wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:02 PM BST

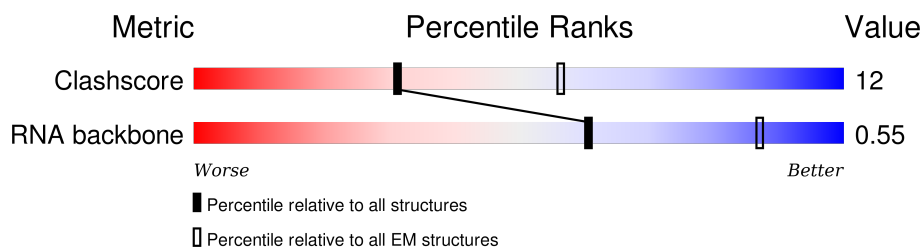|		
PDB ID	:	1ML5
EMDB ID:	:	EMD-1005
Title	:	Structure of the E. coli ribosomal termination complex with release factor 2
Authors	:	Klaholz, B.P.; Pape, T.; Zavialov, A.V.; Myasnikov, A.G.; Orlova, E.V.; Vestergaard, B.; Ehrenberg, M.; van Heel, M.
Deposited on	:	2002-08-30
Resolution	:	14.00 Å(reported)
Based on PDB ID	:	1GQE, 1GIX, 1GIY

1 Overall quality at a glance ⓘ

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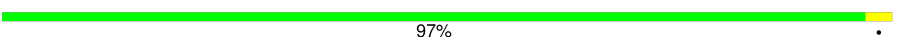*ELECTRON MICROSCOPY*

The reported resolution of this entry is 14.00 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.
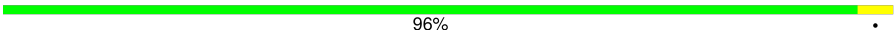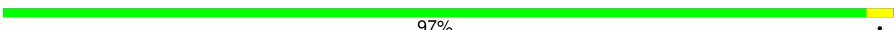
Metric	Percentile Ranks	Value
Clashscore		12
RNA backbone		0.55

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
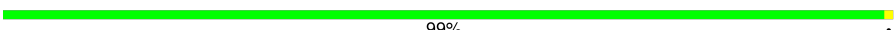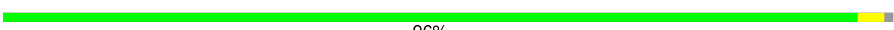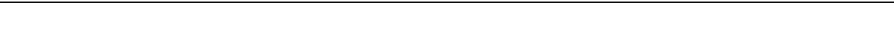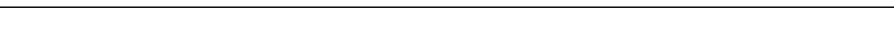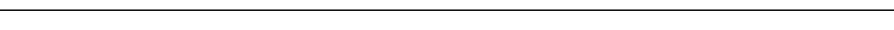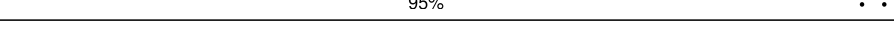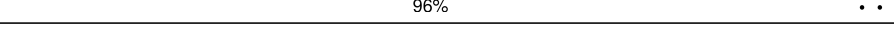
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
RNA backbone	3027	244

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	1522	97% ·
2	B	76	32% 46% 17% 5%
3	C	6	17% 67% 17%
4	a	2916	97% ··
5	b	123	98% ·
6	Z	365	96% ··
7	E	256	90% · 9%
8	F	239	84% · 14%
9	G	209	96% ·
10	H	162	91% · 7%
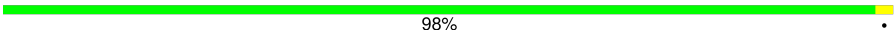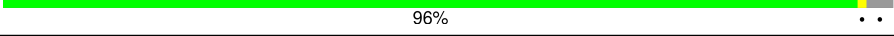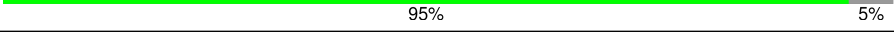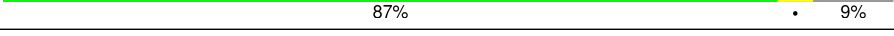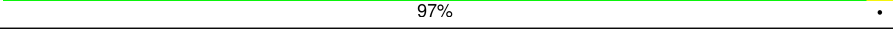
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Mol	Chain	Length	Quality of chain
11	I	101	96%
12	J	156	97%
13	K	138	99%
14	L	128	96%
15	M	105	88% 6% 7%
16	N	129	89% 8%
17	O	135	89% 8%
18	P	126	96%
19	Q	61	87% 11%
20	R	89	94%
21	S	91	90% 9%
22	T	105	95%
23	U	88	80% 17%
24	V	93	86% 14%
25	W	106	92% 7%
26	X	26	92% 8%
27	c	228	95%
28	d	178	96%
29	e	338	55% 43%
30	f	246	75% 23%
31	g	176	67% 31%
32	h	177	92% 7%
33	l	141	94% 6%
34	m	145	79% 19%
35	n	122	97%

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Mol	Chain	Length	Quality of chain
36	o	164	49%　·　49%
37	p	138	98%　·
38	q	186	59%　·　39%
39	r	66	79%　21%
40	s	113	96%　··
41	t	84	90%　10%
42	u	119	88%　·　8%
43	v	94	95%　5%
44	w	70	87%　·　9%
45	x	60	97%　·

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 11392 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 30S 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	1519	Total P 1519 1519		0	1519

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

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

- Molecule 3 is a RNA chain called A- AND P-SITE MESSENGER RNA CODONS.

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

- Molecule 4 is a RNA chain called 50S 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	a	2889	Total P 2889 2889		0	2889

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

Mol	Chain	Residues	Atoms		AltConf	Trace
5	b	123	Total P 123 123		0	123

- Molecule 6 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	Z	362	Total C 362 362		0	362

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms		AltConf	Trace
7	E	234	Total 234	C 234	0	234

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms		AltConf	Trace
8	F	206	Total 206	C 206	0	206

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms		AltConf	Trace
9	G	208	Total 208	C 208	0	208

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms		AltConf	Trace
10	H	150	Total 150	C 150	0	150

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms		AltConf	Trace
11	I	101	Total 101	C 101	0	101

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms		AltConf	Trace
12	J	155	Total 155	C 155	0	155

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms		AltConf	Trace
13	K	138	Total 138	C 138	0	138

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms		AltConf	Trace
14	L	127	Total 127	C 127	0	127

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms		AltConf	Trace
15	M	98	Total 98	C 98	0	98

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms		AltConf	Trace
16	N	119	Total 119	C 119	0	119

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms		AltConf	Trace
17	O	124	Total 124	C 124	0	124

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms		AltConf	Trace
18	P	125	Total 125	C 125	0	125

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms		AltConf	Trace
19	Q	60	Total 60	C 60	0	60

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms		AltConf	Trace
20	R	88	Total 88	C 88	0	88

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms		AltConf	Trace
21	S	83	Total 83	C 83	0	83

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms		AltConf	Trace
22	T	104	Total 104	C 104	0	104

- Molecule 23 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms		AltConf	Trace
23	U	73	Total 73	C 73	0	73

- Molecule 24 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms		AltConf	Trace
24	V	80	Total 80	C 80	0	80

- Molecule 25 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms		AltConf	Trace
25	W	99	Total 99	C 99	0	99

- Molecule 26 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms		AltConf	Trace
26	X	24	Total 24	C 24	0	24

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

Mol	Chain	Residues	Atoms		AltConf	Trace
27	c	224	Total 224	C 224	0	224

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

Mol	Chain	Residues	Atoms		AltConf	Trace
28	d	173	Total 173	C 173	0	173

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

Mol	Chain	Residues	Atoms		AltConf	Trace
29	e	191	Total 191	C 191	0	191

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

Mol	Chain	Residues	Atoms		AltConf	Trace
30	f	189	Total 189	C 189	0	189

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

Mol	Chain	Residues	Atoms		AltConf	Trace
31	g	122	Total 122	C 122	0	122

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

Mol	Chain	Residues	Atoms		AltConf	Trace
32	h	164	Total 164	C 164	0	164

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms		AltConf	Trace
33	l	133	Total 133	C 133	0	133

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms		AltConf	Trace
34	m	117	Total 117	C 117	0	117

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms		AltConf	Trace
35	n	122	Total 122	C 122	0	122

• Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms		AltConf	Trace
36	o	84	Total 84	C 84	0	84

• Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms		AltConf	Trace
37	p	138	Total 138	C 138	0	138

• Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms		AltConf	Trace
38	q	113	Total 113	C 113	0	113

• Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms		AltConf	Trace
39	r	52	Total 52	C 52	0	52

• Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms		AltConf	Trace
40	s	110	Total 110	C 110	0	110

• Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms		AltConf	Trace
41	t	76	Total 76	C 76	0	76

• Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms		AltConf	Trace
42	u	110	Total 110	C 110	0	110

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms		AltConf	Trace
43	v	89	Total 89	C 89	0	89

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms		AltConf	Trace
44	w	64	Total 64	C 64	0	64

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms		AltConf	Trace
45	x	60	Total 60	C 60	0	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. 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: 30S 16S RIBOSOMAL RNA
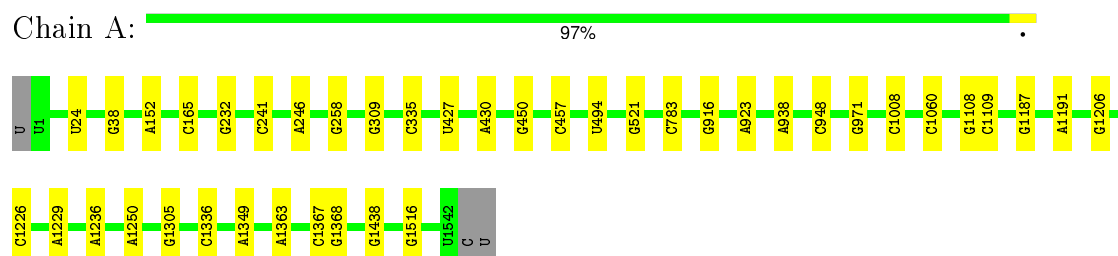
Chain A:

- Molecule 2: T-RNA(PHE)
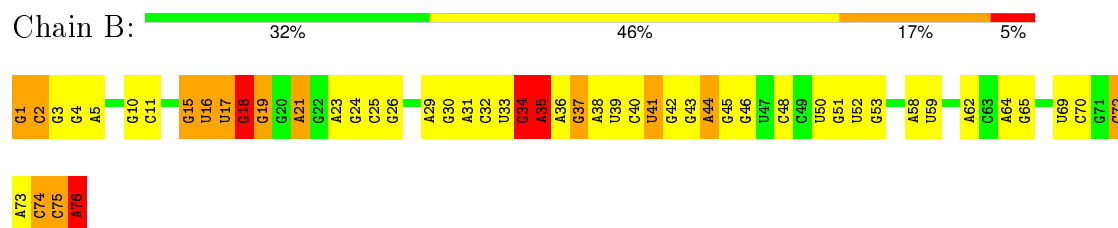
Chain B:

- Molecule 3: A- AND P-SITE MESSENGER RNA CODONS
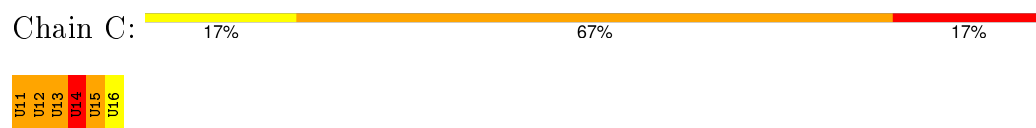
Chain C:

- Molecule 4: 50S 23S RIBOSOMAL RNA
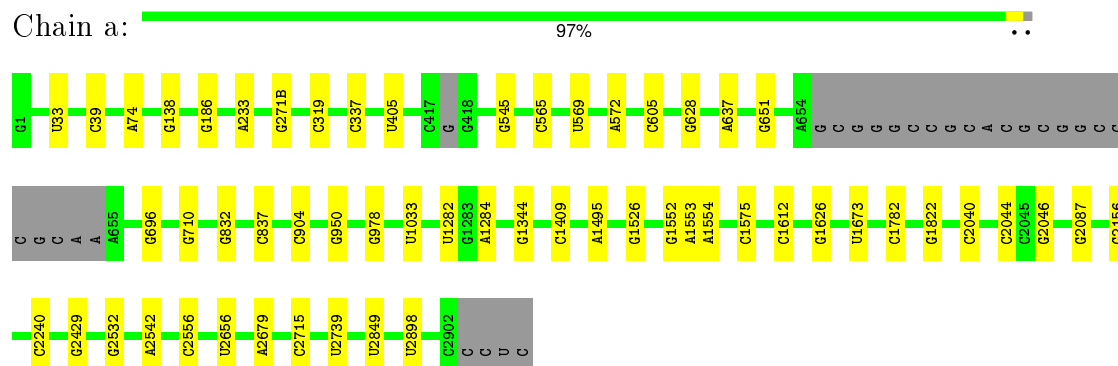
Chain a:

• Molecule 5: 50S 5S RIBOSOMAL RNA

Chain b:

98%

A-1 C32 C42 U120
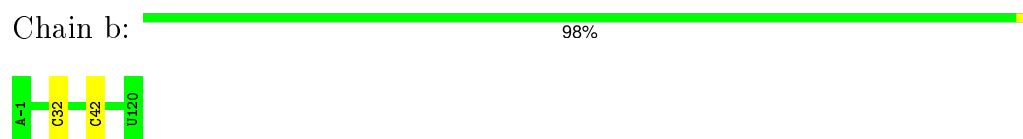
• Molecule 6: Peptide chain release factor 2

Chain Z:

96%

MET PHE GLU I4 D19 G76 Q112 G160 F207 D208 S209 D227 H253 V254 N255 N283 K362 A363 G364 L365
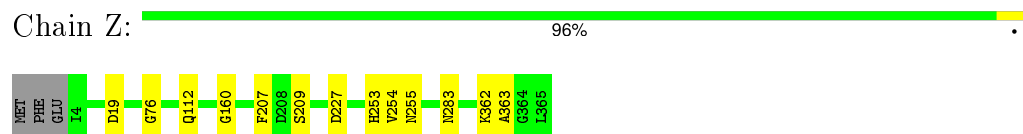
• Molecule 7: 30S RIBOSOMAL PROTEIN S2

Chain E:

90% 9%

MET PRO VAL GLU ILE THR V7 E35 M83 R130 K133 Q240 GLU GLU ALA THR GLU THR PRO GLU GLY GLU SER GLU VAL ALA
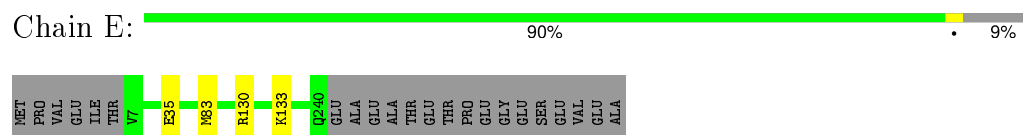
• Molecule 8: 30S RIBOSOMAL PROTEIN S3

Chain F:

84% 14%

MET G2 E19 R40 I57 R88 P174 G194 V207 ILE GLY GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU PRO LYS ALA GLU GLU ARG PRO ARG ARG ARG PRO ALA VAL ARG VAL LYS LYS GLU GLU
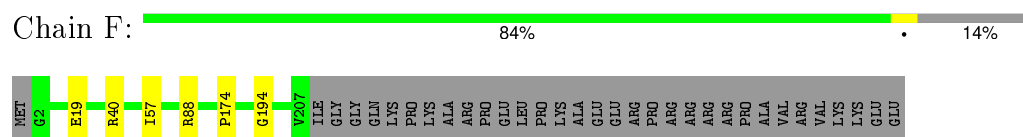
• Molecule 9: 30S RIBOSOMAL PROTEIN S4

Chain G:

96%

MET G2 P7 L21 P40 D102 V133 P142 S152 I204 R209
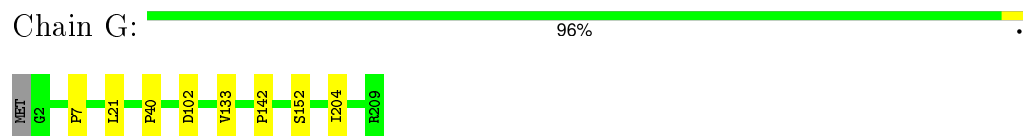
• Molecule 10: 30S RIBOSOMAL PROTEIN S5

Chain H:

91% 7%

MET PRO GLU THR D5 T16 A21 G74 G154 GLU ALA HIS ALA GLN ALA GLN GLY
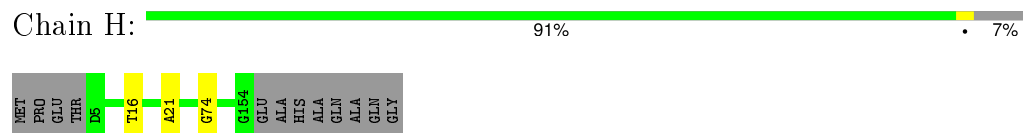
• Molecule 11: 30S RIBOSOMAL PROTEIN S6

Chain I:

96%

M1 Q16 G44 Y50 A101
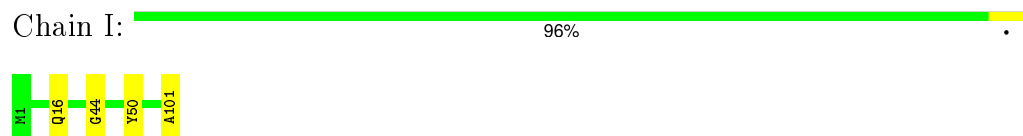
• Molecule 12: 30S RIBOSOMAL PROTEIN S7

Chain J:

97%

MET A2 R3 R4 A7 R143 M144 W156

• Molecule 13: 30S RIBOSOMAL PROTEIN S8

Chain K: 99%

M1 E49 P72 W138
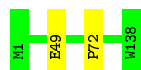
• Molecule 14: 30S RIBOSOMAL PROTEIN S9

Chain L: 96%

MET E2 D60 G68 K113 Y114 R128

• Molecule 15: 30S RIBOSOMAL PROTEIN S10

Chain M: 88% 6% 7%

MET PRO K3 A18 E25 G52 P53 H62 F63 T100 VAL GLY GLY GLY ARG

• Molecule 16: 30S RIBOSOMAL PROTEIN S11

Chain N: 89% 8%

MET ALA LYS LYS PRO SER LYS LYS LYS VAL K11 I32 I48 A72 S101 S129

• Molecule 17: 30S RIBOSOMAL PROTEIN S12

Chain O: 89% 8%

MET VAL ALA LEU P5 V18 V43 E73 K119 A128 ALA LYS THR ALA ALA LYS LYS

• Molecule 18: 30S RIBOSOMAL PROTEIN S13

Chain P: 96%

MET A2 N62 T109 G112 T116 K126

• Molecule 19: 30S RIBOSOMAL PROTEIN S14

Chain Q: 87% 11%

MET A2 A10 P54 G55 V56 R57 K58 A59 S60 W61
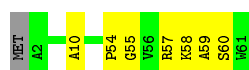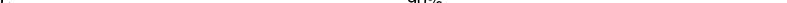
- Molecule 20: 30S RIBOSOMAL PROTEIN S15

Chain R:

- Molecule 21: 30S RIBOSOMAL PROTEIN S16

Chain S:

- Molecule 22: 30S RIBOSOMAL PROTEIN S17

Chain T:

- Molecule 23: 30S RIBOSOMAL PROTEIN S18

Chain U:
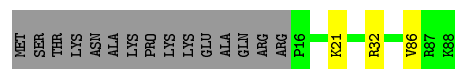
- Molecule 24: 30S RIBOSOMAL PROTEIN S19

Chain V:
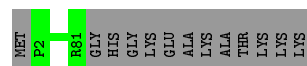
- Molecule 25: 30S RIBOSOMAL PROTEIN S20

Chain W:

- Molecule 26: 30S RIBOSOMAL PROTEIN THX

Chain X:
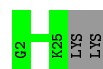
- Molecule 27: 50S RIBOSOMAL PROTEIN L1

Chain c:

PRO LYS HIS GLY K5 I152 I153 G176 F208 T215 I224 S228

• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain d: 96%

Q60 R86 L139 A216 ARG GLY THR LYS TRP P222 G237
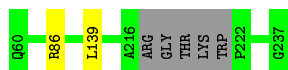
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain e: 55% 43%

PRO GLN PRO SER ARG PRO ARG LYS GLY SER LEU GLY PHE GLY PRO ARG LYS ARG SER THR SER GLU THR PRO ARG PHE ASN TRP PRO SER ASP ASP GLY GLN PRO GLY V38 T49 HIS VAL VAL LEU VAL ASN ASP GLU ASN SER P61 M65 GLU E66 E87 ASP THR

PRO TYR GLY Q93 L112 SER ASP ARG LEU ASP HIS ALA LEU ASP VAL GLU ASP GLN ILE ARG ASP ALA HIS GLY ASP LEU GLY LEU LEU ILE THR HIS VAL PRO ASP ALA VAL PRO SER VAL PRO LYS LYS LYS PRO ASP TYR VAL ASN ASN GLU SER ASN

GLY GLY SER VAL S171 D172 G185 N190 ASP I192 K208 R247 G274 ASP GLU PRO THR VAL ASP GLY GLY PHE VAL ASN TYR GLY ILE VAL ASP G291 K297 K305 R312 PRO A314 Q320 PRO ARG LEU ASP PRO GLU VAL ARG TYR VAL ASN ASN GLU SER ASN

GLN GLY

• Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain f: 75% 23%

M1 D7 LEU ASP GLY N11 P19 H69 VAL PRO LYS LEU ASP GLY ARG ALA ARG R79 K85 P92 L100 D120 ALA LEU VAL ALA ASP ARG GLY HIS GLU PHE ASP ARG ASP GLU GLU VAL PRO V138 R168 ALA ASP GLU THR LYS ILE LYS ALA GLY GLN GLY

SER ALA ARG GLY ARG LYS TYR ARG ARG PRO ALA SER ILE L193 P225 GLY ALA PRO G230 R246
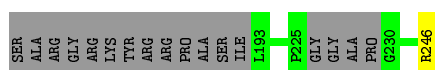
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain g: 67% 31%

SER SER GLU SER GLU SER GLY GLY ASP F10 V22 H29 GLY GLY ARG ASP LEU A35 N36 A37 D39 V73 G107 VAL GLU GLU HIS THR GLU PHE PRO SER GLN GLU TYR ASP PRO SER ILE ILE TYR GLY L128 R156 LEU ASN PRO ALA ASP ALA VAL ALA PHE

ILE GLU THR ASP TYR ASP GLU VAL GLU VAL SER GLU
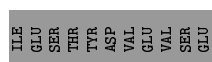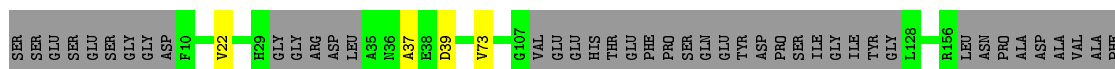
• Molecule 32: 50S RIBOSOMAL PROTEIN L6

Chain h: 92% 7%

SER ARG VAL GLY LYS LYS P7 D56 K100 L170 LYS GLU GLU LYS THR GLY LYS

• Molecule 33: 50S RIBOSOMAL PROTEIN L11

Chain l: 94% • 6%

MET ALA LYS LYS VAL ALA ALA Q8 S89 V140 ASP
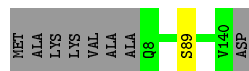
• Molecule 34: 50S RIBOSOMAL PROTEIN L13

Chain m: 79% • 19%

MET SER VAL A4 E28 E34 A44 P88 HIS X90 D110 GLU ASP GLY GLU VAL LEU ASP GLY THR SER LEU ARG LEU ASN ILE LYS PHE VAL T131 A141 ASN LYS THR TRP
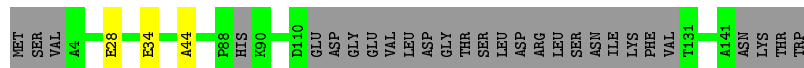
• Molecule 35: 50S RIBOSOMAL PROTEIN L14

Chain n: 97% •

M1 Q4 S14 R64 R94 I122
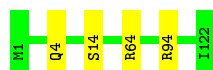
• Molecule 36: 50S RIBOSOMAL PROTEIN L15

Chain o: 49% • 49%

THR SER LYS LYS ARG GLN ARG GLY SER ARG THR HIS GLY GLY SER HIS LYS ASN ARG ARG GLY ALA GLY HIS ARG GLY GLY ARG GLY ASP ALA GLY ARG ASP LYS HIS PHE HIS ASN HIS GLU PRO LEU GLY LYS LYS SER GLY F51 E83 VAL GLU ASP GLY GLY PHE ARG

VAL D92 V96 VAL GLU GLU A100 V108 A111 L145 GLY GLU GLU ARG GLN ALA GLU GLU GLU THR GLU ASP ALA ASP ALA ASP GLU GLU
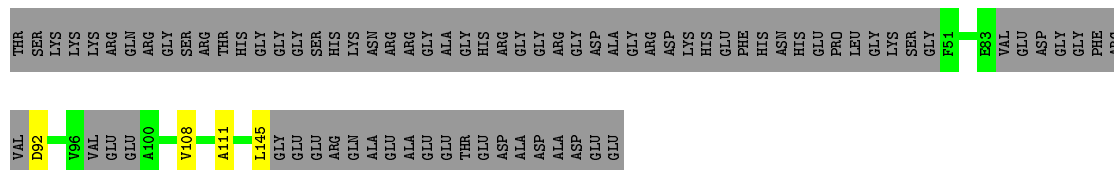
• Molecule 37: 50S RIBOSOMAL PROTEIN L16

Chain p: 98% •

S9 V72 N127 P128 A157
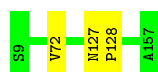
• Molecule 38: 50S RIBOSOMAL PROTEIN L18

Chain q: 59% • 39%

ALA THR GLY PRO ARG TYR LYS VAL P9 L24 R37 T49 LEU GLY P52 E72 ALA P74 T75 G76 ASN MET PRO S80 L86 P111 GLY SER K114 I129 PRO HIS ASN ASP ASP VAL LEU ALA ASP TRP GLN ARG THR ARG GLY ALA HIS ILE ALA GLU TYR ASP GLU

GLN LEU GLU GLU PRO LEU TYR SER GLY ASP PHE ASP ALA ALA ASP LEU PRO GLU HIS PHE ASP GLU LEU ARG GLU THR LEU LEU ASP GLY ASP ILE GLU LEU
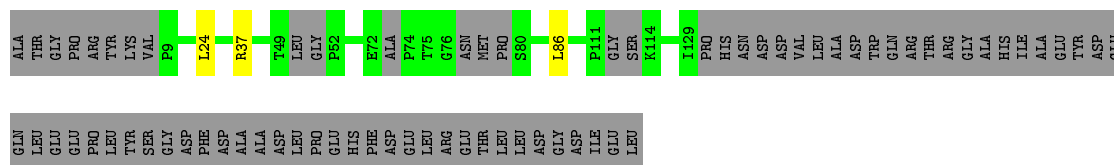
• Molecule 39: 50S RIBOSOMAL PROTEIN L19

Chain r: 79% 21%

PRO ARG THR R4 L42 GLY R44 R56 GLY GLU ALA GLY GLU ALA GLU ASP GLU ALA
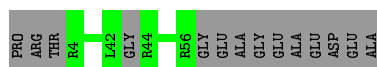
• Molecule 40: 50S RIBOSOMAL PROTEIN L22

Chain s: 96%   • •

M1 K110 HIS GLY LYS

• Molecule 41: 50S RIBOSOMAL PROTEIN L23

Chain t: 90%   10%

S1 F20 GLN N22 D73 ALA Q75 A78 SER ARG ILE GLY VAL PHE
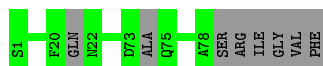
• Molecule 42: 50S RIBOSOMAL PROTEIN L24

Chain u: 88%   •   8%

S1 K6 Y35 G36 GLN ARG ASN V40 A44 V96 L101 E113 SER GLU ASP ASP SER ALA

• Molecule 43: 50S RIBOSOMAL PROTEIN L25

Chain v: 95%   5%

M1 R9 LYS GLU Q12 S17 ARG R19 G32 GLY K34 H80 PRO Y82 A94
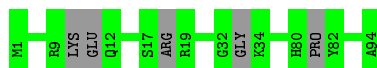
• Molecule 44: 50S RIBOSOMAL PROTEIN L29

Chain w: 87%   •   9%

T1 Q6 E7 R31 ALA V33 R55 D85 LEU GLN GLU ASN GLU
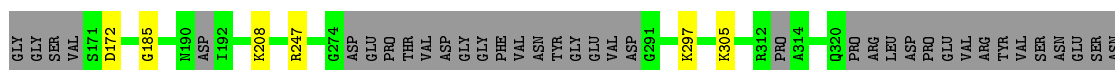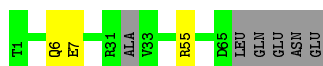
• Molecule 45: 50S RIBOSOMAL PROTEIN L30

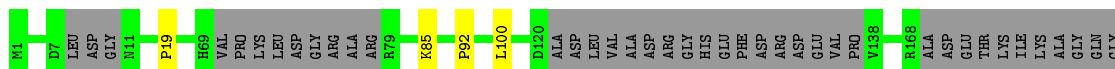Chain x: 97%   •

M1 P16 R55 E60

4 Experimental information ⓘ

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	phase flipping CTF correction of each particle as function of position in the micrograph	Depositor
Microscope	FEI/PHILIPS CM200FEG/ST	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	1000	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 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
2	B	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
3	C	2.34	5/131 (3.8%)	2.47	3/200 (1.5%)
All	All	1.53	12/1618 (0.7%)	1.57	25/2515 (1.0%)

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	B	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	74	C	O3'-P	-26.96	1.28	1.61
2	B	75	C	O3'-P	-25.74	1.30	1.61
2	B	44	A	O3'-P	-16.95	1.40	1.61
2	B	72	C	O3'-P	-15.83	1.42	1.61
3	C	14	U	O3'-P	-12.23	1.46	1.61

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	13	U	P-O3'-C3'	27.70	152.94	119.70
2	B	35	A	P-O3'-C3'	27.03	152.14	119.70
2	B	74	C	O3'-P-O5'	24.45	150.46	104.00
2	B	35	A	OP1-P-O3'	14.59	137.30	105.20
2	B	72	C	O3'-P-O5'	13.95	130.50	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	18	G	Sidechain
2	B	19	G	Sidechain
2	B	62	A	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	1519	0	0	15	24
2	B	1652	0	862	67	29
3	C	120	0	61	11	1
4	a	2889	0	0	0	52
5	b	123	0	0	0	2
6	Z	362	0	0	23	7
7	E	234	0	0	0	4
8	F	206	0	0	2	4
9	G	208	0	0	2	8
10	H	150	0	0	1	2
11	I	101	0	0	0	4
12	J	155	0	0	0	4
13	K	138	0	0	0	2
14	L	127	0	0	3	1
15	M	98	0	0	5	3
16	N	119	0	0	0	4
17	O	124	0	0	1	3
18	P	125	0	0	2	2
19	Q	60	0	0	5	3
20	R	88	0	0	0	4
21	S	83	0	0	0	1
22	T	104	0	0	0	4
23	U	73	0	0	0	3
24	V	80	0	0	0	0
25	W	99	0	0	0	2
26	X	24	0	0	0	0
27	c	224	0	0	0	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	d	173	0	0	0	2
29	e	191	0	0	0	6
30	f	189	0	0	0	5
31	g	122	0	0	0	4
32	h	164	0	0	0	2
33	l	133	0	0	0	1
34	m	117	0	0	0	3
35	n	122	0	0	0	4
36	o	84	0	0	0	4
37	p	138	0	0	0	3
38	q	113	0	0	0	3
39	r	52	0	0	0	0
40	s	110	0	0	0	1
41	t	76	0	0	0	0
42	u	110	0	0	0	6
43	v	89	0	0	0	0
44	w	64	0	0	0	3
45	x	60	0	0	0	2
All	All	11392	0	923	98	117

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 12.

The worst 5 of 98 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)
2:B:73:A:H3'	6:Z:255:ASN:CA	1.33	1.51
1:A:430:A:P	9:G:7:PRO:CA	2.16	1.34
2:B:73:A:C3'	6:Z:255:ASN:CA	2.05	1.33
2:B:1:G:N2	2:B:2:C:H41	1.22	1.32
2:B:1:G:N2	2:B:2:C:N4	1.77	1.30

The worst 5 of 117 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:904:C:P	4:a:2715:C:P[1_657]	0.14	2.06
1:A:241:C:P	29:e:172:ASP:CA[1_435]	0.38	1.82
4:a:1552:G:P	7:E:35:GLU:CA[1_574]	0.41	1.79
2:B:40:5MC:C2	4:a:1673:U:P[1_546]	0.47	1.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:A:P	15:M:53:PRO:CA[1_563]	0.57	1.63

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/1522	-	-
2	B	75/76 (98%)	13 (17%)	3 (4%)
3	C	5/6 (83%)	1 (20%)	0
4	a	0/2916	-	-
5	b	0/123	-	-
All	All	80/4643 (1%)	14 (17%)	3 (3%)

5 of 14 RNA backbone outliers are listed below:

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

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	16	H2U
2	B	18	G
2	B	35	A

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

14 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	B	10	2	18,26,27	1.05	1 (5%)	21,38,41	2.70	4 (19%)
2	H2U	B	16	2	17,21,22	0.80	1 (5%)	23,30,33	1.08	2 (8%)
2	H2U	B	17	2	17,21,22	0.76	0	23,30,33	1.04	2 (8%)
2	M2G	B	26	2	18,27,28	1.23	3 (16%)	22,40,43	2.22	2 (9%)
2	OMC	B	32	2	15,22,23	0.76	0	20,31,34	0.63	0
2	OMG	B	34	3,2	18,26,27	1.26	1 (5%)	21,38,41	2.87	3 (14%)
2	YG	B	37	2	28,42,43	1.01	2 (7%)	28,62,65	2.27	8 (28%)
2	PSU	B	39	2	15,21,22	1.24	2 (13%)	16,30,33	3.40	2 (12%)
2	5MC	B	40	2	14,22,23	0.90	1 (7%)	17,32,35	0.97	2 (11%)
2	7MG	B	46	2	20,26,27	1.12	2 (10%)	23,39,42	2.35	2 (8%)
2	5MC	B	49	2	14,22,23	0.80	0	17,32,35	1.06	2 (11%)
2	5MU	B	54	2	13,22,23	1.07	1 (7%)	16,32,35	4.96	2 (12%)
2	PSU	B	55	2	15,21,22	1.45	3 (20%)	16,30,33	3.22	4 (25%)
2	1MA	B	58	2	15,25,26	3.16	3 (20%)	15,37,40	2.34	2 (13%)

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	B	10	2	-	0/5/27/28	0/3/3/3
2	H2U	B	16	2	-	0/7/38/39	0/2/2/2
2	H2U	B	17	2	-	0/7/38/39	0/2/2/2
2	M2G	B	26	2	-	0/7/29/30	0/3/3/3
2	OMC	B	32	2	-	0/5/27/28	0/2/2/2
2	OMG	B	34	3,2	-	0/5/27/28	0/3/3/3
2	YG	B	37	2	-	0/20/42/43	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	B	39	2	-	0/7/25/26	0/2/2/2
2	5MC	B	40	2	-	0/3/25/26	0/2/2/2
2	7MG	B	46	2	-	0/7/37/38	0/3/3/3
2	5MC	B	49	2	-	0/3/25/26	0/2/2/2
2	5MU	B	54	2	-	0/3/25/26	0/2/2/2
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	1MA	B	58	2	-	0/3/25/26	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39	PSU	C6-C5	-3.25	1.33	1.38
2	B	55	PSU	C6-C5	-2.95	1.34	1.38
2	B	26	M2G	C8-N7	-2.14	1.30	1.34
2	B	40	5MC	C6-C5	-2.14	1.34	1.40
2	B	55	PSU	O4'-C1'	-2.01	1.41	1.44

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	C5-C4-N3	-13.32	114.17	125.35
2	B	34	OMG	C5-C6-N1	-9.40	111.24	123.52
2	B	26	M2G	C5-C6-N1	-9.03	111.72	123.52
2	B	10	2MG	C5-C6-N1	-8.94	111.83	123.52
2	B	46	7MG	C5-C6-N1	-7.36	112.43	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	10	2MG	3	0
2	B	16	H2U	3	0
2	B	17	H2U	3	1
2	B	26	M2G	6	0
2	B	32	OMC	1	0
2	B	34	OMG	4	0
2	B	37	YG	7	2
2	B	39	PSU	1	1
2	B	40	5MC	3	2

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	46	7MG	0	1
2	B	58	1MA	0	1

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.