wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 08:30 PM EDT

PDB ID	:	486D
Title	:	X-RAY CRYSTAL STRUCTURES OF 70S RIBOSOME FUNCTIONAL COMPLEXES
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Deposited on	:	1999-09-09
Resolution	:	7.50 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:

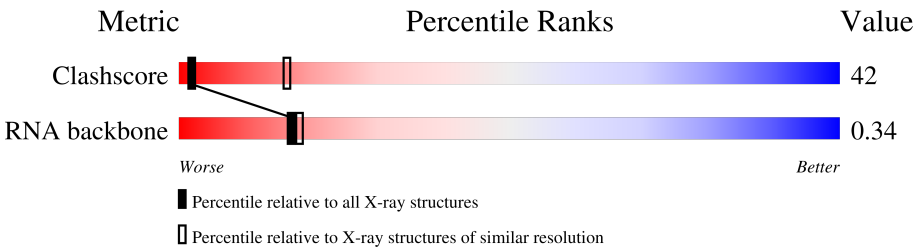
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 7.50 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	1069 (10.00-3.90)
RNA backbone	3102	1079 (11.50-3.00)

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	74	• 14% 45% 41%
2	B	3	33% 67%
3	C	72	22% 57% 21%
4	D	3	67% 33%
5	E	72	• 12% 53% 33%
6	F	85	100%
7	G	33	100%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	M2G	A	26	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4934 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 P-SITE TRNA OF 70S RIBOSOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	74	1603	722	283	524	74	0	0	0

- Molecule 2 is a RNA chain called P-SITE CODON OF 70S RIBOSOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	3	60	27	6	24	3	0	0	0

- Molecule 3 is a RNA chain called A-SITE TRNA OF 70S RIBOSOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	72	1546	692	270	512	72	0	0	0

- Molecule 4 is a RNA chain called A-SITE CODON OF 70S RIBOSOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	3	63	28	10	22	3	0	0	0

- Molecule 5 is a RNA chain called E-SITE TRNA OF 70S RIBOSOME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	E	72	1540	687	269	512	72	0	0	0

- Molecule 6 is a RNA chain called PENULTIMATE STEM OF 16S RRNA IN THE 70S RIBOSOME.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	P			
6	F	85	85	85	0	0	85

- Molecule 7 is a RNA chain called 900 STEM-LOOP OF 16S RRNA IN THE 70S RIBOSOME.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	33	Total P 33 33	0	0	33

- Molecule 8 is IRIDIUM ION (three-letter code: IR) (formula: Ir).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	4	Total Ir 4 4	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. 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: P-SITE TRNA OF 70S RIBOSOME

Chain A: 14% 45% 41%

U1 C2 C3 G4 U5 G6 A7 U8 A9 G10 U11 U12 U13 A14 A15 U16 G17 G18 U19 C20 A21 G22 A23 A24 U25 G26 C27 C28 A29 G30 A31 C32 U33 G34 A35 A36 G37 A38 U39 C40 U41 G42 G43 A44 G45 A46 U48 C49 G50 G51 G52 G53 U54 U55 C56 A57 A58 U59 U60 C61

C62 C63 C64 G65 U66 C67 G68 C69 G70 G71 A72 G73 C74 C75

• Molecule 2: P-SITE CODON OF 70S RIBOSOME

Chain B: 33% 67%

U1 U2 U3

• Molecule 3: A-SITE TRNA OF 70S RIBOSOME

Chain C: 22% 57% 21%

G1 C2 G3 G4 A5 U6 U7 U8 A9 G10 C11 U12 C13 A14 G15 U16 U17 G18 G19 G20 A21 G22 A23 G24 C25 G26 C27 C28 C29 G30 C31 U32 U33 G34 U35 C36 G37 C38 G39 U40 G41 G42 G43 A44 G45 G46 U47 C48 C49 U50 G51 U52 G53 U54 U55 C56 G57 A58 U59 C60

C61 A62 C63 A64 G65 A66 A67 U68 U69 C70 G71 C72

• Molecule 4: A-SITE CODON OF 70S RIBOSOME

Chain D: 67% 33%

G1 U2 C3

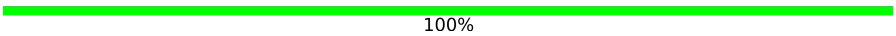
• Molecule 5: E-SITE TRNA OF 70S RIBOSOME

Chain E: 12% 53% 33%

U1 C2 C3 G4 U5 G6 A7 U8 A9 G10 U11 U12 U13 A14 A15 U16 G17 G18 U19 C20 A21 G22 A23 A24 U25 G26 C27 G28 C29 G30 C31 U32 U33 G34 U35 C36 G37 C38 G39 U40 G41 C42 C43 A44 G45 A46 U48 C49 G50 G51 G52 G53 U54 U55 C56 A57 A58 U59 U60 C61

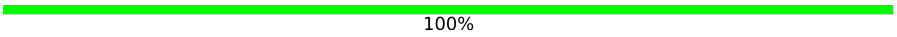
C62 C63 C64 G65 U66 C67 G68 C69 G70 G71 A72 G73

- Molecule 6: PENULTIMATE STEM OF 16S RRNA IN THE 70S RIBOSOME

Chain F: 

There are no outlier residues recorded for this chain.

- Molecule 7: 900 STEM-LOOP OF 16S RRNA IN THE 70S RIBOSOME

Chain G: 

There are no outlier residues recorded for this chain.

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	508.02Å 508.02Å 802.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 7.50	Depositor
% Data completeness (in resolution range)	97.7 ((Not available)-7.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4934	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: OMC, IR, M2G, H2U, 5MU, 1MG, YYG, PSU, 1MA, 5MC, 2MG, 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
1	A	4.10	2/1538 (0.1%)	2.99	185/2393 (7.7%)
2	B	2.23	2/65 (3.1%)	1.08	0/98
3	C	2.94	149/1454 (10.2%)	4.65	377/2259 (16.7%)
4	D	1.19	0/69	2.51	7/105 (6.7%)
5	E	1.30	1/1536 (0.1%)	2.48	161/2393 (6.7%)
All	All	2.98	154/4662 (3.3%)	3.44	730/7248 (10.1%)

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
3	C	0	35

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	U	C1'-N1	151.98	3.76	1.48
3	C	19	G	C6-N1	-17.44	1.27	1.39
3	C	18	G	C8-N7	15.44	1.40	1.30
3	C	42	G	C8-N7	15.08	1.40	1.30
3	C	4	G	C8-N7	13.52	1.39	1.30

The worst 5 of 730 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	U	C6-N1-C1'	-73.97	17.65	121.20
1	A	39	U	O4'-C1'-N1	-20.01	92.19	108.20
3	C	22	G	N3-C4-C5	-19.64	118.78	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	20	G	N3-C4-C5	-19.30	118.95	128.60
3	C	57	G	N3-C4-C5	-19.27	118.97	128.60

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1	G	Sidechain
3	C	2	C	Sidechain
3	C	3	G	Sidechain
3	C	5	A	Sidechain
3	C	6	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	A	1603	0	830	146	0
2	B	60	0	31	4	0
3	C	1546	0	796	61	0
4	D	63	0	33	4	0
5	E	1540	0	784	117	0
6	F	85	0	0	0	0
7	G	33	0	0	0	0
8	F	4	0	0	0	0
All	All	4934	0	2474	309	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 42.

The worst 5 of 309 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:G:H2'	1:A:74:C:C5	1.46	1.48
1:A:67:C:OP1	3:C:4:G:C4'	1.65	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:C:OP1	3:C:4:G:C3'	1.72	1.37
1:A:67:C:OP1	3:C:4:G:C2'	1.73	1.35
1:A:67:C:OP1	3:C:4:G:O2'	1.57	1.20

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	72/74 (97%)	32 (44%)	1 (1%)
2	B	2/3 (66%)	0	0
3	C	69/72 (95%)	15 (21%)	4 (5%)
4	D	2/3 (66%)	1 (50%)	0
5	E	72/72 (100%)	28 (38%)	1 (1%)
6	F	0/85	-	-
7	G	0/33	-	-
All	All	217/342 (63%)	76 (35%)	6 (2%)

5 of 76 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	C
1	A	5	U
1	A	6	G
1	A	9	A
1	A	16	H2U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	46	7MG
3	C	58	1MA
5	E	1	U
3	C	18	G
1	A	1	U

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

29 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	$\#\|Z\| > 2$
3	M2G	C	26	3	20,27,28	1.61	4 (20%)	22,40,43	1.22	3 (13%)
1	H2U	A	19	1	18,21,22	0.78	0	21,30,33	1.11	3 (14%)
1	5MU	A	54	1	19,22,23	0.74	0	28,32,35	1.26	2 (7%)
3	1MA	C	58	3	16,25,26	1.47	4 (25%)	18,37,40	1.73	4 (22%)
5	5MU	E	54	5	19,22,23	0.73	0	28,32,35	1.25	2 (7%)
1	H2U	A	16	1	18,21,22	0.59	0	21,30,33	0.97	2 (9%)
1	M2G	A	26	1	20,27,28	1.17	3 (15%)	22,40,43	1.50	2 (9%)
5	H2U	E	16	5	18,21,22	0.60	0	21,30,33	0.97	2 (9%)
3	H2U	C	17	3	18,21,22	1.21	2 (11%)	21,30,33	1.87	4 (19%)
3	PSU	C	32	3	18,21,22	0.86	1 (5%)	22,30,33	0.98	1 (4%)
3	1MG	C	37	3	18,26,27	1.06	1 (5%)	19,39,42	0.88	1 (5%)
5	1MG	E	37	5	18,26,27	0.98	1 (5%)	19,39,42	0.91	0
1	PSU	A	13	1	18,21,22	0.53	0	22,30,33	0.72	0
5	PSU	E	55	5	18,21,22	0.62	0	22,30,33	0.83	1 (4%)
1	YYG	A	37	1	31,42,43	2.25	7 (22%)	33,62,65	2.42	13 (39%)
5	PSU	E	13	5	18,21,22	0.53	0	22,30,33	0.72	1 (4%)
1	OMC	A	32	1	19,22,23	0.93	1 (5%)	26,31,34	1.98	3 (11%)
3	5MU	C	54	3	19,22,23	1.55	4 (21%)	28,32,35	2.01	7 (25%)
5	H2U	E	19	5	18,21,22	0.78	0	21,30,33	1.11	3 (14%)
3	PSU	C	55	3	18,21,22	1.64	4 (22%)	22,30,33	1.86	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	5MC	C	49	3	18,22,23	1.50	3 (16%)	26,32,35	1.38	4 (15%)
5	PSU	E	32	5	18,21,22	0.54	0	22,30,33	0.78	0
1	5MC	A	40	1	18,22,23	0.54	0	26,32,35	0.83	0
1	5MC	A	49	1	18,22,23	0.57	0	26,32,35	0.95	2 (7%)
1	PSU	A	55	1	18,21,22	0.62	0	22,30,33	0.83	1 (4%)
3	H2U	C	16	3	18,21,22	1.33	3 (16%)	21,30,33	1.78	4 (19%)
3	2MG	C	10	3	18,26,27	1.59	3 (16%)	16,38,41	1.57	3 (18%)
3	7MG	C	46	3	22,26,27	4.07	3 (13%)	29,39,42	2.23	9 (31%)
5	5MC	E	49	5	18,22,23	0.56	0	26,32,35	0.93	2 (7%)

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
3	M2G	C	26	3	-	1/7/29/30	0/3/3/3
1	H2U	A	19	1	-	4/7/38/39	0/2/2/2
1	5MU	A	54	1	-	2/7/25/26	0/2/2/2
3	1MA	C	58	3	-	1/3/25/26	0/3/3/3
5	5MU	E	54	5	-	2/7/25/26	0/2/2/2
1	H2U	A	16	1	-	3/7/38/39	0/2/2/2
1	M2G	A	26	1	-	2/7/29/30	0/3/3/3
5	H2U	E	16	5	-	3/7/38/39	0/2/2/2
3	H2U	C	17	3	-	4/7/38/39	0/2/2/2
3	PSU	C	32	3	-	4/7/25/26	0/2/2/2
3	1MG	C	37	3	-	0/3/25/26	0/3/3/3
5	1MG	E	37	5	-	2/3/25/26	0/3/3/3
1	PSU	A	13	1	-	0/7/25/26	0/2/2/2
5	PSU	E	55	5	-	4/7/25/26	0/2/2/2
1	YYG	A	37	1	-	12/20/42/43	0/3/4/4
5	PSU	E	13	5	-	0/7/25/26	0/2/2/2
1	OMC	A	32	1	-	0/9/27/28	0/2/2/2
3	5MU	C	54	3	-	0/7/25/26	0/2/2/2
5	H2U	E	19	5	-	4/7/38/39	0/2/2/2
3	PSU	C	55	3	-	2/7/25/26	0/2/2/2
3	5MC	C	49	3	-	2/7/25/26	0/2/2/2
5	PSU	E	32	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	40	1	-	0/7/25/26	0/2/2/2
1	5MC	A	49	1	-	2/7/25/26	0/2/2/2
1	PSU	A	55	1	-	4/7/25/26	0/2/2/2
3	H2U	C	16	3	-	4/7/38/39	0/2/2/2
3	2MG	C	10	3	-	0/5/27/28	0/3/3/3
3	7MG	C	46	3	-	2/7/37/38	0/3/3/3
5	5MC	E	49	5	-	2/7/25/26	0/2/2/2

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	46	7MG	C8-N9	-18.11	1.35	1.46
1	A	37	YYG	C2-N2	6.52	1.47	1.35
1	A	37	YYG	O23-C21	5.28	1.43	1.34
1	A	37	YYG	O18-C16	4.58	1.44	1.33
1	A	37	YYG	C3-N3	-4.30	1.37	1.46

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	OMC	CM2-O2'-C2'	8.42	136.62	114.52
1	A	37	YYG	C3-N3-C4	6.42	128.12	116.71
3	C	17	H2U	C4-N3-C2	-5.31	121.39	125.79
1	A	37	YYG	C24-O23-C21	-4.97	109.79	115.66
1	A	37	YYG	O23-C21-N20	4.96	119.50	110.80

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	H2U	O4'-C4'-C5'-O5'
1	A	19	H2U	C3'-C4'-C5'-O5'
1	A	37	YYG	C12-C13-C14-C15
1	A	37	YYG	N20-C21-O23-C24
1	A	37	YYG	O22-C21-O23-C24

There are no ring outliers.

20 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	19	H2U	2	0
1	A	54	5MU	3	0
5	E	54	5MU	3	0
1	A	16	H2U	3	0
1	A	26	M2G	9	0
5	E	16	H2U	3	0
3	C	17	H2U	2	0
3	C	32	PSU	3	0
3	C	37	1MG	8	0
5	E	37	1MG	5	0
1	A	13	PSU	2	0
5	E	55	PSU	4	0
1	A	37	YYG	8	0
5	E	13	PSU	2	0
5	E	19	H2U	2	0
1	A	40	5MC	4	0
1	A	49	5MC	2	0
1	A	55	PSU	4	0
3	C	16	H2U	5	0
5	E	49	5MC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
3	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	44:A	O3'	45:G	P	8.02
1	A	25:U	O3'	26:M2G	P	4.86
1	C	28:C	O3'	29:C	P	4.23
1	C	41:G	O3'	42:G	P	3.71

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.