



wwPDB X-ray Structure Validation Summary Report

Jul 22, 2014 – 08:07 AM EDT

PDB ID : 4V42
Title : Crystal structure of the ribosome at 5.5 Å resolution.
Authors : Yusupov, M.M.; Yusupova, G.Z.; Baucom, A.; Lieberman, K.; Earnest, T.N.;
Cate, J.H.D.; Noller, H.F.
Deposited on : 2001-03-30
Resolution : 5.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

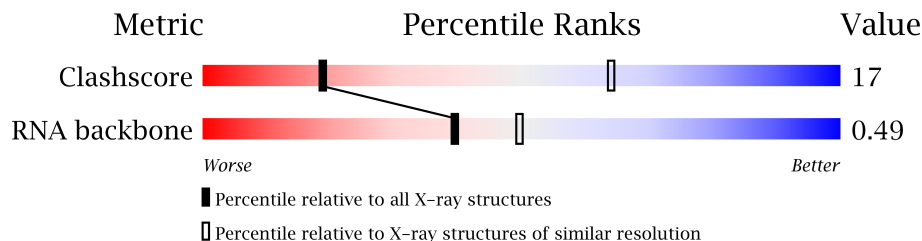
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23489

1 Overall quality at a glance

The reported resolution of this entry is 5.50 Å.



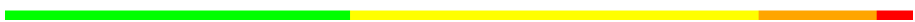










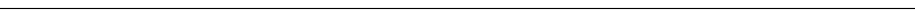

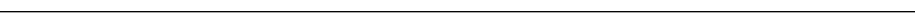


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1008 (7.40-3.52)
RNA backbone	1838	1040 (7.50-2.80)









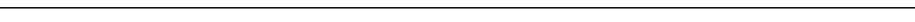













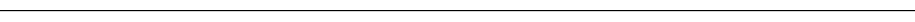

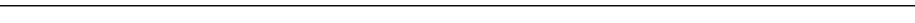






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	AB	76	
2	AC	76	
3	AD	74	
4	A1	6	
5	AE	256	
6	AF	239	
7	AG	209	
8	AH	162	
9	AI	101	
10	AJ	156	
11	AK	138	
12	AL	128	
13	AM	105	
14	AN	129	
15	AO	135	
16	AP	126	
17	AQ	61	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	AR	89	
19	AS	91	
20	AT	105	
21	AU	88	
22	AV	93	
23	AW	106	
24	AX	26	
25	BA	2916	
26	BB	123	
27	BC	228	
28	BD	178	
29	BE	338	
30	BF	246	
31	BG	176	
32	BH	177	
33	BI	128	
33	BJ	128	
34	BK	149	
35	BL	141	
36	BM	145	
37	BN	122	
38	BO	164	
39	BP	138	
40	BQ	186	
41	BR	66	
42	BS	113	
43	BT	84	
44	BU	119	
45	BV	94	
46	BW	70	
47	BX	60	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 14656 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	AA	1519	Total	P	0	0	1519
			1519	1519			

- Molecule 2 is a RNA chain called TRNA(PHE).

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

There are 28 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AC	32	OMC	C	TRNA MODIFICATION	GB 176479
AC	34	OMG	G	TRNA MODIFICATION	GB 176479
AC	37	YG	G	TRNA MODIFICATION	GB 176479
AC	39	PSU	U	TRNA MODIFICATION	GB 176479
AC	40	5MC	C	TRNA MODIFICATION	GB 176479
AC	46	7MG	G	TRNA MODIFICATION	GB 176479
AC	49	5MC	C	TRNA MODIFICATION	GB 176479
AC	54	5MU	U	TRNA MODIFICATION	GB 176479
AC	55	PSU	U	TRNA MODIFICATION	GB 176479
AC	58	1MA	A	TRNA MODIFICATION	GB 176479

- Molecule 3 is a RNA chain called TRNA(PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	AD	74	Total	C	N	O	P	S	0	0	0
			1570	702	269	524	74	1			

- Molecule 4 is a RNA chain called A- AND P-SITE MESSENGER RNA CODONS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A1	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	AE	234	Total	C	0	0	234
			234	234			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
6	AF	206	Total	C	0	0	206
			206	206			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	AG	208	Total	C	0	0	208
			208	208			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	AH	150	Total	C	0	0	150
			150	150			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	AI	101	Total	C	0	0	101
			101	101			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	AJ	155	Total	C	0	0	155
			155	155			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	AK	138	Total	C	0	0	138
			138	138			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	AL	127	Total	C	0	0	127
			127	127			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	AM	98	Total	C	0	0	98
			98	98			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
14	AN	119	Total	C	0	0	119
			119	119			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	AO	124	Total	C	0	0	124
			124	124			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
16	AP	125	Total	C	0	0	125
			125	125			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
17	AQ	60	Total	C	0	0	60
			60	60			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
18	AR	88	Total	C	0	0	88
			88	88			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
19	AS	83	Total	C	0	0	83
			83	83			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
20	AT	104	Total	C	0	0	104
			104	104			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
21	AU	73	Total	C	0	0	73
			73	73			

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	AV	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	AW	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	AX	24	Total C 24 24	0	0	24

- Molecule 25 is a RNA chain called 50S 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	BA	2889	Total P 2889 2889	0	0	2889

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	INSERTION	? 48268

- Molecule 26 is a RNA chain called 50S 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	BB	123	Total P 123 123	0	0	123

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 176261

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	BC	224	Total C 224 224	0	0	224

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	BD	173	Total C 173 173	0	0	173

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	BE	191	Total C 191 191	0	0	191

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BE	113	SER	ASP	CONFLICT	UNP P20279
BE	114	ASP	VAL	CONFLICT	UNP P20279
BE	115	ARG	PRO	CONFLICT	UNP P20279
BE	116	LEU	GLU	CONFLICT	UNP P20279
BE	119	ALA	ASP	CONFLICT	UNP P20279
BE	120	LEU	PRO	CONFLICT	UNP P20279
BE	122	ILE	ALA	CONFLICT	UNP P20279
BE	123	VAL	ALA	CONFLICT	UNP P20279
BE	125	ASP	GLU	CONFLICT	UNP P20279

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	BF	189	Total C 189 189	0	0	189

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	GLU	GLN	CONFLICT	UNP P12735

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	BG	122	Total C 122 122	0	0	122

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	BH	164	Total C 164 164	0	0	164

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	BI	128	Total C 128 128	0	0	128
33	BJ	128	Total C 128 128	0	0	128

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	BK	148	Total C 148 148	0	0	148

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	BL	133	Total C 133 133	0	0	133

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BM	117	Total C 117 117	0	0	117

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	BN	122	Total C 122 122	0	0	122

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BO	84	Total C 84 84	0	0	84

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
39	BP	138	Total	C	0	0	138
			138	138			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
40	BQ	113	Total	C	0	0	113
			113	113			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
41	BR	52	Total	C	0	0	52
			52	52			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
42	BS	110	Total	C	0	0	110
			110	110			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
43	BT	76	Total	C	0	0	76
			76	76			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
44	BU	110	Total	C	0	0	110
			110	110			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
45	BV	89	Total	C	0	0	89
			89	89			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
46	BW	64	Total	C	0	0	64
			64	64			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
47	BX	60	Total	C	0	0	60
			60	60			

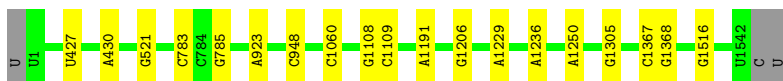
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

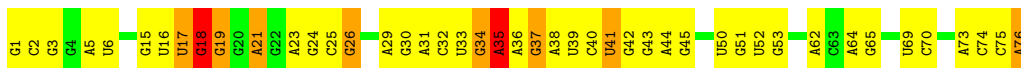
- Molecule 1: 30S 16S RIBOSOMAL RNA

Chain AA: 



- Molecule 2: TRNA(PHE)

Chain AB: 



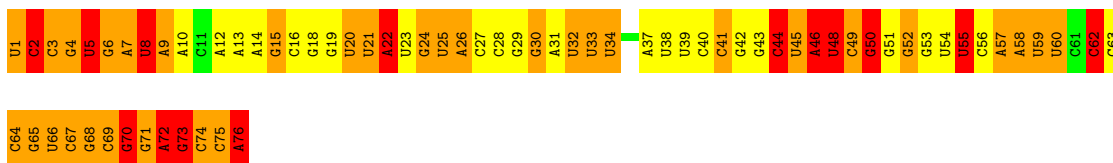
- Molecule 2: TRNA(PHE)

Chain AC: 



- Molecule 3: TRNA(PHE)

Chain AD: 



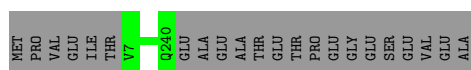
- Molecule 4: A- AND P-SITE MESSENGER RNA CODONS

Chain A1: 



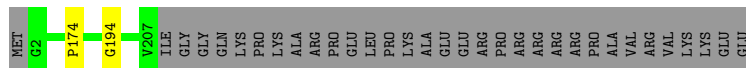
- Molecule 5: 30S RIBOSOMAL PROTEIN S2

Chain AE: 



- Molecule 6: 30S RIBOSOMAL PROTEIN S3

Chain AF:



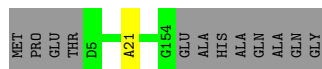
- Molecule 7: 30S RIBOSOMAL PROTEIN S4

Chain AG:



- Molecule 8: 30S RIBOSOMAL PROTEIN S5

Chain AH:



- Molecule 9: 30S RIBOSOMAL PROTEIN S6

Chain AI:

There are no outlier residues recorded for this chain.

- Molecule 10: 30S RIBOSOMAL PROTEIN S7

Chain AJ:



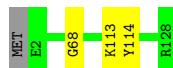
- Molecule 11: 30S RIBOSOMAL PROTEIN S8

Chain AK:

There are no outlier residues recorded for this chain.

- Molecule 12: 30S RIBOSOMAL PROTEIN S9

Chain AL:



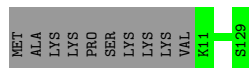
- Molecule 13: 30S RIBOSOMAL PROTEIN S10

Chain AM:



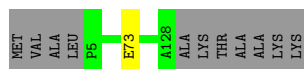
- Molecule 14: 30S RIBOSOMAL PROTEIN S11

Chain AN: 



- Molecule 15: 30S RIBOSOMAL PROTEIN S12

Chain AO: 



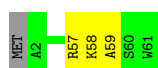
- Molecule 16: 30S RIBOSOMAL PROTEIN S13

Chain AP: 



- Molecule 17: 30S RIBOSOMAL PROTEIN S14

Chain AQ: 



- Molecule 18: 30S RIBOSOMAL PROTEIN S15

Chain AR: 



- Molecule 19: 30S RIBOSOMAL PROTEIN S16

Chain AS: 



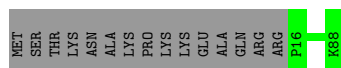
- Molecule 20: 30S RIBOSOMAL PROTEIN S17

Chain AT: 



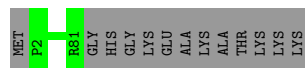
- Molecule 21: 30S RIBOSOMAL PROTEIN S18

Chain AU: 



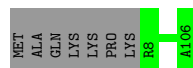
- Molecule 22: 30S RIBOSOMAL PROTEIN S19

Chain AV:



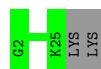
- Molecule 23: 30S RIBOSOMAL PROTEIN S20

Chain AW:



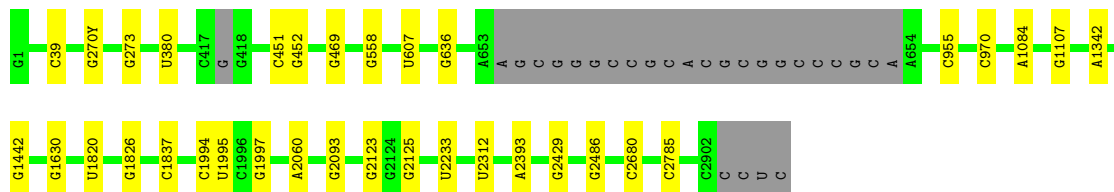
- Molecule 24: 30S RIBOSOMAL PROTEIN THX

Chain AX:



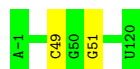
- Molecule 25: 50S 23S RIBOSOMAL RNA

Chain BA:



- Molecule 26: 50S 5S RIBOSOMAL RNA

Chain BB:



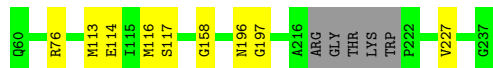
- Molecule 27: 50S RIBOSOMAL PROTEIN L1

Chain BC:



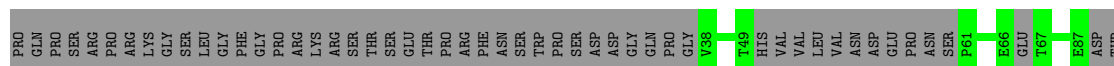
- Molecule 28: 50S RIBOSOMAL PROTEIN L2

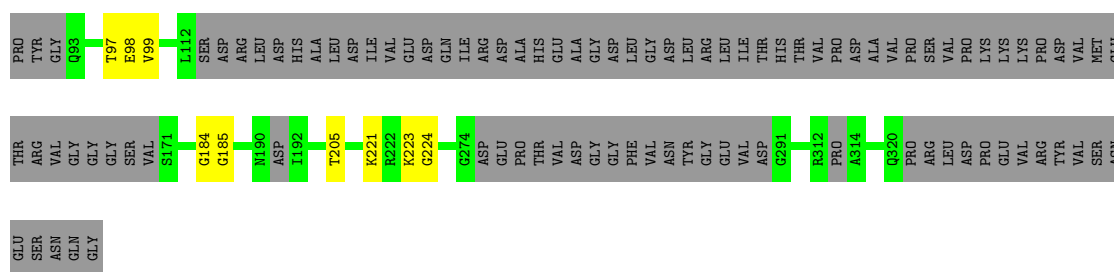
Chain BD: 



- Molecule 29: 50S RIBOSOMAL PROTEIN L3

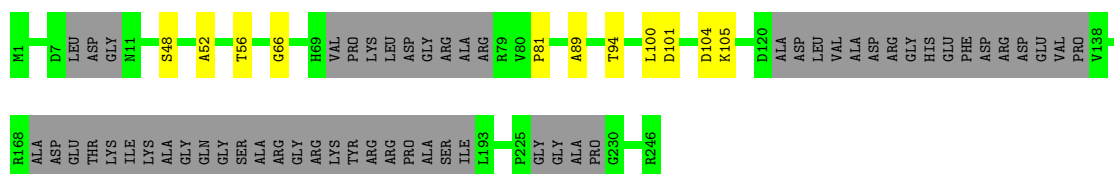
Chain BE: 





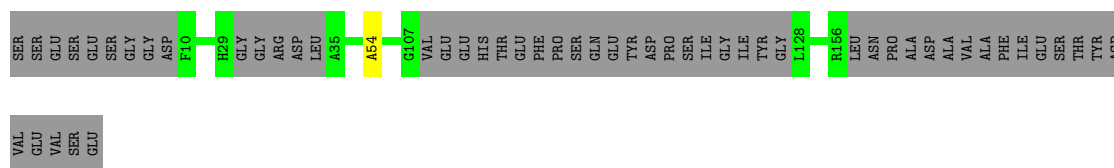
• Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain BF:

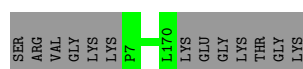


● Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain BG: 



• Molecule 32: 50S RIBOSOMAL PROTEIN L6

[illegible]

- Molecule 33: 50S RIBOSOMAL PROTEIN L7/L12

Chain BI:



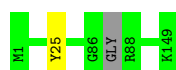
- Molecule 33: 50S RIBOSOMAL PROTEIN L7/L12

Chain B.J: _____

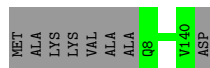
There are no outlier residues recorded for this chain.

● Molecule 34: 50S RIBOSOMAL PROTEIN L9

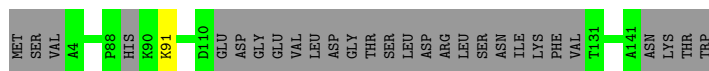
Chain BK: _____



- Molecule 35: 50S RIBOSOMAL PROTEIN L11

Chain BL: 

- Molecule 36: 50S RIBOSOMAL PROTEIN L13

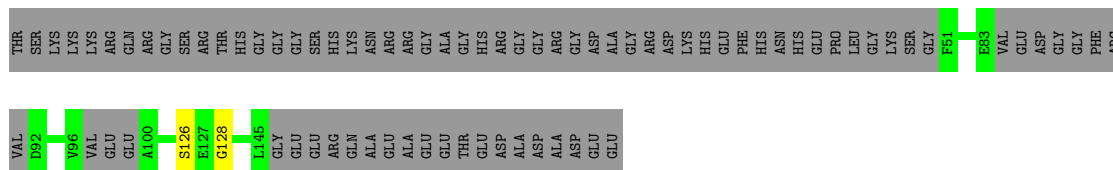
Chain BM: 

- Molecule 37: 50S RIBOSOMAL PROTEIN L14

Chain BN: 

There are no outlier residues recorded for this chain.

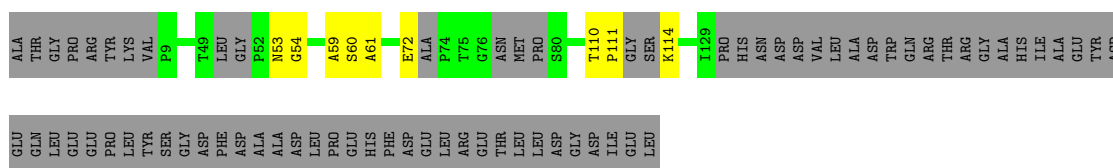
- Molecule 38: 50S RIBOSOMAL PROTEIN L15

Chain BO: 

- Molecule 39: 50S RIBOSOMAL PROTEIN L16

Chain BP: 

- Molecule 40: 50S RIBOSOMAL PROTEIN L18

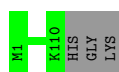
Chain BQ: 

- Molecule 41: 50S RIBOSOMAL PROTEIN L19

Chain BR: 

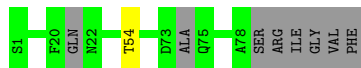
- Molecule 42: 50S RIBOSOMAL PROTEIN L22

Chain BS: 



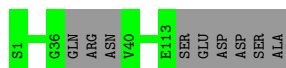
- Molecule 43: 50S RIBOSOMAL PROTEIN L23

Chain BT:



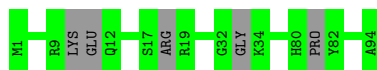
- Molecule 44: 50S RIBOSOMAL PROTEIN L24

Chain BU:



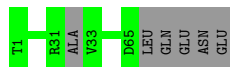
- Molecule 45: 50S RIBOSOMAL PROTEIN L25

Chain BV:



- Molecule 46: 50S RIBOSOMAL PROTEIN L29

Chain BW:



- Molecule 47: 50S RIBOSOMAL PROTEIN L30

Chain BX:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 – 5.50	Depositor
% Data completeness (in resolution range)	95.3 (250.00-5.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	O	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14656	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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, M2G, OMG, H2U, YG, 2MG, 5MC, 1MA, 4SU, 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 > 5$	RMSZ	# $ Z > 5$
2	AB	1.21	4/1486 (0.3%)	1.43	13/2311 (0.6%)
2	AC	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
3	AD	1.95	17/1616 (1.1%)	2.85	154/2512 (6.1%)
4	A1	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	AB	0	3
2	AC	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	AD	33	U	O3'-P	31.20	1.98	1.61
2	AC	74	C	O3'-P	-27.00	1.28	1.61
2	AB	75	C	O3'-P	-26.77	1.29	1.61
2	AC	75	C	O3'-P	-25.61	1.30	1.61
3	AD	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(°)	Ideal(°)
2	AB	35	A	P-O3'-C3'	41.11	169.03	119.70
3	AD	25	U	P-O3'-C3'	31.41	157.40	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	75	C	P-O3'-C3'	-29.51	84.29	119.70
4	A1	3	U	P-O3'-C3'	27.61	152.83	119.70
3	AD	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	AB	18	G	Sidechain
2	AB	19	G	Sidechain
2	AB	62	A	Sidechain
2	AC	18	G	Sidechain
2	AC	19	G	Sidechain

5.2 Close contacts ⓘ

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	AA	1519	0	0	16	0
2	AB	1652	0	862	56	0
2	AC	1652	0	862	53	0
3	AD	1570	0	801	105	0
4	A1	120	0	61	5	0
5	AE	234	0	0	0	0
6	AF	206	0	0	2	0
7	AG	208	0	0	2	0
8	AH	150	0	0	1	0
9	AI	101	0	0	0	0
10	AJ	155	0	0	4	0
11	AK	138	0	0	0	0
12	AL	127	0	0	3	0
13	AM	98	0	0	5	0
14	AN	119	0	0	0	0
15	AO	124	0	0	1	0
16	AP	125	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	AQ	60	0	0	4	0
18	AR	88	0	0	0	0
19	AS	83	0	0	0	0
20	AT	104	0	0	0	0
21	AU	73	0	0	0	0
22	AV	80	0	0	0	0
23	AW	99	0	0	0	0
24	AX	24	0	0	0	0
25	BA	2889	0	0	33	0
26	BB	123	0	0	2	0
27	BC	224	0	0	4	0
28	BD	173	0	0	6	0
29	BE	191	0	0	7	0
30	BF	189	0	0	9	0
31	BG	122	0	0	1	0
32	BH	164	0	0	0	0
33	BI	128	0	0	3	0
33	BJ	128	0	0	0	0
34	BK	148	0	0	1	0
35	BL	133	0	0	0	0
36	BM	117	0	0	1	0
37	BN	122	0	0	0	0
38	BO	84	0	0	2	0
39	BP	138	0	0	2	0
40	BQ	113	0	0	6	0
41	BR	52	0	0	0	0
42	BS	110	0	0	0	0
43	BT	76	0	0	1	0
44	BU	110	0	0	0	0
45	BV	89	0	0	0	0
46	BW	64	0	0	0	0
47	BX	60	0	0	1	0
All	All	14656	0	2586	285	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 17.

The worst 5 of 285 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:BF:100:LEU:CA	30:BF:101:ASP:CA	1.80	1.54
2:AC:1:G:N2	2:AC:2:C:H41	1.22	1.34
1:AA:430:A:P	7:AG:7:PRO:CA	2.16	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:BD:196:ASN:CA	28:BD:197:GLY:CA	2.06	1.31
3:AD:75:C:C2'	3:AD:76:A:H5'	1.59	1.30

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	0/1522	-	-
2	AB	74/76 (97%)	13 (17%)	0
2	AC	75/76 (98%)	13 (17%)	0
25	BA	0/2916	-	-
26	BB	0/123	-	-
3	AD	72/74 (97%)	26 (36%)	0
4	A1	5/6 (83%)	1 (20%)	0
All	All	226/4793 (4%)	53 (23%)	0

5 of 53 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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	2MG	AB	10	2	24,26,27	0.86	1 (4%)	33,38,41	5.59	4 (12%)
2	H2U	AB	16	2	19,21,22	0.90	2 (10%)	27,30,33	1.12	3 (11%)
2	H2U	AB	17	2	19,21,22	0.88	1 (5%)	27,30,33	1.03	2 (7%)
2	M2G	AB	26	2	25,27,28	0.97	1 (4%)	35,40,43	5.57	4 (11%)
2	OMC	AB	32	2	20,22,23	1.00	1 (5%)	25,31,34	0.84	1 (4%)
2	OMG	AB	34	2,4	24,26,27	1.09	2 (8%)	33,38,41	5.37	4 (12%)
2	YG	AB	37	2	40,42,43	1.06	3 (7%)	50,62,65	11.07	12 (24%)
2	PSU	AB	39	2	19,21,22	0.92	0	23,30,33	0.81	0
2	5MC	AB	40	2	20,22,23	1.09	2 (10%)	26,32,35	1.33	3 (11%)
2	7MG	AB	46	2	24,26,27	1.18	4 (16%)	34,39,42	1.92	6 (17%)
2	5MC	AB	49	2	20,22,23	1.60	4 (20%)	26,32,35	1.39	3 (11%)
2	5MU	AB	54	2	20,22,23	1.26	4 (20%)	25,32,35	1.38	3 (12%)
2	PSU	AB	55	2	19,21,22	1.10	2 (10%)	23,30,33	1.02	2 (8%)
2	1MA	AB	58	2	23,25,26	2.91	5 (21%)	32,37,40	1.77	5 (15%)
2	2MG	AC	10	2	24,26,27	0.88	2 (8%)	33,38,41	5.66	4 (12%)
2	H2U	AC	16	2	19,21,22	0.89	2 (10%)	27,30,33	1.12	3 (11%)
2	H2U	AC	17	2	19,21,22	0.89	1 (5%)	27,30,33	1.04	2 (7%)
2	M2G	AC	26	2	25,27,28	0.97	1 (4%)	35,40,43	5.57	4 (11%)
2	OMC	AC	32	2	20,22,23	0.99	1 (5%)	25,31,34	0.85	1 (4%)
2	OMG	AC	34	2,4	24,26,27	1.08	2 (8%)	33,38,41	5.33	4 (12%)
2	YG	AC	37	2	40,42,43	1.07	3 (7%)	50,62,65	11.22	12 (24%)
2	PSU	AC	39	2	19,21,22	0.93	0	23,30,33	0.81	0
2	5MC	AC	40	2	20,22,23	1.08	2 (10%)	26,32,35	1.32	3 (11%)
2	7MG	AC	46	2	24,26,27	1.17	3 (12%)	34,39,42	1.90	6 (17%)
2	5MC	AC	49	2	20,22,23	1.60	4 (20%)	26,32,35	1.41	3 (11%)
2	5MU	AC	54	2	20,22,23	1.24	4 (20%)	25,32,35	1.36	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	AC	55	2	19,21,22	1.09	2 (10%)	23,30,33	1.01	2 (8%)
2	1MA	AC	58	2	23,25,26	2.91	5 (21%)	32,37,40	1.77	5 (15%)
3	H2U	AD	20	3	19,21,22	0.59	1 (5%)	27,30,33	0.75	1 (3%)
3	H2U	AD	21	3	19,21,22	0.68	0	27,30,33	0.69	0
3	5MC	AD	49	3	20,22,23	0.88	1 (5%)	26,32,35	1.86	4 (15%)
3	5MU	AD	54	3	20,22,23	1.22	2 (10%)	25,32,35	1.79	2 (8%)
3	PSU	AD	55	3	19,21,22	1.21	2 (10%)	23,30,33	1.09	2 (8%)
3	4SU	AD	8	3	19,21,22	1.35	1 (5%)	23,30,33	26.94	1 (4%)

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	2MG	AB	10	2	-	0/10/27/28	0/3/3/3
2	H2U	AB	16	2	-	0/8/38/39	0/2/2/2
2	H2U	AB	17	2	-	0/8/38/39	0/2/2/2
2	M2G	AB	26	2	-	0/12/29/30	0/3/3/3
2	OMC	AB	32	2	-	0/8/27/28	0/2/2/2
2	OMG	AB	34	2,4	-	1/10/27/28	0/3/3/3
2	YG	AB	37	2	-	0/25/42/43	0/4/4/4
2	PSU	AB	39	2	-	0/8/25/26	0/2/2/2
2	5MC	AB	40	2	-	0/6/25/26	0/2/2/2
2	7MG	AB	46	2	-	0/8/37/38	0/3/3/3
2	5MC	AB	49	2	-	0/6/25/26	0/2/2/2
2	5MU	AB	54	2	-	0/6/25/26	0/2/2/2
2	PSU	AB	55	2	-	0/8/25/26	0/2/2/2
2	1MA	AB	58	2	-	0/8/25/26	0/3/3/3
2	2MG	AC	10	2	-	0/10/27/28	0/3/3/3
2	H2U	AC	16	2	-	0/8/38/39	0/2/2/2
2	H2U	AC	17	2	-	0/8/38/39	0/2/2/2
2	M2G	AC	26	2	-	0/12/29/30	0/3/3/3
2	OMC	AC	32	2	-	0/8/27/28	0/2/2/2
2	OMG	AC	34	2,4	-	1/10/27/28	0/3/3/3
2	YG	AC	37	2	-	0/25/42/43	0/4/4/4
2	PSU	AC	39	2	-	0/8/25/26	0/2/2/2
2	5MC	AC	40	2	-	0/6/25/26	0/2/2/2
2	7MG	AC	46	2	-	0/8/37/38	0/3/3/3
2	5MC	AC	49	2	-	0/6/25/26	0/2/2/2
2	5MU	AC	54	2	-	0/6/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	AC	55	2	-	0/8/25/26	0/2/2/2
2	1MA	AC	58	2	-	0/8/25/26	0/3/3/3
3	H2U	AD	20	3	-	0/8/38/39	0/2/2/2
3	H2U	AD	21	3	-	0/8/38/39	0/2/2/2
3	5MC	AD	49	3	-	1/6/25/26	0/2/2/2
3	5MU	AD	54	3	-	0/6/25/26	0/2/2/2
3	PSU	AD	55	3	-	0/8/25/26	0/2/2/2
3	4SU	AD	8	3	-	0/6/25/26	0/2/2/2

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AC	58	1MA	C6-N6	10.36	1.48	1.29
2	AB	58	1MA	C6-N6	10.28	1.48	1.29
2	AB	58	1MA	C6-N1	6.94	1.45	1.37
2	AC	58	1MA	C6-N1	6.92	1.45	1.37
3	AD	8	4SU	C5-C4	4.57	1.43	1.38

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	8	4SU	C4-N3-C2	129.19	127.13	121.60
2	AC	37	YG	C6-C5-N7	-75.95	130.20	134.24
2	AB	37	YG	C6-C5-N7	-74.86	130.25	134.24
2	AC	10	2MG	C6-C5-N7	-31.05	129.96	134.14
2	AC	26	M2G	C6-C5-N7	-30.66	130.01	134.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AC	34	OMG	OP2-P-O5'-C5'
2	AB	34	OMG	OP2-P-O5'-C5'
3	AD	49	5MC	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	AD	4
2	AB	1
2	AC	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AB	44:A	O3'	45:G	P	2.49
1	AD	37:A	O3'	38:U	P	2.28
1	AC	25:C	O3'	26:M2G	P	2.12
1	AD	48:U	O3'	49:5MC	P	1.99
1	AD	33:U	O3'	34:U	P	1.98

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.