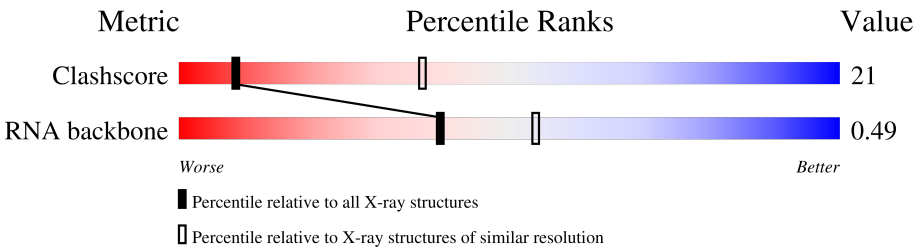
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 7.00 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	1069 (10.00-3.90)
RNA backbone	3102	1078 (10.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1522	99% ·
2	B	76	36% 49% 8% 8%
2	C	76	34% 43% 14% 8%
3	D	74	5% 30% 42% 23%
4	1	36	69% 6% 11% · 11%
5	E	256	91% 9%
6	F	239	85% · 14%
7	G	209	99% ·
8	H	162	92% · 7%

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Mol	Chain	Length	Quality of chain
9	I	101	100%
10	J	156	98%
11	K	138	100%
12	L	128	97%
13	M	105	90% 7%
14	N	129	92% 8%
15	O	135	91% 8%
16	P	126	98%
17	Q	61	93% 5%
18	R	89	99%
19	S	91	91% 9%
20	T	105	99%
21	U	88	83% 17%
22	V	93	86% 14%
23	W	106	93% 7%
24	X	26	92% 8%

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	B	26	-	-	X	-
3	5MC	D	49	-	-	X	-
3	4SU	D	8	-	-	X	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 8935 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
			Total	P			
1	A	1519	1519	1519	0	0	1519

- Molecule 2 is a RNA chain called tRNA(Phe).

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

There are 28 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	32	OMC	C	modified residue	GB 176479
C	34	OMG	G	modified residue	GB 176479
C	37	YG	G	modified residue	GB 176479
C	39	PSU	U	modified residue	GB 176479
C	40	5MC	C	modified residue	GB 176479
C	46	7MG	G	modified residue	GB 176479
C	49	5MC	C	modified residue	GB 176479
C	54	5MU	U	modified residue	GB 176479
C	55	PSU	U	modified residue	GB 176479
C	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	D	74	1570	702	269	524	74	1	0	0	0

- Molecule 4 is a RNA chain called MESSENGER RNA MV36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	1	32	146	54	12	48	32	0	0	26

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
5	E	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	F	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	G	208	208	208	0	0	208

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	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	I	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	J	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	K	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	L	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	M	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	N	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	O	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	P	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	Q	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	R	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	S	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	T	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	U	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	V	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	W	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	X	24	Total C 24 24	0	0	24

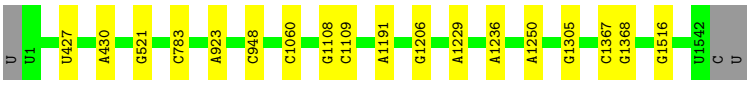
3 Residue-property plots (i)

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. 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.

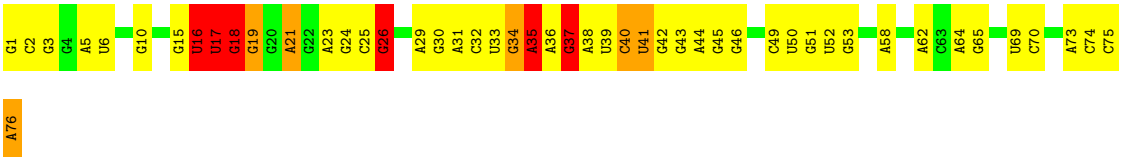
• Molecule 1: 30S 16S ribosomal RNA

Chain A: 99%



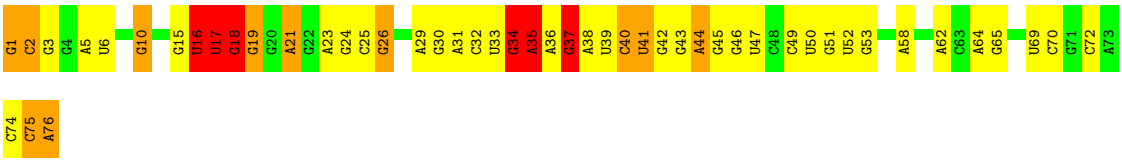
• Molecule 2: tRNA(Phe)

Chain B: 36% 49% 8% 8%



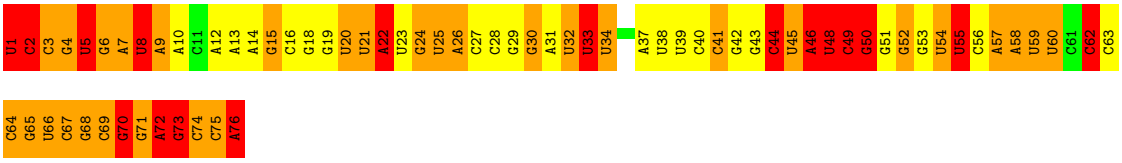
• Molecule 2: tRNA(Phe)

Chain C: 34% 43% 14% 8%



• Molecule 3: tRNA(Phe)

Chain D: 5% 30% 42% 23%



• Molecule 4: MESSENGER RNA MV36

Chain 1: 69% 6% 11% • 11%

G1 U16 U17 U18 U19 U20 U21 A22 C32 A A C U

• Molecule 5: 30S RIBOSOMAL PROTEIN S2

Chain E: 91% 9%

MET PRO VAL GLU ILE THR V7 Q240 GLU ALA GLU ALA THR GLU THR PRO GLU GLY GLU SER GLU VAL GLU ALA

• Molecule 6: 30S RIBOSOMAL PROTEIN S3

Chain F: 85% • 14%

MET G2 P174 G194 V207 ILE GLY GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU PRO LYS ALA GLU GLU ARG PRO ARG ARG ARG ARG PRO ALA VAL ARG VAL LYS LYS GLU GLU

• Molecule 7: 30S RIBOSOMAL PROTEIN S4

Chain G: 99% •

MET G2 P7 P40 R209

• Molecule 8: 30S RIBOSOMAL PROTEIN S5

Chain H: 92% • 7%

MET PRO GLU THR D5 A21 G154 GLU ALA HIS ALA GLN ALA GLN GLY

• Molecule 9: 30S RIBOSOMAL PROTEIN S6

Chain I: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: 30S RIBOSOMAL PROTEIN S7

Chain J: 98% ••

MET A2 S77 N84 W156

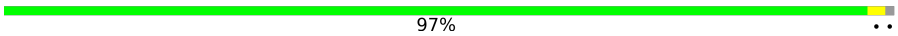
• Molecule 11: 30S RIBOSOMAL PROTEIN S8

Chain K: 100%

There are no outlier residues recorded for this chain.

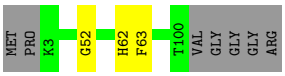
- Molecule 12: 30S RIBOSOMAL PROTEIN S9

Chain L:



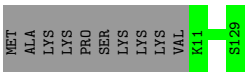
- Molecule 13: 30S RIBOSOMAL PROTEIN S10

Chain M:



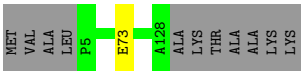
- Molecule 14: 30S RIBOSOMAL PROTEIN S11

Chain N:



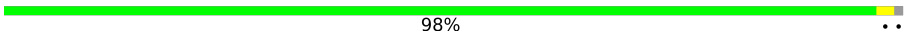
- Molecule 15: 30S RIBOSOMAL PROTEIN S12

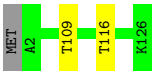
Chain O:



- Molecule 16: 30S RIBOSOMAL PROTEIN S13

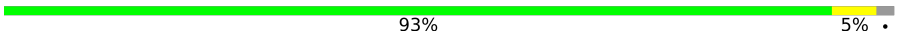
Chain P:

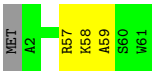




- Molecule 17: 30S RIBOSOMAL PROTEIN S14

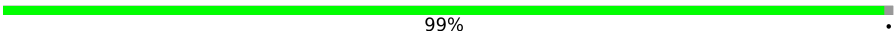
Chain Q:





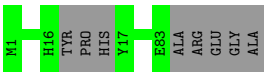
- Molecule 18: 30S RIBOSOMAL PROTEIN S15

Chain R:



- Molecule 19: 30S RIBOSOMAL PROTEIN S16

Chain S: 91% 9%



• Molecule 20: 30S RIBOSOMAL PROTEIN S17

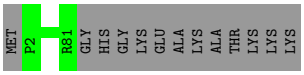
Chain T: 99% •

• Molecule 21: 30S RIBOSOMAL PROTEIN S18

Chain U: 83% 17%

• Molecule 22: 30S RIBOSOMAL PROTEIN S19

Chain V: 86% 14%



• Molecule 23: 30S RIBOSOMAL PROTEIN S20

Chain W: 93% 7%

• Molecule 24: 30S RIBOSOMAL PROTEIN THX

Chain X: 92% 8%

4 Data and refinement statistics (i)

Xtriage (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 – 7.00	Depositor
% Data completeness (in resolution range)	89.5 (250.00-7.00)	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.	Xtriage
Total number of atoms	8935	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: M2G, PSU, 7MG, 1MA, OMC, YG, 4SU, H2U, 5MC, 2MG, OMG, 5MU

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	B	1.21	4/1486 (0.3%)	1.43	13/2311 (0.6%)
2	C	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
3	D	1.95	17/1616 (1.1%)	2.85	154/2512 (6.1%)
4	1	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	B	0	3
2	C	0	3
All	All	0	6

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	33	U	O3'-P	31.20	1.98	1.61
2	C	74	C	O3'-P	-27.00	1.28	1.61
2	B	75	C	O3'-P	-26.77	1.29	1.61
2	C	75	C	O3'-P	-25.61	1.30	1.61
3	D	15	G	O3'-P	24.09	1.90	1.61

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	35	A	P-O3'-C3'	41.11	169.03	119.70
3	D	25	U	P-O3'-C3'	31.41	157.40	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	75	C	P-O3'-C3'	-29.51	84.29	119.70
4	1	18	U	P-O3'-C3'	27.61	152.83	119.70
3	D	8	4SU	O3'-P-O5'	-27.11	52.48	104.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	18	G	Sidechain
2	B	19	G	Sidechain
2	B	62	A	Sidechain
2	C	18	G	Sidechain
2	C	19	G	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	A	1519	0	0	15	0
2	B	1652	0	862	56	0
2	C	1652	0	862	53	0
3	D	1570	0	801	105	0
4	1	146	0	61	6	0
5	E	234	0	0	0	0
6	F	206	0	0	2	0
7	G	208	0	0	2	0
8	H	150	0	0	1	0
9	I	101	0	0	0	0
10	J	155	0	0	4	0
11	K	138	0	0	0	0
12	L	127	0	0	3	0
13	M	98	0	0	5	0
14	N	119	0	0	0	0
15	O	124	0	0	1	0
16	P	125	0	0	2	0
17	Q	60	0	0	4	0
18	R	88	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	83	0	0	0	0
20	T	104	0	0	0	0
21	U	73	0	0	0	0
22	V	80	0	0	0	0
23	W	99	0	0	0	0
24	X	24	0	0	0	0
All	All	8935	0	2586	237	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 21.

The worst 5 of 237 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:C:1:G:N2	2:C:2:C:H41	1.22	1.34
1:A:430:A:P	7:G:7:PRO:CA	2.16	1.32
3:D:75:C:C2'	3:D:76:A:H5'	1.59	1.30
2:C:1:G:N2	2:C:2:C:N4	1.77	1.29
3:D:75:C:H2'	3:D:76:A:C5'	1.62	1.27

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	A	0/1522	-	-
2	B	74/76 (97%)	13 (17%)	3 (4%)
2	C	75/76 (98%)	13 (17%)	3 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	73/74 (98%)	26 (35%)	2 (2%)
4	1	5/36 (13%)	1 (20%)	0
All	All	227/1784 (12%)	53 (23%)	8 (3%)

5 of 53 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	3	G
2	B	17	H2U
2	B	18	G
2	B	19	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	33	U
3	D	1	U
2	C	18	G
2	C	16	H2U
2	C	35	A

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	5MU	B	54	2	19,22,23	0.53	0	28,32,35	0.65	0
2	5MU	C	54	2	19,22,23	0.51	0	28,32,35	0.65	0
2	H2U	B	16	2	18,21,22	0.74	1 (5%)	21,30,33	1.14	2 (9%)
3	PSU	D	55	3	18,21,22	0.62	0	22,30,33	0.83	1 (4%)
2	H2U	C	17	2	18,21,22	0.68	1 (5%)	21,30,33	0.99	2 (9%)
2	OMG	C	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	1MA	C	58	2	16,25,26	2.84	4 (25%)	18,37,40	2.21	5 (27%)
2	YG	C	37	2	31,42,43	0.92	1 (3%)	33,62,65	2.60	10 (30%)
2	1MA	B	58	2	16,25,26	2.83	4 (25%)	18,37,40	2.21	5 (27%)
3	5MU	D	54	3	19,22,23	0.75	0	28,32,35	1.29	2 (7%)
2	PSU	C	55	2	18,21,22	0.72	0	22,30,33	0.85	0
2	5MC	B	40	2	18,22,23	0.45	0	26,32,35	0.70	1 (3%)
2	PSU	C	39	2	18,21,22	0.70	0	22,30,33	0.68	0
2	5MC	C	49	2	18,22,23	0.75	0	26,32,35	0.72	1 (3%)
2	7MG	C	46	2	22,26,27	1.07	2 (9%)	29,39,42	1.20	3 (10%)
2	M2G	B	26	2	20,27,28	1.20	2 (10%)	22,40,43	0.78	0
2	7MG	B	46	2	22,26,27	1.10	2 (9%)	29,39,42	1.21	3 (10%)
2	H2U	C	16	2	18,21,22	0.74	1 (5%)	21,30,33	1.14	2 (9%)
2	OMC	C	32	2	19,22,23	0.47	0	26,31,34	0.57	0
2	5MC	B	49	2	18,22,23	0.75	0	26,32,35	0.73	1 (3%)
3	4SU	D	8	3	18,21,22	0.36	0	26,30,33	0.33	0
2	PSU	B	39	2	18,21,22	0.70	0	22,30,33	0.68	0
3	5MC	D	49	3	18,22,23	0.58	0	26,32,35	0.94	2 (7%)
2	2MG	B	10	2	18,26,27	1.08	2 (11%)	16,38,41	0.74	0
3	H2U	D	20	3	18,21,22	0.31	0	21,30,33	0.69	0
2	OMG	B	34	4,2	18,26,27	1.05	2 (11%)	19,38,41	0.87	1 (5%)
2	5MC	C	40	2	18,22,23	0.45	0	26,32,35	0.70	1 (3%)
3	H2U	D	21	3	18,21,22	0.44	0	21,30,33	0.65	0
2	YG	B	37	2	31,42,43	0.93	1 (3%)	33,62,65	2.59	10 (30%)
2	M2G	C	26	2	20,27,28	1.21	2 (10%)	22,40,43	0.78	0
2	OMC	B	32	2	19,22,23	0.47	0	26,31,34	0.57	0
2	PSU	B	55	2	18,21,22	0.73	0	22,30,33	0.85	0
2	H2U	B	17	2	18,21,22	0.65	0	21,30,33	0.98	1 (4%)
2	2MG	C	10	2	18,26,27	1.10	1 (5%)	16,38,41	0.75	0

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
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	5MU	C	54	2	-	0/7/25/26	0/2/2/2
2	H2U	B	16	2	-	4/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	D	55	3	-	4/7/25/26	0/2/2/2
2	H2U	C	17	2	-	0/7/38/39	0/2/2/2
2	OMG	C	34	4,2	-	1/5/27/28	0/3/3/3
2	1MA	C	58	2	-	0/3/25/26	0/3/3/3
2	YG	C	37	2	-	7/20/42/43	0/3/4/4
2	1MA	B	58	2	-	0/3/25/26	0/3/3/3
3	5MU	D	54	3	-	2/7/25/26	0/2/2/2
2	PSU	C	55	2	-	0/7/25/26	0/2/2/2
2	5MC	B	40	2	-	1/7/25/26	0/2/2/2
2	PSU	C	39	2	-	0/7/25/26	0/2/2/2
2	5MC	C	49	2	-	0/7/25/26	0/2/2/2
2	7MG	C	46	2	-	2/7/37/38	0/3/3/3
2	M2G	B	26	2	-	0/7/29/30	0/3/3/3
2	7MG	B	46	2	-	2/7/37/38	0/3/3/3
2	H2U	C	16	2	-	4/7/38/39	0/2/2/2
2	OMC	C	32	2	-	0/9/27/28	0/2/2/2
2	5MC	B	49	2	-	0/7/25/26	0/2/2/2
3	4SU	D	8	3	-	0/7/25/26	0/2/2/2
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
3	5MC	D	49	3	-	2/7/25/26	0/2/2/2
2	2MG	B	10	2	-	0/5/27/28	0/3/3/3
3	H2U	D	20	3	-	2/7/38/39	0/2/2/2
2	OMG	B	34	4,2	-	1/5/27/28	0/3/3/3
2	5MC	C	40	2	-	1/7/25/26	0/2/2/2
3	H2U	D	21	3	-	2/7/38/39	0/2/2/2
2	YG	B	37	2	-	8/20/42/43	0/3/4/4
2	M2G	C	26	2	-	0/7/29/30	0/3/3/3
2	OMC	B	32	2	-	0/9/27/28	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	H2U	B	17	2	-	1/7/38/39	0/2/2/2
2	2MG	C	10	2	-	0/5/27/28	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	58	1MA	C6-N6	8.07	1.48	1.27
2	B	58	1MA	C6-N6	8.02	1.48	1.27
2	C	58	1MA	C2-N3	6.91	1.37	1.29
2	B	58	1MA	C2-N3	6.90	1.37	1.29
2	C	26	M2G	C5-C6	-3.12	1.41	1.47

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	37	YG	C11-C12-N1	8.57	111.36	106.53
2	B	37	YG	C11-C12-N1	8.54	111.35	106.53
2	C	37	YG	C24-O23-C21	6.29	123.08	115.66
2	B	37	YG	C24-O23-C21	6.26	123.05	115.66
2	C	58	1MA	CM1-N1-C6	-5.20	112.39	120.27

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	16	H2U	O4'-C1'-N1-C2
2	B	16	H2U	O4'-C1'-N1-C6
2	B	16	H2U	C2'-C1'-N1-C6
2	B	37	YG	C12-C13-C14-C15
2	B	37	YG	C15-C16-O18-C19

There are no ring outliers.

22 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	16	H2U	5	0
3	D	55	PSU	3	0
2	C	17	H2U	4	0
2	C	34	OMG	3	0
2	C	37	YG	7	0
3	D	54	5MU	2	0
2	B	40	5MC	3	0
2	C	39	PSU	1	0
2	B	26	M2G	14	0
2	C	16	H2U	4	0
2	C	32	OMC	1	0
3	D	8	4SU	9	0
2	B	39	PSU	1	0
3	D	49	5MC	8	0
3	D	20	H2U	2	0
2	B	34	OMG	2	0
2	C	40	5MC	3	0
2	B	37	YG	7	0
2	C	26	M2G	6	0
2	B	32	OMC	1	0
2	B	17	H2U	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	10	2MG	3	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	D	10
2	B	4
2	C	4
4	1	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	21:U	O3'	22:A	P	4.04
1	B	44:A	O3'	45:G	P	2.49
1	D	37:A	O3'	38:U	P	2.28
1	C	25:C	O3'	26:M2G	P	2.12
1	D	48:U	O3'	49:5MC	P	1.99

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.