wwPDB EM Map/Model Validation Report (i)

Aug 22, 2014 – 03:50 PM BST

PDB ID	:	4CXH
EMDB ID:	:	EMD-2624
Title	:	Regulation of the mammalian elongation cycle by 40S subunit rolling: a eukaryotic-specific ribosome rearrangement
Authors	:	Budkevich, T.V.; Giesebrecht, J.; Behrmann, E.; Loerke, J.; Ramrath, D.J.F.; Mielke, T.; Ismer, J.; Hildebrand, P.; Tung, C.-S.; Nierhaus, K.H.; Sanbonmatsu, K.Y.; Spahn, C.M.T.
Deposited on	:	2014-04-07
Resolution	:	8.90 Å(reported)

This is a wwPDB validation report for a publicly released PDB 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/ValidationPDFNotes.html

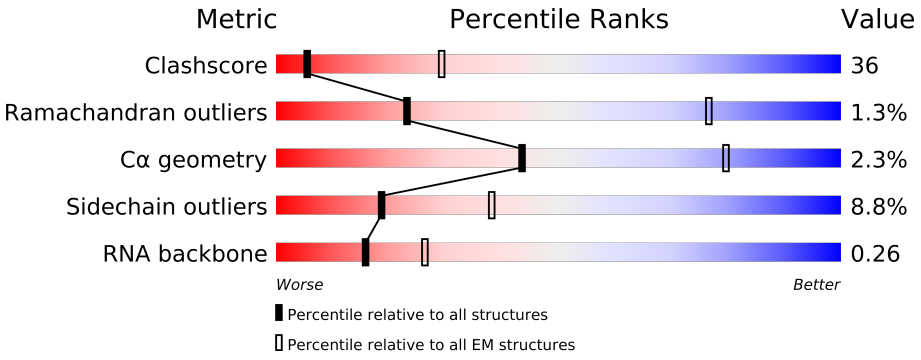
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Percentile statistics	:	23426
Cα geometry	:	trunk23477
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk23477

1 Overall quality at a glance

The reported resolution of this entry is 8.90 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	99129	735
Ramachandran outliers	96105	539
Cα geometry	96347	682
Sidechain outliers	96047	526
RNA backbone	2807	214

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

Mol	Chain	Length	Quality of chain
1	1	135	
2	2	50	
3	A	437	
4	X	143	
5	Y	76	
6	a	48	
7	b	17	
8	c	19	
9	x	28	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12270 atoms, of which 0 are hydrogen and 0 are deuterium.

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 18S RRNA - H44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	135	2890	1288	527	940	135	0	0

- Molecule 2 is a RNA chain called 28S RRNA - H89.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	50	1057	471	176	360	50	0	0

- Molecule 3 is a protein called ELONGATION FACTOR 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	427	3272	2104	570	585	13	0	0

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	134	1047	663	205	177	2	0	0

- Molecule 5 is a RNA chain called TRANSFER RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	Y	76	1636	737	290	532	76	1	0	0

- Molecule 6 is a RNA chain called 18S RRNA - H5-H14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	a	48	1024	458	192	326	48	0	0

- Molecule 7 is a RNA chain called 18S RRNA - H8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	17	Total	C	N	O	P	0	0
			363	162	63	121	17		

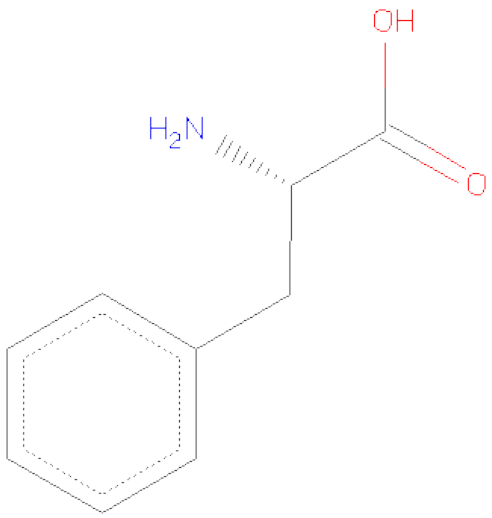
- Molecule 8 is a RNA chain called 28S RRNA - H95.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	19	Total	C	N	O	P	0	0
			410	183	78	130	19		

- Molecule 9 is a RNA chain called MESSENGER RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	x	28	Total	C	N	O	P	0	0
			560	252	56	224	28		

- Molecule 10 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



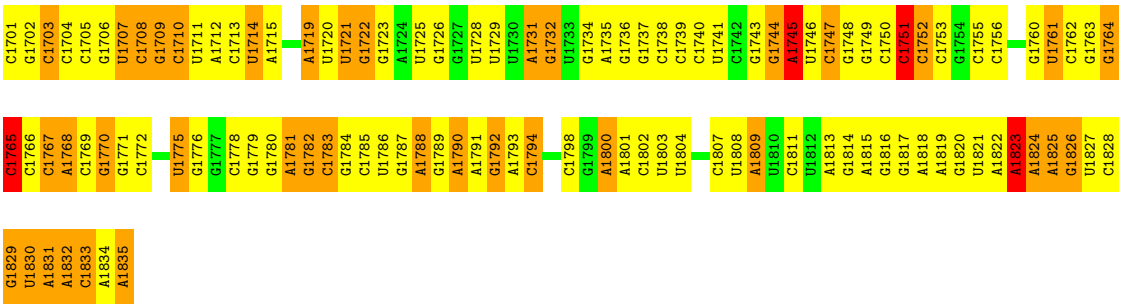
Mol	Chain	Residues	Atoms				AltConf
10	Y	1	Total	C	N	O	0
			11	9	1	1	

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: 18S RRNA - H44

Chain 1:

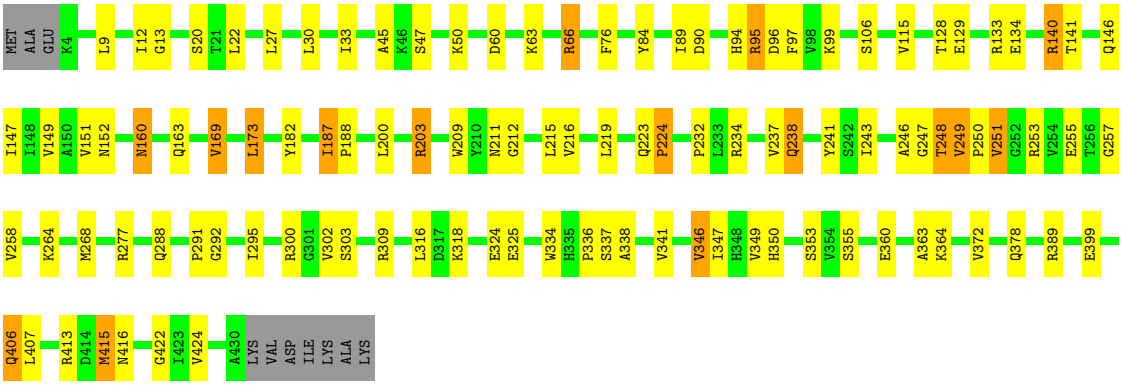


- Molecule 2: 28S RRNA - H89

Chain 2:

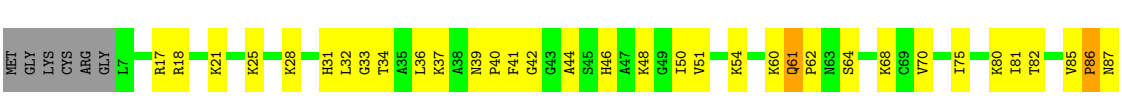
- Molecule 3: ELONGATION FACTOR 1A

Chain A:



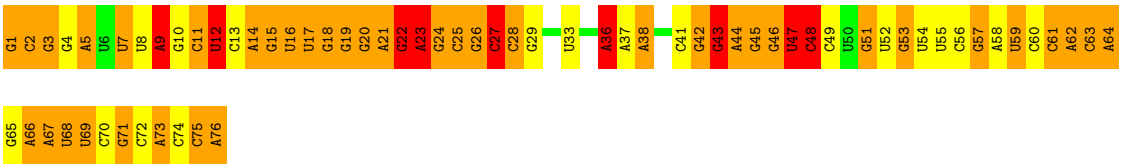
- Molecule 4: 40S RIBOSOMAL PROTEIN US12

Chain X:



• Molecule 5: TRANSFER RNA

Chain Y:



• Molecule 6: 18S RRNA - H5-H14

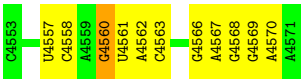
Chain a:

• Molecule 7: 18S RRNA - H8

Chain b:

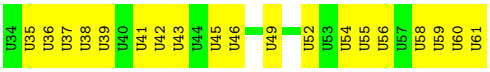
• Molecule 8: 28S RRNA - H95

Chain c:



• Molecule 9: MESSENGER RNA

Chain x:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\mathring{A}^2)$	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 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, H2U, MIA, 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	1	0.33	0/3232	0.77	0/5039
2	2	0.34	0/1177	0.81	0/1831
3	A	0.44	0/3346	0.62	0/4542
4	X	0.46	0/1064	0.70	0/1421
5	Y	0.49	1/1550 (0.1%)	1.95	67/2410 (2.8%)
6	a	0.37	0/1145	0.83	1/1782 (0.1%)
7	b	0.36	0/405	0.78	0/629
8	c	0.35	0/459	0.86	1/714 (0.1%)
9	x	0.42	1/615 (0.2%)	1.25	11/948 (1.2%)
All	All	0.40	2/12993 (0.0%)	1.00	80/19316 (0.4%)

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	1	0	1
5	Y	1	1
9	x	1	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	1	G	OP3-P	-5.70	1.54	1.61
9	x	60	U	O3'-P	5.01	1.67	1.61

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	22	G	O4'-C1'-N9	29.41	131.72	108.20
5	Y	21	A	N9-C1'-C2'	-20.11	87.86	114.00
5	Y	22	G	N9-C1'-C2'	-18.95	89.37	114.00
5	Y	71	G	O4'-C1'-N9	-17.36	94.31	108.20
5	Y	48	C	O4'-C1'-N1	15.05	120.24	108.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	Y	36	A	C3'
9	x	58	U	C3'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	1823	A	Sidechain
5	Y	33	U	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2890	0	1462	156	0
2	2	1057	0	535	63	0
3	A	3272	0	3294	119	0
4	X	1047	0	1110	46	0
5	Y	1636	0	846	197	0
6	a	1024	0	525	0	0
7	b	363	0	182	0	0
8	c	410	0	207	0	0
9	x	560	0	278	0	0
10	Y	11	0	8	4	0
All	All	12270	0	8447	512	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

The worst 5 of 512 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:241:TYR:CG	5:Y:76:A:H4'	1.25	1.72
3:A:336:PRO:CG	5:Y:53:G:H5'	1.17	1.56
3:A:336:PRO:CB	5:Y:53:G:H5"	1.42	1.47
3:A:336:PRO:CB	5:Y:53:G:C5'	1.97	1.41
3:A:336:PRO:CG	5:Y:53:G:C5'	1.95	1.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
3	A	425/437 (97%)	414 (97%)	11 (3%)	0	100 100
4	X	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	3 38
All	All	557/580 (96%)	534 (96%)	16 (3%)	7 (1%)	23 69

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	61	GLN
4	X	106	GLY
4	X	107	ARG
4	X	116	PRO
4	X	33	GLY

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 X-ray entries followed by that with respect to entries of similar resolution. 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
3	A	344/372 (92%)	309 (90%)	35 (10%)	10 45
4	X	108/115 (94%)	103 (95%)	5 (5%)	36 76
All	All	452/487 (93%)	412 (91%)	40 (9%)	19 53

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	187	ILE
3	A	237	VAL
4	X	31	HIS
3	A	211	ASN
3	A	238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	348	HIS
4	X	77	ASN
4	X	61	GLN
3	A	315	HIS
4	X	31	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	134/135 (99%)	57 (42%)	7 (5%)
2	2	49/50 (98%)	28 (57%)	4 (8%)
5	Y	74/76 (97%)	30 (40%)	7 (9%)
6	a	47/48 (97%)	32 (68%)	0
7	b	16/17 (94%)	10 (62%)	0
8	c	18/19 (94%)	11 (61%)	0
9	x	27/28 (96%)	15 (55%)	0
All	All	365/373 (97%)	183 (50%)	18 (4%)

5 of 183 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	1702	G
1	1	1703	C
1	1	1707	U

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Mol	Chain	Res	Type
1	1	1708	C
1	1	1709	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	4387	G
2	2	4388	A
5	Y	22	G
1	1	1834	A
2	2	4374	A

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

11 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	$\#\|Z\| > 2$
5	2MG	Y	10	5	24,26,27	1.15	2 (8%)	33,38,41	12.76	7 (21%)
5	H2U	Y	16	5	19,21,22	1.00	1 (5%)	27,30,33	2.83	9 (33%)
5	H2U	Y	17	5	19,21,22	0.88	2 (10%)	27,30,33	2.06	5 (18%)
5	M2G	Y	26	5	25,27,28	1.77	6 (24%)	35,40,43	14.45	16 (45%)
5	OMC	Y	32	5	20,22,23	1.18	3 (15%)	25,31,34	0.89	2 (8%)
5	MIA	Y	37	9,5	29,31,32	1.02	2 (6%)	41,44,47	1.58	6 (14%)
5	7MG	Y	46	5	24,26,27	3.04	4 (16%)	34,39,42	3.42	11 (32%)
5	5MC	Y	49	5	20,22,23	1.29	5 (25%)	26,32,35	2.90	6 (23%)
5	5MU	Y	54	5	20,22,23	5.48	5 (25%)	24,32,35	4.00	9 (37%)
5	PSU	Y	55	5	19,21,22	1.66	4 (21%)	23,30,33	5.21	9 (39%)
5	1MA	Y	58	5	23,25,26	1.21	2 (8%)	32,37,40	1.08	2 (6%)

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
5	2MG	Y	10	5	-	0/10/27/28	0/3/3/3
5	H2U	Y	16	5	-	1/8/38/39	0/2/2/2
5	H2U	Y	17	5	-	0/8/38/39	0/2/2/2
5	M2G	Y	26	5	-	1/12/29/30	0/3/3/3
5	OMC	Y	32	5	-	0/8/27/28	0/2/2/2
5	MIA	Y	37	9,5	-	0/16/33/34	0/3/3/3
5	7MG	Y	46	5	-	0/8/37/38	0/3/3/3
5	5MC	Y	49	5	-	0/6/25/26	0/2/2/2
5	5MU	Y	54	5	-	0/6/25/26	0/2/2/2
5	PSU	Y	55	5	-	0/8/25/26	0/2/2/2
5	1MA	Y	58	5	-	0/8/25/26	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	54	5MU	C5M-C5	-23.90	1.02	1.51
5	Y	46	7MG	C8-N9	-11.49	1.37	1.46
5	Y	46	7MG	CM7-N7	7.93	1.58	1.46
5	Y	26	M2G	P-OP1	4.19	1.51	1.46
5	Y	26	M2G	C5-C4	4.18	1.49	1.40

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	26	M2G	C6-C5-N7	-83.26	129.81	134.24
5	Y	10	2MG	C6-C5-N7	-72.23	130.39	134.24
5	Y	55	PSU	N1-C2-N3	-16.56	114.97	128.53
5	Y	55	PSU	C5-C4-N3	-12.99	114.73	125.33
5	Y	46	7MG	C2'-C1'-N9	-12.86	85.08	114.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	26	M2G	C2'-C1'-N9-C8
5	Y	16	H2U	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
10	PHE	Y	77	5	11,11,12	1.11	1 (9%)	13,13,15	2.57	3 (23%)

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
10	PHE	Y	77	5	-	1/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Y	77	PHE	CA-N	-2.64	1.39	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Y	77	PHE	CB-CA-C	-5.97	101.15	111.50
10	Y	77	PHE	CG-CB-CA	-4.94	102.95	114.19
10	Y	77	PHE	O-C-CA	-4.65	113.81	125.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Y	77	PHE	O-C-CA-CB

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

5.9 Trace-atom model geometry

5.9.1 Abnormal distances between consecutive trace-atoms (i)

The following table provides a summary of the distances observed between consecutive Cα atoms (in protein chains) or P atoms (in RNA or DNA chains).

Mol	Chain	Analysed	Outliers
1	1	134/135 (99.3%)	3/134 (2.2%)
2	2	49/50 (98.0%)	1/49 (2.0%)
3	A	426/437 (97.5%)	0/426 (0.0%)
4	X	133/143 (93.0%)	0/133 (0.0%)
5	Y	75/76 (98.7%)	1/75 (1.3%)
6	a	47/48 (97.9%)	0/47 (0.0%)
7	b	16/17 (94.1%)	0/16 (0.0%)
8	c	18/19 (94.7%)	0/18 (0.0%)
9	x	27/28 (96.4%)	1/27 (3.7%)
All	All	925/953 (97.1%)	6/925 (0.6%)

5 of 6 trace-atom distance outliers are listed below:

Mol	Chain	Res	Type	Error type	Distance error
5	Y	43	G	short	0.59
9	x	35	U	short	0.46
1	1	1751	C	short	0.25
2	2	4380	U	short	0.05
1	1	1745	A	short	0.03

5.9.2 Cα torsion geometry

The following table provides a summary of the Cα pseudo-geometry for proteins. The "Percentiles" column lists the percent Cα pseudo-geometry outliers 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
3	A	424/437 (97%)	276 (65%)	137 (32%)	11 (3%)	35 73
4	X	131/143 (92%)	88 (67%)	41 (31%)	2 (2%)	68 93
All	All	555/580 (96%)	364 (66%)	178 (32%)	13 (2%)	43 79

5 of 13 Cα pseudo-geometry outliers are listed below:

Mol	Chain	Res	Type
3	A	324	GLU
3	A	12	ILE
3	A	378	GLN
3	A	422	GLY
4	X	86	PRO