



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 4, 2017 – 03:12 PM EST

PDB ID : 6AZ1
EMDB ID: : EMD-7024
Title : Cryo-EM structure of the small subunit of Leishmania ribosome bound to paromomycin
Authors : Shalev-Benami, M.; Zhang, Y.; Rozenberg, H.; Matzov, D.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on : unknown
Resolution : 2.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

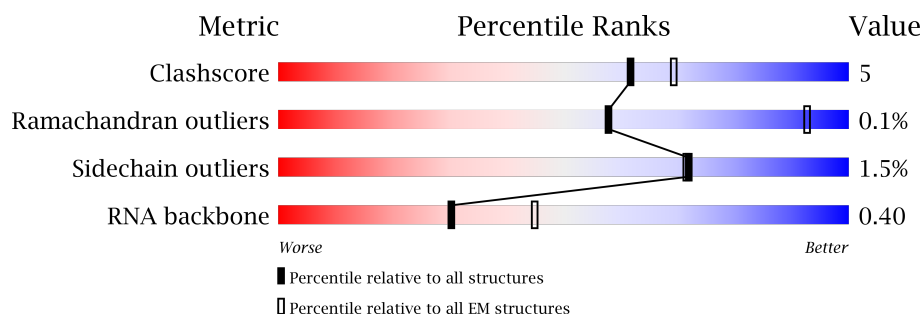
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.








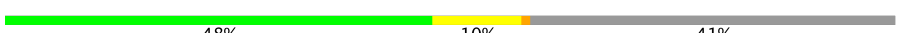











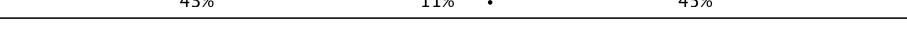







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	264	68% 17% 15%
2	B	246	75% 11% 14%
3	C	219	81% 16% .
4	D	190	88% 7% .
5	E	273	80% 15% 5%
6	F	265	73% 10% 17%
7	G	249	84% 11% . .
8	H	190	88% 8% . .

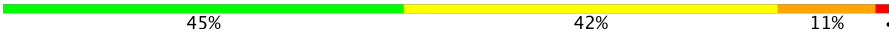


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Mol	Chain	Length	Quality of chain
9	I	200	
10	J	130	
11	K	220	
12	L	149	
13	M	116	
14	N	153	
15	O	144	
16	P	143	
17	Q	141	
18	R	153	
19	S	57	
20	T	151	
21	U	173	
22	V	143	
23	W	152	
24	X	179	
25	Y	159	
26	Z	137	
27	a	120	
28	b	112	
29	c	86	
30	d	87	
31	e	66	
32	f	152	
33	g	312	

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Mol	Chain	Length	Quality of chain
34	1	2203	
35	2	76	
36	3	77	
37	4	76	
38	5	13	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	OMG	1	509	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 80594 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 protein called Ribosomal protein s1e.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	3	0
			1829	1147	350	320	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	GLY	conflict	UNP E9BRS2

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	211	Total	C	N	O	S	2	0
			1676	1066	306	292	12		

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	212	Total	C	N	O	S	5	0
			1668	1059	307	289	13		

- Molecule 4 is a protein called ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	182	Total	C	N	O	S	1	0
			1504	948	304	244	8		

- Molecule 5 is a protein called ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	2	0
			2029	1292	395	333	9		

- Molecule 6 is a protein called ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	220	Total	C	N	O	S	0	0
			1656	1062	298	286	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	4	THR	ALA	conflict	UNP E9BNF0
F	8	GLN	-	insertion	UNP E9BNF0
F	10	ALA	ASN	conflict	UNP E9BNF0
F	12	ALA	GLY	conflict	UNP E9BNF0
F	13	ALA	VAL	conflict	UNP E9BNF0
F	14	ASP	GLU	conflict	UNP E9BNF0
F	15	VAL	ALA	conflict	UNP E9BNF0

- Molecule 7 is a protein called ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	238	Total	C	N	O	S	1	0
			1796	1123	366	304	3		

- Molecule 8 is a protein called ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	184	Total	C	N	O	S	1	0
			1438	893	283	255	7		

- Molecule 9 is a protein called ribosomal protein S7e.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	200	Total	C	N	O	S	0	0
			1613	1033	303	270	7		

- Molecule 10 is a protein called ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	129	Total	C	N	O	S	0	0
			1014	643	188	175	8		

- Molecule 11 is a protein called ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	183	Total	C	N	O	S	0	0
			1403	885	294	222	2		

- Molecule 12 is a protein called ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1127	724	209	191	3		

- Molecule 13 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	102	Total	C	N	O	S	1	0
			809	505	149	153	2		

- Molecule 14 is a protein called ribosomal protein S10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	91	Total	C	N	O	S	1	0
			728	473	127	123	5		

- Molecule 15 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	137	Total	C	N	O	S	2	0
			1032	637	205	183	7		

- Molecule 16 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	142	Total	C	N	O	S	3	0
			1134	716	229	186	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	18	ARG	CYS	conflict	UNP E9BFB6
P	34	ALA	SER	conflict	UNP E9BFB6
P	36	LYS	ARG	conflict	UNP E9BFB6
P	127	SER	ASN	conflict	UNP E9BFB6

- Molecule 17 is a protein called ribosomal protein S12e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O	S	0	0
			746	462	130	149	5		

- Molecule 18 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	142	Total	C	N	O	S	0	0
			1080	680	210	186	4		

- Molecule 19 is a protein called ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	54	Total	C	N	O	S	0	0
			441	272	90	73	6		

- Molecule 20 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	142	Total	C	N	O	S	0	0
			1153	727	228	190	8		

- Molecule 21 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	156	Total	C	N	O	S	0	0
			1241	786	249	201	5		

- Molecule 22 is a protein called ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	122	Total	C	N	O	S	1	0
			935	587	187	156	5		

- Molecule 23 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	110	Total	C	N	O	S	0	0
			822	530	158	130	4		

- Molecule 24 is a protein called ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	152	Total	C	N	O	S	1	0
			1202	765	235	198	4		

- Molecule 25 is a protein called ribosomal protein S21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	88	Total	C	N	O	S	0	0
			664	409	122	129	4		

- Molecule 26 is a protein called ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	127	Total	C	N	O	S	1	0
			1032	664	199	166	3		

- Molecule 27 is a protein called ribosomal protein S25e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	72	Total	C	N	O	S	0	0
			544	348	94	99	3		

- Molecule 28 is a protein called ribosomal protein S26e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	103	Total	C	N	O	S	0	0
			796	496	164	129	7		

- Molecule 29 is a protein called ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	84	Total	C	N	O	S	0	0
			656	407	128	113	8		

- Molecule 30 is a protein called ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	65	Total	C	N	O	S	0	0
			466	286	94	82	4		

- Molecule 31 is a protein called ribosomal protein S30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	59	Total	C	N	O	S	0	0
			449	280	97	71	1		

- Molecule 32 is a protein called ribosomal protein S31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	60	Total	C	N	O	S	0	0
			385	242	71	69	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	5	ILE	VAL	conflict	UNP E9BTC5

- Molecule 33 is a protein called LACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	300	Total	C	N	O	S	1	0
			2240	1410	395	423	12		

- Molecule 34 is a RNA chain called ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	1760	Total	C	N	O	P	0	0
			37613	16832	6780	12242	1759		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1539	M1Y	U	conflict	GB 322500086
1	1543	C4J	U	conflict	GB 322500086

- Molecule 35 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	76	Total	C	N	O	P	0	0
			1626	729	290	531	75		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1	G	-	expression tag	GB 1229082179

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Chain	Residue	Modelled	Actual	Comment	Reference
2	2	C	-	expression tag	GB 1229082179
2	3	G	-	expression tag	GB 1229082179
2	70	C	G	conflict	GB 1229082179

- Molecule 36 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	77	Total	C	N	O	P	0	0
			1639	732	297	534	76		

- Molecule 37 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	G	-	expression tag	GB 1229082179
4	2	C	-	expression tag	GB 1229082179
4	3	G	-	expression tag	GB 1229082179
4	70	C	G	conflict	GB 1229082179

- Molecule 38 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	12	Total	C	N	O	P	0	0
			251	113	43	83	12		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

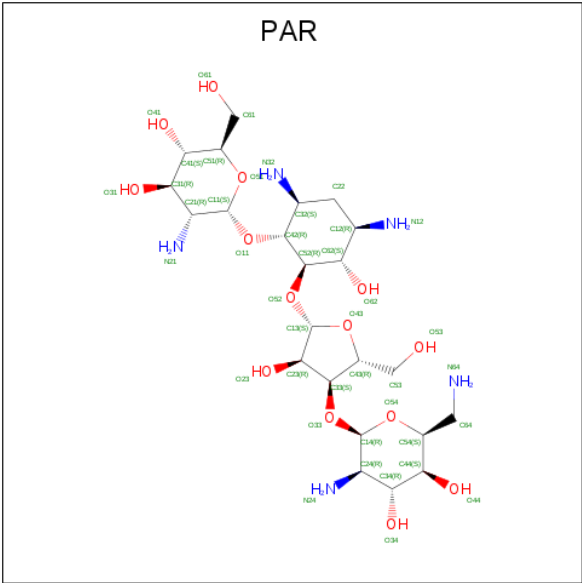
Mol	Chain	Residues	Atoms		AltConf
39	1	20	Total	Mg	0
			20	20	
39	D	1	Total	Mg	0
			1	1	
39	C	1	Total	Mg	0
			1	1	
39	5	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
39	S	1	Total	Mg	0
			1	1	

- Molecule 40 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				AltConf
40	1	1	Total	C	N	O	0
			252	138	30	84	
40	1	1	Total	C	N	O	0
			252	138	30	84	
40	1	1	Total	C	N	O	0
			252	138	30	84	
40	1	1	Total	C	N	O	0
			252	138	30	84	
40	1	1	Total	C	N	O	0
			252	138	30	84	
40	1	1	Total	C	N	O	0
			252	138	30	84	

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	D	2	Total	O	0
			2	2	
41	E	1	Total	O	0
			1	1	

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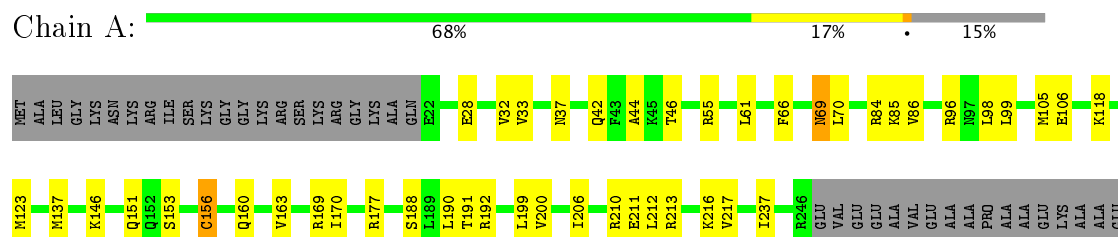
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Mol	Chain	Residues	Atoms		AltConf
41	F	3	Total 3	O 3	0
41	G	1	Total 1	O 1	0
41	H	1	Total 1	O 1	0
41	K	1	Total 1	O 1	0
41	L	1	Total 1	O 1	0
41	M	3	Total 3	O 3	0
41	O	1	Total 1	O 1	0
41	P	6	Total 6	O 6	0
41	R	2	Total 2	O 2	0
41	S	1	Total 1	O 1	0
41	T	4	Total 4	O 4	0
41	X	4	Total 4	O 4	0
41	Y	1	Total 1	O 1	0
41	Z	1	Total 1	O 1	0
41	b	1	Total 1	O 1	0
41	c	2	Total 2	O 2	0
41	f	1	Total 1	O 1	0
41	1	217	Total 217	O 217	0
41	2	2	Total 2	O 2	0
41	3	3	Total 3	O 3	0
41	5	3	Total 3	O 3	0

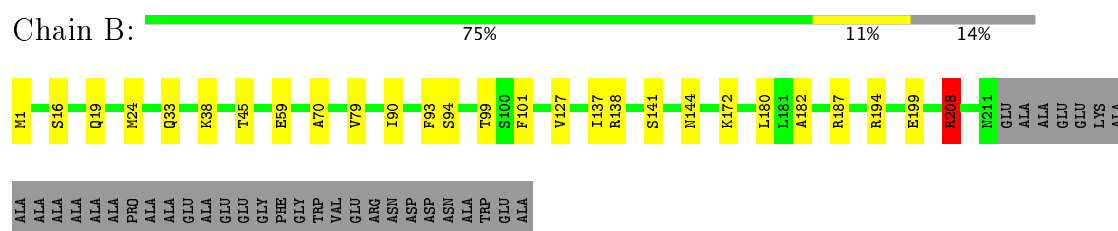
3 Residue-property plots

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

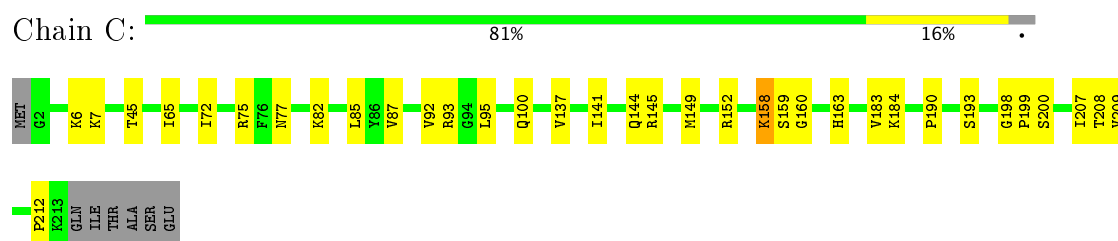
- Molecule 1: Ribosomal protein s1e



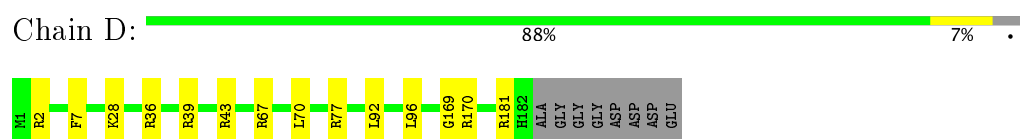
- Molecule 2: ribosomal protein S2



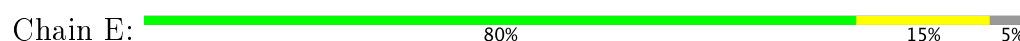
- Molecule 3: ribosomal protein S3



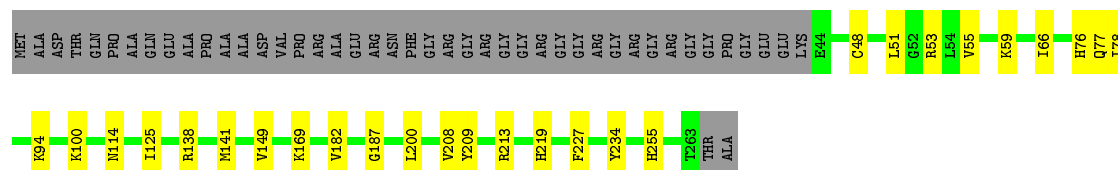
- Molecule 4: ribosomal protein S4



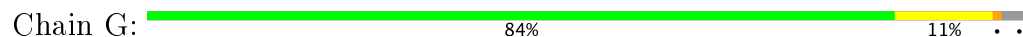
- Molecule 5: ribosomal protein S4e



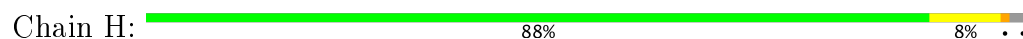
- Molecule 6: ribosomal protein S5



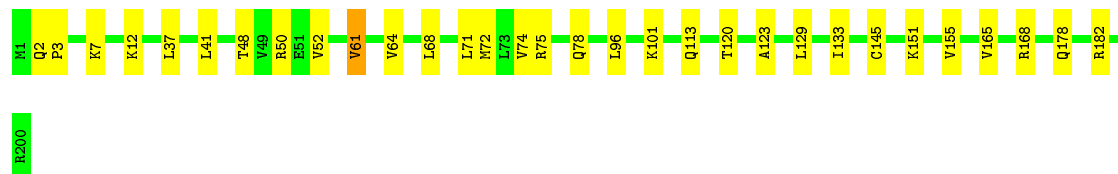
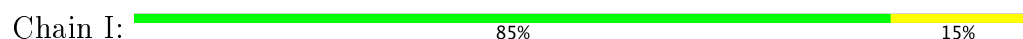
- Molecule 7: ribosomal protein S6e



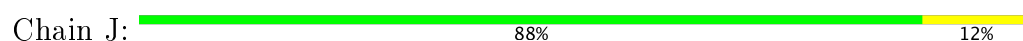
- Molecule 8: ribosomal protein S7



- Molecule 9: ribosomal protein S7e

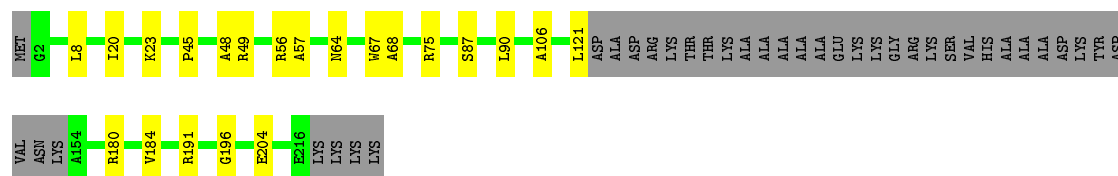


- Molecule 10: ribosomal protein S8




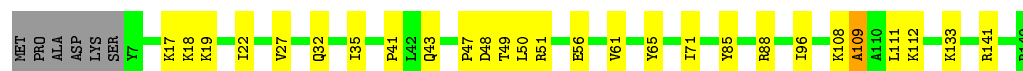
- Molecule 11: ribosomal protein S8e

Chain K: 



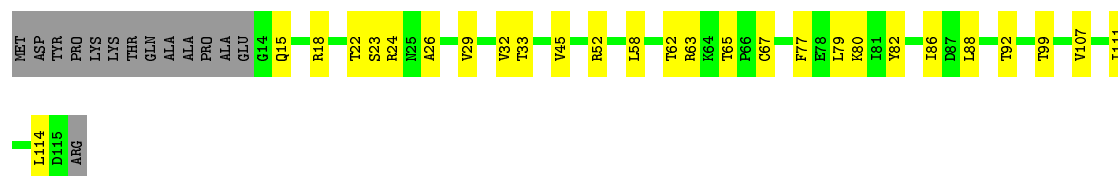
- Molecule 12: ribosomal protein S9

Chain L: 



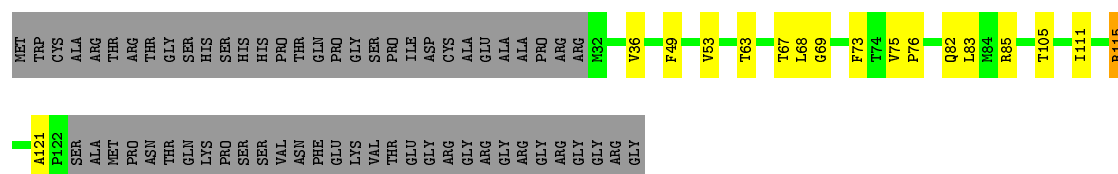
- Molecule 13: ribosomal protein S10

Chain M: 




- Molecule 14: ribosomal protein S10e

Chain N: 



- Molecule 15: ribosomal protein S11

Chain O: 



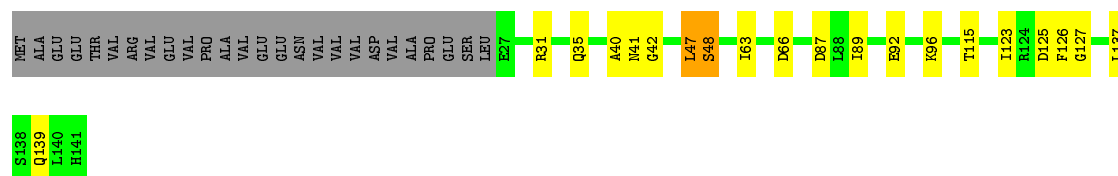
- Molecule 16: ribosomal protein S12

Chain P: 




- Molecule 17: ribosomal protein S12e

Chain Q: 



- Molecule 18: ribosomal protein S13

Chain R: 




- Molecule 19: ribosomal protein S14

Chain S: 




- Molecule 20: ribosomal protein S15

Chain T: 



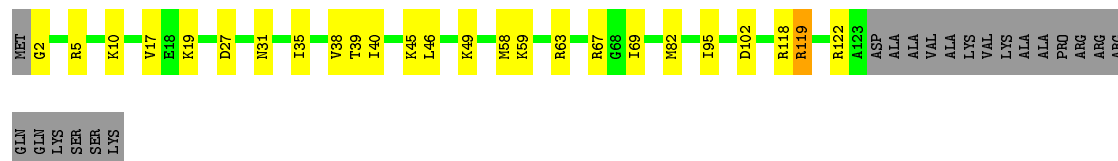
- Molecule 21: ribosomal protein S17

Chain U: 



- Molecule 22: ribosomal protein S17e

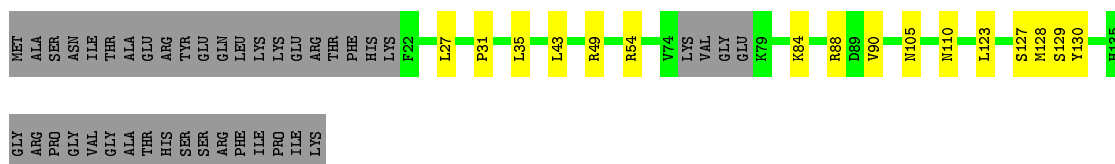
Chain V: 



- Molecule 23: ribosomal protein S19

Chain W: 





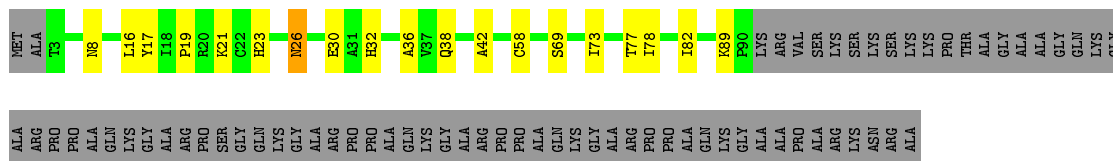
- Molecule 24: ribosomal protein S19e

Chain X: 77% 8% 15%



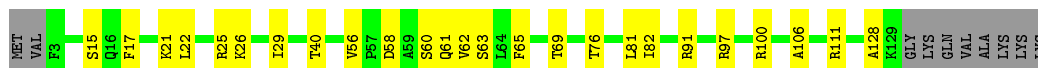
- Molecule 25: ribosomal protein S21e

Chain Y: 43% 11% 45%



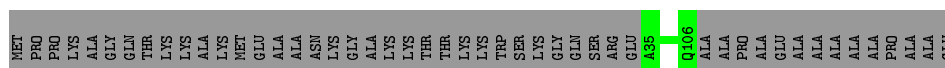
- Molecule 26: ribosomal protein S24e

Chain Z: 74% 18% 7%



- Molecule 27: ribosomal protein S25e

Chain a: 60% 40%



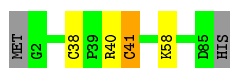
- Molecule 28: ribosomal protein S26e

Chain b: 88% 8%



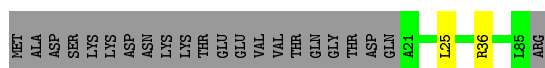
- Molecule 29: ribosomal protein S27e

Chain c: 93% 7%




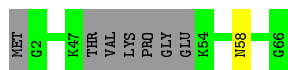
- Molecule 30: ribosomal protein S28e

Chain d:  72% 25%



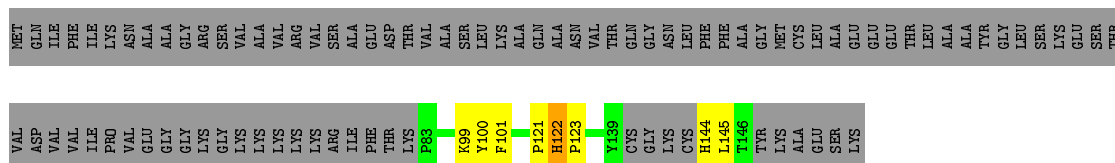
- Molecule 31: ribosomal protein S30e

Chain e:  88% 11%



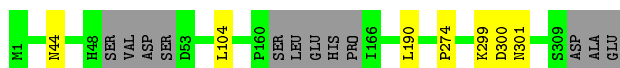
- Molecule 32: ribosomal protein S31e

Chain f:  34% 5% 61%



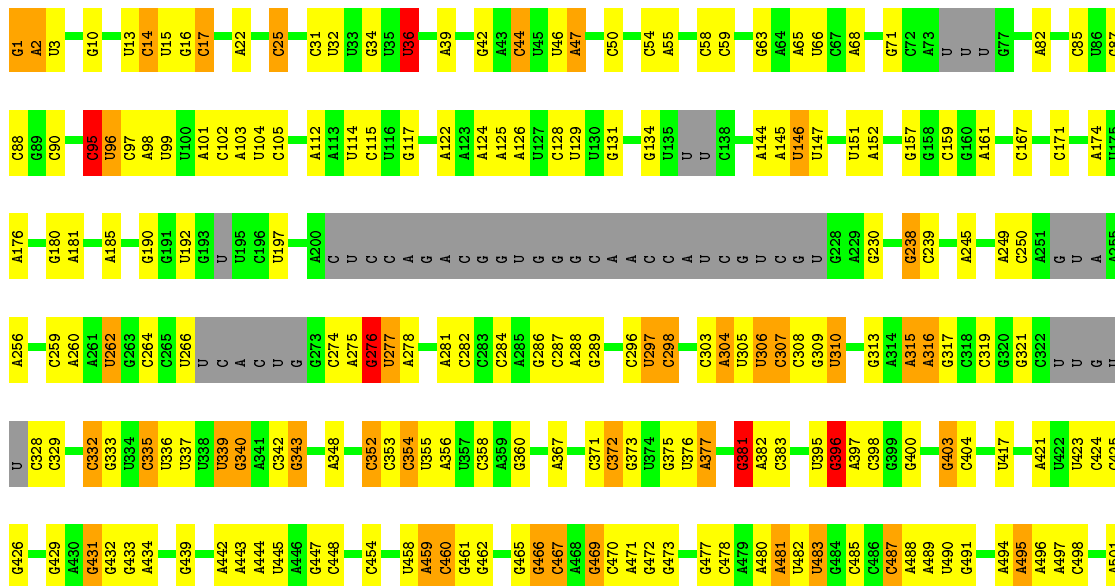
- Molecule 33: LACK1

Chain g:  94%

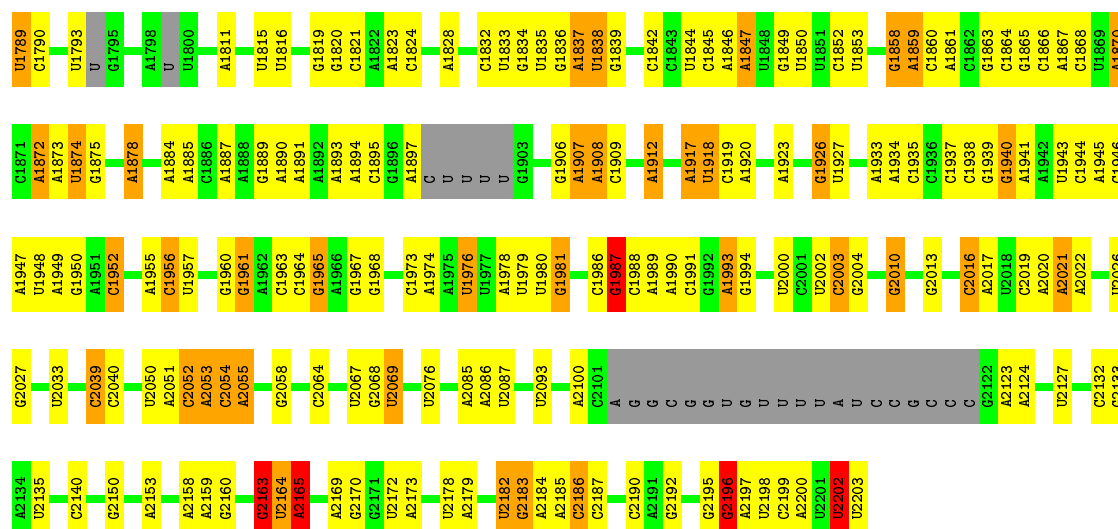


- Molecule 34: ribosomal RNA 18S

Chain 1:  42% 28% 8% 20%

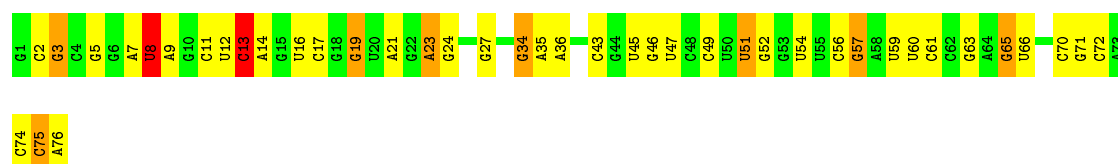


A1723	C1634	A1465	G1551	G1241	C1141	G	G	U	C657	A731	U569	A502
G1724	U1635	G1466	G1552	A1242	G1142	C	U	C	U658	U732	A570	C503
A	U1636	A	G1553	U1243	C	C	U	C	G659	G	A571	
A	U1637	C	A1554	G1244	A1145	G	C	C	U660	U	A572	U506
A	U1638	C	C1473	C	A1146	C	U	C	U661	G	C573	G507
C	U1639	G	U1559	A1248	A1147	A	G	U	G662	G	C574	A508
C	G1639	C	C	G1249	C	C	C	U	C575	U	C575	G509
C	G1640	C	C	A1250	A1152	C	U	U	G663	U738	A576	G510
C	U1641	C	C	G1251	A1153	G	U	U	C576	C	U577	
C	C1642	A	U1566	A1252	C	C	U	G	A668	C740	C578	G513
C	G1643	A1485	C	U1257	C1157	C	U	U	A669	C741	C579	C514
C	U1653	C1486	C	U	U	C	U	G	A670	C742	A580	
G	U1654	A1489	C	C1263	A1160	G	G	A	G671	A		A516
C	A1571	C	A	C1263	A1161	U	U	U	U672	U	G588	
C	C1572	A1490	C	G	A1162	C	C	U	U675	U	U589	G520
G	A1573	G	G	G1270	C1271	C	C	U	U676	C	A590	A521
G	G1574	A1493	C	A1272	A1173	A	C	U	C676	C	A591	A522
G	U1657	C	C	C	U	C	C	U	A685	U750	C592	A523
G	U1658	C	C	C	C	C	C	U	C686	G	A593	U524
G	U1659	C	C	C	C	C	C	U	U687	C	A594	A525
U	G1664	G1498	C	C1275	U1179	C	U	U	G688	G	G600	U529
U	A1576	C	U1577	C1276	C1180	C	U	G	U689	G	G601	U
U	G1578	C1500	C	G1277	C1181	C	U	U	G690	U759	A602	G
U	A1579	G	A	A1277	A1182	C	C	U	U691	C	A604	C
U	U1666	G1501	U	G1278	G1183	C	C	U	C692	C	U607	U
U	U1667	G1502	U	U1279	C1184	C	C	U	U693	C	U608	C
A	C1668	A1503	C	C	C	C	C	U	U694	C		C
C			C	C	C	C	C	U	G695	C		C
C	U1671	G1507	C	A1280	G1188	G	C	A972	U694	U		C
C	C1672	C1508	C	C1281	C1189	C	C	U	G695	C	A605	A
A	A1673	C	C	U1287	C1190	U	U	G	U696	U	G606	G
C			U	G1288	A1191	C	C	U	U697	C	U607	U
C	G1677	C	U	A1289	U1192	C	U	U	G	C763		C
U	A1678	C	U	C	C	C	C	U	C	A		C
U	G1679	A1594	C	U1290	U1196	C	C	U	C	A	C614	A
U	G1680	C	U	A1291	C	C	C	U	G	U	C615	U
C	A1681	U1520	C	G1295	A1199	C	C	U	C	U	A616	U
C	G1682	G1521	C	C	C	C	C	U	U	U	A617	U
C		G1522	C	U1298	C1206	C	C	A	U	U	C618	G
C	C1686	A1523	C	C	U1207	C	C	G	U	A	A619	G
G1760	A1687	G1524	U1425	U	C1212	C	C	G	A	C	C620	A
G1761	U1426	C1525	U1426	C	A1213	C	G	U	U	A770	C621	U
A1762	C1694	G1530	U	G	C1216	C	C	U	U	C771	C622	U
			U	C	A1217	C	A	U	C	A772	C623	G
G1765	U1698	U1533	C	C	U1365	C	C	U	C	A773	C624	U
G	A1699	C1534	C	C	C1368	C	C	U	G	C775	C625	C
G1700	U1610	U1535	C	C	U1369	C	C	U	U	A776	C626	A
U1610	U1610	A1536	C	C	U1370	U	C	C	U	A	U627	U553
A1702	U1703	U1537	G1615	U1537	U1371	C	C	U	U	G	A628	U554
G1770	U1703	U1538	A1616	C	U	C	C	U	C	U	A629	C555
A1771	A1706	?1539	A1617	?1539	U	C	C	U	G	U716	U630	C555
U1773	U1773	A1541	U1618	G1540	C	C	C	U	U	A	U631	A556
A1709	U1709	A1542	G1619	C	U1449	C	C	U	U	C	C632	A557
U1775	U1775	C1543	G1620	U1443	A1452	C	C	U	U	A	U558	G559
U1776	G1712	C1544	G1621	U1444	C1455	C	U	U	U	A783	C722	G562
U1777	C1713	A1545	G1622	U1445	U1455	C	U	A	C	C784	C723	G563
	C1714	U1546	C1626	G1460	A1546	C	C	A	G	G785	A724	A643
G1782	G1715	C1547	U1628	G1461	U1547	C	C	C	U	G786	U725	G564
C1783	A1716	G1462	U1628	G1462	C	C	C	U	G	G787	G	A564
	U1717	C1548	U1628	G1463	C	C	U	U	G	A788	U727	A565
A1787	A1718	C1549	G1629	U1463	U1463	C	C	U	U	U790	C729	U567
U1789				U1464	A1464	C	C	U	U	G791	G565	U569



• Molecule 35: tRNA-Phe

Chain 2: 45% 42% 11%



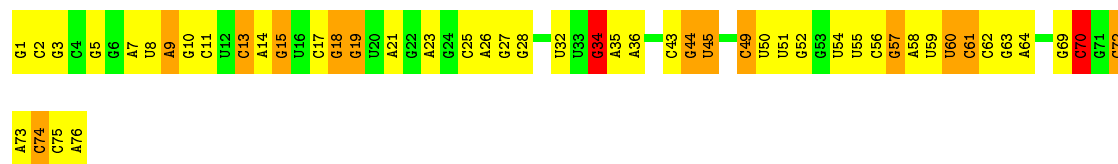
• Molecule 36: P-site tRNA

Chain 3: 62% 30% 8%



• Molecule 37: E-site tRNA

Chain 4: 34% 46% 17%



• Molecule 38: mRNA

Chain 5: 54% 38% 8%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	141028	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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, PAR, OMG, OMU, MA6, MIA, MG, 5MC, M1Y, 4OC, 7MG, A2M, C4J

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.52	0/1860	0.69	2/2503 (0.1%)
10	J	0.64	0/1031	0.64	0/1382
11	K	0.55	0/1425	0.68	0/1916
12	L	0.53	0/1148	0.68	1/1543 (0.1%)
13	M	0.41	0/819	0.69	0/1109
14	N	0.48	0/753	0.62	0/1024
15	O	0.57	0/1047	0.67	1/1408 (0.1%)
16	P	0.51	0/1163	0.75	4/1554 (0.3%)
17	Q	0.30	0/749	0.81	3/1028 (0.3%)
18	R	0.44	0/1099	0.65	0/1489
19	S	0.49	0/446	0.73	0/591
2	B	0.53	0/1713	0.64	1/2316 (0.0%)
20	T	0.60	0/1176	0.73	0/1577
21	U	0.60	0/1270	0.66	0/1710
22	V	0.40	0/945	0.60	0/1267
23	W	0.40	0/841	0.56	0/1144
24	X	0.51	0/1236	0.67	0/1659
25	Y	0.52	0/674	0.64	0/914
26	Z	0.47	0/1056	0.67	0/1407
27	a	0.45	0/549	0.66	0/743
28	b	0.68	1/813 (0.1%)	0.80	1/1092 (0.1%)
29	c	0.65	0/669	0.72	1/897 (0.1%)
3	C	0.46	0/1700	0.64	0/2274
30	d	0.41	0/468	0.76	1/630 (0.2%)
31	e	0.45	0/456	0.57	0/603
32	f	0.29	0/393	0.68	1/540 (0.2%)
33	g	0.44	0/2294	0.72	3/3131 (0.1%)
34	1	1.06	0/41155	1.23	426/64074 (0.7%)
35	2	0.46	0/1783	0.98	6/2776 (0.2%)
36	3	0.59	0/1831	1.04	8/2853 (0.3%)
37	4	0.43	1/1809 (0.1%)	1.16	22/2819 (0.8%)
38	5	1.00	0/279	1.29	3/431 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	D	0.48	0/1533	0.62	1/2057 (0.0%)
5	E	0.50	0/2074	0.70	1/2797 (0.0%)
6	F	0.51	0/1692	0.62	0/2295
7	G	0.41	0/1823	0.65	2/2449 (0.1%)
8	H	0.47	0/1460	0.68	1/1959 (0.1%)
9	I	0.58	0/1644	0.68	1/2217 (0.0%)
All	All	0.82	2/84876 (0.0%)	1.02	490/124178 (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
12	L	0	1
15	O	0	1
16	P	0	3
17	Q	0	1
19	S	0	2
2	B	0	2
21	U	0	2
26	Z	0	1
29	c	0	2
32	f	0	4
33	g	0	1
All	All	0	20

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	78	CYS	CB-SG	6.89	1.94	1.82
37	4	75	C	C1'-N1	5.14	1.56	1.48

The worst 5 of 490 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	78	CYS	CA-CB-SG	13.35	138.02	114.00
34	1	1956	C	N1-C2-O2	13.04	126.72	118.90
34	1	1973	C	N1-C2-O2	11.17	125.60	118.90
34	1	1956	C	N3-C2-O2	-10.96	114.23	121.90
34	1	1510	C	C2-N1-C1'	10.23	130.05	118.80

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	208[A]	ARG	Peptide
2	B	208[B]	ARG	Peptide
12	L	109	ALA	Peptide
15	O	97	ARG	Peptide
16	P	86	PRO	Peptide

5.2 Too-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 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	1829	0	1914	28	0
2	B	1676	0	1713	16	0
3	C	1668	0	1738	22	0
4	D	1504	0	1573	10	0
5	E	2029	0	2121	24	0
6	F	1656	0	1699	15	0
7	G	1796	0	1827	20	0
8	H	1438	0	1466	10	0
9	I	1613	0	1674	17	0
10	J	1014	0	1044	11	0
11	K	1403	0	1451	15	0
12	L	1127	0	1181	17	0
13	M	809	0	849	21	0
14	N	728	0	691	9	0
15	O	1032	0	1055	14	0
16	P	1134	0	1204	15	0
17	Q	746	0	647	10	0
18	R	1080	0	1067	12	0
19	S	441	0	451	13	0
20	T	1153	0	1219	13	0
21	U	1241	0	1255	8	0
22	V	935	0	961	21	0
23	W	822	0	801	13	0
24	X	1202	0	1230	9	0
25	Y	664	0	657	11	0
26	Z	1032	0	1101	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	a	544	0	566	0	0
28	b	796	0	810	0	0
29	c	656	0	661	0	0
30	d	466	0	476	0	0
31	e	449	0	476	0	0
32	f	385	0	293	0	0
33	g	2240	0	2094	0	0
34	1	37613	0	19015	314	0
35	2	1626	0	834	10	0
36	3	1639	0	837	8	0
37	4	1619	0	822	14	0
38	5	251	0	130	1	0
39	1	20	0	0	0	0
39	5	1	0	0	0	0
39	C	1	0	0	0	0
39	D	1	0	0	0	0
39	S	1	0	0	0	0
40	1	252	0	269	13	0
41	1	217	0	0	8	0
41	2	2	0	0	0	0
41	3	3	0	0	0	0
41	5	3	0	0	0	0
41	D	2	0	0	0	0
41	E	1	0	0	0	0
41	F	3	0	0	0	0
41	G	1	0	0	0	0
41	H	1	0	0	0	0
41	K	1	0	0	0	0
41	L	1	0	0	0	0
41	M	3	0	0	0	0
41	O	1	0	0	0	0
41	P	6	0	0	1	0
41	R	2	0	0	0	0
41	S	1	0	0	0	0
41	T	4	0	0	0	0
41	X	4	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	1	0
41	b	1	0	0	0	0
41	c	2	0	0	0	0
41	f	1	0	0	0	0
All	All	80594	0	59872	608	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 608 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)
34:1:489:A:N1	34:1:509:OMG:CM2	1.87	1.37
40:1:2305:PAR:O43	40:1:2305:PAR:C13	1.63	1.25
40:1:2302:PAR:C13	40:1:2302:PAR:O43	1.64	1.22
40:1:2304:PAR:O43	40:1:2304:PAR:C13	1.63	1.16
34:1:576:A:O2'	34:1:577:U:H5'	1.47	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/264 (86%)	209 (92%)	17 (8%)	0	100	100
2	B	211/246 (86%)	200 (95%)	11 (5%)	0	100	100
3	C	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	32	60
4	D	181/190 (95%)	176 (97%)	5 (3%)	0	100	100
5	E	260/273 (95%)	246 (95%)	14 (5%)	0	100	100
6	F	218/265 (82%)	206 (94%)	12 (6%)	0	100	100
7	G	237/249 (95%)	222 (94%)	15 (6%)	0	100	100
8	H	181/190 (95%)	173 (96%)	8 (4%)	0	100	100
9	I	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
10	J	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
11	K	179/220 (81%)	170 (95%)	9 (5%)	0	100	100
12	L	141/149 (95%)	127 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	101/116 (87%)	94 (93%)	7 (7%)	0	100	100
14	N	90/153 (59%)	85 (94%)	5 (6%)	0	100	100
15	O	137/144 (95%)	128 (93%)	9 (7%)	0	100	100
16	P	143/143 (100%)	134 (94%)	8 (6%)	1 (1%)	25	53
17	Q	113/141 (80%)	107 (95%)	6 (5%)	0	100	100
18	R	140/153 (92%)	131 (94%)	9 (6%)	0	100	100
19	S	52/57 (91%)	50 (96%)	2 (4%)	0	100	100
20	T	140/151 (93%)	132 (94%)	8 (6%)	0	100	100
21	U	154/173 (89%)	141 (92%)	13 (8%)	0	100	100
22	V	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
23	W	106/152 (70%)	100 (94%)	6 (6%)	0	100	100
24	X	151/179 (84%)	141 (93%)	10 (7%)	0	100	100
25	Y	86/159 (54%)	85 (99%)	1 (1%)	0	100	100
26	Z	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
27	a	70/120 (58%)	68 (97%)	2 (3%)	0	100	100
28	b	101/112 (90%)	96 (95%)	5 (5%)	0	100	100
29	c	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
30	d	63/87 (72%)	61 (97%)	2 (3%)	0	100	100
31	e	55/66 (83%)	52 (94%)	3 (6%)	0	100	100
32	f	56/152 (37%)	40 (71%)	14 (25%)	2 (4%)	4	9
33	g	295/312 (95%)	264 (90%)	30 (10%)	1 (0%)	44	73
All	All	4756/5531 (86%)	4466 (94%)	285 (6%)	5 (0%)	58	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	87	ASN
32	f	123	PRO
32	f	122	HIS
3	C	190	PRO
33	g	274	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/223 (88%)	191 (97%)	6 (3%)	46	76
2	B	180/202 (89%)	176 (98%)	4 (2%)	57	84
3	C	176/184 (96%)	172 (98%)	4 (2%)	56	84
4	D	158/164 (96%)	156 (99%)	2 (1%)	73	91
5	E	207/225 (92%)	203 (98%)	4 (2%)	62	87
6	F	170/208 (82%)	168 (99%)	2 (1%)	75	92
7	G	171/208 (82%)	166 (97%)	5 (3%)	48	77
8	H	149/159 (94%)	146 (98%)	3 (2%)	60	86
9	I	173/187 (92%)	170 (98%)	3 (2%)	66	88
10	J	108/111 (97%)	108 (100%)	0	100	100
11	K	130/176 (74%)	130 (100%)	0	100	100
12	L	113/120 (94%)	112 (99%)	1 (1%)	82	94
13	M	93/104 (89%)	93 (100%)	0	100	100
14	N	72/129 (56%)	70 (97%)	2 (3%)	49	79
15	O	103/113 (91%)	98 (95%)	5 (5%)	29	58
16	P	117/116 (101%)	113 (97%)	4 (3%)	42	73
17	Q	60/119 (50%)	60 (100%)	0	100	100
18	R	106/130 (82%)	105 (99%)	1 (1%)	82	94
19	S	47/49 (96%)	45 (96%)	2 (4%)	33	64
20	T	124/132 (94%)	123 (99%)	1 (1%)	85	95
21	U	128/150 (85%)	127 (99%)	1 (1%)	85	95
22	V	91/124 (73%)	88 (97%)	3 (3%)	43	73
23	W	78/131 (60%)	78 (100%)	0	100	100
24	X	122/147 (83%)	120 (98%)	2 (2%)	68	89
25	Y	72/117 (62%)	68 (94%)	4 (6%)	25	51
26	Z	109/118 (92%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	58/95 (61%)	58 (100%)	0	100	100
28	b	81/93 (87%)	78 (96%)	3 (4%)	39	70
29	c	72/76 (95%)	70 (97%)	2 (3%)	49	79
30	d	46/75 (61%)	45 (98%)	1 (2%)	57	84
31	e	43/54 (80%)	42 (98%)	1 (2%)	56	84
32	f	26/126 (21%)	24 (92%)	2 (8%)	15	34
33	g	232/266 (87%)	229 (99%)	3 (1%)	73	91
All	All	3812/4631 (82%)	3741 (98%)	71 (2%)	72	87

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	133	ILE
15	O	136[A]	LYS
31	e	58	ASN
12	L	133	LYS
15	O	59[A]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	11	GLN
16	P	63	ASN
31	e	60	GLN
12	L	32	GLN
14	N	82	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	1	1725/2203 (78%)	551 (31%)	35 (2%)
35	2	74/76 (97%)	29 (39%)	2 (2%)
36	3	76/77 (98%)	20 (26%)	0
37	4	75/76 (98%)	34 (45%)	2 (2%)
38	5	11/13 (84%)	2 (18%)	0
All	All	1961/2445 (80%)	636 (32%)	39 (1%)

5 of 636 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	1	2	A
34	1	3	U
34	1	14	C
34	1	17	C
34	1	22	A

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	1	915	A
34	1	1250	A
35	2	34	G
34	1	1108	A
34	1	1145	A

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

37 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	$\# Z > 2$
34	OMC	1	115	34	15,22,23	1.24	2 (13%)	19,31,34	1.27	2 (10%)
34	OMG	1	1464	34	18,26,27	1.66	3 (16%)	22,38,41	2.24	6 (27%)
34	OMG	1	1478	34	18,26,27	1.66	4 (22%)	22,38,41	2.18	4 (18%)
34	M1Y	1	1539	34	16,22,23	2.33	5 (31%)	21,32,35	2.59	5 (23%)
34	C4J	1	1543	34	16,29,30	1.82	4 (25%)	20,42,45	0.86	0
34	5MC	1	1544	34	15,22,23	1.40	3 (20%)	17,32,35	0.93	2 (11%)
34	OMG	1	1550	34	18,26,27	1.19	3 (16%)	22,38,41	2.22	6 (27%)
34	OMU	1	1621	34	14,22,23	1.18	1 (7%)	18,31,34	3.03	3 (16%)
34	OMG	1	1623	34	18,26,27	1.76	4 (22%)	22,38,41	2.07	3 (13%)
34	OMG	1	1647	34	18,26,27	1.76	4 (22%)	22,38,41	2.13	4 (18%)
34	OMU	1	1777	34	14,22,23	1.26	2 (14%)	18,31,34	2.98	3 (16%)
34	OMC	1	18	34	15,22,23	1.08	2 (13%)	19,31,34	1.30	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	OMG	1	1829	34	18,26,27	1.81	5 (27%)	22,38,41	2.10	3 (13%)
34	OMU	1	1833	34	14,22,23	0.89	1 (7%)	18,31,34	3.02	3 (16%)
34	OMG	1	1865	34	18,26,27	1.76	4 (22%)	22,38,41	2.14	4 (18%)
34	OMC	1	1866	34	15,22,23	1.35	2 (13%)	19,31,34	1.41	2 (10%)
34	OMU	1	1979	34	14,22,23	0.97	1 (7%)	18,31,34	2.81	2 (11%)
34	7MG	1	1995	36,34	20,26,27	1.52	3 (15%)	22,39,42	1.81	3 (13%)
34	A2M	1	2021	34	18,25,26	2.49	2 (11%)	20,36,39	1.37	5 (25%)
34	OMU	1	2048	34	14,22,23	1.04	2 (14%)	18,31,34	2.93	3 (16%)
34	4OC	1	2059	34	16,23,24	0.68	0	19,32,35	0.89	1 (5%)
34	5MC	1	2061	34	15,22,23	1.43	3 (20%)	17,32,35	1.12	2 (11%)
34	OMC	1	2140	34	15,22,23	0.76	0	19,31,34	1.26	2 (10%)
34	OMG	1	2151	34	18,26,27	1.69	2 (11%)	22,38,41	2.15	4 (18%)
34	MA6	1	2184	34	16,26,27	1.14	2 (12%)	18,38,41	3.53	4 (22%)
34	MA6	1	2185	34	16,26,27	1.13	1 (6%)	18,38,41	4.09	5 (27%)
34	A2M	1	28	34	18,25,26	2.45	3 (16%)	20,36,39	1.15	2 (10%)
34	OMU	1	33	34	14,22,23	1.29	2 (14%)	18,31,34	2.88	3 (16%)
34	OMC	1	38	34	15,22,23	1.00	1 (6%)	19,31,34	1.29	2 (10%)
34	A2M	1	479	34	18,25,26	2.43	3 (16%)	20,36,39	1.15	2 (10%)
34	OMG	1	509	34	18,26,27	1.24	2 (11%)	22,38,41	2.17	6 (27%)
34	OMU	1	661	34	14,22,23	1.08	1 (7%)	18,31,34	2.80	3 (16%)
34	A2M	1	668	34	18,25,26	2.89	4 (22%)	20,36,39	1.11	2 (10%)
34	OMU	1	8	34	14,22,23	1.06	0	18,31,34	2.77	3 (16%)
34	A2M	1	912	34	18,25,26	0.97	1 (5%)	20,36,39	1.71	2 (10%)
34	A2M	1	98	34	18,25,26	2.42	2 (11%)	20,36,39	1.23	3 (15%)
35	MIA	2	37	35	23,31,32	1.17	3 (13%)	25,44,47	1.32	3 (12%)

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
34	OMC	1	115	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1464	34	-	0/5/27/28	0/3/3/3
34	OMG	1	1478	34	-	0/5/27/28	0/3/3/3
34	MIY	1	1539	34	-	0/7/25/26	0/2/2/2
34	C4J	1	1543	34	-	0/12/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	5MC	1	1544	34	-	0/3/25/26	0/2/2/2
34	OMG	1	1550	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1621	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1623	34	-	0/5/27/28	0/3/3/3
34	OMG	1	1647	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1777	34	-	0/5/27/28	0/2/2/2
34	OMC	1	18	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1829	34	-	0/5/27/28	0/3/3/3
34	OMU	1	1833	34	-	0/5/27/28	0/2/2/2
34	OMG	1	1865	34	-	0/5/27/28	0/3/3/3
34	OMC	1	1866	34	-	0/5/27/28	0/2/2/2
34	OMU	1	1979	34	-	0/5/27/28	0/2/2/2
34	7MG	1	1995	36,34	-	0/7/37/38	0/3/3/3
34	A2M	1	2021	34	-	0/5/27/28	0/3/3/3
34	OMU	1	2048	34	-	0/5/27/28	0/2/2/2
34	4OC	1	2059	34	-	0/7/29/30	0/2/2/2
34	5MC	1	2061	34	-	0/3/25/26	0/2/2/2
34	OMC	1	2140	34	-	0/5/27/28	0/2/2/2
34	OMG	1	2151	34	-	0/5/27/28	0/3/3/3
34	MA6	1	2184	34	-	0/7/29/30	0/3/3/3
34	MA6	1	2185	34	-	0/7/29/30	0/3/3/3
34	A2M	1	28	34	-	0/5/27/28	0/3/3/3
34	OMU	1	33	34	-	0/5/27/28	0/2/2/2
34	OMC	1	38	34	-	0/5/27/28	0/2/2/2
34	A2M	1	479	34	-	0/5/27/28	0/3/3/3
34	OMG	1	509	34	-	0/5/27/28	0/3/3/3
34	OMU	1	661	34	-	0/5/27/28	0/2/2/2
34	A2M	1	668	34	-	0/5/27/28	0/3/3/3
34	OMU	1	8	34	-	0/5/27/28	0/2/2/2
34	A2M	1	912	34	-	0/5/27/28	0/3/3/3
34	A2M	1	98	34	-	0/5/27/28	0/3/3/3
35	MIA	2	37	35	-	0/11/33/34	0/3/3/3

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	668	A2M	O5'-C5'	-10.58	1.30	1.44
34	1	2021	A2M	O5'-C5'	-9.40	1.31	1.44
34	1	98	A2M	O5'-C5'	-9.32	1.31	1.44
34	1	28	A2M	O5'-C5'	-9.22	1.31	1.44
34	1	479	A2M	O5'-C5'	-8.81	1.32	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	2185	MA6	N3-C2-N1	-11.47	118.87	128.86
34	1	2185	MA6	N1-C6-N6	-10.86	105.47	117.00
34	1	2184	MA6	N3-C2-N1	-9.86	120.27	128.86
34	1	2184	MA6	N1-C6-N6	-9.23	107.20	117.00
34	1	1539	M1Y	C5-C4-N3	-8.20	118.71	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	1	1464	OMG	2	0
34	1	1621	OMU	2	0
34	1	1777	OMU	1	0
34	1	1979	OMU	2	0
34	1	2021	A2M	1	0
34	1	2184	MA6	1	0
34	1	2185	MA6	2	0
34	1	509	OMG	12	0
34	1	661	OMU	1	0
34	1	912	A2M	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 for Mogul analysis.

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
40	PAR	1	2302	-	45,45,45	3.60	9 (20%)	60,67,67	1.44	12 (20%)
40	PAR	1	2303	34	45,45,45	3.51	10 (22%)	60,67,67	1.85	11 (18%)
40	PAR	1	2304	-	45,45,45	3.65	9 (20%)	60,67,67	1.50	9 (15%)
40	PAR	1	2305	-	45,45,45	3.43	8 (17%)	60,67,67	1.54	11 (18%)
40	PAR	1	2306	-	45,45,45	3.52	9 (20%)	60,67,67	1.34	7 (11%)
40	PAR	1	2307	-	45,45,45	3.56	9 (20%)	60,67,67	1.12	2 (3%)

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
40	PAR	1	2302	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2303	34	-	1/18/94/94	0/4/4/4
40	PAR	1	2304	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2305	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2306	-	-	0/18/94/94	0/4/4/4
40	PAR	1	2307	-	-	0/18/94/94	0/4/4/4

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1	2304	PAR	C13-C23	-17.05	1.30	1.52
40	1	2302	PAR	C13-C23	-16.50	1.31	1.52
40	1	2307	PAR	C13-C23	-16.35	1.31	1.52
40	1	2303	PAR	C13-C23	-15.92	1.32	1.52
40	1	2306	PAR	C13-C23	-15.90	1.32	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	2303	PAR	C14-O33-C33	-6.50	102.17	118.00
40	1	2303	PAR	C31-C41-C51	-4.43	102.41	110.22
40	1	2304	PAR	C14-O33-C33	-3.72	108.93	118.00
40	1	2302	PAR	O11-C11-C21	-3.38	101.78	108.20
40	1	2304	PAR	C13-O52-C52	-3.14	110.34	118.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	1	2303	PAR	C52-O52-C13-C23

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	1	2302	PAR	1	0
40	1	2303	PAR	1	0
40	1	2304	PAR	3	0
40	1	2305	PAR	3	0
40	1	2306	PAR	3	0
40	1	2307	PAR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	960:C	O3'	961:U	P	10.63