



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 24, 2017 – 09:31 AM EDT

PDB ID : 5LZA
EMDB ID: : EMD-4121
Title : Structure of the 70S ribosome with SECIS-mRNA and P-site tRNA (Initial complex, IC)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : unknown
Resolution : 3.60 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-20029824

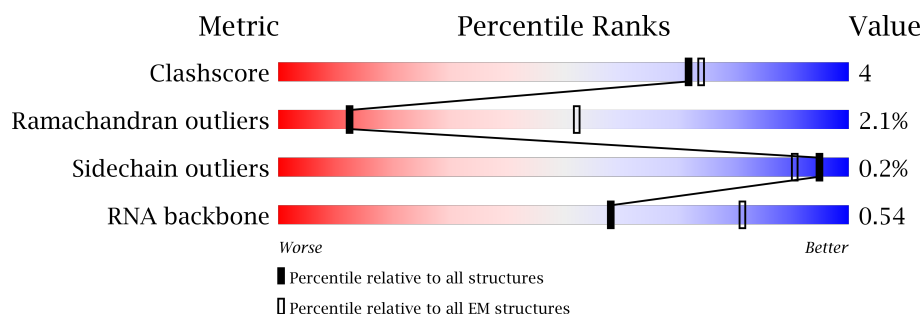
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.





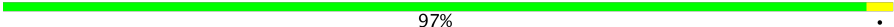

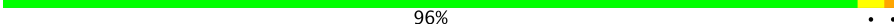
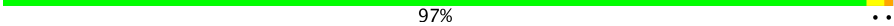
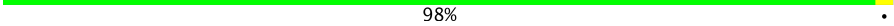
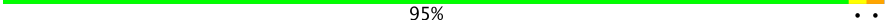
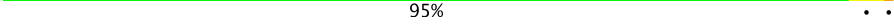

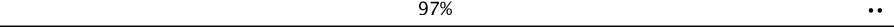
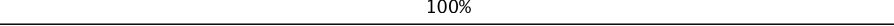
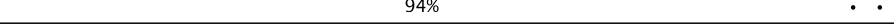












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	1539	74% 24% .
2	b	218	96% ..
3	c	206	100%
4	d	205	99% .
5	e	157	94% ..
6	f	100	93% 5% .
7	g	151	97% ..
8	h	129	98% .







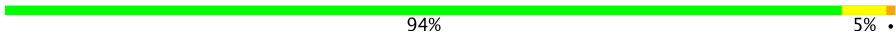















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Mol	Chain	Length	Quality of chain
9	i	127	 94% 6%
10	j	98	 93% 5% .
11	k	116	 97% .
12	l	123	 91% 8% .
13	m	114	 96% . .
14	n	100	 97% . .
15	o	88	 98% .
16	p	82	 95% . .
17	q	80	 95% . .
18	r	65	 91% 8% .
19	s	79	 97% . .
20	t	85	 100%
21	u	65	 94% . .
22	v	77	 68% 31% .
23	x	48	 52% 48%
24	A	2903	 61% 31% 8% .
25	B	120	 63% 29% 7% .
26	C	271	 84% 16%
27	D	209	 84% 16%
28	E	201	 86% 14%
29	F	177	 82% 18% .
30	G	176	 82% 15% . .
31	I	141	 89% 10% .
32	H	149	 91% 9% .
33	J	142	 87% 13%

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Mol	Chain	Length	Quality of chain
34	K	122	 77% 20% .
35	L	143	 85% 13% ..
36	M	136	 85% 15%
37	N	120	 89% 11%
38	O	116	 92% 7% .
39	P	114	 84% 16%
40	Q	117	 94% 5% .
41	R	103	 84% 16%
42	S	110	 88% 12%
43	T	93	 88% 12%
44	U	102	 85% 13% .
45	V	94	 84% 16%
46	W	75	 83% 17%
47	X	77	 84% 16%
48	Y	63	 86% 13% .
49	Z	58	 98%
50	0	56	 89% 9% .
51	1	50	 76% 20% .
52	2	46	 83% 17%
53	3	64	 88% 11% .
54	4	38	 87% 11% .
55	6	66	 79% 20% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
24	G7M	A	2069	X	-	-	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 146037 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	4	0
			33119	14778	6072	10726	1543		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2900	Total	C	N	O	P	1	0
			62296	27797	11464	20134	2901		

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	U	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 50 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

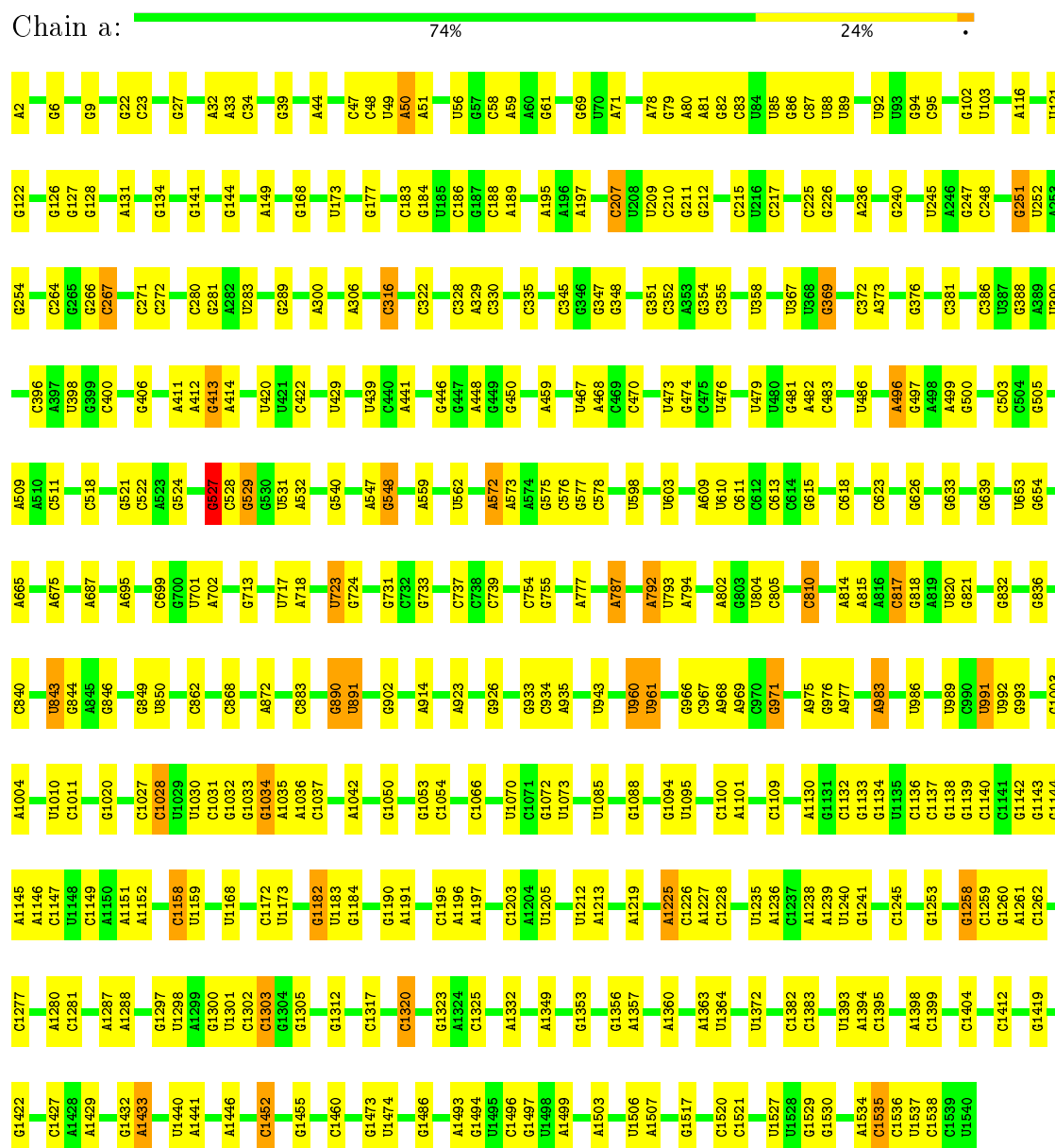
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total 1	Zn 1	0
56	6	1	Total 1	Zn 1	0

3 Residue-property plots

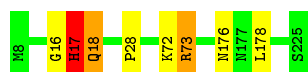
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: 16S ribosomal RNA



- Molecule 2: 30S ribosomal protein S2

Chain b:  96% ..



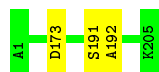
- Molecule 3: 30S ribosomal protein S3

Chain c:  100%



- Molecule 4: 30S ribosomal protein S4

Chain d:  99% .



- Molecule 5: 30S ribosomal protein S5

Chain e:  94% ..



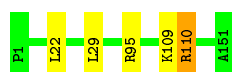
- Molecule 6: 30S ribosomal protein S6

Chain f:  93% 5% .



- Molecule 7: 30S ribosomal protein S7

Chain g:  97% ..



- Molecule 8: 30S ribosomal protein S8

Chain h:  98% .



- Molecule 9: 30S ribosomal protein S9

Chain i:  94% 6%



- Molecule 10: 30S ribosomal protein S10

Chain j: 93% 5% .



- Molecule 11: 30S ribosomal protein S11

Chain k: 97% .



- Molecule 12: 30S ribosomal protein S12

Chain l: 91% 8% .



- Molecule 13: 30S ribosomal protein S13

Chain m: 96% . .



- Molecule 14: 30S ribosomal protein S14

Chain n: 97% . .



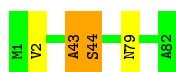
- Molecule 15: 30S ribosomal protein S15

Chain o: 98% .



- Molecule 16: 30S ribosomal protein S16

Chain p: 95% . .



- Molecule 17: 30S ribosomal protein S17

Chain q:  95% ..



- Molecule 18: 30S ribosomal protein S18

Chain r:  91% 8% .



- Molecule 19: 30S ribosomal protein S19

Chain s:  97% ..



- Molecule 20: 30S ribosomal protein S20

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 30S ribosomal protein S21

Chain u:  94% . .



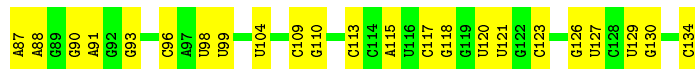
- Molecule 22: fMet-tRNA^{fMet}

Chain v:  68% 31% .



- Molecule 23: SECIS mRNA

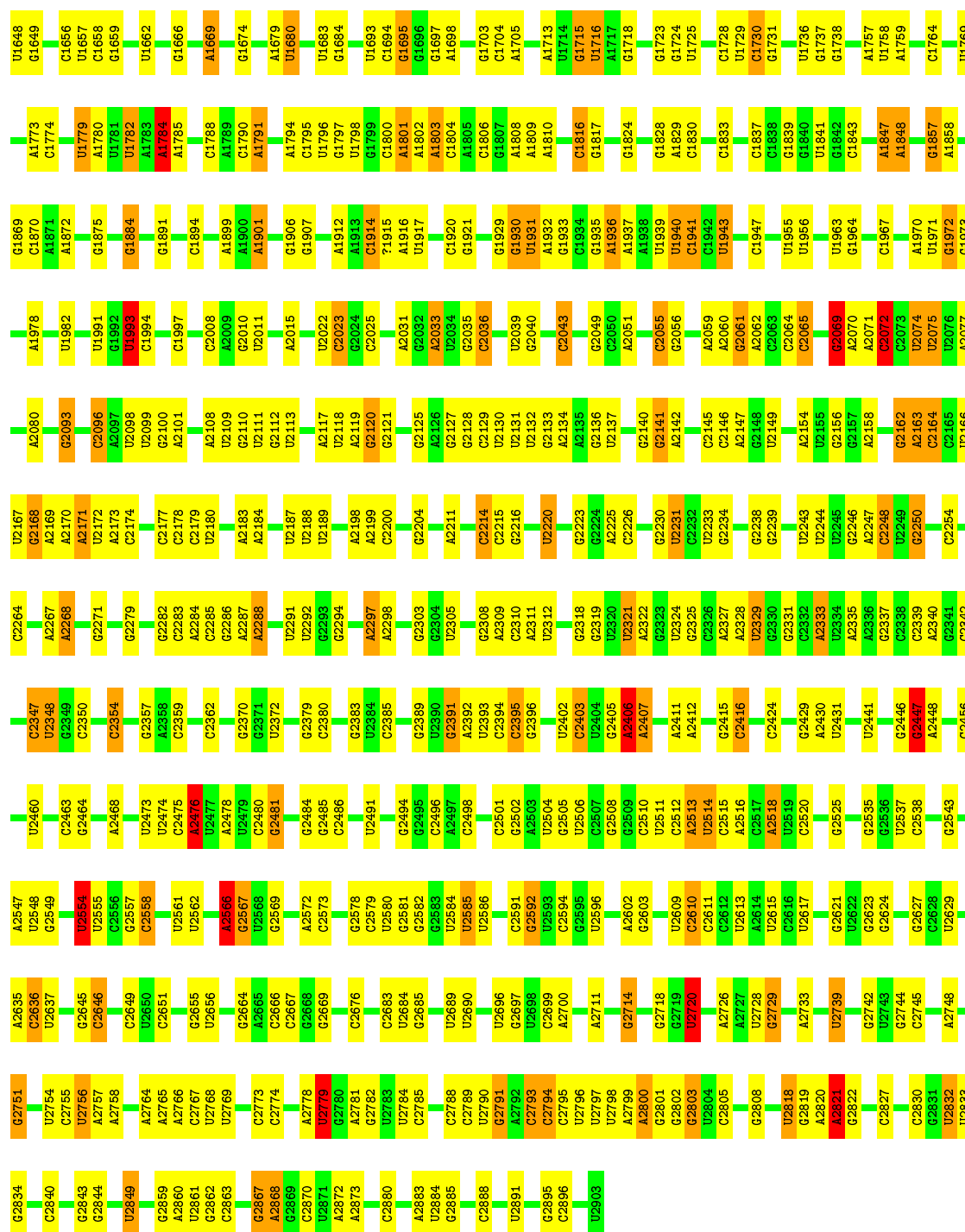
Chain x:  52% 48%



- Molecule 24: 23S ribosomal RNA

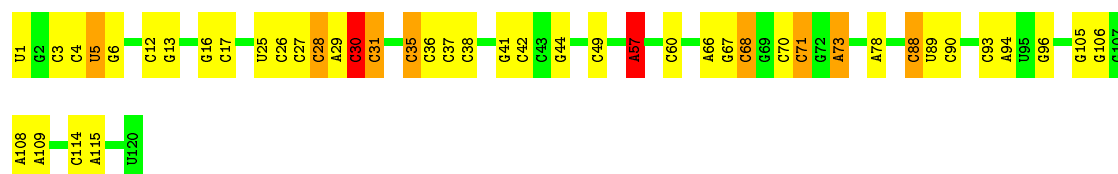
Chain A:  61% 31% 8% .

G1514	G1416	G1317	G1223	U1130	C1043	U846	C736	A627	C542	A412	U306	C208	G1
A1515	G1421	C1323	U1224	G1131	C1044	U847	G737	A632	G543	A415	G307	G214	G7
G1516	G1424	G1324	G1225	U1132	C1045	A849	G738	A633	U545	U416	A309	G215	C8
U1523	G1425	U1325	C1233	C1135	A1046	G856	A739	C635	U546	C420	A310	A216	G9
G1524	C1428	U1326	G1236	G1136	G1047	G857	C740	C636	A547	G424	A311	A219	C11
A1525	C1429	A1237	A1237	G1137	C1053	G858	U741	G636	G548	G424	C314	G220	U12
C1526	C1432	G1332	A1237	G1138	A1054	G859	A743	A637	G549	G424	C314	A221	A13
G1529	G1432	U1340	A1247	G1139	A1057	A866	U746	U639	G555	C435	G317	A222	A14
C1533	A1433	G1341	G1248	U1140	C961	A867	U747	C640	A556	G438	C318	U223	G15
U1534	A1434	A1342	U1249	U1141	G962	C867	U747		A557	A439	G319	A224	A16
A1535	G1435	G1343	G1250	A1142	C965	U868		A643	C557	G438	G320	U225	G17
C1536	G1436	C1344	C1251	A1143	C966	G869	A752	A644	G558	A439	A321	C225	A18
G1436	C1436	C1345	G1252	A1143	C967	U870	A752	C645	G559	A443	A322	C228	U19
C1437	C1437	C1346	A1253	A1151	C968	U871	C758	U646	C560	C444	C323	C229	U20
G1538	C1438	C1348	A1256	A1156	C969	U872	A764	G647	A563	C445	G327	U234	A28
U1539	U1443	A1353	G1257	A1159	U970	A877	A764	A654	A563	C445	G327	U234	A28
G1444	G1444	A1354	C1257	U1159	A973	A878	G771	A655	U566	C455	U328	A241	C32
C1446	C1446	G1259	G1259	A1067	G974	A878	G771	G656	U566	C455	A329	A241	C33
C1451	A1359	U1359	U1263	G1162	A983	G882	G774	U657	A572	A457	A330	U243	G35
C1454	G1360	G1361	A1264	A1165	A984	G883	G775	U657	A573	G458	C335	U244	G39
G1455	C1362	C1362	A1264	A1165	A985	U884	G776	C680	A574	G458	C335	U244	G40
C1566	A1365	A1269	A1269	A1169	C985	C885	G780	A668	A575	G469	A346	C245	G43
G1567	U1458	C1270	A1270	G989	G989	U	G781	G669	C581	G481	U349	G247	G44
C1568	G1459	A1271	C1075	A990	A990	C	A782	A670	A582	A482	A444	C248	G45
A1569	U1460	A1272	C1076	C991	C991	C	A783	C671	G583	A483	C353	G250	G46
C1461	U1461	U1273	A1077	C992	C992	C890	G784	C872	C584	C484	C353	A251	G46
U1570	C1461	A1274	U1078	U1175	U1078	G891	G785	C673	G585		G359	A251	G46
U1578	U1466	G1372	A1275	C995	C995	A892	G785	C673	G585		G359	A251	G46
U1584	U1474	C1376	A1276	A1178	A1080	C893	A789	A674	U588	C490	U360	A255	U50
C1585	G1475	A1377	C1278	C993	U082	U894	A794	A676	A361	G491	C361	A256	G51
C1600	G1478	U1379	G1279	U999	U083	A896	C795	A677	G589	G496	C363	C257	A52
G1601	G1482	A1383	A1287	G1182	A1084	C897	A800	C680	A592	U499	C364	G266	A53
A1614	U1487	C1386	G1288	U1183	A1085	A900	A800	U686	U593	G500	U365	C269	U62
C1615	A1616	A1387	C1290	U1188	A1088	C901	G805	U686	C595	A503	C366	A270	A63
U1624	A1490	U1396	U1294	A1189	A1089	C908	C806	C687	C595	A504	U369	G276	U67
G1627	C1493	C1399	G1300	G1190	U1097	A909	U807	C691	U598	A505	G370	A277	A71
G1628	C1499	U1402	A1301	G1191	U1097	A910	C812	C692	G600	A505	A371	A278	U72
U1629	G1500	A1403	A1302	C1200	C1104	A911	U813	A693	G600	G506	G372	A279	A73
G1633	A1504	C1404	A1303	A1205	U1105	C912	C814	U694	A603	C509	U373	U280	A74
A1634	A1505	U1406	C1305	G1206	G1110	C919	A819	G695	A603	C510	C383	C281	G75
U1636	U1506	G1407	C1306	A1206	A1111	A928	A819	C695	A608	U511	A384	A282	G75
A1637	C1507	G1410	G1311	G1210	G1112	U929	G831	C717	A609	C512	C385	G283	G61
G1643	A1508	G1410	U1312	C1211	G1116	A933	U832	U720	A613	C522	C386	G284	G61
C1646	A1509	U1412	U1313	A1213	G1116	U934	A833	A721	A614	C522	C386	U284	G61
U1647	G1510	C1414	C1314	U1119	U1119	C935	G834	A721	A621	A522	U387	G285	A84
C1648	U1513	C1414	U1315	C1221	U1119	U934	A844	G729	A621	A522	U387	G285	A84
U1649	U1514	C1414	U1315	C1221	U1119	U934	A844	G729	A621	A522	U387	G285	A84

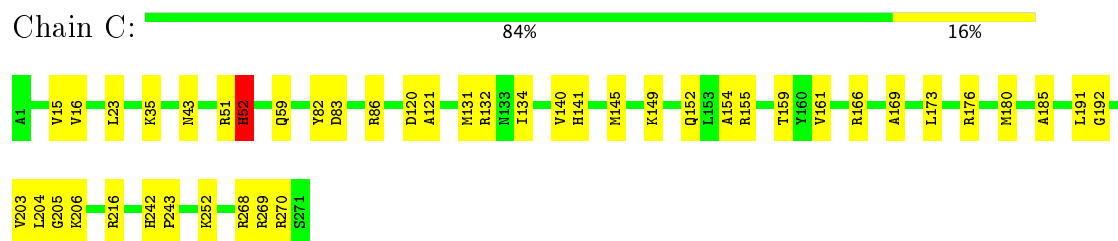


- Molecule 25: 5S ribosomal RNA

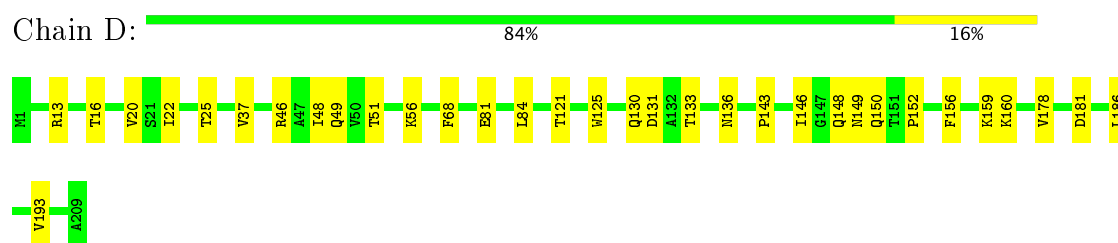
Chain B:



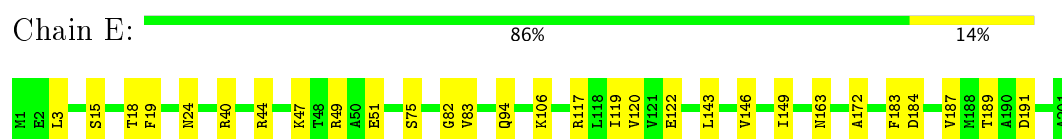
- Molecule 26: 50S ribosomal protein L2



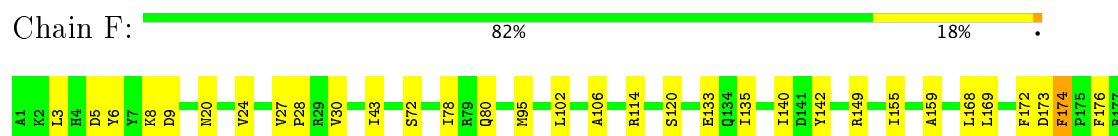
- Molecule 27: 50S ribosomal protein L3



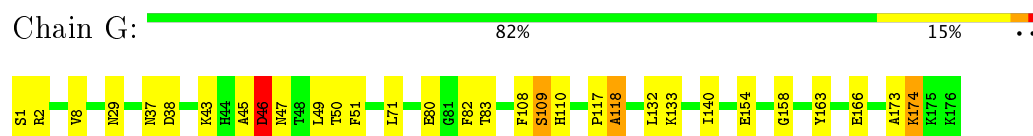
- Molecule 28: 50S ribosomal protein L4



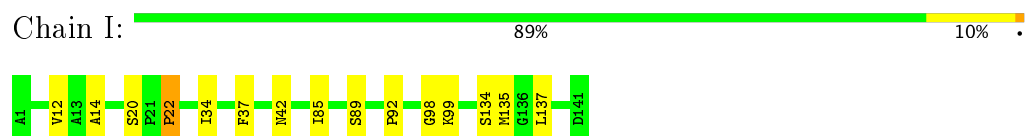
- Molecule 29: 50S ribosomal protein L5



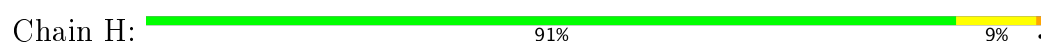
- Molecule 30: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L9





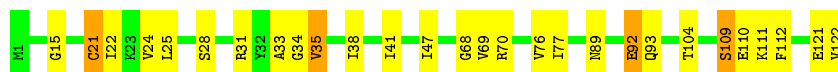
- Molecule 33: 50S ribosomal protein L13

Chain J: 87% 13%



- Molecule 34: 50S ribosomal protein L14

Chain K: 77% 20% .



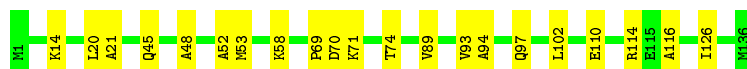
- Molecule 35: 50S ribosomal protein L15

Chain L: 85% 13% ..



- Molecule 36: 50S ribosomal protein L16

Chain M: 85% 15%



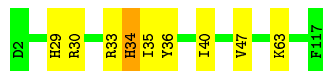
- Molecule 37: 50S ribosomal protein L17

Chain N: 89% 11%



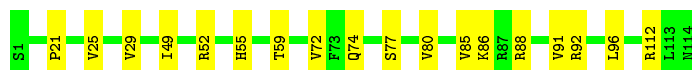
- Molecule 38: 50S ribosomal protein L18

Chain O: 92% 7% .



- Molecule 39: 50S ribosomal protein L19

Chain P: 84% 16%




- Molecule 40: 50S ribosomal protein L20

Chain Q:  94% 5%




- Molecule 41: 50S ribosomal protein L21

Chain R:  84% 16%




- Molecule 42: 50S ribosomal protein L22

Chain S:  88% 12%




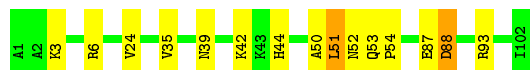
- Molecule 43: 50S ribosomal protein L23

Chain T:  88% 12%




- Molecule 44: 50S ribosomal protein L24

Chain U:  85% 13%




- Molecule 45: 50S ribosomal protein L25

Chain V:  84% 16%




- Molecule 46: 50S ribosomal protein L27

Chain W:  83% 17%



- Molecule 47: 50S ribosomal protein L28

Chain X:  84% 16%



- Molecule 48: 50S ribosomal protein L29

Chain Y:  86% 13%




- Molecule 49: 50S ribosomal protein L30

Chain Z:  98%



- Molecule 50: 50S ribosomal protein L32

Chain 0:  89% 9%




- Molecule 51: 50S ribosomal protein L33

Chain 1:  76% 20%




- Molecule 52: 50S ribosomal protein L34

Chain 2:  83% 17%




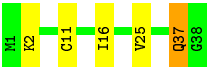
- Molecule 53: 50S ribosomal protein L35

Chain 3:  88% 11%

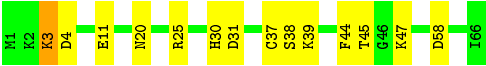


- Molecule 54: 50S ribosomal protein L36

Chain 4:  87% 11%



- Molecule 55: 50S ribosomal protein L31



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	75176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (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: 5MU, 3TD, ZN, OMG, 5MC, MA6, G7M, OMC, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 1MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.61	4/36803 (0.0%)	1.26	322/57406 (0.6%)
10	j	0.37	0/797	0.74	0/1077
11	k	0.40	0/886	0.71	0/1195
12	l	0.43	0/969	0.82	2/1300 (0.2%)
13	m	0.46	0/893	0.78	3/1193 (0.3%)
14	n	0.45	0/806	0.66	1/1074 (0.1%)
15	o	0.40	0/722	0.61	0/964
16	p	0.45	0/659	0.70	1/884 (0.1%)
17	q	0.45	0/658	0.78	1/881 (0.1%)
18	r	0.42	0/512	0.70	0/689
19	s	0.41	0/653	0.75	1/877 (0.1%)
2	b	0.43	0/1736	0.66	3/2338 (0.1%)
20	t	0.42	0/671	0.60	0/888
21	u	0.53	0/501	0.84	1/668 (0.1%)
22	v	0.55	1/1747 (0.1%)	1.29	19/2721 (0.7%)
23	x	0.58	1/1145 (0.1%)	1.09	1/1781 (0.1%)
24	A	0.66	9/69196 (0.0%)	1.26	616/107943 (0.6%)
25	B	0.59	1/2873 (0.0%)	1.25	29/4478 (0.6%)
26	C	0.48	0/2122	0.73	1/2852 (0.0%)
27	D	0.44	0/1586	0.67	0/2134
28	E	0.43	0/1571	0.63	0/2113
29	F	0.43	0/1435	0.71	2/1926 (0.1%)
3	c	0.40	0/1652	0.60	0/2225
30	G	0.42	0/1343	0.67	4/1816 (0.2%)
31	I	0.38	0/1046	0.61	0/1410
32	H	0.38	0/1122	0.63	0/1515
33	J	0.46	0/1152	0.61	0/1551
34	K	0.46	0/948	0.69	0/1268
35	L	0.44	0/1054	0.74	1/1403 (0.1%)
36	M	0.46	0/1093	0.72	1/1460 (0.1%)
37	N	0.44	0/974	0.65	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	O	0.42	0/902	0.59	0/1209
39	P	0.45	0/929	0.67	0/1242
4	d	0.43	0/1665	0.62	0/2227
40	Q	0.47	0/960	0.60	1/1278 (0.1%)
41	R	0.45	0/829	0.72	0/1107
42	S	0.40	0/864	0.62	0/1156
43	T	0.40	0/745	0.63	0/994
44	U	0.44	0/788	0.78	2/1051 (0.2%)
45	V	0.40	0/766	0.60	0/1025
46	W	0.41	0/582	0.62	0/769
47	X	0.38	0/635	0.59	0/848
48	Y	0.42	0/510	0.64	0/677
49	Z	0.40	0/453	0.60	0/605
5	e	0.44	0/1170	0.80	2/1573 (0.1%)
50	o	0.41	0/450	0.72	0/599
51	1	0.42	0/417	0.84	1/554 (0.2%)
52	2	0.41	0/380	0.67	0/498
53	3	0.47	0/513	0.65	0/676
54	4	0.67	1/303 (0.3%)	0.78	0/397
55	6	0.42	0/532	0.62	0/709
6	f	0.49	0/836	0.83	2/1128 (0.2%)
7	g	0.43	0/1196	0.70	3/1602 (0.2%)
8	h	0.42	0/989	0.66	0/1326
9	i	0.41	0/1034	0.69	0/1375
All	All	0.59	17/157773 (0.0%)	1.14	1020/235956 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
10	j	0	5
12	l	0	1
13	m	0	1
16	p	0	1
17	q	0	2
18	r	0	3
19	s	0	1
2	b	0	4
21	u	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	A	2	0
26	C	0	1
28	E	0	1
30	G	0	3
32	H	0	2
34	K	0	3
35	L	0	4
42	S	0	1
44	U	0	3
48	Y	0	1
5	e	0	4
50	0	0	2
51	1	0	1
53	3	0	1
6	f	0	1
7	g	0	2
8	h	0	1
9	i	0	1
All	All	4	51

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	x	87	A	OP3-P	-10.73	1.48	1.61
24	A	1	G	OP3-P	-10.59	1.48	1.61
25	B	1	U	OP3-P	-10.53	1.48	1.61
22	v	1	C	OP3-P	-10.52	1.48	1.61
1	a	2	A	OP3-P	-10.51	1.48	1.61

The worst 5 of 1020 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1313	U	N3-C2-O2	-14.71	111.90	122.20
24	A	2072	C	C6-N1-C2	-14.04	114.69	120.30
1	a	89	U	C5-C4-O4	-13.94	117.53	125.90
1	a	529	G	C5-C6-O6	-13.71	120.38	128.60
24	A	62	U	N1-C2-O2	13.14	132.00	122.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'

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Mol	Chain	Res	Type	Atom
24	A	2069	G7M	C4',C3'

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain,Peptide
2	b	72	LYS	Peptide
5	e	76	ASN	Peptide
5	e	88	HIS	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	33119	0	16685	0	0
2	b	1705	0	1732	0	0
3	c	1625	0	1699	0	0
4	d	1643	0	1710	0	0
5	e	1157	0	1199	0	0
6	f	818	0	808	0	0
7	g	1182	0	1240	0	0
8	h	979	0	1034	0	0
9	i	1022	0	1070	0	0
10	j	787	0	828	0	0
11	k	870	0	878	0	0
12	l	955	0	1019	0	0
13	m	884	0	944	0	0
14	n	794	0	836	0	0
15	o	714	0	737	0	0
16	p	649	0	666	0	0
17	q	649	0	691	0	0
18	r	505	0	502	0	0
19	s	638	0	665	0	0
20	t	665	0	714	0	0
21	u	496	0	486	0	0
22	v	1644	0	840	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	x	1025	0	518	0	0
24	A	62296	0	31354	335	0
25	B	2570	0	1301	10	0
26	C	2083	0	2157	28	0
27	D	1565	0	1616	24	0
28	E	1552	0	1619	18	0
29	F	1411	0	1447	17	0
30	G	1323	0	1374	14	0
31	I	1032	0	1088	7	0
32	H	1111	0	1148	5	0
33	J	1129	0	1162	13	0
34	K	939	0	1012	15	0
35	L	1045	0	1117	16	0
36	M	1074	0	1157	9	0
37	N	961	0	1000	8	0
38	O	892	0	923	4	0
39	P	917	0	965	11	0
40	Q	947	0	1022	7	0
41	R	816	0	839	10	0
42	S	857	0	922	7	0
43	T	739	0	807	5	0
44	U	780	0	834	5	0
45	V	753	0	780	9	0
46	W	575	0	592	8	0
47	X	625	0	655	9	0
48	Y	509	0	543	6	0
49	Z	449	0	491	1	0
50	0	444	0	461	4	0
51	1	410	0	440	9	0
52	2	377	0	418	6	0
53	3	504	0	574	5	0
54	4	302	0	341	3	0
55	6	523	0	522	8	0
56	4	1	0	0	0	0
56	6	1	0	0	0	0
All	All	146037	0	98182	557	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 4.

The worst 5 of 557 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)
30:G:83:THR:HA	30:G:132:LEU:O	1.83	0.79
39:P:88:ARG:HE	39:P:112:ARG:HH21	1.32	0.76
30:G:132:LEU:HB3	30:G:140:ILE:HD11	1.69	0.74
24:A:243:U:OP2	53:3:7:ARG:NH1	2.20	0.73
39:P:59:THR:HG22	39:P:72:VAL:HG12	1.70	0.72

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	
2	b	216/218 (99%)	189 (88%)	23 (11%)	4 (2%)	9	50
3	c	204/206 (99%)	190 (93%)	13 (6%)	1 (0%)	32	73
4	d	203/205 (99%)	187 (92%)	14 (7%)	2 (1%)	18	62
5	e	155/157 (99%)	134 (86%)	16 (10%)	5 (3%)	5	38
6	f	98/100 (98%)	82 (84%)	10 (10%)	6 (6%)	2	22
7	g	149/151 (99%)	135 (91%)	11 (7%)	3 (2%)	9	49
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	22	65
9	i	125/127 (98%)	104 (83%)	15 (12%)	6 (5%)	2	27
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	31
11	k	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	6	43
12	l	121/123 (98%)	98 (81%)	14 (12%)	9 (7%)	1	16
13	m	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	6	42
14	n	98/100 (98%)	83 (85%)	13 (13%)	2 (2%)	9	49
15	o	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	7	46
16	p	80/82 (98%)	71 (89%)	6 (8%)	3 (4%)	4	34
17	q	78/80 (98%)	66 (85%)	10 (13%)	2 (3%)	6	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	63/65 (97%)	57 (90%)	2 (3%)	4 (6%)	1	21
19	s	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	14	57
20	t	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
21	u	63/65 (97%)	50 (79%)	9 (14%)	4 (6%)	1	21
26	C	269/271 (99%)	246 (91%)	20 (7%)	3 (1%)	17	61
27	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	32	73
28	E	199/201 (99%)	184 (92%)	12 (6%)	3 (2%)	12	55
29	F	175/177 (99%)	158 (90%)	13 (7%)	4 (2%)	7	46
30	G	174/176 (99%)	157 (90%)	11 (6%)	6 (3%)	4	38
31	I	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	8	47
32	H	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	6	42
33	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	K	120/122 (98%)	105 (88%)	10 (8%)	5 (4%)	3	31
35	L	141/143 (99%)	129 (92%)	9 (6%)	3 (2%)	8	48
36	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8	47
37	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
38	O	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	10	51
39	P	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	20	64
40	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
41	R	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	9	49
42	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
43	T	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	4	38
44	U	100/102 (98%)	89 (89%)	6 (6%)	5 (5%)	2	26
45	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	13	56
47	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
48	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
49	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
50	0	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	9	50
51	1	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	8	48
52	2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	7	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	11	53
54	4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	42
55	6	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	11	53
All	All	5717/5817 (98%)	5150 (90%)	447 (8%)	120 (2%)	12	48

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	18	GLN
2	b	73	ARG
4	d	192	ALA
5	e	77	ASN

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	
2	b	180/180 (100%)	178 (99%)	2 (1%)	78	91
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	171 (99%)	1 (1%)	89	96
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	80	91
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	78 (99%)	1 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	64 (98%)	1 (2%)	70	89
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
26	C	216/216 (100%)	215 (100%)	1 (0%)	91	97
27	D	164/164 (100%)	164 (100%)	0	100	100
28	E	165/165 (100%)	165 (100%)	0	100	100
29	F	148/148 (100%)	148 (100%)	0	100	100
30	G	137/137 (100%)	137 (100%)	0	100	100
31	I	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	J	116/116 (100%)	116 (100%)	0	100	100
34	K	103/103 (100%)	102 (99%)	1 (1%)	80	91
35	L	102/102 (100%)	101 (99%)	1 (1%)	80	91
36	M	109/109 (100%)	109 (100%)	0	100	100
37	N	100/100 (100%)	100 (100%)	0	100	100
38	O	86/86 (100%)	86 (100%)	0	100	100
39	P	99/99 (100%)	99 (100%)	0	100	100
40	Q	89/89 (100%)	89 (100%)	0	100	100
41	R	84/84 (100%)	84 (100%)	0	100	100
42	S	93/93 (100%)	93 (100%)	0	100	100
43	T	80/80 (100%)	80 (100%)	0	100	100
44	U	83/83 (100%)	83 (100%)	0	100	100
45	V	78/78 (100%)	78 (100%)	0	100	100
46	W	57/57 (100%)	57 (100%)	0	100	100
47	X	67/67 (100%)	66 (98%)	1 (2%)	70	89
48	Y	55/55 (100%)	55 (100%)	0	100	100
49	Z	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	0	47/47 (100%)	46 (98%)	1 (2%)	59	85
51	1	45/45 (100%)	45 (100%)	0	100	100
52	2	38/38 (100%)	38 (100%)	0	100	100
53	3	51/51 (100%)	51 (100%)	0	100	100
54	4	34/34 (100%)	34 (100%)	0	100	100
55	6	59/59 (100%)	59 (100%)	0	100	100
All	All	4728/4751 (100%)	4717 (100%)	11 (0%)	95	99

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	n	34	ASN
16	p	2	VAL
35	L	27	LEU
12	l	33	CYS
34	K	21	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
26	C	44	ASN
27	D	49	GLN
37	N	62	ASN
20	t	12	GLN
37	N	81	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1531/1539 (99%)	260 (16%)	0
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	21 (44%)	0
24	A	2893/2903 (99%)	540 (18%)	34 (1%)
25	B	119/120 (99%)	17 (14%)	3 (2%)
All	All	4666/4687 (99%)	853 (18%)	37 (0%)

5 of 853 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	1211	C
24	A	1458	U
25	B	3	C
24	A	1212	G
24	A	1251	C

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

39 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	$\# Z > 2$
24	6MZ	A	1618	24	18,25,26	1.10	1 (5%)	16,36,39	3.01	4 (25%)
24	2MG	A	1835	24	19,26,27	1.18	2 (10%)	20,38,41	2.62	8 (40%)
24	PSU	A	1911	24	16,21,22	1.49	3 (18%)	20,30,33	3.58	6 (30%)
24	3TD	A	1915	24	16,22,23	3.20	7 (43%)	19,32,35	1.72	4 (21%)
24	PSU	A	1917	24	16,21,22	1.42	3 (18%)	20,30,33	3.49	6 (30%)
24	5MU	A	1939	24	14,22,23	0.97	2 (14%)	16,32,35	2.17	3 (18%)
24	5MC	A	1962	24	15,22,23	1.23	1 (6%)	17,32,35	1.89	4 (23%)
24	6MZ	A	2030	24	18,25,26	1.12	1 (5%)	16,36,39	3.30	4 (25%)
24	G7M	A	2069	24	19,26,27	1.26	2 (10%)	19,39,42	2.57	6 (31%)
24	OMG	A	2251	24,22	18,26,27	1.21	2 (11%)	22,38,41	1.98	6 (27%)
24	2MG	A	2445	24	19,26,27	1.14	2 (10%)	20,38,41	2.33	7 (35%)
24	H2U	A	2449	24	17,21,22	1.16	2 (11%)	21,30,33	2.28	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PSU	A	2457	24	16,21,22	1.82	5 (31%)	20,30,33	3.45	6 (30%)
24	OMC	A	2498	24	15,22,23	0.88	1 (6%)	19,31,34	0.77	0
24	2MA	A	2503	24	18,25,26	1.52	3 (16%)	17,37,40	1.95	2 (11%)
24	PSU	A	2504	24	16,21,22	1.36	2 (12%)	20,30,33	3.62	6 (30%)
24	OMU	A	2552	24	14,22,23	0.86	1 (7%)	18,31,34	2.04	1 (5%)
24	PSU	A	2580	24	16,21,22	1.61	5 (31%)	20,30,33	3.51	6 (30%)
24	PSU	A	2604	24	16,21,22	1.43	2 (12%)	20,30,33	3.66	7 (35%)
24	PSU	A	2605	24	16,21,22	1.35	2 (12%)	20,30,33	3.36	6 (30%)
24	1MG	A	745	24	18,26,27	1.53	3 (16%)	18,39,42	1.85	3 (16%)
24	PSU	A	746	24	16,21,22	1.33	1 (6%)	20,30,33	3.65	6 (30%)
24	5MU	A	747	24	14,22,23	0.75	1 (7%)	16,32,35	2.37	2 (12%)
24	PSU	A	955	24	16,21,22	1.76	4 (25%)	20,30,33	3.46	7 (35%)
1	2MG	a	1207	1	19,26,27	1.27	3 (15%)	20,38,41	2.17	8 (40%)
1	4OC	a	1402	1	16,23,24	0.83	1 (6%)	19,32,35	1.38	1 (5%)
1	5MC	a	1407	1	15,22,23	1.39	1 (6%)	17,32,35	0.93	1 (5%)
1	UR3	a	1498	1	14,22,23	0.88	1 (7%)	16,32,35	0.84	0
1	2MG	a	1516	1	19,26,27	1.17	2 (10%)	20,38,41	2.30	8 (40%)
1	MA6	a	1518	1	16,26,27	1.01	1 (6%)	18,38,41	2.45	5 (27%)
1	MA6	a	1519	1	16,26,27	0.94	1 (6%)	18,38,41	2.64	6 (33%)
1	PSU	a	516	1	16,21,22	1.42	2 (12%)	20,30,33	3.44	6 (30%)
1	G7M	a	527	1	19,26,27	1.61	2 (10%)	19,39,42	2.98	11 (57%)
1	2MG	a	966	1	19,26,27	1.22	2 (10%)	20,38,41	2.33	8 (40%)
1	5MC	a	967	1	15,22,23	1.35	1 (6%)	17,32,35	1.09	2 (11%)
22	H2U	v	20	22	17,21,22	1.01	2 (11%)	21,30,33	1.76	3 (14%)
22	5MU	v	54	22	14,22,23	0.71	0	16,32,35	2.26	3 (18%)
22	PSU	v	55	22	16,21,22	1.20	2 (12%)	20,30,33	3.53	8 (40%)
22	4SU	v	8	22	14,21,22	1.34	1 (7%)	15,30,33	1.32	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
24	6MZ	A	1618	24	-	0/5/27/28	0/3/3/3
24	2MG	A	1835	24	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	A	1911	24	-	0/7/25/26	0/2/2/2
24	3TD	A	1915	24	-	1/7/25/26	0/2/2/2
24	PSU	A	1917	24	-	0/7/25/26	0/2/2/2
24	5MU	A	1939	24	-	0/3/25/26	0/2/2/2
24	5MC	A	1962	24	-	0/3/25/26	0/2/2/2
24	6MZ	A	2030	24	-	0/5/27/28	0/3/3/3
24	G7M	A	2069	24	2/2/5/5	0/3/25/26	0/3/3/3
24	OMG	A	2251	24,22	-	0/5/27/28	0/3/3/3
24	2MG	A	2445	24	-	0/5/27/28	0/3/3/3
24	H2U	A	2449	24	-	0/7/38/39	0/2/2/2
24	PSU	A	2457	24	-	0/7/25/26	0/2/2/2
24	OMC	A	2498	24	-	0/5/27/28	0/2/2/2
24	2MA	A	2503	24	-	0/3/25/26	0/3/3/3
24	PSU	A	2504	24	-	0/7/25/26	0/2/2/2
24	OMU	A	2552	24	-	0/5/27/28	0/2/2/2
24	PSU	A	2580	24	-	0/7/25/26	0/2/2/2
24	PSU	A	2604	24	-	0/7/25/26	0/2/2/2
24	PSU	A	2605	24	-	0/7/25/26	0/2/2/2
24	1MG	A	745	24	-	0/3/25/26	0/3/3/3
24	PSU	A	746	24	-	0/7/25/26	0/2/2/2
24	5MU	A	747	24	-	0/3/25/26	0/2/2/2
24	PSU	A	955	24	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	0/3/25/26	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	5MC	a	967	1	-	0/3/25/26	0/2/2/2
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
22	5MU	v	54	22	-	0/3/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/3/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	2457	PSU	C5-C1'	-5.58	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	955	PSU	C5-C1'	-5.37	1.47	1.52
24	A	2580	PSU	C5-C1'	-4.62	1.48	1.52
24	A	1911	PSU	C5-C1'	-4.45	1.48	1.52
22	v	8	4SU	C4-S4	-4.11	1.59	1.67

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	746	PSU	N1-C2-N3	-10.82	120.61	128.40
24	A	2605	PSU	N1-C2-N3	-9.86	121.31	128.40
24	A	2580	PSU	C5-C4-N3	-9.61	117.54	125.43
22	v	55	PSU	N1-C2-N3	-9.55	121.53	128.40
24	A	2604	PSU	N1-C2-N3	-9.40	121.64	128.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	2069	G7M	C4'
24	A	2069	G7M	C3'
1	a	527	G7M	C4'
1	a	527	G7M	C3'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1915	3TD	O4'-C1'-C5-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1915	3TD	1	0
24	A	1917	PSU	1	0
24	A	2580	PSU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.