



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3DEG  
EMDB ID: : EMD-1524  
Title : Complex of elongating Escherichia coli 70S ribosome and EF4(LepA)-GMPPNP  
Authors : Connell, S.R.; Topf, M.; Qin, Y.; Wilson, D.N.; Mielke, T.; Fucini, P.; Nierhaus, K.H.; Spahn, C.M.T.  
Deposited on : 2008-06-10  
Resolution : 10.90 Å(reported)  
Based on PDB ID : 2i2p, 2i2t, 3cb4, 1gix, 2j01

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

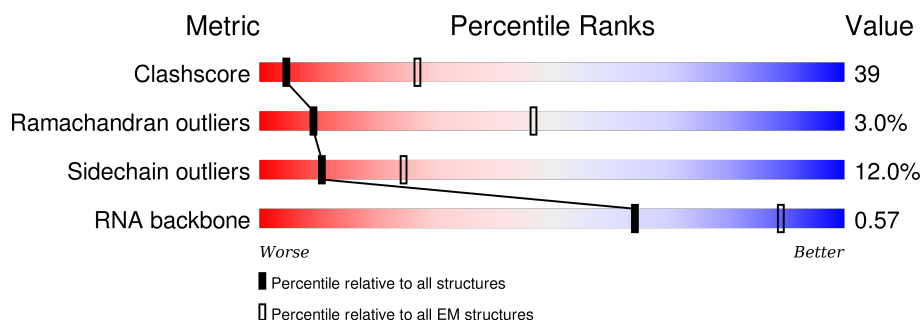
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.90 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.




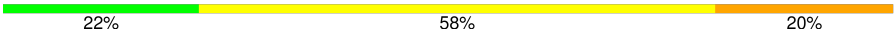

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	76	32% 49% 14% 5%
2	B	77	27% 48% 23% .
3	E	16	38% 56% 6%
4	F	12	75% 25%
5	G	70	30% 56% 10% .
6	I	29	45% 55%
7	J	18	44% 50% 6%
8	K	15	33% 60% 7%

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Mol	Chain	Length	Quality of chain
9	C	545	
10	D	123	
11	H	141	

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

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

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 12950 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 A/L-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

- Molecule 2 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	77	Total	C	N	O	P	0	0
			1645	733	297	538	77		

- Molecule 3 is a RNA chain called 30S RNA helix 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	16	Total	C	N	O	P	0	0
			345	154	65	110	16		

- Molecule 4 is a RNA chain called 30S RNA helix 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	12	Total	C	N	O	P	0	0
			256	114	46	84	12		

- Molecule 5 is a RNA chain called 50S RNA helix 42-44.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	70	Total	C	N	O	P	0	0
			1498	670	276	482	70		

- Molecule 6 is a RNA chain called 50S RNA helix 95.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	29	Total	C	N	O	P	0	0
			625	278	116	202	29		

- Molecule 7 is a RNA chain called 50S RNA helix 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	18	Total	C	N	O	P	0	0
			384	171	67	128	18		

- Molecule 8 is a RNA chain called 50S RNA helix 92.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	15	Total	C	N	O	P	0	0
			316	141	52	108	15		

- Molecule 9 is a protein called GTP-binding protein lepA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	545	Total	C	N	O	S	0	0
			4242	2671	726	824	21		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 11 is a protein called 50S ribosomal protein L11.

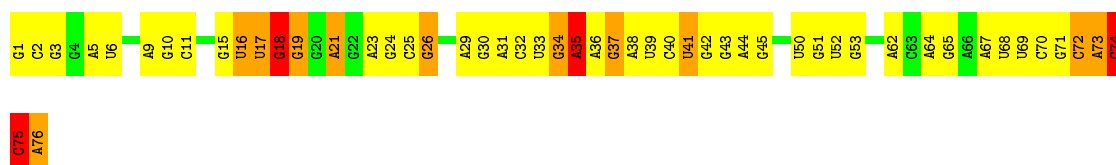
Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

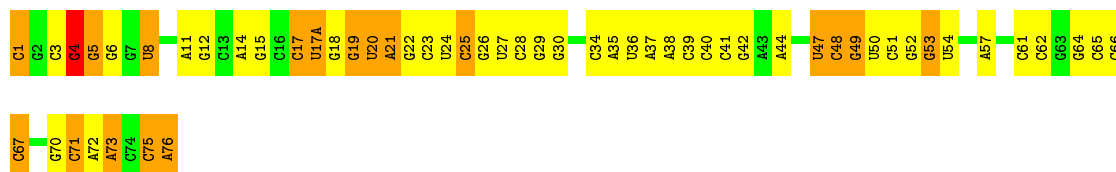
#### • Molecule 1: A/L-tRNA

Chain A:



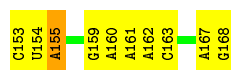
#### • Molecule 2: P-tRNA

Chain B:



#### • Molecule 3: 30S RNA helix 8

Chain E:



#### • Molecule 4: 30S RNA helix 14

Chain F:



#### • Molecule 5: 50S RNA helix 42-44

Chain G:



A1111  
G1112

- Molecule 6: 50S RNA helix 95

Chain I:  45% 55%

C2646 C2649 U2650 C2651 C2655 C2659 A2660 C2661 C2662 C2663 C2664 C2666 C2667 C2668 C2669 A2670 C2671 U2672 C2673 C2674

- Molecule 7: 50S RNA helix 71

Chain J:  44% 50% 6%

U1944 G1945 U1946 C1947 G1948 G1949 U1955 U1956 C1957 C1958 C1959 A1960 C1961

- Molecule 8: 50S RNA helix 92

Chain K:  33% 60% 7%

A2547 U2548 U2552 C2553 U2554 U2555 C2556 C2557 C2558 C2559 A2560 U2561

- Molecule 9: GTP-binding protein lepA

Chain C:  57% 34% 7%

M1 K2 M3 I4 R5 N6 S8 I9 I10 A11 H12 I13 D14 H15 G16 K17 S18 T19 L20 S21 D22 R23 I24 I25 Q26 L27 C28 G29 G30 L31 S32 D33 R34 E35 M36 Q38 V40 L41 D42 S43 M44 D45 L46 E47 R48 E49 R50 G51 I52 T53 I54 K55 A56 Q57 S58 E59

Q72 L73 M74 F75 P79 G80 H81 V82 D83 F84 S85 S86 Y101 V102 D103 Q106 E109 A110 Q111 T112 L113 C116 Y117 M120 D123 N131 K132 Y153 I160 L173 L176 P181 P182 P183 E188 L191 Q192 A193 L194 I195 I196 Y203 L204


L210 R211 N214 K219 G220 D221 V225 M226 S227 T228 G229 Q230 A234 T241 P242 D246 R247 T248 C252 G253 E254 V255 L262 I265 H266 G267 A268 T273 L274 L276 L285 K289 K290 P291 K292 P293 Q294 V295 Y296 A297 L298 L299 L317 S318 L319

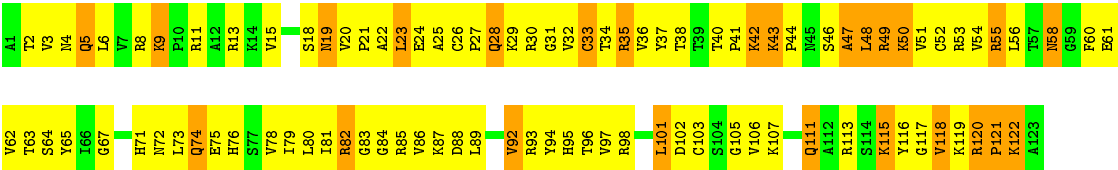
R320 S323 E327 P328 E329 S330 S331 S332 S333 A333 L334 C340 L343 G344 L345 L346 H347 P348 E349 I350 R354 L355 E358 T365 A367 P368 T369 V370 V371 V372 E373 V374 V384 L390 N394 L399 R400 B401 P402 L409 L410 P411 A412 Q412 L413 Y414 L415 G416 N417

V418 I419 T420 L421 K425 R426 M431 M432 M433 Y434 M437 Q438 V439 A440 L441 T442 M447 A448 E449 V450 L451 L452 D453 F454 F455 D456 R457 L458 A459 S460 T461 S462 G463 G464 Y465 A466 L468 D469 Y470 F475 Q476 A477 S478 D479 M480 V481 R482 V483 D484 W485 L486 L487 N488

R491 A494 L495 T499 H500 R501 D502 M503 S504 Q505 N506 R507 L511 K516 I519 P520 R521 Q522 Q523 T526 Q529 T534 H535 A538 R539 S540 T541 V542 K543 Q544 L545

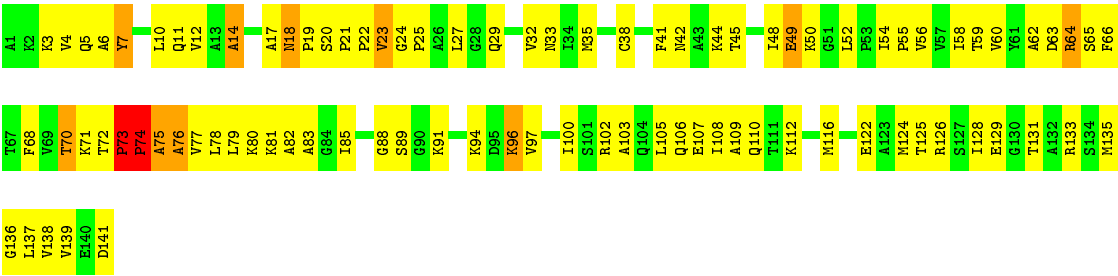
- Molecule 10: 30S ribosomal protein S12

Chain D:  22% 58% 20%



- Molecule 11: 50S ribosomal protein L11

Chain H: 36% 55% 7%





## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.97	2/1486 (0.1%)	1.34	8/2311 (0.3%)
10	D	0.22	0/969	0.46	0/1300
11	H	0.63	5/1046 (0.5%)	0.74	5/1410 (0.4%)
2	B	0.52	1/1814 (0.1%)	0.72	0/2825
3	E	0.21	0/386	0.71	0/600
4	F	0.27	0/285	0.76	0/442
5	G	0.67	5/1677 (0.3%)	0.82	8/2612 (0.3%)
6	I	0.27	0/699	0.74	0/1089
7	J	0.24	0/428	0.72	0/665
8	K	0.23	0/351	0.75	0/544
9	C	0.60	4/4312 (0.1%)	1.04	45/5844 (0.8%)
All	All	0.59	17/13453 (0.1%)	0.92	66/19642 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	7	3
11	H	0	1
2	B	0	2
5	G	0	4
9	C	1	11
All	All	8	21

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	OMG	O3'-P	19.74	1.84	1.61
5	G	1086	A	C5-C6	-16.32	1.26	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1088	A	C6-N1	-10.50	1.28	1.35
9	C	480	MET	C-N	8.63	1.53	1.34
5	G	1060	U	C2-N3	7.75	1.43	1.37

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	A	P-O3'-C3'	41.08	168.99	119.70
1	A	34	OMG	O3'-P-O5'	19.74	141.51	104.00
9	C	14	ASP	CB-CA-C	17.60	145.59	110.40
9	C	13	ILE	C-N-CA	-17.05	79.07	121.70
9	C	13	ILE	N-CA-C	12.32	144.26	111.00

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	73	A	C2'
1	A	74	C	C4',C1'
1	A	75	C	C4',C2',C3'
1	A	76	A	C4'
9	C	13	ILE	CA

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	G	Sidechain
1	A	19	G	Sidechain
1	A	62	A	Sidechain
2	B	25	C	Sidechain
2	B	4	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	1652	0	857	153	0
2	B	1645	0	838	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	345	0	174	12	0
4	F	256	0	131	1	0
5	G	1498	0	757	64	0
6	I	625	0	314	23	0
7	J	384	0	193	27	0
8	K	316	0	161	9	0
9	C	4242	0	4236	417	0
10	D	955	0	1019	126	0
11	H	1032	0	1088	122	0
All	All	12950	0	9768	893	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 39.

The worst 5 of 893 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:71:G:P	9:C:543:LYS:HE3	1.19	1.65
9:C:110:ALA:HB2	9:C:465:TYR:CD2	1.11	1.63
1:A:69:U:C5'	9:C:539:ARG:HD2	1.22	1.56
9:C:26:GLN:CG	9:C:34:ARG:HB3	1.40	1.47
9:C:26:GLN:CD	9:C:34:ARG:HG2	1.31	1.45

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	C	543/545 (100%)	507 (93%)	31 (6%)	5 (1%)	21 67
10	D	121/123 (98%)	80 (66%)	30 (25%)	11 (9%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	H	139/141 (99%)	115 (83%)	16 (12%)	8 (6%)	2	27
All	All	803/809 (99%)	702 (87%)	77 (10%)	24 (3%)	9	42

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	488	ASN
10	D	42	LYS
11	H	18	ASN
9	C	291	VAL
9	C	293	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	C	465/465 (100%)	407 (88%)	58 (12%)	6	30
10	D	103/103 (100%)	83 (81%)	20 (19%)	2	12
11	H	109/109 (100%)	106 (97%)	3 (3%)	51	78
All	All	677/677 (100%)	596 (88%)	81 (12%)	11	31

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	C	415	LEU
9	C	468	LEU
10	D	111	GLN
9	C	419	ILE
9	C	449	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
9	C	505	GLN
9	C	523	GLN
10	D	111	GLN
9	C	395	ASN
11	H	29	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	74/76 (97%)	16 (21%)	6 (8%)
2	B	76/77 (98%)	18 (23%)	0
3	E	15/16 (93%)	1 (6%)	0
4	F	11/12 (91%)	1 (9%)	0
5	G	69/70 (98%)	9 (13%)	0
6	I	28/29 (96%)	0	0
7	J	17/18 (94%)	1 (5%)	0
8	K	14/15 (93%)	1 (7%)	0
All	All	304/313 (97%)	47 (15%)	6 (1%)

5 of 47 RNA backbone outliers are listed below:

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

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	35	A
1	A	75	C
1	A	73	A
1	A	18	G
1	A	74	C

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

15 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
1	2MG	A	10	1	18,26,27	1.06	1 (5%)	21,38,41	2.70	4 (19%)
1	H2U	A	16	1	17,21,22	0.80	1 (5%)	23,30,33	1.08	2 (8%)
1	H2U	A	17	1	17,21,22	0.74	0	23,30,33	1.01	2 (8%)
1	M2G	A	26	1	18,27,28	1.22	3 (16%)	22,40,43	2.21	2 (9%)
1	OMC	A	32	1	15,22,23	0.75	0	20,31,34	0.63	0
1	OMG	A	34	1	18,26,27	1.26	1 (5%)	21,38,41	2.87	3 (14%)
1	YG	A	37	1	28,42,43	1.02	1 (3%)	28,62,65	2.27	8 (28%)
1	PSU	A	39	1	15,21,22	1.24	2 (13%)	16,30,33	3.38	2 (12%)
1	5MC	A	40	1	14,22,23	0.90	1 (7%)	17,32,35	0.98	2 (11%)
1	7MG	A	46	1	20,26,27	1.12	2 (10%)	23,39,42	2.37	2 (8%)
1	5MC	A	49	1	14,22,23	0.80	0	17,32,35	1.04	2 (11%)
1	5MU	A	54	1	13,22,23	1.10	1 (7%)	16,32,35	5.04	2 (12%)
1	PSU	A	55	1	15,21,22	1.47	3 (20%)	16,30,33	3.20	4 (25%)
1	1MA	A	58	1	15,25,26	3.12	3 (20%)	15,37,40	2.35	2 (13%)
2	5MU	B	54	2	13,22,23	1.10	2 (15%)	16,32,35	4.75	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	10	1	-	0/5/27/28	0/3/3/3
1	H2U	A	16	1	-	0/7/38/39	0/2/2/2
1	H2U	A	17	1	-	0/7/38/39	0/2/2/2
1	M2G	A	26	1	-	0/7/29/30	0/3/3/3
1	OMC	A	32	1	-	0/5/27/28	0/2/2/2
1	OMG	A	34	1	-	0/5/27/28	0/3/3/3
1	YG	A	37	1	-	0/20/42/43	0/4/4/4
1	PSU	A	39	1	-	0/7/25/26	0/2/2/2
1	5MC	A	40	1	-	0/3/25/26	0/2/2/2
1	7MG	A	46	1	-	0/7/37/38	0/3/3/3
1	5MC	A	49	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	A	54	1	-	0/3/25/26	0/2/2/2
1	PSU	A	55	1	-	0/7/25/26	0/2/2/2
1	1MA	A	58	1	-	0/3/25/26	0/3/3/3
2	5MU	B	54	2	-	0/3/25/26	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	PSU	C6-C5	-3.29	1.33	1.38
1	A	55	PSU	C6-C5	-2.96	1.34	1.38
1	A	40	5MC	C6-C5	-2.17	1.34	1.40
1	A	26	M2G	C8-N7	-2.12	1.30	1.34
2	B	54	5MU	C6-C5	-2.12	1.34	1.40

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	5MU	C5-C4-N3	-13.51	114.01	125.35
2	B	54	5MU	C5-C4-N3	-11.85	115.40	125.35
1	A	34	OMG	C5-C6-N1	-9.39	111.25	123.52
1	A	26	M2G	C5-C6-N1	-8.99	111.78	123.52
1	A	10	2MG	C5-C6-N1	-8.93	111.85	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	2MG	1	0
1	A	16	H2U	3	0
1	A	17	H2U	3	0
1	A	26	M2G	13	0
1	A	32	OMC	1	0
1	A	34	OMG	1	0
1	A	37	YG	7	0
1	A	39	PSU	1	0
1	A	40	5MC	3	0
2	B	54	5MU	2	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.