wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:59 PM BST

PDB ID	:	1FCW
Title	:	TRNA POSITIONS DURING THE ELONGATION CYCLE
Authors	:	Agrawal, R.K.; Spahn, C.M.T.; Penczek, P.; Grassucci, R.A.; Nierhaus, K.H.; Frank, J.
Deposited on	:	2000-07-19
Resolution	:	17.00 Å(reported)

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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

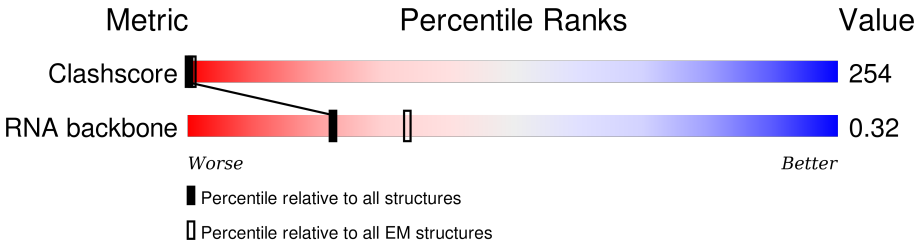
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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)	EM structures (#Entries)
Clashscore	114402	924
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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	76	12% 59% 29%
1	B	76	• 9% 59% 30%
1	C	76	• 32% 37% 28%
1	D	76	• 16% 54% 28%
1	E	76	• 14% 57% 26%

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	H2U	A	16	-	-	X	-
1	H2U	A	17	-	-	X	-
1	M2G	A	26	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	OMC	A	32	-	-	X	-
1	OMG	A	34	-	-	X	-
1	YG	A	37	X	-	X	-
1	PSU	A	39	-	-	X	-
1	5MC	A	40	-	-	X	-
1	7MG	A	46	-	-	X	-
1	5MC	A	49	-	-	X	-
1	5MU	A	54	-	-	X	-
1	PSU	A	55	-	-	X	-
1	1MA	A	58	-	-	X	-
1	2MG	B	10	-	-	X	-
1	H2U	B	16	-	-	X	-
1	H2U	B	17	-	-	X	-
1	M2G	B	26	-	-	X	-
1	OMC	B	32	-	-	X	-
1	OMG	B	34	-	-	X	-
1	YG	B	37	X	-	X	-
1	PSU	B	39	-	-	X	-
1	5MC	B	40	-	-	X	-
1	7MG	B	46	-	-	X	-
1	5MC	B	49	-	-	X	-
1	5MU	B	54	-	-	X	-
1	PSU	B	55	-	-	X	-
1	1MA	B	58	-	-	X	-
1	YG	C	37	X	-	-	-
1	2MG	D	10	-	-	X	-
1	H2U	D	17	-	-	X	-
1	M2G	D	26	-	-	X	-
1	YG	D	37	X	-	-	-
1	7MG	D	46	-	-	X	-
1	5MC	D	49	-	-	X	-
1	5MU	D	54	-	-	X	-
1	PSU	D	55	-	-	X	-
1	1MA	D	58	-	-	X	-
1	H2U	E	17	-	-	X	-
1	YG	E	37	X	-	-	-
1	5MC	E	49	-	-	X	-
1	5MU	E	54	-	-	X	-
1	1MA	E	58	-	-	X	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8260 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 TRNAPHE.

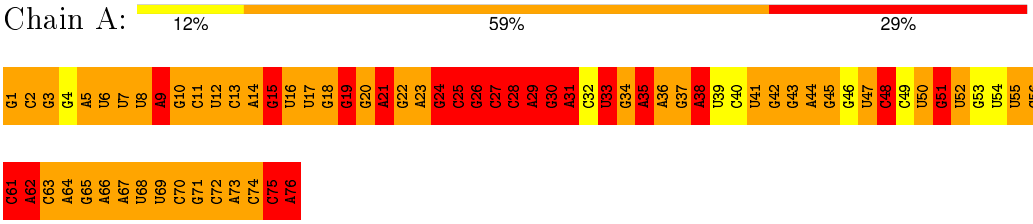
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	B	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	C	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	D	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		
1	E	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

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.

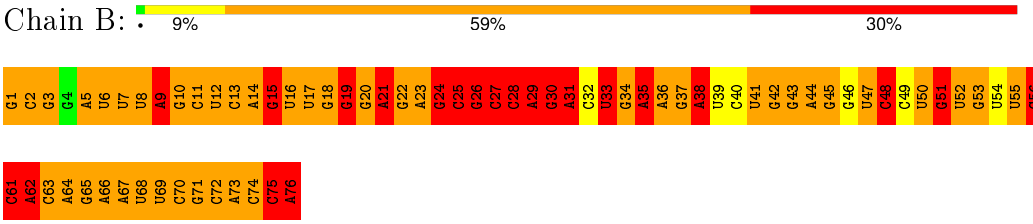
- Molecule 1: TRNAPHE

Chain A:



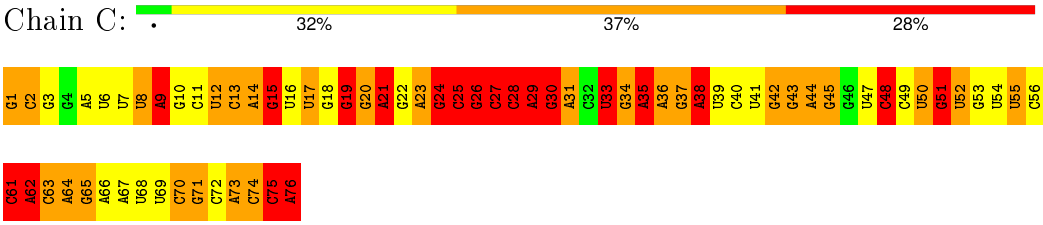
- Molecule 1: TRNAPHE

Chain B:



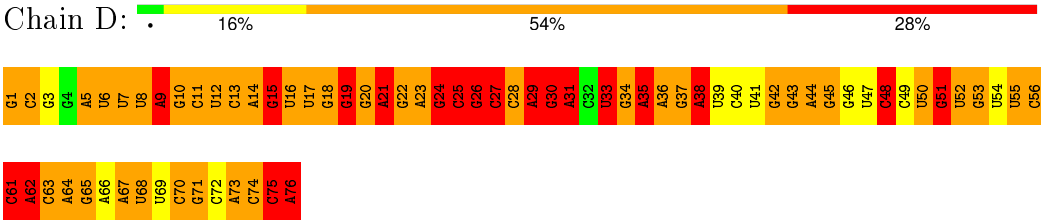
- Molecule 1: TRNAPHE

Chain C:



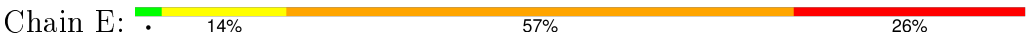
- Molecule 1: TRNAPHE

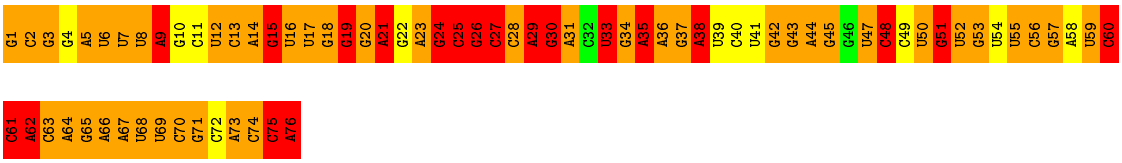
Chain D:



- Molecule 1: TRNAPHE

Chain E:




G1
C2
G3
G4
A5
U6
U7
U8
A9
G10
C11
U12
C13
A14
G15
U16
U17
C18
G19
G20
A21
G22
A23
G24
C25
G26
C27
C28
A29
G30
A31
C32
U33
G34
A35
A36
G37
A38
U39
C40
U41
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
A73
C74
C75
A76

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	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 ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1200.	Depositor
Maximum defocus (nm)	2200.	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	1.34	2/1487 (0.1%)	2.55	176/2315 (7.6%)
1	B	1.33	2/1487 (0.1%)	2.55	176/2315 (7.6%)
1	C	1.33	3/1487 (0.2%)	2.55	175/2315 (7.6%)
1	D	1.33	2/1487 (0.1%)	2.55	178/2315 (7.7%)
1	E	1.32	3/1487 (0.2%)	2.55	175/2315 (7.6%)
All	All	1.33	12/7435 (0.2%)	2.55	880/11575 (7.6%)

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
1	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
1	E	1	0
All	All	5	0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	U	C4-O4	5.57	1.28	1.23
1	B	59	U	C4-O4	5.56	1.28	1.23
1	D	59	U	C4-O4	5.54	1.28	1.23
1	E	19	G	C2'-C1'	-5.53	1.47	1.53
1	E	59	U	C4-O4	5.37	1.27	1.23

The worst 5 of 880 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	18	G	P-O3'-C3'	13.16	135.49	119.70
1	B	18	G	P-O3'-C3'	13.13	135.45	119.70
1	D	18	G	P-O3'-C3'	13.03	135.33	119.70
1	E	18	G	P-O3'-C3'	13.02	135.32	119.70
1	C	18	G	P-O3'-C3'	12.99	135.29	119.70

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	37	YG	C15
1	B	37	YG	C15
1	C	37	YG	C15
1	D	37	YG	C15
1	E	37	YG	C15

There are no planarity outliers.

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	737	2017	0
1	B	1652	0	728	2071	0
1	C	1652	0	860	140	0
1	D	1652	0	814	809	0
1	E	1652	0	810	805	0
All	All	8260	0	3949	3083	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 254.

The worst 5 of 3083 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:B:73:A:P	1:C:75:C:H3'	1.34	1.68
1:A:70:C:C4'	1:B:69:U:H3'	1.23	1.63
1:A:37:YG:C8	1:B:36:A:H2'	1.20	1.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:C:H2'	1:B:29:A:C5'	1.28	1.60
1:A:37:YG:C13	1:B:37:YG:H142	1.19	1.60

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	75/76 (98%)	28 (37%)	1 (1%)
1	B	75/76 (98%)	29 (38%)	1 (1%)
1	C	75/76 (98%)	28 (37%)	1 (1%)
1	D	75/76 (98%)	28 (37%)	1 (1%)
1	E	75/76 (98%)	28 (37%)	1 (1%)
All	All	375/380 (98%)	141 (37%)	5 (1%)

5 of 141 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	15	G
1	A	16	H2U
1	A	17	H2U
1	A	19	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	75	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	75	C
1	C	75	C
1	D	75	C
1	E	75	C

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

70 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	1.19	2 (11%)	21,38,41	3.48	5 (23%)
1	H2U	A	16	1	17,21,22	0.74	0	23,30,33	1.13	2 (8%)
1	H2U	A	17	1	17,21,22	0.67	0	23,30,33	0.82	0
1	M2G	A	26	1	18,27,28	1.09	2 (11%)	22,40,43	2.92	8 (36%)
1	OMC	A	32	1	15,22,23	1.13	1 (6%)	20,31,34	2.07	3 (15%)
1	OMG	A	34	1	18,26,27	1.33	4 (22%)	21,38,41	2.81	4 (19%)
1	YG	A	37	1	28,42,43	2.94	5 (17%)	28,62,65	2.54	10 (35%)
1	PSU	A	39	1	15,21,22	1.46	3 (20%)	16,30,33	3.58	1 (6%)
1	5MC	A	40	1	14,22,23	0.85	1 (7%)	17,32,35	1.11	1 (5%)
1	7MG	A	46	1	20,26,27	1.77	3 (15%)	23,39,42	1.94	2 (8%)
1	5MC	A	49	1	14,22,23	0.93	1 (7%)	17,32,35	1.19	1 (5%)
1	5MU	A	54	1	13,22,23	1.13	2 (15%)	16,32,35	3.07	2 (12%)
1	PSU	A	55	1	15,21,22	1.52	3 (20%)	16,30,33	3.81	3 (18%)
1	1MA	A	58	1	15,25,26	1.23	1 (6%)	15,37,40	1.53	3 (20%)
1	2MG	B	10	1	18,26,27	1.20	2 (11%)	21,38,41	3.48	5 (23%)
1	H2U	B	16	1	17,21,22	0.72	0	23,30,33	1.13	2 (8%)
1	H2U	B	17	1	17,21,22	0.67	0	23,30,33	0.82	0
1	M2G	B	26	1	18,27,28	1.10	2 (11%)	22,40,43	2.92	8 (36%)
1	OMC	B	32	1	15,22,23	1.13	1 (6%)	20,31,34	2.07	3 (15%)
1	OMG	B	34	1	18,26,27	1.32	4 (22%)	21,38,41	2.81	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	YG	B	37	1	28,42,43	2.93	5 (17%)	28,62,65	2.54	10 (35%)
1	PSU	B	39	1	15,21,22	1.45	3 (20%)	16,30,33	3.57	1 (6%)
1	5MC	B	40	1	14,22,23	0.86	1 (7%)	17,32,35	1.11	1 (5%)
1	7MG	B	46	1	20,26,27	1.77	3 (15%)	23,39,42	1.95	2 (8%)
1	5MC	B	49	1	14,22,23	0.93	1 (7%)	17,32,35	1.19	1 (5%)
1	5MU	B	54	1	13,22,23	1.13	2 (15%)	16,32,35	3.08	2 (12%)
1	PSU	B	55	1	15,21,22	1.53	3 (20%)	16,30,33	3.80	3 (18%)
1	1MA	B	58	1	15,25,26	1.23	1 (6%)	15,37,40	1.53	3 (20%)
1	2MG	C	10	1	18,26,27	1.19	3 (16%)	21,38,41	3.45	5 (23%)
1	H2U	C	16	1	17,21,22	0.72	0	23,30,33	1.15	2 (8%)
1	H2U	C	17	1	17,21,22	0.67	0	23,30,33	0.84	0
1	M2G	C	26	1	18,27,28	1.08	2 (11%)	22,40,43	2.93	8 (36%)
1	OMC	C	32	1	15,22,23	1.13	1 (6%)	20,31,34	2.07	3 (15%)
1	OMG	C	34	1	18,26,27	1.32	3 (16%)	21,38,41	2.85	4 (19%)
1	YG	C	37	1	28,42,43	2.91	5 (17%)	28,62,65	2.53	10 (35%)
1	PSU	C	39	1	15,21,22	1.47	3 (20%)	16,30,33	3.54	1 (6%)
1	5MC	C	40	1	14,22,23	0.90	1 (7%)	17,32,35	1.11	1 (5%)
1	7MG	C	46	1	20,26,27	1.77	3 (15%)	23,39,42	1.93	2 (8%)
1	5MC	C	49	1	14,22,23	0.93	1 (7%)	17,32,35	1.21	1 (5%)
1	5MU	C	54	1	13,22,23	1.09	1 (7%)	16,32,35	3.07	2 (12%)
1	PSU	C	55	1	15,21,22	1.53	3 (20%)	16,30,33	3.81	3 (18%)
1	1MA	C	58	1	15,25,26	1.25	2 (13%)	15,37,40	1.51	3 (20%)
1	2MG	D	10	1	18,26,27	1.19	2 (11%)	21,38,41	3.47	5 (23%)
1	H2U	D	16	1	17,21,22	0.74	0	23,30,33	1.14	2 (8%)
1	H2U	D	17	1	17,21,22	0.67	0	23,30,33	0.81	0
1	M2G	D	26	1	18,27,28	1.10	2 (11%)	22,40,43	2.93	8 (36%)
1	OMC	D	32	1	15,22,23	1.14	1 (6%)	20,31,34	2.07	3 (15%)
1	OMG	D	34	1	18,26,27	1.33	3 (16%)	21,38,41	2.83	4 (19%)
1	YG	D	37	1	28,42,43	2.92	5 (17%)	28,62,65	2.55	10 (35%)
1	PSU	D	39	1	15,21,22	1.44	3 (20%)	16,30,33	3.54	1 (6%)
1	5MC	D	40	1	14,22,23	0.93	1 (7%)	17,32,35	1.10	1 (5%)
1	7MG	D	46	1	20,26,27	1.76	3 (15%)	23,39,42	1.91	2 (8%)
1	5MC	D	49	1	14,22,23	0.91	1 (7%)	17,32,35	1.20	1 (5%)
1	5MU	D	54	1	13,22,23	1.10	1 (7%)	16,32,35	3.09	2 (12%)
1	PSU	D	55	1	15,21,22	1.54	3 (20%)	16,30,33	3.80	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	1MA	D	58	1	15,25,26	1.23	2 (13%)	15,37,40	1.52	3 (20%)
1	2MG	E	10	1	18,26,27	1.19	3 (16%)	21,38,41	3.47	5 (23%)
1	H2U	E	16	1	17,21,22	0.69	0	23,30,33	1.14	2 (8%)
1	H2U	E	17	1	17,21,22	0.68	0	23,30,33	0.84	0
1	M2G	E	26	1	18,27,28	1.08	2 (11%)	22,40,43	2.91	8 (36%)
1	OMC	E	32	1	15,22,23	1.15	1 (6%)	20,31,34	2.08	3 (15%)
1	OMG	E	34	1	18,26,27	1.34	3 (16%)	21,38,41	2.83	4 (19%)
1	YG	E	37	1	28,42,43	2.92	5 (17%)	28,62,65	2.54	10 (35%)
1	PSU	E	39	1	15,21,22	1.47	3 (20%)	16,30,33	3.54	1 (6%)
1	5MC	E	40	1	14,22,23	0.92	1 (7%)	17,32,35	1.09	1 (5%)
1	7MG	E	46	1	20,26,27	1.74	3 (15%)	23,39,42	1.93	2 (8%)
1	5MC	E	49	1	14,22,23	0.96	1 (7%)	17,32,35	1.20	1 (5%)
1	5MU	E	54	1	13,22,23	1.10	1 (7%)	16,32,35	3.04	2 (12%)
1	PSU	E	55	1	15,21,22	1.53	3 (20%)	16,30,33	3.78	3 (18%)
1	1MA	E	58	1	15,25,26	1.26	1 (6%)	15,37,40	1.52	3 (20%)

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	1/1/8/9	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
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
1	2MG	B	10	1	-	0/5/27/28	0/3/3/3
1	H2U	B	16	1	-	0/7/38/39	0/2/2/2
1	H2U	B	17	1	-	0/7/38/39	0/2/2/2

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	YG	C3-N3	-8.65	1.37	1.49
1	B	37	YG	C3-N3	-8.60	1.37	1.49
1	E	37	YG	C3-N3	-8.53	1.37	1.49
1	D	37	YG	C3-N3	-8.53	1.37	1.49
1	C	37	YG	C3-N3	-8.45	1.37	1.49

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	2MG	CM2-N2-C2	-12.83	108.60	123.03
1	B	10	2MG	CM2-N2-C2	-12.81	108.62	123.03
1	E	10	2MG	CM2-N2-C2	-12.73	108.72	123.03
1	D	10	2MG	CM2-N2-C2	-12.72	108.73	123.03
1	C	10	2MG	CM2-N2-C2	-12.60	108.86	123.03

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	37	YG	C15
1	D	37	YG	C15
1	A	37	YG	C15
1	C	37	YG	C15
1	E	37	YG	C15

There are no torsion outliers.

There are no ring outliers.

62 monomers are involved in 984 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	2MG	4	0
1	A	16	H2U	25	0
1	A	17	H2U	34	0
1	A	26	M2G	19	0
1	A	32	OMC	35	0
1	A	34	OMG	35	0
1	A	37	YG	119	0
1	A	39	PSU	40	0
1	A	40	5MC	83	0
1	A	46	7MG	28	0
1	A	49	5MC	8	0
1	A	54	5MU	8	0
1	A	55	PSU	18	0
1	A	58	1MA	32	0
1	B	10	2MG	25	0
1	B	16	H2U	16	0
1	B	17	H2U	30	0
1	B	26	M2G	14	0
1	B	32	OMC	36	0
1	B	34	OMG	50	0
1	B	37	YG	106	0
1	B	39	PSU	42	0
1	B	40	5MC	65	0
1	B	46	7MG	45	0
1	B	49	5MC	32	0
1	B	54	5MU	10	0
1	B	55	PSU	7	0
1	B	58	1MA	32	0
1	C	17	H2U	2	0
1	C	26	M2G	4	0
1	C	34	OMG	2	0
1	C	37	YG	8	0
1	C	39	PSU	4	0
1	C	40	5MC	4	0
1	C	49	5MC	2	0
1	C	54	5MU	2	0
1	C	55	PSU	2	0
1	C	58	1MA	3	0
1	D	10	2MG	12	0
1	D	16	H2U	6	0
1	D	17	H2U	13	0
1	D	26	M2G	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	34	OMG	2	0
1	D	37	YG	8	0
1	D	39	PSU	4	0
1	D	40	5MC	4	0
1	D	46	7MG	22	0
1	D	49	5MC	18	0
1	D	54	5MU	15	0
1	D	55	PSU	11	0
1	D	58	1MA	47	0
1	E	16	H2U	6	0
1	E	17	H2U	55	0
1	E	26	M2G	4	0
1	E	34	OMG	2	0
1	E	37	YG	8	0
1	E	39	PSU	4	0
1	E	40	5MC	4	0
1	E	49	5MC	39	0
1	E	54	5MU	23	0
1	E	55	PSU	5	0
1	E	58	1MA	28	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.