



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 07:33 PM EST

PDB ID : 3JBU
EMDB ID : EMD-6483
Title : Mechanisms of Ribosome Stalling by SecM at Multiple Elongation Steps
Authors : Zhang, J.; Pan, X.J.; Yan, K.G.; Sun, S.; Gao, N.; Sui, S.F.
Deposited on : 2015-10-16
Resolution : 3.64 Å(reported)
Based on initial model : 4V7T

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

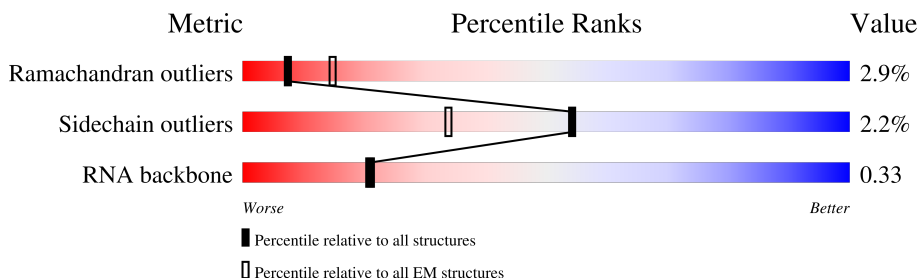
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	241	
2	C	233	
3	D	206	
4	E	167	
5	F	131	
6	G	156	
7	H	130	
8	I	130	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	U	71	
21	0	78	
22	1	63	
23	2	59	
24	3	57	
25	4	55	
26	6	46	
27	7	65	
28	8	38	
29	c	273	
30	d	209	
31	e	201	
32	f	179	
33	g	177	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	h	149	
35	j	142	
36	k	123	
37	l	144	
38	m	136	
39	n	127	
40	o	117	
41	p	115	
42	q	118	
43	r	103	
44	s	110	
45	t	100	
46	u	104	
47	w	94	
48	y	85	
49	z	87	
50	A	1542	
51	X	11	
52	a	120	
53	b	2904	
54	v	76	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 143334 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	113	Total	C	N	O	S	0	0
			876	541	177	155	3		

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	79	ARG	GLN	conflict	UNP P0ADZ4

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	135	Total	C	N	O	S	0	0
			1063	680	201	176	6		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 49 is a protein called SecM-glycine.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	z	26	Total	C	N	O	0	0
			203	129	33	41		

- Molecule 50 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	A	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	X	11	Total	C	N	O	P	0	0
			232	103	39	79	11		

- Molecule 52 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	118	Total	C	N	O	P	0	0
			2528	1126	464	821	117		

- Molecule 53 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	b	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

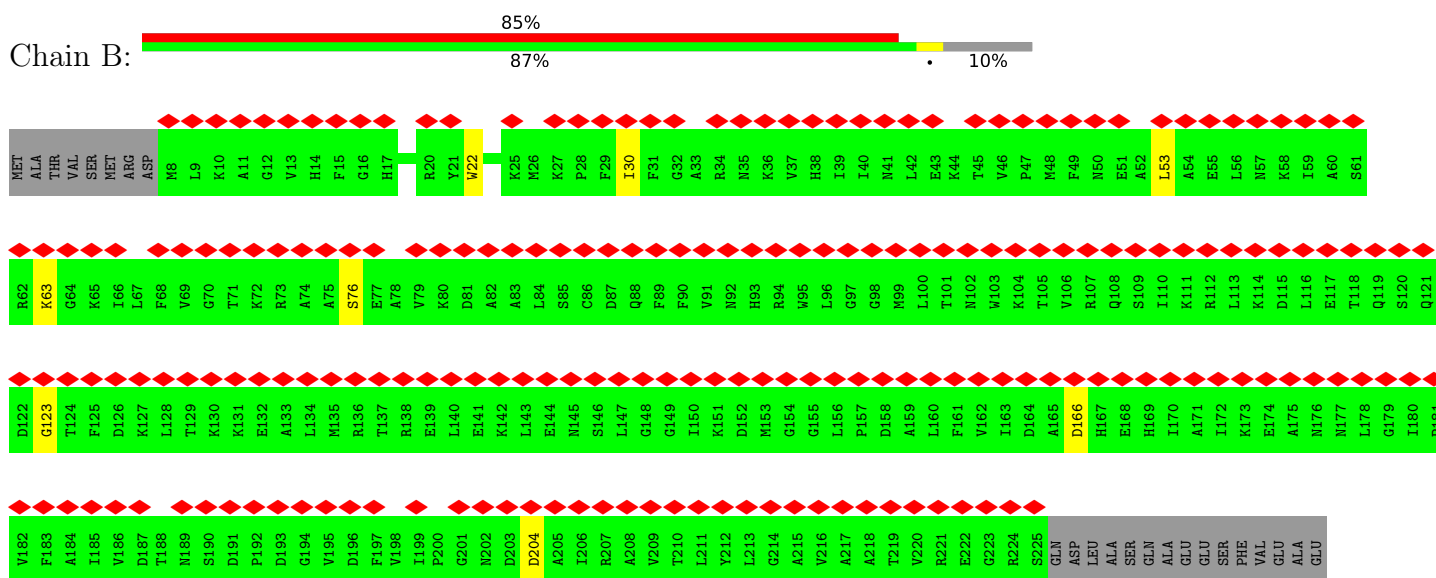
- Molecule 54 is a RNA chain called glycine-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	76	Total	C	N	O	P	0	0
			1623	722	291	534	76		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 30S ribosomal protein S2

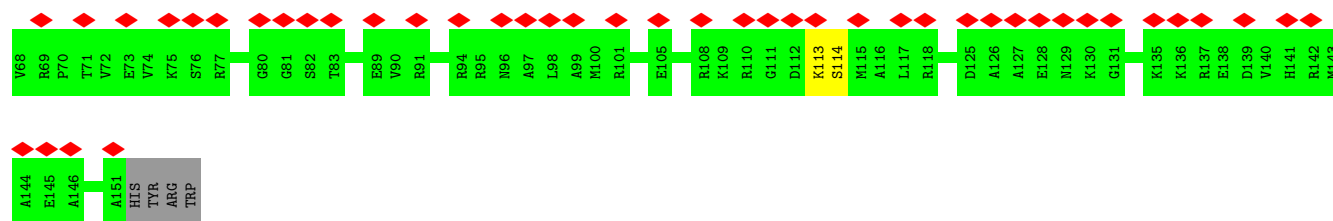


R183	K184	P185	E186	R187	S188	D189	L190	S191	A192	D193	I194	N195	E196	H197	L198	I199	L202	Y203	S204	K205																																						
M123	V124	N125	G126	R127	V128	V129	M130	I131	A132	S133	V134	Q135	V136	S137	P138	M139	D140	V141	Y142	S143	I144	E145	E146	K147	A148	K149	K150	Q151	S152	R153	V154	K155	A156	A157	L158	E159	L160	A161	E162	Q163	R164	E165	K166	P167	T168	W169	L170	E171	V172	D173	A174	G175	K176	M177	E178	G179	T180	F181
R62	I63	V64	G65	V66	L67	E68	R69	Q70	F71	R72	N73	Y74	Y75	K76	E77	A78	R79	L80	L81	K82	G83	H84	T85	G86	E87	K88	L89	L90	A91	L92	L93	E94	G95	R96	L97	D98	N99	Q100	V101	Y102	R103	M104	G105	F106	G107	A108	T109	R110	A111	E112	A113	R114	Q115	L116	H119	K120	A121	I122
A1	R2	Y3	L4	K7	L8	S11	R12	R13	E14	G15	T16	D17	L18	F19	L20	K21	S22	G23	V24	R25	A26	T27	L28	D28	T29	K30	C31	L32	R33	L34	E35	A36	P37	Q38	Q39	R40	G41	A42	R43	K44	P45	R46	L47	S48	D49	V50	G51	V52	Q53	L54	R55	E56	K57	Q58	K59	V60	R61	

Met	ALA	HIS	ILE	GLU	LYS	GLN	ALA	GLY	E9	L10	Q11	E12	K13	L14	I15	A16	V17	M18	R19	G27	F30	S31	F32	T33	A34	L35	T36	V37	D40	G41	N42	G43	R44	V45	G46	F47	G48	K51	A52	R53	E54	V55	P56	A57	A58	I59	Q60	K61	A62	M63	E64	K65	A66	R67	R68
M69	M70	I71	M72	V73	A74	L75	M76	M77	G78	G81	V84	K85	G86	M87	H88	T89	G90	S91	R92	V93	F94	M95	Q96	P97	A98	S99	E100	G101	T102	G103	I104	I105	A106	G107	G108	A109	V113	L114	E115	V116	A117	G118	V119	H120	M121	K125	A126	Y127	G128	S129	T130	N134	V135		
A138	T139	I140	D141	G142	L143	E144	M145	M146	M147	S148	P149	E150	A153	A154	K155	R156	G157	K158	SER	VAL	GLU	GLU	ILE	LEU	GLY	LYS																													

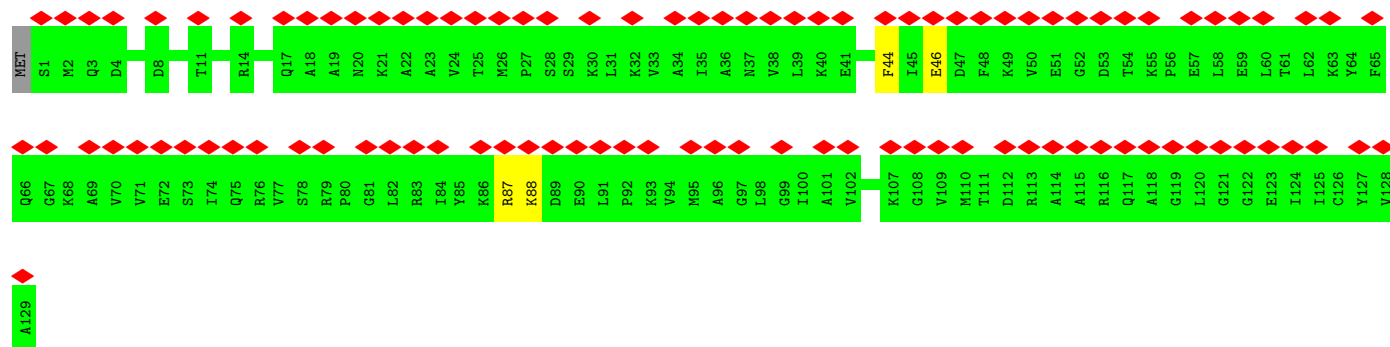
E98	A99	S100	PRO	MET	VAL	LYS	ALA	LYS	ASP	ARG	GLU	ARG	ARG	GLU	ARG	ARG	ASP	ASP	PHE	ALA	ASN	THR	ALA	ASP	ASP	ALA	ASP	GLY	GLY	ASP	SER	GLU															
R1	R2	H9	D13	E16	Q17	E23	R24	Y25	A28	T29	T30	G31	A32	E33	G34	X35	I36	H37	E40	D41	R44	R45	O46	L47	A48	H55	K56	A57	E69	D72	R79	F80	N81	D82	A83	V84	I85	R88	V89	H90	R91	T92	K93	H94	A95	V96	T97

[illegible]



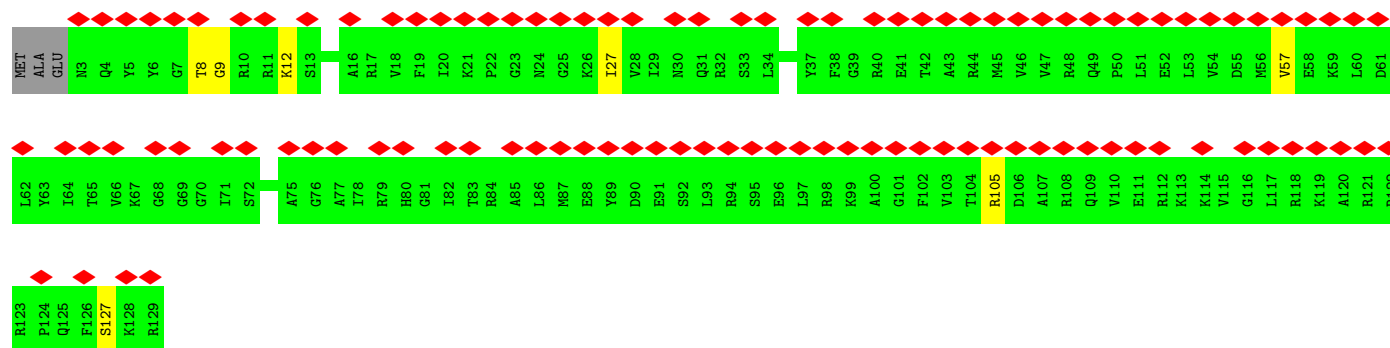
• Molecule 7: 30S ribosomal protein S8

Chain H: 76% 96%



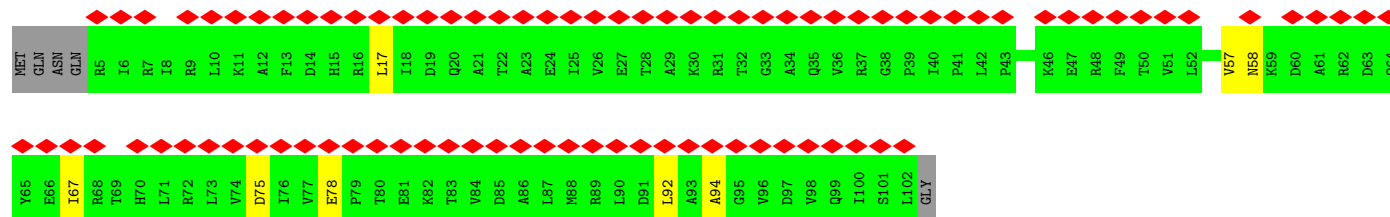
• Molecule 8: 30S ribosomal protein S9

Chain I: 80% 92% 5%

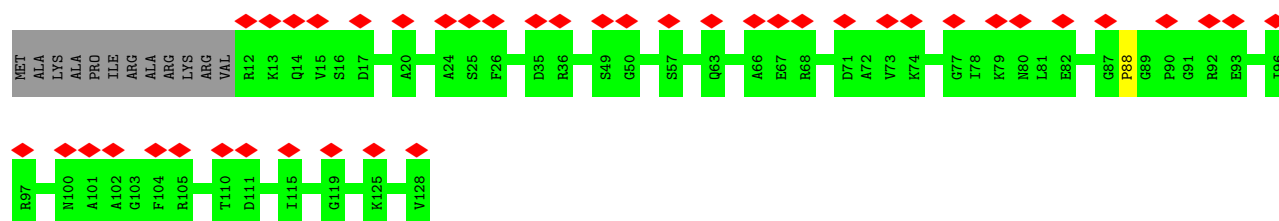
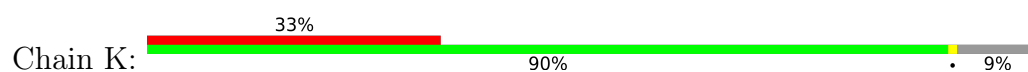


• Molecule 9: 30S ribosomal protein S10

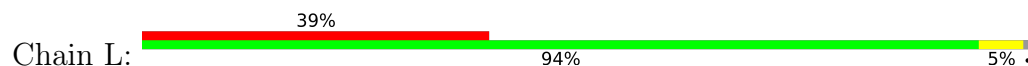
Chain J: 85% 87% 8% 5%



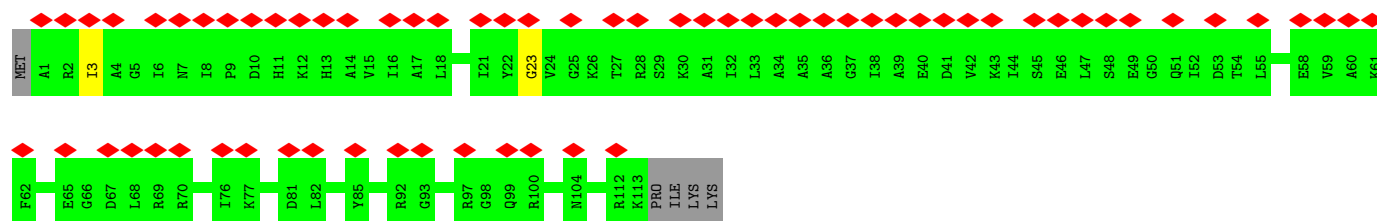
• Molecule 10: 30S ribosomal protein S11



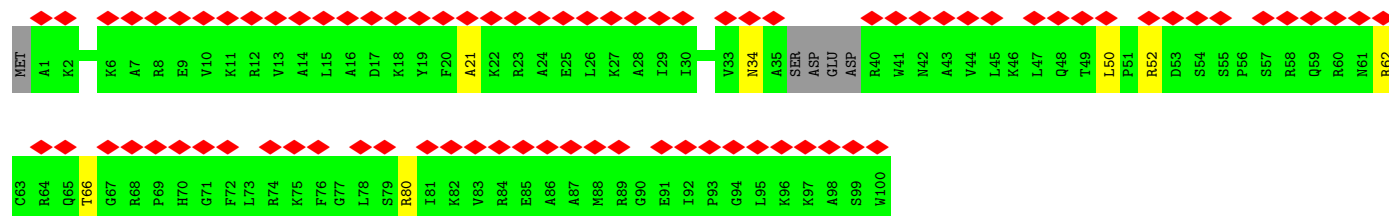
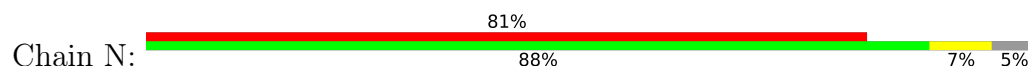
- Molecule 11: 30S ribosomal protein S12



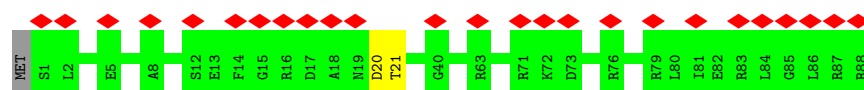
- Molecule 12: 30S ribosomal protein S13



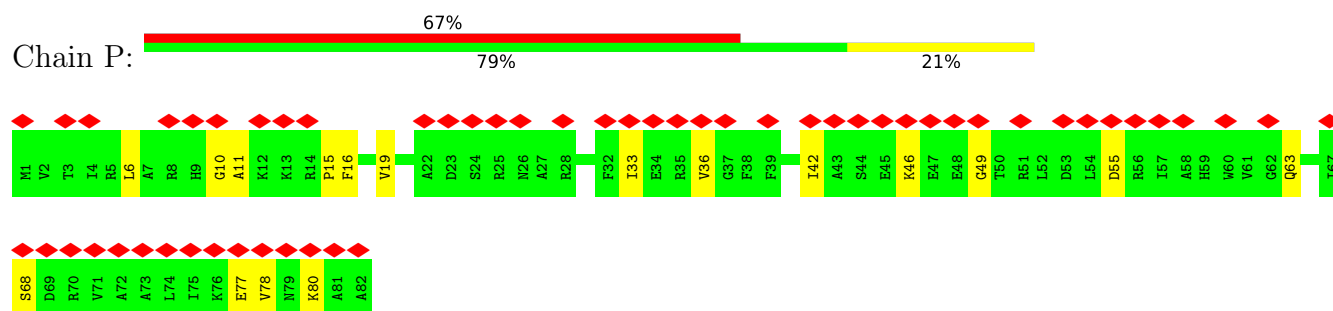
- Molecule 13: 30S ribosomal protein S14



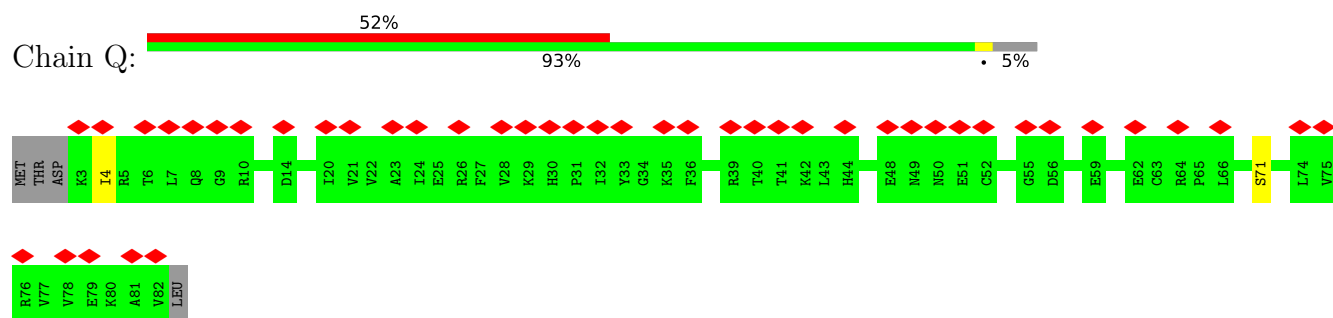
- Molecule 14: 30S ribosomal protein S15



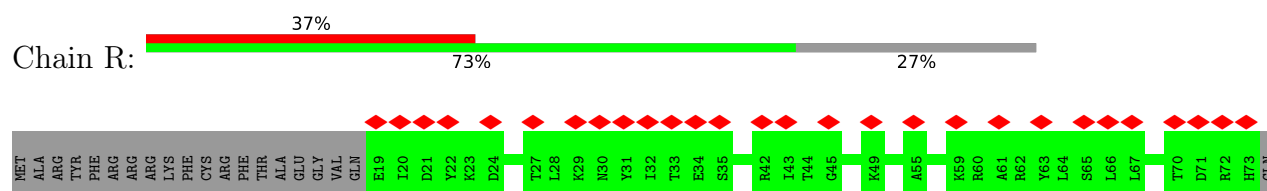
- Molecule 15: 30S ribosomal protein S16



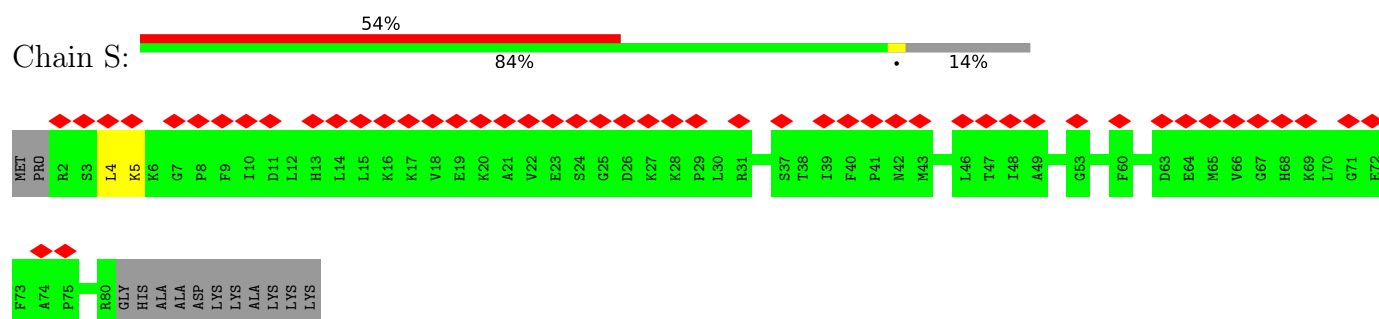
- Molecule 16: 30S ribosomal protein S17



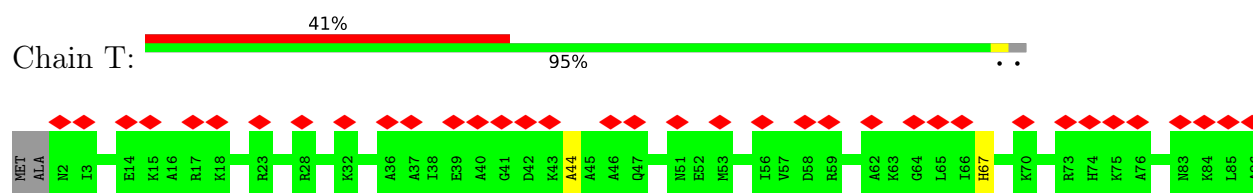
- Molecule 17: 30S ribosomal protein S18



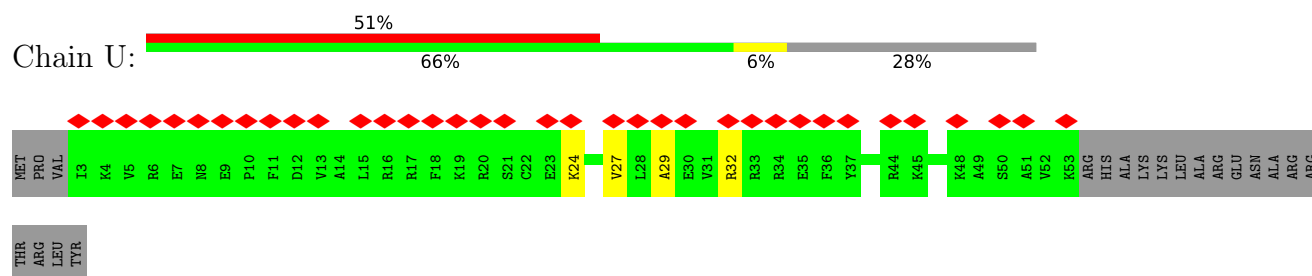
- Molecule 18: 30S ribosomal protein S19



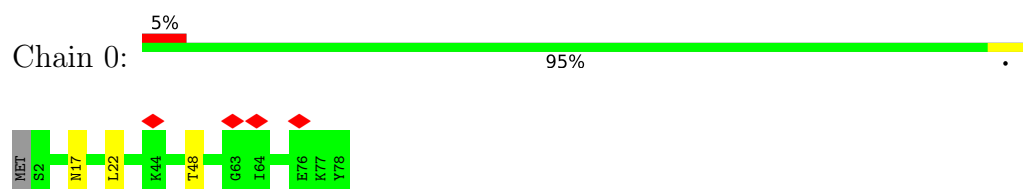
- Molecule 19: 30S ribosomal protein S20



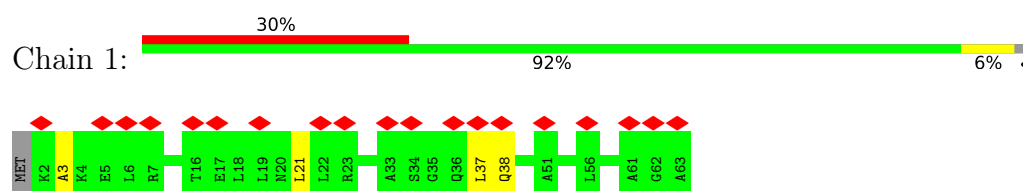
- Molecule 20: 30S ribosomal protein S21



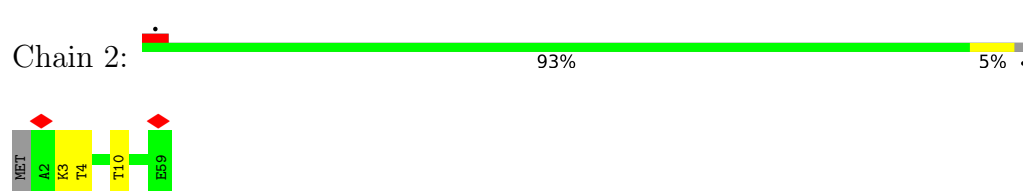
- Molecule 21: 50S ribosomal protein L28



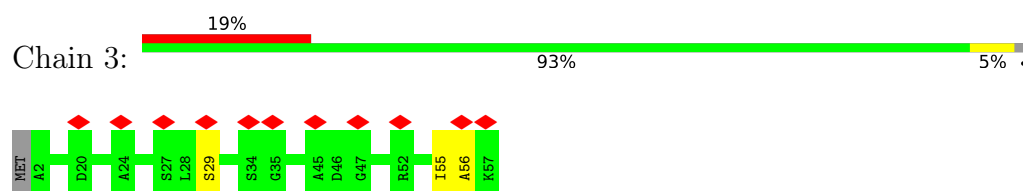
- Molecule 22: 50S ribosomal protein L29



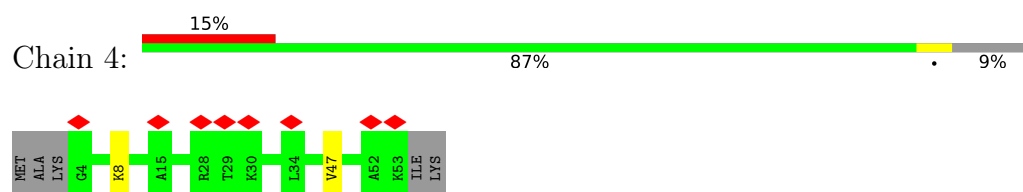
- Molecule 23: 50S ribosomal protein L30



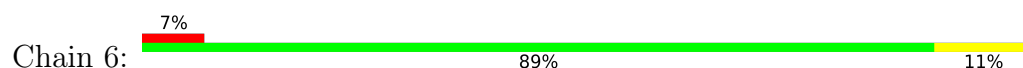
- Molecule 24: 50S ribosomal protein L32

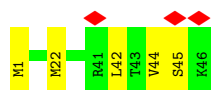


- Molecule 25: 50S ribosomal protein L33

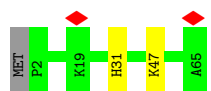


- Molecule 26: 50S ribosomal protein L34

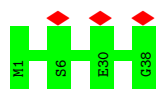




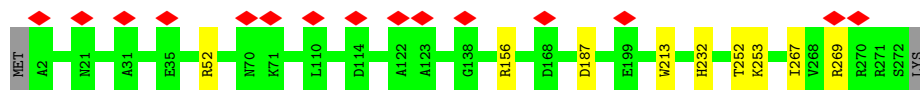
- Molecule 27: 50S ribosomal protein L35



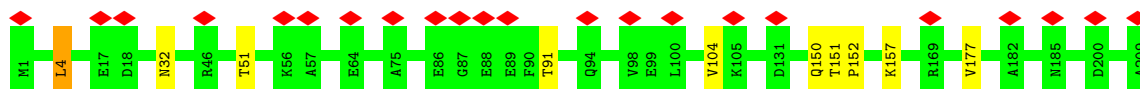
- Molecule 28: 50S ribosomal protein L36



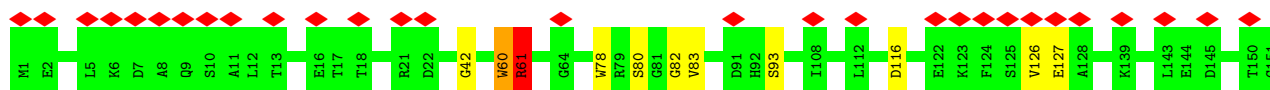
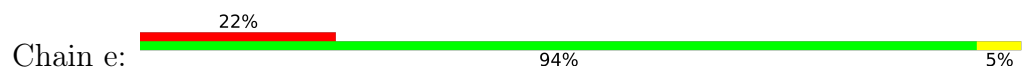
- Molecule 29: 50S ribosomal protein L2



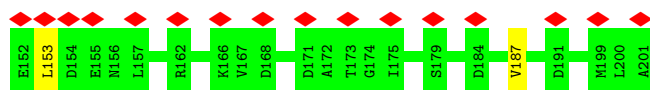
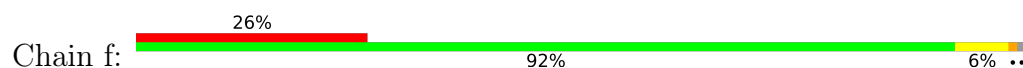
- Molecule 30: 50S ribosomal protein L3

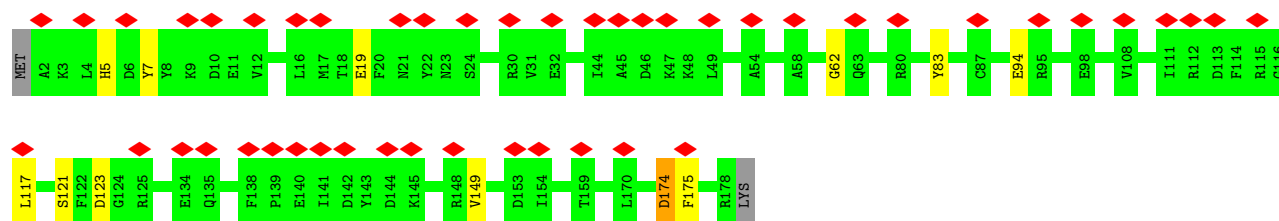


- Molecule 31: 50S ribosomal protein L4



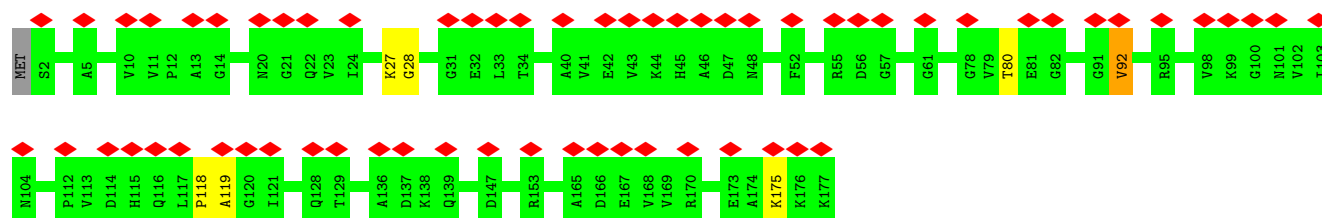
- Molecule 32: 50S ribosomal protein L5





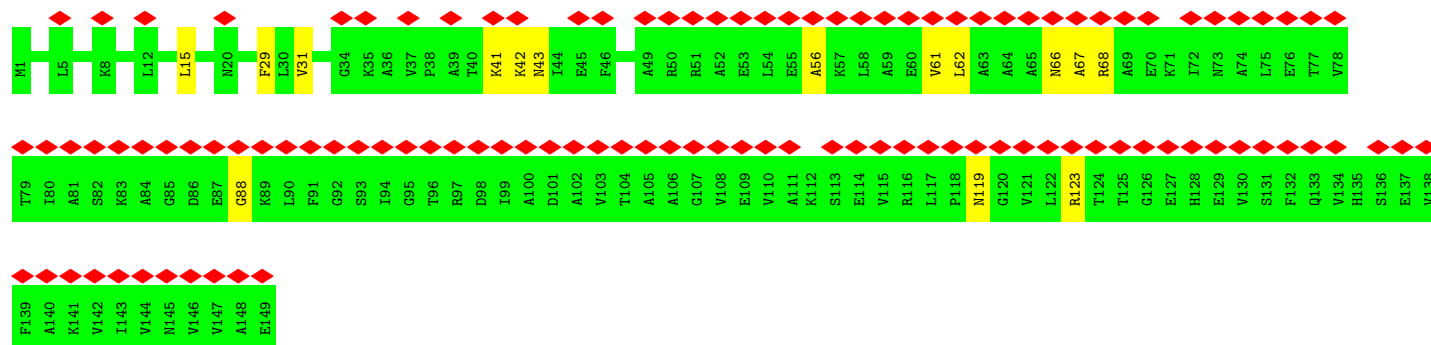
- Molecule 33: 50S ribosomal protein L6

Chain g: 36% 95%



- Molecule 34: 50S ribosomal protein L9

Chain h: 74% 90% 10%



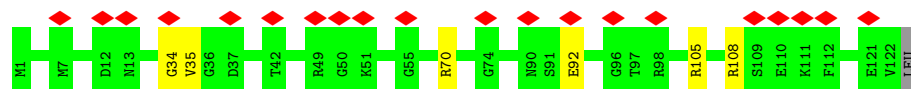
- Molecule 35: 50S ribosomal protein L13

Chain j: 8% 96%

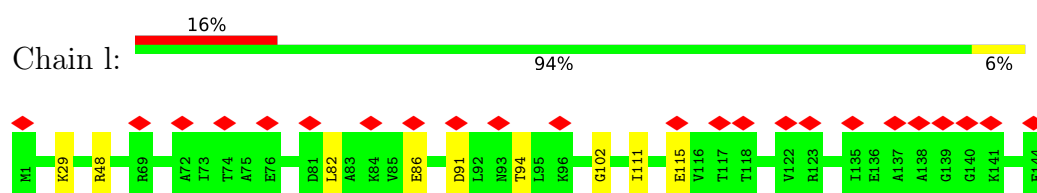


- Molecule 36: 50S ribosomal protein L14

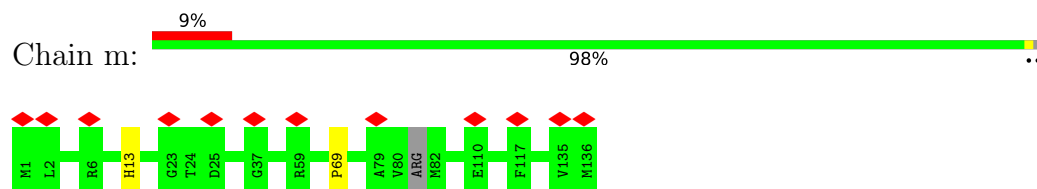
Chain k: 16% 94% 5%



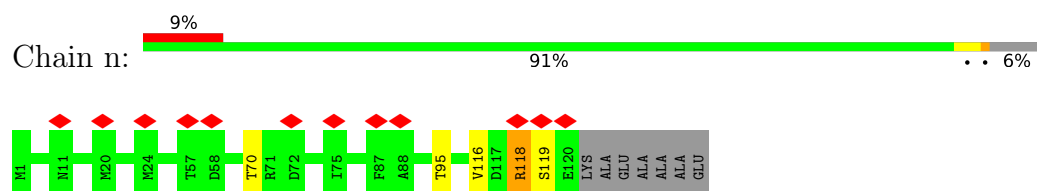
- Molecule 37: 50S ribosomal protein L15



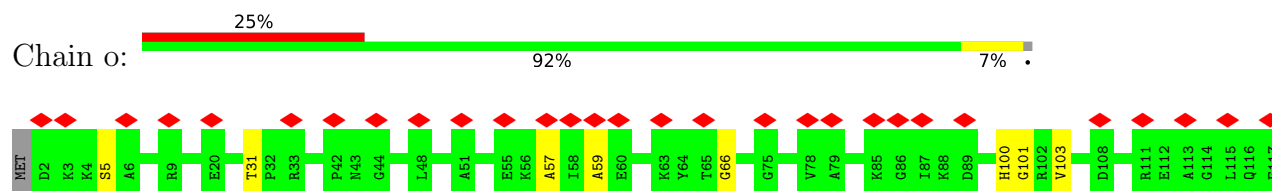
- Molecule 38: 50S ribosomal protein L16



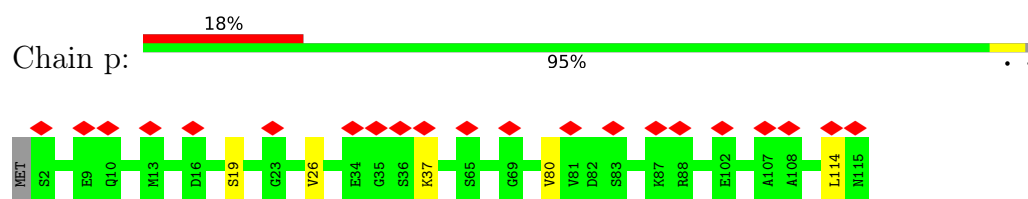
- Molecule 39: 50S ribosomal protein L17



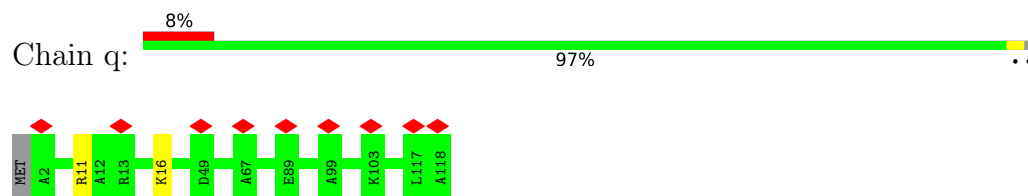
- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19

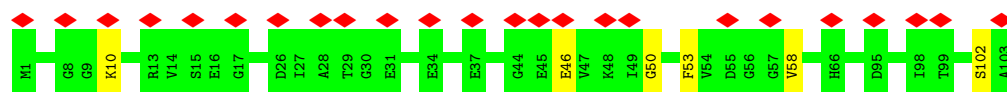


- Molecule 42: 50S ribosomal protein L20

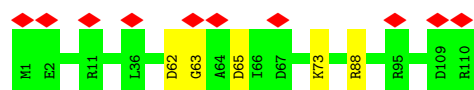


- Molecule 43: 50S ribosomal protein L21

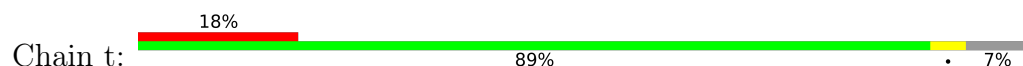




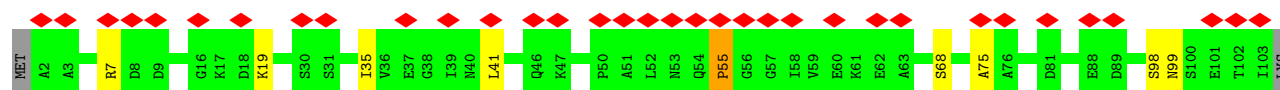
- Molecule 44: 50S ribosomal protein L22



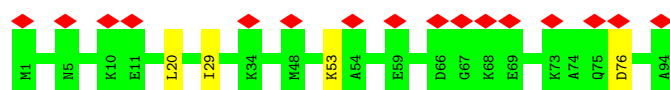
- Molecule 45: 50S ribosomal protein L23



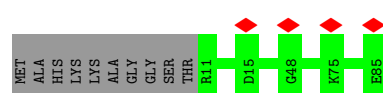
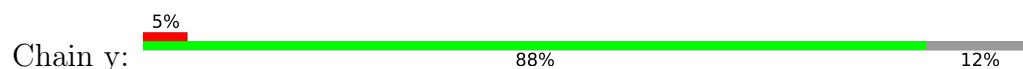
- Molecule 46: 50S ribosomal protein L24



- Molecule 47: 50S ribosomal protein L25



- Molecule 48: 50S ribosomal protein L27

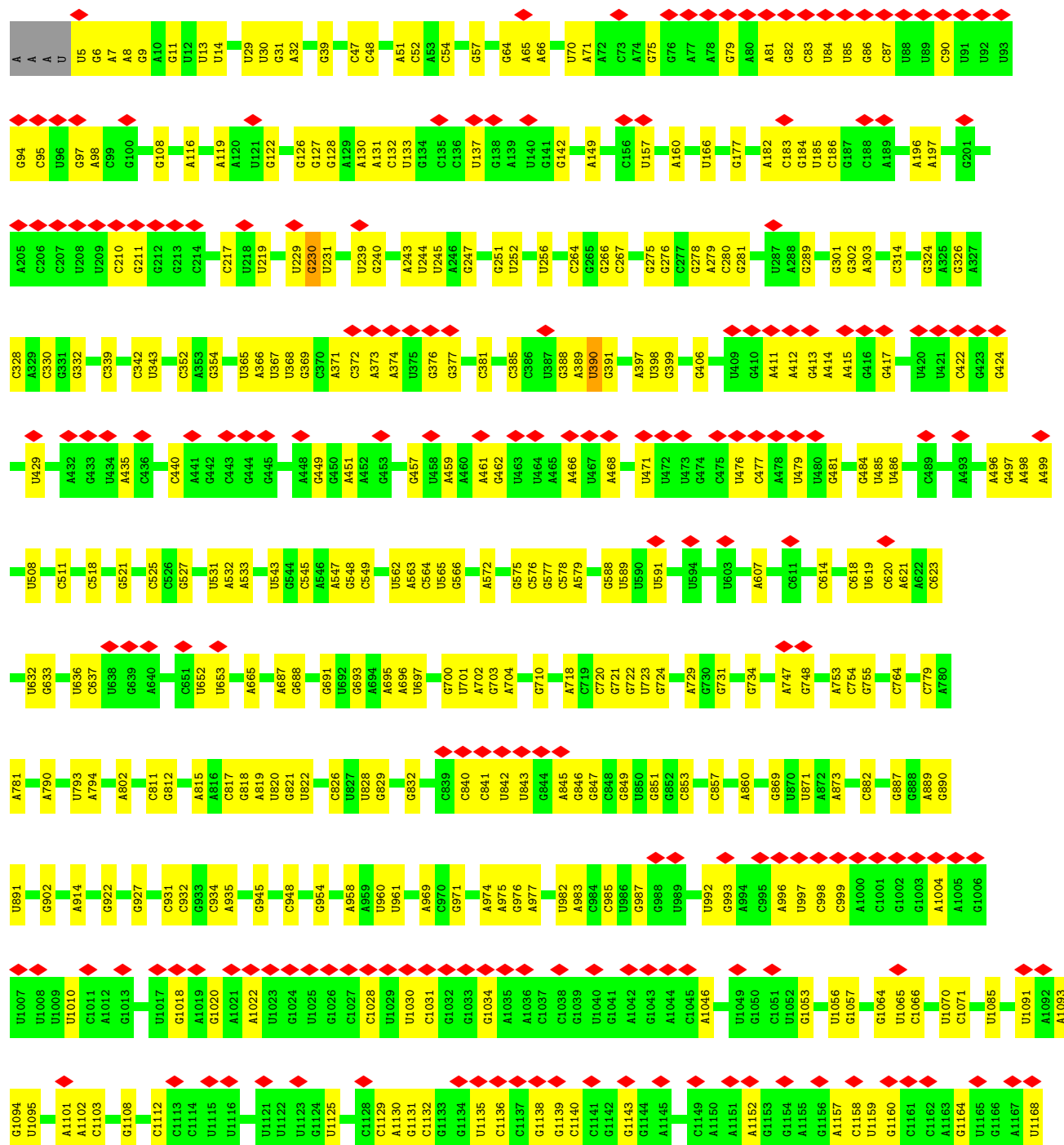


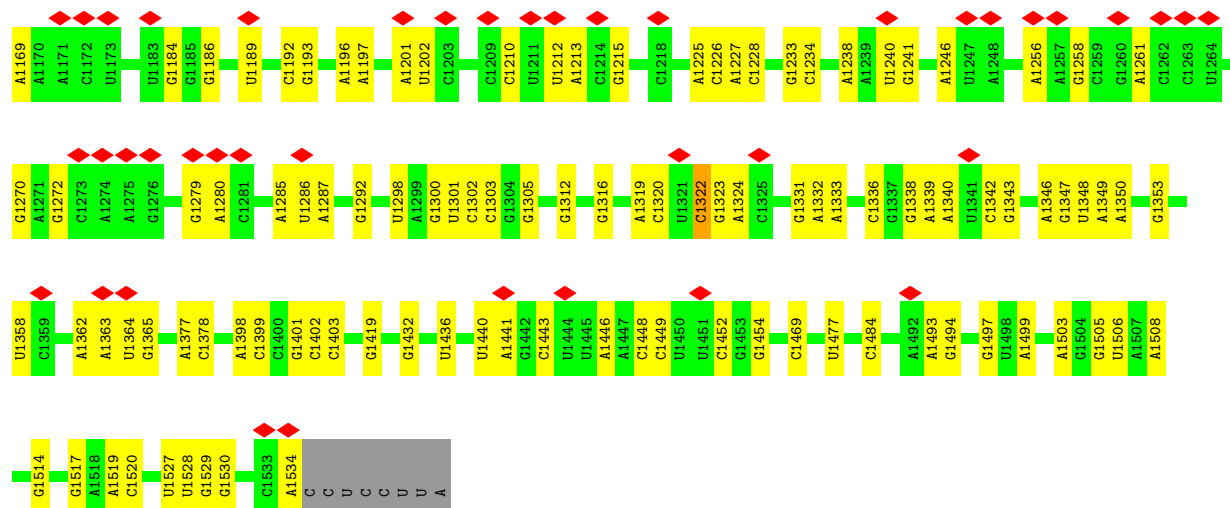
- Molecule 49: SecM-glycine



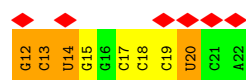
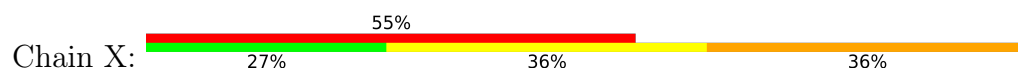


● Molecule 50: 16S rRNA

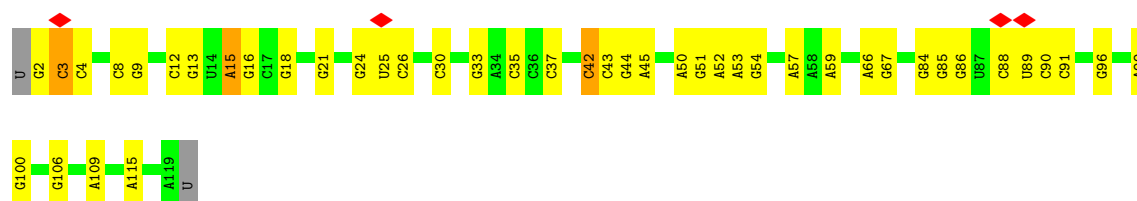




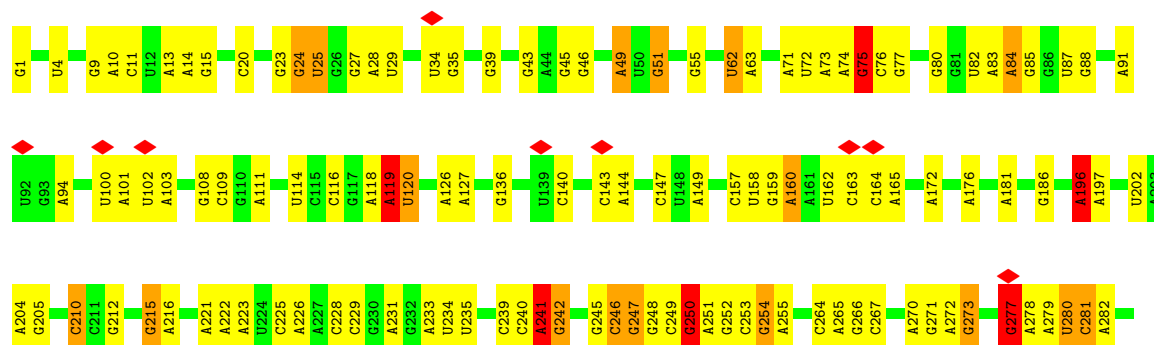
• Molecule 51: mRNA



• Molecule 52: 5S rRNA

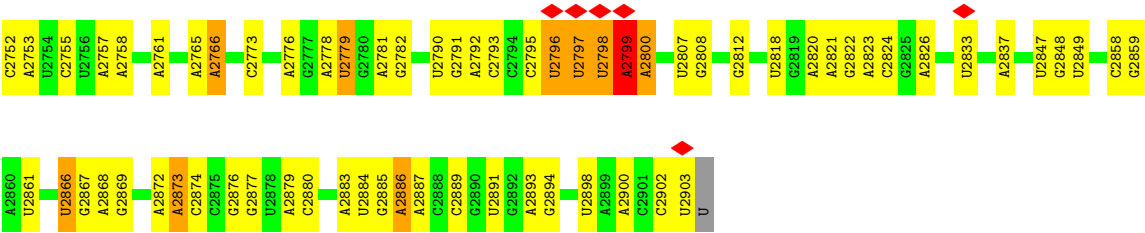


• Molecule 53: 23S rRNA

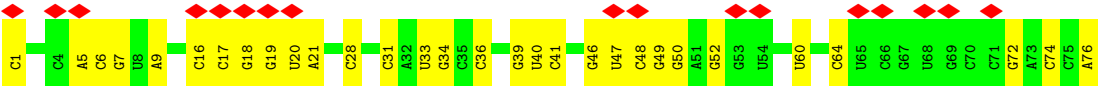




G1540	G1541	G1542	A1552	A1553	U1554	G1555	G1556	G1557	G1558	U1559	U1562	A1566	G1567	G1568	A1569	A1570	A1571	A1572	U1576	G1577	U1578	A1583	U1584	C1585	C1592	C1595	A1598	U1599	C1600	G1601	U1602	A1603	C1606	C1607	A1608	A1609	A1610	C1612	C1615	A1616	C1617	A1618	U1624	G1631	A1632	G1633											
A1634	A1635		G1643	G1644	G1645	U1646	U1647	U1648	G1649	G1653	A1654	A1655	A1656	U1657	G1658	G1659	G1660	G1661	U1662	G1663	G1667	A1668	A1669	G1674	C1675	A1678		U1687	U1689	C1693	C1694	G1695	G1696	G1697	A1698	G1699	A1700	G1703	C1704	A1705	G1706	G1707	G1710	A1713	U1714	G1715	U1725										
C1726	C1727	C1728	U1729	C1730	G1731	C1732	G1733	G1738	A1739	A1746	G1750	A1754	A1755	G1756	A1757	U1758	A1759	C1760	C1761	A1762	G1763	C1764	U1765	G1766	A1773	C1774	U1775	G1776	A1780	A1783	A1784	A1785	A1786	A1787	G1792	C1793	A1794	C1800	A1801	A1802	A1803	C1804	G1807	A1808	A1809	A1810	G1811	G1814									
A1815	C1816	G1817	G1823	G1824	U1825	G1826	A1829	C1833	G1839	G1840	C1843	G1846	A1847	A1848	G1849	A1858	U1859	G1860	G1861	G1862	U1865	A1866	G1867	C1868	G1869	A1870	A1871	A1872	G1873	A1890	G1897	C1905	G1906	G1907	C1908	A1913	C1914	U1915	A1916	U1917	A1918	A1919	C1924	A1927	A1928												
G1929	G1930	U1931	A1932	A1936	A1937	A1938	U1939	U1940	C1941	C1942	C1943	U1944	U1951	A1952	G1953	G1954	U1955	U1963	G1964	C1965	A1966	C1967	G1968	A1969	U1970	U1971	G1972	G1975	G1980	A1981	U1982	U1991	G1992	U1993	C1996	C1997	A1998	C1999	U2007	G2012	A2013	A2014	A2015	U2016	A2019	A2020	C2021	U2022	C2023								
G2024	C2025	A2030	A2031	G2032	A2033	U2034	G2035	C2036	C2043	G2046	A2051	A2052	G2053	A2054	G2055	G2056	A2060	G2061	C2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	A2077	A2080	G2083	G2087	A2088	U2092	G2093	A2094	G2100	A2101	G2102	C2103	C2104	U2105	U2106	G2107	A2108	U2109	G2110	U2111	G2112	U2113									
A2114	G2115	G2116	A2117	U2118	U2119	G2120	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	C2143	G2144	C2145	C2146	A2147	G2148	U2149	C2150	U2151	G2152	A2153	A2154	U2155	G2156	G2157	A2158	G2159	C2160	C2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174
C2175	A2176	C2177	C2178	U2180	U2181	U2182	A2183	A2184	U2185	G2186	U2187	G2193	A2198	A2199	U2202	U2203	G2204	A2205	C2206	C2207	U2210	A2211	U2212	U2213	C2214	C2215	A2225	G2230	G2238	G2239	U2243	U2249	G2250	G2251	G2252	G2255	U2256	C2257	C2258	U2259	U2265	A2266	A2267	A2268	G2271	U2272											
A2273	A2274	C2275	G2276	G2279	G2282	C2283	G2286	A2287	A2288	G2289	A2297	G2304	U2305	C2306	G2307	G2308	A2309	G2319	U2320	U2321	A2322	G2323	U2324	U2329	G2330	G2331	C2332	A2333	U2334	A2335	A2336	C2339	A2340	U2344	G2345	A2346	C2347	C2350	G2351	G2356	A2366	G2371	A2377	A2378	G2379												
G2382	G2383	U2384	C2385	A2388	G2396	U2397	U2398	G2399	G2400	U2401	U2402	C2403	A2406	A2407	G2410	A2411	C2420	U2423	A2424	A2425	A2426	G2427	G2428	G2429	A2430	U2431	A2434	A2439	C2440	U2441	G2444	G2445	G2446	U2447	A2448	U2449	A2450	A2451	G2452	A2453	G2454	G2455	G2458	A2459	U2460	C2465	G2466										
C2467	G2472	C2475	A2476	U2477	A2478	G2481	G2484	G2490	U2491	U2492	A2497	C2498	G2502	G2505	G2509	C2510	U2513	C2517	A2518	U2519	G2525	G2526	C2527	U2528	G2529	A2530	A2534	G2535	G2536	A2541	A2542	G2543	G2544	A2547	C2551	U2554	U2555	C2556	U2562	U2563	A2564																
A2565	A2566	G2567	A2572	G2573	C2574	G2575	G2576	A2577	G2578	G2581	G2582	G2583	U2584	U2585	U2586	A2587	G2588	U2589	A2590	C2593	G2594	G2595	U2596	G2597	C2598	A2599	A2600	C2601	U2613	A2614	U2615	G2621	G2625	U2629	A2632	G2633	A2634	G2638	A2639	G2640	G2641	A2650	G2651														
C2646	A2654	G2655	U2656	A2657	C2658	G2659	A2660	A2661	A2662	G2663	G2673	G2677	G2685	G2688	U2689	U2690	C2691	C2699	G2702	C2703	U2707	C2712	U2713	G2714	C2715	C2716	C2717	G2718	G2719	G2722	U2727	U2728	G2729	A2733	G2735	A2736	G2737	A2738	G2744	U2745	U2746	G2747	A2750	G2751													



• Molecule 54: glycine-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60354	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	37878	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.29	0/1735	0.51	0/2338
2	C	0.33	0/1651	0.55	0/2225
3	D	0.34	0/1665	0.55	0/2227
4	E	0.38	0/1118	0.56	0/1504
5	F	0.32	0/835	0.56	0/1128
6	G	0.31	0/1187	0.53	0/1591
7	H	0.35	0/989	0.55	0/1326
8	I	0.32	0/1034	0.61	0/1375
9	J	0.33	0/796	0.59	0/1077
10	K	0.30	0/893	0.53	0/1205
11	L	0.36	0/969	0.59	0/1300
12	M	0.31	0/884	0.52	0/1181
13	N	0.34	0/785	0.54	0/1043
14	O	0.33	0/724	0.54	0/966
15	P	0.29	0/659	0.49	0/884
16	Q	0.34	0/657	0.53	0/881
17	R	0.37	0/462	0.58	0/621
18	S	0.32	0/652	0.55	0/877
19	T	0.33	0/671	0.52	0/888
20	U	0.33	0/430	0.63	0/570
21	0	0.38	0/635	0.67	0/848
22	1	0.37	0/502	0.65	0/667
23	2	0.39	0/453	0.61	0/605
24	3	0.41	0/450	0.73	0/599
25	4	0.38	0/416	0.58	0/554
26	6	0.44	0/380	0.77	0/498
27	7	0.37	0/513	0.62	0/676
28	8	0.38	0/303	0.74	0/397
29	c	0.39	0/2121	0.70	1/2852 (0.0%)
30	d	0.38	0/1586	0.63	1/2134 (0.0%)
31	e	0.39	0/1571	0.62	1/2113 (0.0%)
32	f	0.39	0/1434	0.66	0/1926
33	g	0.37	0/1343	0.56	0/1816
34	h	0.37	0/1122	0.68	5/1515 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	j	0.37	0/1152	0.58	0/1551
36	k	0.38	0/947	0.68	1/1268 (0.1%)
37	l	0.38	0/1062	0.68	0/1413
38	m	0.38	0/1081	0.63	0/1443
39	n	0.39	0/973	0.67	0/1301
40	o	0.39	0/902	0.70	0/1209
41	p	0.37	0/929	0.66	0/1242
42	q	0.39	0/960	0.69	1/1278 (0.1%)
43	r	0.40	0/829	0.67	1/1107 (0.1%)
44	s	0.35	0/864	0.67	1/1156 (0.1%)
45	t	0.40	0/744	0.66	1/994 (0.1%)
46	u	0.39	0/787	0.67	0/1051
47	w	0.36	0/766	0.58	0/1025
48	y	0.37	0/576	0.60	0/762
49	z	0.49	0/206	0.83	2/277 (0.7%)
50	A	0.87	6/36762 (0.0%)	0.86	20/57350 (0.0%)
51	X	1.07	4/257 (1.6%)	0.91	0/396
52	a	0.45	1/2824 (0.0%)	0.93	7/4402 (0.2%)
53	b	0.55	52/69800 (0.1%)	1.03	441/108892 (0.4%)
54	v	0.36	1/1812 (0.1%)	0.85	4/2822 (0.1%)
All	All	0.60	64/155858 (0.0%)	0.89	487/233346 (0.2%)

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
11	L	0	1
23	2	0	1
29	c	0	1
30	d	0	1
36	k	0	1
37	l	0	1
43	r	0	1
52	a	0	1
53	b	0	72
All	All	0	80

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	A	230	G	C6-N1	60.83	1.82	1.39
50	A	230	G	N3-C4	58.56	1.76	1.35
50	A	230	G	C2-N3	55.19	1.76	1.32
50	A	230	G	N1-C2	53.83	1.80	1.37
50	A	230	G	C5-C4	53.10	1.75	1.38
50	A	230	G	C5-C6	39.86	1.82	1.42
53	b	1087	G	O3'-P	16.62	1.81	1.61
53	b	2055	C	O3'-P	16.06	1.80	1.61
53	b	1055	G	O5'-C5'	11.59	1.62	1.44
53	b	1349	C	C4-N4	-10.90	1.24	1.33
53	b	2131	U	N1-C2	10.86	1.48	1.38
51	X	12	G	OP3-P	-10.81	1.48	1.61
53	b	2131	U	C4-C5	10.37	1.52	1.43
53	b	1	G	OP3-P	-10.10	1.49	1.61
54	v	1	C	OP3-P	-9.99	1.49	1.61
53	b	1088	A	O5'-C5'	9.14	1.59	1.44
53	b	2455	G	O3'-P	-8.96	1.50	1.61
53	b	1057	A	O3'-P	8.87	1.71	1.61
53	b	1349	C	N3-C4	-8.77	1.27	1.33
53	b	1055	G	C5'-C4'	8.63	1.61	1.51
53	b	1103	A	O3'-P	8.44	1.71	1.61
53	b	2056	G	O3'-P	-8.42	1.51	1.61
53	b	1087	G	C3'-O3'	8.37	1.53	1.42
53	b	2451	A	O3'-P	-8.29	1.51	1.61
53	b	1088	A	C5'-C4'	8.16	1.61	1.51
53	b	1078	U	O3'-P	7.67	1.70	1.61
53	b	2109	U	N1-C6	7.65	1.44	1.38
53	b	1349	C	N1-C2	7.42	1.47	1.40
53	b	2109	U	N3-C4	7.30	1.45	1.38
53	b	1086	A	O3'-P	7.06	1.69	1.61
53	b	780	G	O3'-P	6.73	1.69	1.61
53	b	1349	C	C2-N3	-6.71	1.30	1.35
53	b	2575	C	O3'-P	6.70	1.69	1.61
53	b	2178	C	O3'-P	6.62	1.69	1.61
52	a	2	G	O3'-P	6.58	1.69	1.61
53	b	1349	C	C2-O2	6.37	1.30	1.24
53	b	400	G	O3'-P	6.33	1.68	1.61
51	X	14	U	C1'-N1	6.21	1.58	1.48
53	b	569	U	O3'-P	-5.96	1.54	1.61
53	b	1100	C	O3'-P	5.93	1.68	1.61
53	b	1055	G	P-O5'	5.89	1.65	1.59
53	b	401	A	O5'-C5'	5.86	1.53	1.44
53	b	1661	G	O3'-P	5.81	1.68	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	b	2446	G	O3'-P	5.80	1.68	1.61
53	b	1826	G	O3'-P	5.80	1.68	1.61
53	b	1080	A	N1-C2	5.78	1.39	1.34
53	b	1088	A	P-O5'	5.73	1.65	1.59
53	b	778	G	O3'-P	5.66	1.68	1.61
53	b	1773	A	O3'-P	5.48	1.67	1.61
53	b	979	A	O3'-P	5.46	1.67	1.61
53	b	1054	A	O3'-P	5.46	1.67	1.61
53	b	1054	A	C3'-O3'	5.40	1.49	1.42
53	b	87	U	O3'-P	5.37	1.67	1.61
51	X	13	C	C1'-N1	5.37	1.56	1.48
53	b	247	G	O3'-P	-5.29	1.54	1.61
53	b	514	A	N3-C4	5.28	1.38	1.34
53	b	2384	U	O3'-P	5.26	1.67	1.61
53	b	1088	A	O4'-C1'	5.24	1.48	1.41
53	b	2444	G	O3'-P	-5.20	1.54	1.61
53	b	1060	U	O3'-P	5.17	1.67	1.61
53	b	779	U	O3'-P	5.16	1.67	1.61
53	b	2109	U	C2-O2	5.12	1.26	1.22
53	b	2330	G	O3'-P	5.11	1.67	1.61
51	X	20	U	C1'-N1	5.09	1.56	1.48

All (487) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	A	230	G	N7-C8-N9	21.72	123.96	113.10
50	A	230	G	C2-N3-C4	19.69	121.75	111.90
50	A	230	G	N3-C4-N9	18.99	137.39	126.00
53	b	1509	A	N9-C1'-C2'	17.94	137.32	114.00
53	b	1275	A	N9-C1'-C2'	17.27	136.46	114.00
53	b	1943	U	N1-C1'-C2'	16.93	136.01	114.00
53	b	1102	C	N1-C1'-C2'	16.51	135.47	114.00
54	v	74	C	O3'-P-O5'	-15.69	74.20	104.00
53	b	1060	U	N1-C1'-C2'	15.38	134.00	114.00
53	b	2092	U	N1-C1'-C2'	14.95	133.43	114.00
54	v	74	C	OP2-P-O3'	14.00	136.01	105.20
53	b	1395	A	N9-C1'-C2'	13.75	131.88	114.00
53	b	1204	A	N9-C1'-C2'	13.69	131.79	114.00
53	b	2455	G	P-O3'-C3'	-13.40	103.62	119.70
50	A	230	G	N3-C4-C5	-13.17	122.02	128.60
50	A	230	G	N1-C2-N3	-12.74	116.26	123.90
53	b	1079	C	N1-C1'-C2'	-12.69	97.50	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	1272	A	N9-C1'-C2'	12.39	130.10	114.00
53	b	250	G	N9-C1'-C2'	12.34	130.04	114.00
53	b	1349	C	N1-C2-O2	12.22	126.23	118.90
50	A	230	G	N9-C4-C5	-12.10	100.56	105.40
53	b	2597	G	N9-C1'-C2'	12.03	129.64	114.00
53	b	2613	U	N1-C1'-C2'	11.68	129.18	114.00
53	b	1205	A	N9-C1'-C2'	11.56	129.03	114.00
50	A	230	G	C4-C5-N7	-11.46	106.22	110.80
53	b	2118	U	O4'-C1'-N1	11.29	117.23	108.20
53	b	2210	U	N1-C1'-C2'	11.25	128.63	114.00
53	b	2178	C	N1-C1'-C2'	-11.23	99.40	114.00
53	b	1667	G	N9-C1'-C2'	-11.15	99.50	114.00
53	b	2449	U	N1-C1'-C2'	-11.08	99.60	114.00
53	b	1069	A	O4'-C1'-N9	10.94	116.95	108.20
53	b	1349	C	C2-N1-C1'	10.93	130.82	118.80
53	b	2799	A	N9-C1'-C2'	10.93	128.20	114.00
53	b	1080	A	C8-N9-C1'	-10.92	108.05	127.70
53	b	782	A	N9-C1'-C2'	10.73	127.94	114.00
53	b	1080	A	C4-N9-C1'	10.63	145.43	126.30
53	b	1349	C	N3-C4-N4	-10.61	110.57	118.00
52	a	3	C	C4'-C3'-O3'	10.55	134.09	113.00
53	b	1080	A	O4'-C1'-N9	10.47	116.57	108.20
53	b	2161	C	N1-C1'-C2'	10.33	127.43	114.00
53	b	119	A	N9-C1'-C2'	10.26	127.33	114.00
53	b	2517	C	N1-C1'-C2'	-10.20	100.73	114.00
53	b	2798	U	N1-C1'-C2'	10.19	127.25	114.00
53	b	1266	G	O4'-C1'-N9	10.17	116.33	108.20
53	b	1299	G	C2'-C3'-O3'	9.94	131.37	109.50
53	b	614	A	N9-C1'-C2'	9.92	126.89	114.00
53	b	246	C	N1-C1'-C2'	9.64	126.53	114.00
53	b	1616	A	N9-C1'-C2'	9.54	126.39	114.00
53	b	1079	C	C6-N1-C1'	-9.52	109.38	120.80
53	b	1349	C	C6-N1-C1'	-9.49	109.42	120.80
53	b	973	A	N9-C1'-C2'	9.43	126.26	114.00
53	b	877	A	N9-C1'-C2'	-9.41	101.65	112.00
54	v	74	C	P-O3'-C3'	-9.38	108.44	119.70
53	b	2161	C	O4'-C1'-N1	9.29	115.63	108.20
53	b	1225	G	N9-C1'-C2'	9.16	125.91	114.00
53	b	456	C	N1-C1'-C2'	9.13	125.86	114.00
53	b	25	U	N1-C1'-C2'	9.09	125.82	114.00
53	b	2282	G	N9-C1'-C2'	-9.05	102.05	112.00
53	b	788	A	N9-C1'-C2'	-9.03	102.07	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	1395	A	O4'-C1'-N9	8.84	115.27	108.20
53	b	1055	G	C8-N9-C1'	-8.83	115.52	127.00
53	b	1088	A	C5'-C4'-O4'	8.83	119.69	109.10
53	b	640	C	N1-C1'-C2'	8.81	125.46	114.00
53	b	959	A	N9-C1'-C2'	8.81	125.46	114.00
53	b	1458	U	N1-C1'-C2'	8.81	125.46	114.00
53	b	979	A	N9-C1'-C2'	-8.81	102.31	112.00
53	b	1088	A	O4'-C1'-N9	-8.79	101.17	108.20
53	b	457	A	N9-C1'-C2'	8.77	125.40	114.00
53	b	2451	A	P-O3'-C3'	8.75	130.20	119.70
53	b	1522	A	N9-C1'-C2'	8.72	125.33	114.00
53	b	479	A	C4'-C3'-O3'	-8.68	91.18	109.40
53	b	983	A	N9-C1'-C2'	8.68	125.28	114.00
53	b	2505	G	P-O3'-C3'	-8.67	109.30	119.70
50	A	230	G	C5-C6-N1	8.63	115.81	111.50
53	b	2467	C	N1-C1'-C2'	-8.61	102.53	112.00
53	b	401	A	P-O5'-C5'	8.53	134.54	120.90
53	b	49	A	N9-C1'-C2'	8.43	124.96	114.00
53	b	242	G	N9-C1'-C2'	-8.41	102.75	112.00
53	b	1084	A	N9-C1'-C2'	8.36	124.86	114.00
53	b	1097	U	O4'-C1'-N1	8.31	114.85	108.20
53	b	544	C	N1-C1'-C2'	8.29	124.78	114.00
53	b	2750	A	O4'-C1'-N9	-8.27	101.58	108.20
53	b	2779	U	N1-C1'-C2'	8.25	124.72	114.00
53	b	931	U	N1-C1'-C2'	8.24	124.72	114.00
53	b	1272	A	O4'-C1'-N9	-8.24	101.61	108.20
53	b	1055	G	O5'-C5'-C4'	8.22	127.32	111.70
53	b	1773	A	C2'-C3'-O3'	8.22	127.58	109.50
53	b	1952	A	N9-C1'-C2'	8.15	124.60	114.00
53	b	2596	U	N1-C1'-C2'	8.12	124.56	114.00
53	b	1970	A	N9-C1'-C2'	8.12	124.55	114.00
53	b	2250	G	N9-C1'-C2'	8.10	124.54	114.00
53	b	618	G	N9-C1'-C2'	8.08	124.50	114.00
53	b	1055	G	C5'-C4'-O4'	8.08	118.79	109.10
53	b	1055	G	C4-N9-C1'	8.04	136.96	126.50
53	b	1265	A	N9-C1'-C2'	8.01	124.41	114.00
53	b	1103	A	C2'-C3'-O3'	8.01	127.12	109.50
53	b	2178	C	C2'-C3'-O3'	8.00	127.11	109.50
53	b	858	G	N9-C1'-C2'	-7.98	103.22	112.00
53	b	2162	G	O4'-C1'-N9	7.89	114.51	108.20
53	b	1459	G	N9-C1'-C2'	7.88	124.25	114.00
53	b	1143	A	N9-C1'-C2'	7.84	124.19	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	A	1158	C	N1-C2-O2	7.83	123.60	118.90
53	b	388	G	O4'-C1'-N9	7.82	114.46	108.20
53	b	1087	G	C4'-C3'-O3'	7.82	128.64	113.00
53	b	783	A	O4'-C1'-N9	7.81	114.44	108.20
53	b	1459	G	C1'-O4'-C4'	-7.79	103.67	109.90
53	b	241	A	N9-C1'-C2'	7.77	124.10	114.00
53	b	2056	G	OP2-P-O3'	7.76	122.28	105.20
53	b	1079	C	C2-N1-C1'	7.74	127.32	118.80
53	b	1392	A	N9-C1'-C2'	7.72	124.04	114.00
53	b	160	A	N9-C1'-C2'	7.72	124.03	114.00
53	b	1301	A	O4'-C1'-N9	7.71	114.37	108.20
53	b	1057	A	N9-C1'-C2'	-7.71	103.52	112.00
53	b	801	G	O4'-C1'-N9	-7.70	102.04	108.20
53	b	2128	G	N9-C1'-C2'	7.66	123.95	114.00
53	b	1567	G	N9-C1'-C2'	7.63	123.93	114.00
53	b	787	C	N1-C1'-C2'	7.63	123.92	114.00
53	b	979	A	C2'-C3'-O3'	7.63	126.28	109.50
53	b	108	G	N9-C1'-C2'	-7.62	103.61	112.00
53	b	2211	A	N9-C1'-C2'	7.57	123.84	114.00
53	b	72	U	N1-C1'-C2'	7.55	123.81	114.00
53	b	2172	U	C4'-C3'-O3'	7.55	128.09	113.00
53	b	2458	G	N9-C1'-C2'	-7.53	103.72	112.00
53	b	1088	A	C8-N9-C1'	-7.51	114.18	127.70
50	A	230	G	N3-C2-N2	7.51	125.16	119.90
34	h	62	LEU	N-CA-C	7.50	131.26	111.00
53	b	281	C	N1-C1'-C2'	7.50	123.75	114.00
53	b	783	A	C4'-C3'-O3'	7.49	127.97	113.00
53	b	1087	G	P-O3'-C3'	7.47	128.66	119.70
53	b	417	C	N1-C1'-C2'	-7.46	103.79	112.00
53	b	2117	A	N9-C1'-C2'	7.42	123.65	114.00
53	b	2211	A	O4'-C1'-N9	-7.41	102.28	108.20
53	b	603	A	N9-C1'-C2'	7.39	123.61	114.00
53	b	639	U	N1-C1'-C2'	7.39	123.61	114.00
50	A	1158	C	C2-N1-C1'	7.38	126.92	118.80
53	b	1102	C	C6-N1-C1'	-7.33	112.00	120.80
53	b	1054	A	O4'-C1'-N9	7.32	114.05	108.20
53	b	2645	G	N9-C1'-C2'	-7.32	103.95	112.00
53	b	1088	A	C2'-C3'-O3'	7.29	125.55	109.50
53	b	1055	G	P-O5'-C5'	7.29	132.57	120.90
53	b	2051	A	N9-C1'-C2'	-7.26	104.02	112.00
53	b	1300	G	O4'-C1'-N9	-7.25	102.40	108.20
53	b	247	G	N9-C1'-C2'	7.24	123.41	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	277	G	C2'-C3'-O3'	7.22	125.39	109.50
53	b	1967	C	N1-C1'-C2'	7.22	123.39	114.00
53	b	1057	A	C2'-C3'-O3'	7.22	125.38	109.50
53	b	2439	A	N9-C1'-C2'	-7.21	104.07	112.00
29	c	156	ARG	NE-CZ-NH2	-7.20	116.70	120.30
53	b	1300	G	N9-C1'-C2'	7.20	123.36	114.00
53	b	957	C	N1-C1'-C2'	7.16	123.31	114.00
53	b	242	G	O4'-C1'-N9	7.14	113.91	108.20
53	b	2541	A	C2'-C3'-O3'	7.13	125.19	109.50
53	b	2178	C	C4'-C3'-O3'	7.12	127.23	113.00
53	b	1076	C	N1-C1'-C2'	7.10	123.23	114.00
53	b	1055	G	N9-C1'-C2'	7.10	123.23	114.00
53	b	2160	C	O4'-C1'-N1	7.08	113.87	108.20
53	b	574	A	N9-C1'-C2'	7.07	123.19	114.00
53	b	603	A	O4'-C1'-N9	-7.06	102.56	108.20
53	b	2455	G	OP2-P-O3'	7.05	120.70	105.20
53	b	1698	A	N9-C1'-C2'	7.02	123.13	114.00
53	b	1088	A	C4'-C3'-O3'	-7.02	94.66	109.40
53	b	500	G	N9-C1'-C2'	-7.02	104.28	112.00
53	b	574	A	O4'-C1'-N9	-7.01	102.59	108.20
53	b	2205	A	C2'-C3'-O3'	7.00	124.90	113.70
53	b	2796	U	N1-C1'-C2'	6.98	123.07	114.00
53	b	873	C	C2'-C3'-O3'	6.98	124.86	113.70
53	b	1349	C	N3-C2-O2	-6.98	117.02	121.90
53	b	1392	A	O4'-C1'-N9	6.97	113.78	108.20
53	b	2661	G	N9-C1'-C2'	6.94	123.02	114.00
53	b	158	U	N1-C1'-C2'	6.89	122.96	114.00
53	b	559	G	N9-C1'-C2'	-6.87	104.44	112.00
53	b	2702	G	C2'-C3'-O3'	6.85	124.66	113.70
53	b	1156	A	N9-C1'-C2'	6.85	122.90	114.00
53	b	1080	A	C5'-C4'-O4'	6.83	117.30	109.10
34	h	61	VAL	N-CA-C	6.83	129.45	111.00
53	b	1918	A	N9-C1'-C2'	-6.83	104.49	112.00
53	b	1377	G	N9-C1'-C2'	6.81	122.86	114.00
53	b	1069	A	C1'-O4'-C4'	-6.81	104.45	109.90
53	b	215	G	N9-C1'-C2'	6.80	122.84	114.00
53	b	564	C	N1-C1'-C2'	6.80	122.84	114.00
53	b	1080	A	C1'-O4'-C4'	-6.77	104.48	109.90
53	b	2879	A	N9-C1'-C2'	6.77	122.80	114.00
53	b	2304	G	C2'-C3'-O3'	6.76	124.52	113.70
53	b	2012	G	C2'-C3'-O3'	6.76	124.52	113.70
53	b	2530	A	N9-C1'-C2'	6.75	122.78	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	783	A	O5'-P-OP1	-6.74	99.64	105.70
53	b	2425	A	N9-C1'-C2'	6.73	122.75	114.00
53	b	544	C	O4'-C1'-N1	6.72	113.58	108.20
53	b	2455	G	OP1-P-O3'	-6.70	90.46	105.20
53	b	388	G	C1'-O4'-C4'	-6.70	104.54	109.90
53	b	1078	U	C2'-C3'-O3'	6.69	124.41	113.70
53	b	2272	U	N1-C1'-C2'	6.69	122.70	114.00
53	b	2162	G	C1'-O4'-C4'	-6.69	104.55	109.90
52	a	15	A	N9-C1'-C2'	6.68	122.68	114.00
53	b	2118	U	C1'-O4'-C4'	-6.66	104.57	109.90
53	b	1508	A	N9-C1'-C2'	6.64	122.63	114.00
53	b	2797	U	O4'-C1'-C2'	-6.64	99.16	105.80
53	b	2518	A	O4'-C1'-N9	-6.61	102.91	108.20
53	b	2589	A	C2'-C3'-O3'	6.60	124.26	113.70
53	b	1349	C	C5'-C4'-O4'	6.57	116.98	109.10
53	b	1311	G	N9-C1'-C2'	-6.56	104.78	112.00
53	b	2127	G	N9-C1'-C2'	6.56	122.53	114.00
53	b	1098	A	C2'-C3'-O3'	6.54	124.16	113.70
53	b	1392	A	C1'-O4'-C4'	-6.52	104.69	109.90
53	b	241	A	O4'-C1'-N9	-6.48	103.02	108.20
53	b	1301	A	C1'-O4'-C4'	-6.47	104.72	109.90
53	b	2564	A	N9-C1'-C2'	6.46	122.39	114.00
53	b	387	U	N1-C1'-C2'	6.45	122.38	114.00
50	A	1158	C	N3-C2-O2	-6.42	117.40	121.90
53	b	1023	U	C5'-C4'-O4'	6.40	116.78	109.10
53	b	450	G	N9-C1'-C2'	-6.38	104.98	112.00
53	b	477	A	N9-C1'-C2'	6.35	122.25	114.00
53	b	986	C	N1-C1'-C2'	6.35	122.25	114.00
53	b	1348	C	C4'-C3'-O3'	6.33	125.67	113.00
53	b	1080	A	O4'-C4'-C3'	-6.33	97.67	104.00
53	b	87	U	C2'-C3'-O3'	6.32	123.81	113.70
53	b	464	U	N1-C1'-C2'	6.31	122.20	114.00
53	b	877	A	O4'-C4'-C3'	-6.30	97.70	104.00
53	b	1087	G	O4'-C1'-N9	6.28	113.23	108.20
53	b	196	A	O4'-C1'-N9	6.27	113.21	108.20
53	b	1704	C	C2'-C3'-O3'	6.25	123.70	113.70
52	a	3	C	OP1-P-O3'	6.25	118.94	105.20
53	b	2798	U	O4'-C1'-N1	6.25	113.20	108.20
53	b	448	U	N1-C1'-C2'	-6.24	105.14	112.00
53	b	1055	G	O5'-P-OP1	6.24	118.19	110.70
53	b	1773	A	N9-C1'-C2'	-6.23	105.15	112.00
53	b	674	G	N9-C1'-C2'	-6.22	105.16	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	z	15	THR	C-N-CD	6.21	141.45	128.40
53	b	2178	C	C4'-C3'-C2'	-6.21	96.39	102.60
53	b	2822	G	N9-C1'-C2'	6.20	122.06	114.00
53	b	2873	A	O4'-C1'-N9	6.19	113.15	108.20
53	b	2178	C	O4'-C4'-C3'	-6.19	97.81	104.00
53	b	1496	A	N9-C1'-C2'	6.18	122.04	114.00
53	b	1618	A	N9-C1'-C2'	6.18	122.03	114.00
53	b	2848	G	N9-C1'-C2'	-6.18	105.21	112.00
53	b	1103	A	N9-C1'-C2'	-6.16	105.22	112.00
53	b	2128	G	C4'-C3'-O3'	6.14	125.29	113.00
53	b	2889	C	N1-C1'-C2'	6.14	121.99	114.00
34	h	67	ALA	N-CA-C	6.14	127.59	111.00
53	b	458	G	O4'-C1'-N9	6.14	113.11	108.20
53	b	1266	G	C1'-O4'-C4'	-6.14	104.99	109.90
53	b	1927	A	N9-C1'-C2'	6.13	121.97	114.00
53	b	2750	A	C5'-C4'-O4'	6.13	116.46	109.10
53	b	1459	G	O4'-C1'-N9	6.12	113.10	108.20
52	a	66	A	C2'-C3'-O3'	6.12	123.49	113.70
50	A	390	U	N3-C2-O2	-6.11	117.92	122.20
53	b	273	G	N9-C1'-C2'	6.11	121.94	114.00
53	b	2336	A	N9-C1'-C2'	6.11	121.94	114.00
53	b	2446	G	N9-C1'-C2'	-6.10	105.29	112.00
53	b	576	U	N1-C1'-C2'	6.09	121.92	114.00
53	b	1125	G	N9-C1'-C2'	6.09	121.92	114.00
53	b	786	C	N1-C1'-C2'	6.07	121.90	114.00
53	b	801	G	C2'-C3'-O3'	6.07	123.42	113.70
53	b	2431	U	N1-C1'-C2'	-6.07	105.33	112.00
53	b	2800	A	C4'-C3'-O3'	6.07	125.13	113.00
53	b	1088	A	P-O5'-C5'	6.06	130.60	120.90
53	b	1033	U	C3'-C2'-C1'	6.04	106.33	101.50
50	A	365	U	C2-N1-C1'	6.04	124.94	117.70
53	b	1395	A	C1'-O4'-C4'	-6.02	105.08	109.90
53	b	1980	G	N9-C1'-C2'	-6.02	105.38	112.00
53	b	1756	G	C5'-C4'-O4'	6.02	116.32	109.10
53	b	974	G	O4'-C1'-N9	6.01	113.01	108.20
53	b	1400	U	N1-C1'-C2'	6.01	121.81	114.00
53	b	2210	U	O4'-C1'-N1	-6.01	103.39	108.20
53	b	454	A	N9-C1'-C2'	5.99	121.79	114.00
53	b	914	G	N9-C1'-C2'	-5.99	105.41	112.00
53	b	1675	C	N1-C1'-C2'	5.99	121.78	114.00
53	b	2798	U	C1'-O4'-C4'	-5.98	105.11	109.90
53	b	385	C	N1-C1'-C2'	5.98	121.78	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	2249	U	N1-C1'-C2'	-5.98	105.43	112.00
53	b	800	A	N9-C1'-C2'	5.97	121.77	114.00
31	e	61	ARG	N-CA-C	5.97	127.12	111.00
53	b	1600	C	N1-C1'-C2'	5.97	121.76	114.00
53	b	2654	A	N9-C1'-C2'	5.97	121.76	114.00
53	b	877	A	C4'-C3'-C2'	-5.97	96.63	102.60
53	b	2567	G	N9-C1'-C2'	5.96	121.75	114.00
30	d	4	LEU	CB-CG-CD1	5.96	121.13	111.00
53	b	253	C	N1-C1'-C2'	-5.95	105.45	112.00
53	b	1698	A	O4'-C1'-N9	-5.94	103.45	108.20
53	b	1057	A	C4'-C3'-O3'	5.94	124.88	113.00
53	b	2271	G	N9-C1'-C2'	5.93	121.71	114.00
53	b	196	A	N9-C1'-C2'	-5.93	105.48	112.00
53	b	1249	U	N1-C1'-C2'	5.93	121.71	114.00
53	b	465	G	N9-C1'-C2'	5.92	121.69	114.00
53	b	479	A	N9-C1'-C2'	5.91	121.69	114.00
53	b	1756	G	C5'-C4'-C3'	5.91	125.46	116.00
53	b	2131	U	C5-C6-N1	-5.91	119.75	122.70
53	b	2025	C	N1-C1'-C2'	5.90	121.67	114.00
53	b	1057	A	C4'-C3'-C2'	-5.89	96.71	102.60
53	b	1078	U	N1-C1'-C2'	5.89	121.65	114.00
53	b	1204	A	O4'-C1'-N9	-5.88	103.50	108.20
53	b	608	A	N9-C1'-C2'	5.88	121.64	114.00
53	b	1253	A	N9-C1'-C2'	5.87	121.63	114.00
53	b	1814	G	N9-C1'-C2'	5.86	121.61	114.00
53	b	51	G	N9-C1'-C2'	-5.86	105.56	112.00
53	b	2329	U	N1-C1'-C2'	-5.85	105.56	112.00
53	b	2161	C	C1'-O4'-C4'	-5.84	105.23	109.90
53	b	2180	U	O4'-C1'-C2'	-5.84	99.96	105.80
53	b	877	A	C5'-C4'-O4'	5.83	116.10	109.10
53	b	2307	G	N9-C1'-C2'	5.83	121.58	114.00
53	b	2873	A	C1'-O4'-C4'	-5.83	105.24	109.90
53	b	1272	A	C4-N9-C1'	-5.83	115.81	126.30
53	b	84	A	N9-C1'-C2'	-5.83	105.59	112.00
53	b	1070	A	N9-C1'-C2'	5.83	121.57	114.00
53	b	1100	C	C4'-C3'-O3'	5.83	124.65	113.00
53	b	1056	G	N9-C1'-C2'	5.82	121.57	114.00
53	b	1495	A	N9-C1'-C2'	5.82	121.57	114.00
53	b	2750	A	N9-C1'-C2'	5.81	121.55	114.00
53	b	390	U	N1-C1'-C2'	-5.81	105.61	112.00
53	b	2160	C	O4'-C4'-C3'	-5.80	98.20	104.00
53	b	1087	G	C5'-C4'-C3'	5.79	125.26	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	411	G	N9-C1'-C2'	5.79	121.52	114.00
53	b	985	C	N1-C1'-C2'	5.78	121.52	114.00
52	a	33	G	N9-C1'-C2'	-5.77	105.65	112.00
53	b	1058	U	O4'-C1'-N1	5.77	112.82	108.20
53	b	704	G	N9-C1'-C2'	-5.77	105.65	112.00
53	b	1055	G	O5'-P-OP2	-5.77	100.50	105.70
53	b	1348	C	N1-C1'-C2'	-5.77	105.65	112.00
53	b	1801	A	N9-C1'-C2'	5.77	121.50	114.00
53	b	2172	U	O4'-C1'-N1	5.77	112.82	108.20
53	b	1103	A	O4'-C1'-N9	5.77	112.81	108.20
53	b	1996	C	N1-C1'-C2'	5.77	121.50	114.00
53	b	1761	C	N1-C1'-C2'	5.76	121.49	114.00
53	b	2340	A	C8-N9-C1'	-5.76	117.33	127.70
53	b	2151	U	C4'-C3'-O3'	5.76	124.51	113.00
53	b	75	G	O4'-C1'-C2'	-5.75	100.05	105.80
53	b	2178	C	O4'-C1'-N1	5.74	112.79	108.20
53	b	1133	A	O4'-C1'-N9	5.73	112.79	108.20
53	b	1678	A	N9-C1'-C2'	-5.73	105.70	112.00
49	z	16	PRO	CB-CA-C	5.73	126.32	112.00
53	b	479	A	C2'-C3'-O3'	5.72	122.86	113.70
53	b	1401	G	N9-C1'-C2'	5.69	121.40	114.00
53	b	400	G	N9-C1'-C2'	5.68	121.39	114.00
52	a	42	C	N1-C1'-C2'	5.68	121.38	114.00
50	A	1158	C	C6-N1-C2	-5.67	118.03	120.30
53	b	400	G	C2'-C3'-O3'	5.67	122.77	113.70
53	b	280	U	N1-C1'-C2'	5.66	121.36	114.00
53	b	1060	U	C3'-C2'-C1'	-5.66	96.97	101.50
44	s	88	ARG	NE-CZ-NH1	-5.66	117.47	120.30
53	b	1754	A	N9-C1'-C2'	5.66	121.36	114.00
53	b	447	A	N9-C1'-C2'	-5.65	105.79	112.00
53	b	1057	A	O4'-C1'-C2'	-5.64	100.16	105.80
53	b	1839	G	O4'-C1'-C2'	-5.64	100.16	105.80
53	b	2551	C	N1-C1'-C2'	-5.64	105.80	112.00
53	b	423	A	N9-C1'-C2'	5.64	121.33	114.00
53	b	1097	U	C5'-C4'-O4'	5.61	115.84	109.10
53	b	830	G	N9-C1'-C2'	5.61	121.29	114.00
53	b	1098	A	O4'-C4'-C3'	-5.60	98.40	104.00
53	b	1103	A	C4'-C3'-C2'	-5.58	97.02	102.60
53	b	845	A	C4'-C3'-O3'	5.58	124.15	113.00
50	A	365	U	N1-C2-O2	5.57	126.70	122.80
53	b	196	A	C1'-O4'-C4'	-5.56	105.45	109.90
53	b	877	A	C4'-C3'-O3'	5.54	124.09	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	2266	A	N9-C1'-C2'	5.53	121.19	114.00
53	b	544	C	C1'-O4'-C4'	-5.53	105.48	109.90
53	b	410	G	C2'-C3'-O3'	5.53	122.54	113.70
53	b	1055	G	C3'-C2'-C1'	5.53	105.92	101.50
53	b	1069	A	O4'-C1'-C2'	-5.53	100.27	105.80
53	b	2252	G	N9-C1'-C2'	-5.52	105.93	112.00
53	b	531	C	N1-C1'-C2'	5.52	121.17	114.00
53	b	777	G	C2'-C3'-O3'	5.52	122.53	113.70
53	b	2877	G	N9-C1'-C2'	-5.52	105.93	112.00
53	b	866	A	O4'-C1'-C2'	-5.51	100.29	105.80
53	b	1234	U	N1-C1'-C2'	5.51	121.16	114.00
53	b	1758	U	N1-C1'-C2'	5.50	121.15	114.00
53	b	2211	A	C4'-C3'-O3'	-5.50	97.86	109.40
53	b	62	U	O4'-C1'-N1	5.49	112.59	108.20
53	b	791	C	N1-C1'-C2'	5.48	121.13	114.00
53	b	571	U	O4'-C1'-N1	5.47	112.58	108.20
53	b	1023	U	C5'-C4'-C3'	5.47	124.76	116.00
53	b	2590	A	C5'-C4'-O4'	5.47	115.67	109.10
53	b	2172	U	C2'-C3'-O3'	-5.47	97.47	109.50
53	b	1104	C	C5'-C4'-O4'	5.46	115.66	109.10
53	b	1287	A	N9-C1'-C2'	5.46	121.09	114.00
50	A	230	G	C4-N9-C1'	5.46	133.59	126.50
53	b	1239	G	N9-C1'-C2'	-5.45	106.00	112.00
53	b	2152	G	C5'-C4'-O4'	5.45	115.64	109.10
53	b	979	A	C4'-C3'-C2'	-5.45	97.15	102.60
53	b	1204	A	O4'-C4'-C3'	-5.45	98.55	104.00
53	b	1054	A	C4'-C3'-O3'	5.44	123.88	113.00
53	b	372	G	O4'-C1'-N9	5.43	112.55	108.20
53	b	2340	A	C4-N9-C1'	5.43	136.07	126.30
53	b	9	G	C2'-C3'-O3'	5.42	122.37	113.70
53	b	1032	A	N9-C1'-C2'	-5.42	106.04	112.00
53	b	2656	U	N1-C1'-C2'	-5.42	106.04	112.00
53	b	2160	C	N1-C1'-C2'	-5.41	106.05	112.00
53	b	2614	A	N9-C1'-C2'	-5.40	106.06	112.00
53	b	119	A	O4'-C1'-N9	-5.40	103.88	108.20
53	b	388	G	O4'-C4'-C3'	-5.38	98.62	104.00
53	b	1969	A	N9-C1'-C2'	5.37	120.98	114.00
53	b	2173	A	O5'-P-OP2	-5.37	100.87	105.70
53	b	401	A	C5'-C4'-O4'	5.36	115.53	109.10
53	b	2152	G	C8-N9-C1'	-5.35	120.05	127.00
53	b	805	G	N9-C1'-C2'	5.34	120.94	114.00
53	b	1205	A	C4'-C3'-O3'	-5.34	98.18	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	910	A	N9-C1'-C2'	5.34	120.94	114.00
53	b	1103	A	O4'-C4'-C3'	-5.34	98.66	104.00
53	b	2449	U	O4'-C1'-N1	5.33	112.47	108.20
53	b	1865	U	N1-C1'-C2'	-5.33	106.14	112.00
53	b	2288	A	N9-C1'-C2'	5.33	120.92	114.00
53	b	1058	U	N1-C1'-C2'	5.32	120.92	114.00
53	b	1081	U	O4'-C4'-C3'	-5.32	98.68	104.00
53	b	1569	A	N9-C1'-C2'	5.32	120.91	114.00
53	b	2866	U	N1-C1'-C2'	5.31	120.91	114.00
50	A	230	G	C6-C5-N7	5.31	133.58	130.40
53	b	1425	G	N9-C1'-C2'	5.31	120.90	114.00
53	b	925	A	N9-C1'-C2'	-5.29	106.18	112.00
53	b	583	G	N9-C1'-C2'	-5.29	106.18	112.00
53	b	1238	G	C2'-C3'-O3'	5.29	122.16	113.70
53	b	801	G	C5'-C4'-O4'	5.29	115.45	109.10
36	k	70	ARG	NE-CZ-NH2	-5.28	117.66	120.30
53	b	1079	C	C3'-C2'-C1'	5.28	105.72	101.50
53	b	2869	G	N9-C1'-C2'	5.26	120.84	114.00
53	b	157	C	N1-C1'-C2'	5.26	120.83	114.00
53	b	531	C	O4'-C1'-N1	-5.25	104.00	108.20
53	b	934	U	C5'-C4'-O4'	5.25	115.40	109.10
53	b	1585	C	N1-C1'-C2'	5.25	120.83	114.00
53	b	1461	C	N1-C1'-C2'	5.25	120.82	114.00
53	b	2128	G	O4'-C1'-C2'	-5.24	100.56	105.80
53	b	1204	A	C4'-C3'-O3'	-5.23	98.41	109.40
53	b	674	G	C4'-C3'-C2'	-5.23	97.37	102.60
53	b	2238	G	N9-C1'-C2'	5.23	120.80	114.00
53	b	1102	C	C2-N1-C1'	5.22	124.55	118.80
50	A	1322	C	C2-N1-C1'	5.22	124.54	118.80
53	b	2127	G	O4'-C1'-N9	-5.21	104.03	108.20
53	b	989	G	N9-C1'-C2'	-5.21	106.27	112.00
53	b	1088	A	C1'-O4'-C4'	5.21	114.07	109.90
34	h	66	ASN	N-CA-C	5.20	125.05	111.00
53	b	365	U	C4'-C3'-O3'	5.20	123.40	113.00
53	b	1238	G	N9-C1'-C2'	-5.20	106.28	112.00
53	b	1583	A	N9-C1'-C2'	-5.19	106.29	112.00
53	b	2340	A	N9-C1'-C2'	5.19	120.75	114.00
53	b	372	G	C1'-O4'-C4'	-5.19	105.75	109.90
53	b	1393	A	N9-C1'-C2'	5.19	120.74	114.00
53	b	782	A	C4'-C3'-O3'	-5.17	98.54	109.40
53	b	1344	U	N1-C1'-C2'	5.17	120.71	114.00
52	a	3	C	P-O3'-C3'	-5.16	113.50	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	q	11	ARG	NE-CZ-NH2	-5.16	117.72	120.30
53	b	250	G	O4'-C1'-N9	-5.16	104.08	108.20
53	b	43	G	N9-C1'-C2'	5.15	120.70	114.00
53	b	1133	A	C1'-O4'-C4'	-5.15	105.78	109.90
53	b	2020	A	N9-C1'-C2'	-5.15	106.33	112.00
53	b	783	A	O4'-C4'-C3'	-5.15	98.85	104.00
53	b	1224	U	N1-C1'-C2'	5.15	120.69	114.00
54	v	33	U	P-O3'-C3'	5.14	125.87	119.70
50	A	754	C	C2-N1-C1'	5.14	124.45	118.80
53	b	2174	C	N1-C1'-C2'	5.14	120.68	114.00
53	b	395	U	N1-C1'-C2'	-5.13	106.36	112.00
53	b	1801	A	O4'-C1'-N9	-5.13	104.10	108.20
53	b	809	G	N9-C1'-C2'	5.12	120.66	114.00
45	t	3	ARG	NE-CZ-NH1	5.12	122.86	120.30
53	b	2210	U	C4'-C3'-O3'	-5.12	98.66	109.40
53	b	1780	A	N9-C1'-C2'	5.11	120.65	114.00
53	b	1801	A	C4'-C3'-O3'	-5.10	98.70	109.40
53	b	2330	G	O4'-C1'-C2'	-5.10	100.70	105.80
53	b	2384	U	C3'-C2'-C1'	5.09	105.58	101.50
53	b	2180	U	N1-C1'-C2'	-5.09	106.40	112.00
53	b	24	G	N9-C1'-C2'	5.09	120.62	114.00
53	b	450	G	C2'-C3'-O3'	5.09	121.84	113.70
53	b	356	G	N9-C1'-C2'	5.08	120.61	114.00
53	b	2518	A	N9-C1'-C2'	5.08	120.61	114.00
53	b	995	C	N1-C1'-C2'	5.08	120.61	114.00
43	r	10	LYS	CD-CE-NZ	5.08	123.38	111.70
53	b	877	A	C2'-C3'-O3'	5.08	121.83	113.70
53	b	1427	A	N9-C1'-C2'	5.08	120.60	114.00
53	b	1815	A	N9-C1'-C2'	5.08	120.60	114.00
53	b	2576	G	N9-C1'-C2'	5.08	120.60	114.00
53	b	254	G	N9-C1'-C2'	-5.07	106.43	112.00
53	b	1330	C	N1-C1'-C2'	5.07	120.59	114.00
53	b	1804	C	C2'-C3'-O3'	5.07	121.81	113.70
53	b	1266	G	O4'-C1'-C2'	-5.06	100.74	105.80
34	h	31	VAL	C-N-CD	-5.06	109.47	120.60
53	b	2150	C	O4'-C1'-C2'	-5.06	100.74	105.80
53	b	436	C	C5'-C4'-O4'	5.06	115.17	109.10
53	b	2750	A	C2'-C3'-O3'	5.06	121.79	113.70
53	b	2588	G	N9-C1'-C2'	-5.06	106.44	112.00
53	b	2282	G	O4'-C1'-C2'	-5.05	100.75	105.80
53	b	873	C	N1-C1'-C2'	-5.05	106.45	112.00
53	b	896	A	O4'-C4'-C3'	-5.05	98.95	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	b	120	U	N1-C1'-C2'	5.03	120.53	114.00
53	b	914	G	C4'-C3'-C2'	-5.03	97.57	102.60
53	b	896	A	N9-C1'-C2'	-5.02	106.47	112.00
53	b	94	A	C4-N9-C1'	5.02	135.34	126.30
53	b	2169	A	C3'-C2'-C1'	5.02	105.51	101.50
53	b	2238	G	O4'-C1'-N9	-5.02	104.19	108.20
53	b	2497	A	N9-C1'-C2'	-5.02	106.48	112.00
53	b	94	A	C8-N9-C1'	-5.00	118.69	127.70

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	2	3	LYS	Peptide
11	L	71	HIS	Peptide
52	a	45	A	Sidechain
53	b	1057	A	Sidechain
53	b	1060	U	Sidechain
53	b	1069	A	Sidechain
53	b	1079	C	Sidechain
53	b	1088	A	Sidechain
53	b	1102	C	Sidechain
53	b	1103	A	Sidechain
53	b	1104	C	Sidechain
53	b	1143	A	Sidechain
53	b	1186	G	Sidechain
53	b	119	A	Sidechain
53	b	1204	A	Sidechain
53	b	1225	G	Sidechain
53	b	1266	G	Sidechain
53	b	1272	A	Sidechain
53	b	1275	A	Sidechain
53	b	1300	G	Sidechain
53	b	1392	A	Sidechain
53	b	1395	A	Sidechain
53	b	1509	A	Sidechain
53	b	1667	G	Sidechain
53	b	1678	A	Sidechain
53	b	1698	A	Sidechain
53	b	1759	A	Sidechain
53	b	1774	C	Sidechain
53	b	1829	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	b	1927	A	Sidechain
53	b	1943	U	Sidechain
53	b	196	A	Sidechain
53	b	2092	U	Sidechain
53	b	210	C	Sidechain
53	b	2118	U	Sidechain
53	b	2159	G	Sidechain
53	b	2160	C	Sidechain
53	b	2161	C	Sidechain
53	b	2178	C	Sidechain
53	b	2210	U	Sidechain
53	b	2211	A	Sidechain
53	b	2282	G	Sidechain
53	b	2330	G	Sidechain
53	b	241	A	Sidechain
53	b	242	G	Sidechain
53	b	2449	U	Sidechain
53	b	246	C	Sidechain
53	b	247	G	Sidechain
53	b	25	U	Sidechain
53	b	250	G	Sidechain
53	b	2517	C	Sidechain
53	b	2518	A	Sidechain
53	b	2564	A	Sidechain
53	b	2590	A	Sidechain
53	b	2597	G	Sidechain
53	b	2615	U	Sidechain
53	b	2750	A	Sidechain
53	b	2766	A	Sidechain
53	b	277	G	Sidechain
53	b	2796	U	Sidechain
53	b	2799	A	Sidechain
53	b	2886	A	Sidechain
53	b	388	G	Sidechain
53	b	574	A	Sidechain
53	b	603	A	Sidechain
53	b	674	G	Sidechain
53	b	75	G	Sidechain
53	b	779	U	Sidechain
53	b	782	A	Sidechain
53	b	783	A	Sidechain
53	b	788	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	b	801	G	Sidechain
53	b	959	A	Sidechain
53	b	973	A	Sidechain
53	b	979	A	Sidechain
29	c	232	HIS	Peptide
30	d	151	THR	Peptide
36	k	34	GLY	Peptide
37	l	102	GLY	Peptide
43	r	50	GLY	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	B	216/241 (90%)	186 (86%)	22 (10%)	8 (4%)	3	28
2	C	204/233 (88%)	173 (85%)	22 (11%)	9 (4%)	2	23
3	D	203/206 (98%)	179 (88%)	19 (9%)	5 (2%)	5	35
4	E	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	3	30
5	F	98/131 (75%)	82 (84%)	12 (12%)	4 (4%)	3	25
6	G	148/156 (95%)	128 (86%)	15 (10%)	5 (3%)	3	30
7	H	127/130 (98%)	111 (87%)	12 (9%)	4 (3%)	4	32
8	I	125/130 (96%)	99 (79%)	20 (16%)	6 (5%)	2	21
9	J	96/103 (93%)	77 (80%)	11 (12%)	8 (8%)	1	10
10	K	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	17	56
11	L	121/124 (98%)	100 (83%)	16 (13%)	5 (4%)	3	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	111/118 (94%)	100 (90%)	9 (8%)	2 (2%)	8	42
13	N	92/101 (91%)	78 (85%)	7 (8%)	7 (8%)	1	12
14	O	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	37
15	P	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	6
16	Q	78/84 (93%)	67 (86%)	9 (12%)	2 (3%)	5	34
17	R	53/75 (71%)	49 (92%)	4 (8%)	0	100	100
18	S	77/92 (84%)	66 (86%)	9 (12%)	2 (3%)	5	34
19	T	83/87 (95%)	78 (94%)	3 (4%)	2 (2%)	6	36
20	U	49/71 (69%)	39 (80%)	6 (12%)	4 (8%)	1	10
21	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
22	1	60/63 (95%)	51 (85%)	7 (12%)	2 (3%)	4	30
23	2	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	8	42
24	3	54/57 (95%)	49 (91%)	3 (6%)	2 (4%)	3	28
25	4	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
26	6	44/46 (96%)	41 (93%)	1 (2%)	2 (4%)	2	22
27	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
28	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
29	c	269/273 (98%)	252 (94%)	16 (6%)	1 (0%)	34	70
30	d	207/209 (99%)	195 (94%)	10 (5%)	2 (1%)	15	54
31	e	199/201 (99%)	186 (94%)	5 (2%)	8 (4%)	3	26
32	f	175/179 (98%)	154 (88%)	15 (9%)	6 (3%)	3	30
33	g	174/177 (98%)	139 (80%)	30 (17%)	5 (3%)	4	33
34	h	147/149 (99%)	120 (82%)	19 (13%)	8 (5%)	2	19
35	j	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	11	47
36	k	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	9	43
37	l	142/144 (99%)	128 (90%)	9 (6%)	5 (4%)	3	29
38	m	131/136 (96%)	125 (95%)	5 (4%)	1 (1%)	19	58
39	n	118/127 (93%)	111 (94%)	4 (3%)	3 (2%)	5	35
40	o	114/117 (97%)	107 (94%)	2 (2%)	5 (4%)	2	23
41	p	112/115 (97%)	106 (95%)	5 (4%)	1 (1%)	17	56
42	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	r	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	15	54
44	s	108/110 (98%)	103 (95%)	2 (2%)	3 (3%)	5	33
45	t	91/100 (91%)	82 (90%)	6 (7%)	3 (3%)	4	30
46	u	100/104 (96%)	82 (82%)	12 (12%)	6 (6%)	1	17
47	w	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
48	y	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
49	z	24/87 (28%)	21 (88%)	3 (12%)	0	100	100
All	All	5497/5903 (93%)	4898 (89%)	440 (8%)	159 (3%)	7	33

All (159) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	SER
2	C	7	ASN
2	C	61	LYS
4	E	99	SER
4	E	146	MET
5	F	98	GLU
8	I	127	SER
9	J	58	ASN
13	N	80	ARG
15	P	11	ALA
15	P	80	LYS
18	S	4	LEU
19	T	44	ALA
22	1	3	ALA
24	3	56	ALA
26	6	44	VAL
30	d	152	PRO
31	e	61	ARG
31	e	153	LEU
32	f	62	GLY
32	f	123	ASP
33	g	119	ALA
34	h	41	LYS
35	j	81	ILE
37	l	111	ILE
39	n	70	THR
39	n	119	SER
44	s	65	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	u	7	ARG
2	C	63	ILE
3	D	125	ASN
5	F	94	HIS
7	H	44	PHE
7	H	46	GLU
8	I	8	THR
8	I	27	ILE
9	J	17	LEU
9	J	57	VAL
9	J	67	ILE
9	J	94	ALA
11	L	24	GLU
11	L	88	ASP
12	M	3	ILE
13	N	52	ARG
13	N	66	THR
14	O	21	THR
15	P	10	GLY
15	P	16	PHE
15	P	36	VAL
16	Q	71	SER
18	S	5	LYS
19	T	67	HIS
20	U	32	ARG
24	3	55	ILE
29	c	253	LYS
33	g	92	VAL
34	h	68	ARG
34	h	119	ASN
34	h	123	ARG
35	j	25	LEU
36	k	35	VAL
37	l	29	LYS
37	l	115	GLU
40	o	59	ALA
41	p	114	LEU
44	s	62	ASP
44	s	63	GLY
45	t	38	ALA
46	u	19	LYS
46	u	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	22	TRP
1	B	63	LYS
1	B	123	GLY
2	C	106	ARG
2	C	111	ASP
2	C	145	ALA
3	D	194	ILE
4	E	142	GLY
5	F	85	ILE
6	G	4	ARG
6	G	15	PRO
6	G	113	LYS
7	H	88	LYS
10	K	88	PRO
13	N	21	ALA
13	N	50	LEU
15	P	49	GLY
15	P	78	VAL
20	U	24	LYS
32	f	121	SER
32	f	175	PHE
34	h	15	LEU
36	k	108	ARG
37	l	82	LEU
37	l	86	GLU
40	o	66	GLY
45	t	17	SER
1	B	204	ASP
2	C	129	PHE
3	D	47	LEU
4	E	103	GLY
4	E	147	ASN
5	F	48	ALA
6	G	114	SER
9	J	75	ASP
11	L	46	SER
11	L	60	PHE
12	M	23	GLY
13	N	62	ARG
14	O	20	ASP
20	U	29	ALA
22	1	37	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	2	4	THR
26	6	45	SER
31	e	80	SER
31	e	127	GLU
32	f	174	ASP
38	m	69	PRO
39	n	118	ARG
40	o	57	ALA
40	o	100	HIS
46	u	75	ALA
46	u	98	SER
1	B	53	LEU
3	D	119	HIS
7	H	87	ARG
9	J	78	GLU
9	J	92	LEU
11	L	76	HIS
31	e	42	GLY
31	e	60	TRP
33	g	118	PRO
33	g	175	LYS
34	h	56	ALA
43	r	53	PHE
1	B	166	ASP
3	D	4	LEU
8	I	12	LYS
13	N	34	ASN
31	e	82	GLY
34	h	29	PHE
45	t	18	GLU
2	C	154	GLY
8	I	57	VAL
15	P	42	ILE
30	d	104	VAL
32	f	149	VAL
8	I	9	GLY
20	U	27	VAL
31	e	83	VAL
33	g	28	GLY
1	B	30	ILE
2	C	107	LYS
6	G	54	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	Q	4	ILE
15	P	15	PRO
34	h	88	GLY
40	o	101	GLY
46	u	55	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	B	180/199 (90%)	180 (100%)	0	100	100
2	C	170/190 (90%)	170 (100%)	0	100	100
3	D	172/173 (99%)	172 (100%)	0	100	100
4	E	113/126 (90%)	113 (100%)	0	100	100
5	F	87/112 (78%)	87 (100%)	0	100	100
6	G	123/129 (95%)	123 (100%)	0	100	100
7	H	104/105 (99%)	104 (100%)	0	100	100
8	I	105/107 (98%)	104 (99%)	1 (1%)	76	88
9	J	86/90 (96%)	86 (100%)	0	100	100
10	K	90/99 (91%)	90 (100%)	0	100	100
11	L	103/104 (99%)	103 (100%)	0	100	100
12	M	91/96 (95%)	91 (100%)	0	100	100
13	N	79/84 (94%)	79 (100%)	0	100	100
14	O	76/77 (99%)	76 (100%)	0	100	100
15	P	65/65 (100%)	57 (88%)	8 (12%)	4	25
16	Q	74/78 (95%)	74 (100%)	0	100	100
17	R	48/65 (74%)	48 (100%)	0	100	100
18	S	70/79 (89%)	70 (100%)	0	100	100
19	T	65/66 (98%)	65 (100%)	0	100	100
20	U	44/61 (72%)	44 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	0	67/68 (98%)	64 (96%)	3 (4%)	27	61
22	1	54/55 (98%)	52 (96%)	2 (4%)	34	65
23	2	48/49 (98%)	47 (98%)	1 (2%)	53	77
24	3	47/48 (98%)	46 (98%)	1 (2%)	53	77
25	4	45/49 (92%)	43 (96%)	2 (4%)	28	62
26	6	38/38 (100%)	35 (92%)	3 (8%)	12	43
27	7	51/52 (98%)	49 (96%)	2 (4%)	32	64
28	8	34/34 (100%)	34 (100%)	0	100	100
29	c	216/218 (99%)	210 (97%)	6 (3%)	43	71
30	d	164/164 (100%)	157 (96%)	7 (4%)	29	62
31	e	165/165 (100%)	158 (96%)	7 (4%)	30	62
32	f	148/150 (99%)	141 (95%)	7 (5%)	26	60
33	g	137/138 (99%)	134 (98%)	3 (2%)	52	76
34	h	114/114 (100%)	112 (98%)	2 (2%)	59	80
35	j	116/116 (100%)	113 (97%)	3 (3%)	46	73
36	k	103/104 (99%)	101 (98%)	2 (2%)	57	79
37	l	103/103 (100%)	100 (97%)	3 (3%)	42	71
38	m	108/109 (99%)	107 (99%)	1 (1%)	78	89
39	n	100/103 (97%)	97 (97%)	3 (3%)	41	70
40	o	86/87 (99%)	83 (96%)	3 (4%)	36	67
41	p	99/100 (99%)	95 (96%)	4 (4%)	31	64
42	q	89/90 (99%)	88 (99%)	1 (1%)	73	87
43	r	84/84 (100%)	81 (96%)	3 (4%)	35	66
44	s	93/93 (100%)	92 (99%)	1 (1%)	73	87
45	t	80/84 (95%)	80 (100%)	0	100	100
46	u	83/85 (98%)	79 (95%)	4 (5%)	25	59
47	w	78/78 (100%)	74 (95%)	4 (5%)	24	58
48	y	56/63 (89%)	56 (100%)	0	100	100
49	z	21/62 (34%)	9 (43%)	12 (57%)	0	0
All	All	4572/4808 (95%)	4473 (98%)	99 (2%)	54	76

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	105	ARG
15	P	6	LEU
15	P	19	VAL
15	P	33	ILE
15	P	46	LYS
15	P	55	ASP
15	P	63	GLN
15	P	68	SER
15	P	77	GLU
21	0	17	ASN
21	0	22	LEU
21	0	48	THR
22	1	21	LEU
22	1	38	GLN
23	2	10	THR
24	3	29	SER
25	4	8	LYS
25	4	47	VAL
26	6	1	MET
26	6	22	MET
26	6	42	LEU
27	7	31	HIS
27	7	47	LYS
29	c	52	ARG
29	c	187	ASP
29	c	213	TRP
29	c	252	THR
29	c	267	ILE
29	c	269	ARG
30	d	4	LEU
30	d	32	ASN
30	d	51	THR
30	d	91	THR
30	d	150	GLN
30	d	157	LYS
30	d	177	VAL
31	e	60	TRP
31	e	61	ARG
31	e	78	TRP
31	e	93	SER
31	e	116	ASP
31	e	126	VAL
31	e	187	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	f	5	HIS
32	f	7	TYR
32	f	19	GLU
32	f	83	TYR
32	f	94	GLU
32	f	117	LEU
32	f	174	ASP
33	g	27	LYS
33	g	80	THR
33	g	92	VAL
34	h	42	LYS
34	h	43	ASN
35	j	30	THR
35	j	131	ASN
35	j	142	ILE
36	k	92	GLU
36	k	105	ARG
37	l	48	ARG
37	l	91	ASP
37	l	94	THR
38	m	13	HIS
39	n	95	THR
39	n	116	VAL
39	n	118	ARG
40	o	5	SER
40	o	31	THR
40	o	103	VAL
41	p	19	SER
41	p	26	VAL
41	p	37	LYS
41	p	80	VAL
42	q	16	LYS
43	r	46	GLU
43	r	58	VAL
43	r	102	SER
44	s	73	LYS
46	u	35	ILE
46	u	41	LEU
46	u	55	PRO
46	u	68	SER
47	w	20	LEU
47	w	29	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	w	53	LYS
47	w	76	ASP
49	z	4	GLN
49	z	6	LEU
49	z	7	ILE
49	z	8	SER
49	z	9	GLU
49	z	12	LEU
49	z	13	PHE
49	z	18	TRP
49	z	21	GLN
49	z	23	GLN
49	z	25	ILE
49	z	26	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	HIS
1	B	167	HIS
1	B	176	ASN
2	C	68	HIS
2	C	175	HIS
3	D	115	GLN
4	E	82	HIS
4	E	88	HIS
4	E	121	ASN
5	F	37	HIS
5	F	68	GLN
5	F	81	ASN
7	H	3	GLN
8	I	30	ASN
8	I	74	GLN
8	I	125	GLN
9	J	70	HIS
10	K	27	ASN
10	K	28	ASN
10	K	39	ASN
11	L	4	ASN
11	L	45	ASN
11	L	58	ASN
11	L	76	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	90	HIS
13	N	34	ASN
14	O	45	HIS
14	O	50	HIS
15	P	26	ASN
15	P	29	ASN
15	P	59	HIS
15	P	63	GLN
16	Q	44	HIS
16	Q	49	ASN
16	Q	50	ASN
18	S	56	HIS
19	T	69	ASN
21	0	16	ASN
22	1	41	HIS
22	1	45	GLN
27	7	31	HIS
28	8	37	GLN
31	e	46	GLN
31	e	115	GLN
32	f	127	ASN
33	g	22	GLN
33	g	38	ASN
34	h	20	ASN
34	h	28	ASN
34	h	43	ASN
39	n	3	HIS
39	n	73	ASN
42	q	37	GLN
44	s	7	HIS
44	s	15	GLN
44	s	61	ASN
46	u	74	ASN
48	y	57	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	A	1530/1542 (99%)	427 (27%)	36 (2%)
51	X	11/11 (100%)	7 (63%)	2 (18%)
52	a	116/120 (96%)	40 (34%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	b	2902/2904 (99%)	1211 (41%)	0
54	v	75/76 (98%)	27 (36%)	0
All	All	4634/4653 (99%)	1712 (36%)	38 (0%)

All (1712) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	A	6	G
50	A	7	A
50	A	8	A
50	A	9	G
50	A	11	G
50	A	13	U
50	A	29	U
50	A	31	G
50	A	32	A
50	A	39	G
50	A	47	C
50	A	48	C
50	A	51	A
50	A	52	C
50	A	54	C
50	A	57	G
50	A	65	A
50	A	70	U
50	A	71	A
50	A	75	G
50	A	79	G
50	A	81	A
50	A	82	G
50	A	83	C
50	A	84	U
50	A	85	U
50	A	86	G
50	A	87	C
50	A	90	C
50	A	95	C
50	A	97	G
50	A	98	A
50	A	108	G
50	A	116	A
50	A	119	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	122	G
50	A	126	G
50	A	127	G
50	A	128	G
50	A	130	A
50	A	131	A
50	A	133	U
50	A	137	U
50	A	142	G
50	A	149	A
50	A	157	U
50	A	160	A
50	A	166	U
50	A	177	G
50	A	182	A
50	A	183	C
50	A	184	G
50	A	185	U
50	A	186	C
50	A	196	A
50	A	197	A
50	A	210	C
50	A	211	G
50	A	217	C
50	A	219	U
50	A	229	U
50	A	230	G
50	A	231	U
50	A	239	U
50	A	240	G
50	A	243	A
50	A	244	U
50	A	245	U
50	A	247	G
50	A	251	G
50	A	252	U
50	A	256	U
50	A	264	C
50	A	266	G
50	A	267	C
50	A	275	G
50	A	276	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	278	G
50	A	280	C
50	A	281	G
50	A	289	G
50	A	302	G
50	A	303	A
50	A	314	C
50	A	324	G
50	A	326	G
50	A	328	C
50	A	330	C
50	A	332	G
50	A	339	C
50	A	342	C
50	A	343	U
50	A	352	C
50	A	354	G
50	A	366	A
50	A	367	U
50	A	368	U
50	A	369	G
50	A	371	A
50	A	372	C
50	A	373	A
50	A	374	A
50	A	376	G
50	A	377	G
50	A	381	C
50	A	385	C
50	A	388	G
50	A	389	A
50	A	390	U
50	A	391	G
50	A	397	A
50	A	398	U
50	A	399	G
50	A	406	G
50	A	411	A
50	A	412	A
50	A	413	G
50	A	414	A
50	A	415	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	417	G
50	A	422	C
50	A	424	G
50	A	429	U
50	A	435	A
50	A	440	C
50	A	449	G
50	A	451	A
50	A	457	G
50	A	459	A
50	A	461	A
50	A	462	G
50	A	466	A
50	A	468	A
50	A	471	U
50	A	476	U
50	A	477	C
50	A	479	U
50	A	481	G
50	A	484	G
50	A	485	U
50	A	486	U
50	A	496	A
50	A	498	A
50	A	499	A
50	A	508	U
50	A	511	C
50	A	518	C
50	A	521	G
50	A	525	C
50	A	527	G
50	A	531	U
50	A	532	A
50	A	533	A
50	A	543	U
50	A	545	C
50	A	547	A
50	A	548	G
50	A	549	C
50	A	562	U
50	A	563	A
50	A	564	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	565	U
50	A	566	G
50	A	572	A
50	A	575	G
50	A	576	C
50	A	577	G
50	A	578	C
50	A	579	A
50	A	588	G
50	A	589	U
50	A	591	U
50	A	607	A
50	A	614	C
50	A	618	C
50	A	619	U
50	A	620	C
50	A	621	A
50	A	623	C
50	A	632	U
50	A	633	G
50	A	636	U
50	A	637	C
50	A	652	U
50	A	653	U
50	A	665	A
50	A	687	A
50	A	688	G
50	A	691	G
50	A	693	G
50	A	695	A
50	A	696	A
50	A	697	U
50	A	700	G
50	A	701	U
50	A	702	A
50	A	703	G
50	A	704	A
50	A	710	G
50	A	718	A
50	A	720	C
50	A	721	G
50	A	722	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	723	U
50	A	724	G
50	A	729	A
50	A	731	G
50	A	734	G
50	A	747	A
50	A	748	G
50	A	753	A
50	A	755	G
50	A	764	C
50	A	779	C
50	A	781	A
50	A	790	A
50	A	793	U
50	A	794	A
50	A	802	A
50	A	812	G
50	A	815	A
50	A	817	C
50	A	818	G
50	A	819	A
50	A	820	U
50	A	821	G
50	A	822	U
50	A	826	C
50	A	828	U
50	A	829	G
50	A	832	G
50	A	841	C
50	A	842	U
50	A	843	U
50	A	845	A
50	A	846	G
50	A	847	G
50	A	849	G
50	A	851	G
50	A	853	C
50	A	857	C
50	A	860	A
50	A	869	G
50	A	871	U
50	A	873	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	882	C
50	A	887	G
50	A	889	A
50	A	890	G
50	A	891	U
50	A	902	G
50	A	914	A
50	A	922	G
50	A	927	G
50	A	931	C
50	A	932	C
50	A	934	C
50	A	935	A
50	A	945	G
50	A	948	C
50	A	954	G
50	A	958	A
50	A	960	U
50	A	961	U
50	A	969	A
50	A	971	G
50	A	974	A
50	A	975	A
50	A	976	G
50	A	977	A
50	A	982	U
50	A	983	A
50	A	985	C
50	A	987	G
50	A	992	U
50	A	993	G
50	A	996	A
50	A	997	U
50	A	998	C
50	A	999	C
50	A	1004	A
50	A	1010	U
50	A	1018	G
50	A	1020	G
50	A	1022	A
50	A	1028	C
50	A	1030	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	1031	C
50	A	1034	G
50	A	1046	A
50	A	1053	G
50	A	1056	U
50	A	1057	G
50	A	1064	G
50	A	1065	U
50	A	1066	C
50	A	1070	U
50	A	1071	C
50	A	1085	U
50	A	1091	U
50	A	1093	A
50	A	1094	G
50	A	1095	U
50	A	1101	A
50	A	1102	A
50	A	1103	C
50	A	1108	G
50	A	1112	C
50	A	1125	U
50	A	1130	A
50	A	1131	G
50	A	1132	C
50	A	1135	U
50	A	1136	C
50	A	1138	G
50	A	1139	G
50	A	1140	C
50	A	1143	G
50	A	1152	A
50	A	1157	A
50	A	1159	U
50	A	1160	G
50	A	1164	G
50	A	1168	U
50	A	1169	A
50	A	1184	G
50	A	1186	G
50	A	1189	U
50	A	1192	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	1193	G
50	A	1196	A
50	A	1197	A
50	A	1201	A
50	A	1202	U
50	A	1210	C
50	A	1212	U
50	A	1213	A
50	A	1215	G
50	A	1225	A
50	A	1226	C
50	A	1227	A
50	A	1228	C
50	A	1233	G
50	A	1234	C
50	A	1238	A
50	A	1240	U
50	A	1241	G
50	A	1246	A
50	A	1256	A
50	A	1258	G
50	A	1261	A
50	A	1270	G
50	A	1272	G
50	A	1279	G
50	A	1280	A
50	A	1285	A
50	A	1286	U
50	A	1287	A
50	A	1292	G
50	A	1298	U
50	A	1300	G
50	A	1301	U
50	A	1302	C
50	A	1303	C
50	A	1305	G
50	A	1312	G
50	A	1316	G
50	A	1319	A
50	A	1320	C
50	A	1322	C
50	A	1323	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	1324	A
50	A	1331	G
50	A	1333	A
50	A	1336	C
50	A	1338	G
50	A	1339	A
50	A	1340	A
50	A	1342	C
50	A	1343	G
50	A	1346	A
50	A	1347	G
50	A	1348	U
50	A	1349	A
50	A	1350	A
50	A	1353	G
50	A	1358	U
50	A	1362	A
50	A	1363	A
50	A	1364	U
50	A	1365	G
50	A	1378	C
50	A	1398	A
50	A	1399	C
50	A	1401	G
50	A	1402	C
50	A	1403	C
50	A	1419	G
50	A	1432	G
50	A	1436	U
50	A	1440	U
50	A	1441	A
50	A	1443	C
50	A	1446	A
50	A	1448	C
50	A	1449	C
50	A	1452	C
50	A	1454	G
50	A	1469	C
50	A	1477	U
50	A	1484	C
50	A	1493	A
50	A	1494	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	A	1497	G
50	A	1499	A
50	A	1503	A
50	A	1505	G
50	A	1506	U
50	A	1508	A
50	A	1514	G
50	A	1517	G
50	A	1519	A
50	A	1520	C
50	A	1528	U
50	A	1529	G
50	A	1530	G
50	A	1534	A
51	X	13	C
51	X	14	U
51	X	15	G
51	X	17	C
51	X	18	C
51	X	19	C
51	X	20	U
52	a	3	C
52	a	4	C
52	a	8	C
52	a	9	G
52	a	12	C
52	a	13	G
52	a	15	A
52	a	16	G
52	a	18	G
52	a	21	G
52	a	24	G
52	a	25	U
52	a	26	C
52	a	30	C
52	a	35	C
52	a	37	C
52	a	42	C
52	a	43	C
52	a	44	G
52	a	50	A
52	a	51	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	a	52	A
52	a	53	A
52	a	54	G
52	a	57	A
52	a	59	A
52	a	67	G
52	a	84	G
52	a	85	G
52	a	86	G
52	a	88	C
52	a	89	U
52	a	90	C
52	a	91	C
52	a	96	G
52	a	99	A
52	a	100	G
52	a	106	G
52	a	109	A
52	a	115	A
53	b	4	U
53	b	10	A
53	b	11	C
53	b	13	A
53	b	14	A
53	b	15	G
53	b	20	C
53	b	23	G
53	b	24	G
53	b	27	G
53	b	28	A
53	b	29	U
53	b	34	U
53	b	35	G
53	b	39	G
53	b	45	G
53	b	46	G
53	b	49	A
53	b	51	G
53	b	55	G
53	b	62	U
53	b	63	A
53	b	71	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	73	A
53	b	74	A
53	b	75	G
53	b	76	C
53	b	77	G
53	b	80	G
53	b	82	U
53	b	83	A
53	b	84	A
53	b	85	G
53	b	88	G
53	b	91	A
53	b	100	U
53	b	101	A
53	b	102	U
53	b	103	A
53	b	109	C
53	b	111	A
53	b	114	U
53	b	116	C
53	b	118	A
53	b	119	A
53	b	120	U
53	b	126	A
53	b	127	A
53	b	136	G
53	b	140	C
53	b	143	C
53	b	144	A
53	b	147	C
53	b	149	A
53	b	159	G
53	b	160	A
53	b	162	U
53	b	163	C
53	b	164	C
53	b	165	A
53	b	172	A
53	b	176	A
53	b	181	A
53	b	186	G
53	b	196	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	197	A
53	b	202	U
53	b	204	A
53	b	205	G
53	b	210	C
53	b	212	G
53	b	215	G
53	b	216	A
53	b	221	A
53	b	222	A
53	b	223	A
53	b	225	C
53	b	226	A
53	b	228	C
53	b	229	C
53	b	231	A
53	b	233	A
53	b	234	U
53	b	235	U
53	b	239	C
53	b	240	C
53	b	241	A
53	b	245	G
53	b	248	G
53	b	249	C
53	b	250	G
53	b	251	A
53	b	252	G
53	b	254	G
53	b	255	A
53	b	264	C
53	b	265	A
53	b	266	G
53	b	267	C
53	b	270	A
53	b	271	G
53	b	272	A
53	b	273	G
53	b	277	G
53	b	278	A
53	b	279	A
53	b	280	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	281	C
53	b	282	A
53	b	289	G
53	b	294	A
53	b	298	G
53	b	299	A
53	b	300	A
53	b	307	G
53	b	309	A
53	b	310	A
53	b	311	A
53	b	322	A
53	b	323	C
53	b	324	A
53	b	326	G
53	b	329	G
53	b	330	A
53	b	331	C
53	b	332	A
53	b	333	G
53	b	338	G
53	b	344	A
53	b	345	A
53	b	346	A
53	b	349	U
53	b	353	C
53	b	355	U
53	b	356	G
53	b	358	U
53	b	359	G
53	b	361	G
53	b	362	A
53	b	364	C
53	b	366	C
53	b	368	A
53	b	369	U
53	b	370	G
53	b	371	A
53	b	372	G
53	b	373	U
53	b	374	A
53	b	375	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	385	C
53	b	386	G
53	b	387	U
53	b	388	G
53	b	391	A
53	b	392	U
53	b	396	G
53	b	400	G
53	b	401	A
53	b	402	A
53	b	403	U
53	b	405	U
53	b	406	G
53	b	409	G
53	b	411	G
53	b	412	A
53	b	413	C
53	b	418	C
53	b	419	U
53	b	421	C
53	b	422	A
53	b	424	G
53	b	425	G
53	b	431	U
53	b	434	U
53	b	435	C
53	b	436	C
53	b	442	G
53	b	443	A
53	b	446	G
53	b	447	A
53	b	448	U
53	b	449	A
53	b	451	U
53	b	452	G
53	b	454	A
53	b	455	C
53	b	456	C
53	b	457	A
53	b	461	C
53	b	465	G
53	b	466	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	475	C
53	b	477	A
53	b	479	A
53	b	480	A
53	b	481	G
53	b	483	A
53	b	489	G
53	b	490	C
53	b	491	G
53	b	492	A
53	b	502	A
53	b	503	A
53	b	504	A
53	b	505	A
53	b	508	A
53	b	509	C
53	b	510	C
53	b	518	G
53	b	519	U
53	b	521	U
53	b	526	A
53	b	527	C
53	b	529	A
53	b	530	G
53	b	531	C
53	b	532	A
53	b	538	A
53	b	544	C
53	b	545	U
53	b	546	U
53	b	547	A
53	b	548	G
53	b	549	G
53	b	550	C
53	b	559	G
53	b	560	C
53	b	563	A
53	b	568	U
53	b	569	U
53	b	572	A
53	b	573	U
53	b	574	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	575	A
53	b	584	C
53	b	586	A
53	b	587	C
53	b	588	U
53	b	603	A
53	b	604	G
53	b	607	U
53	b	608	A
53	b	612	G
53	b	613	A
53	b	614	A
53	b	615	U
53	b	617	G
53	b	618	G
53	b	621	A
53	b	622	G
53	b	625	G
53	b	627	A
53	b	628	G
53	b	631	A
53	b	632	A
53	b	636	G
53	b	637	A
53	b	642	U
53	b	644	A
53	b	646	U
53	b	647	G
53	b	651	G
53	b	652	U
53	b	653	U
53	b	654	A
53	b	655	A
53	b	656	G
53	b	657	U
53	b	659	G
53	b	662	G
53	b	664	G
53	b	668	A
53	b	670	A
53	b	671	C
53	b	672	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	675	A
53	b	686	U
53	b	696	G
53	b	701	G
53	b	704	G
53	b	705	A
53	b	707	G
53	b	711	G
53	b	713	G
53	b	715	A
53	b	716	A
53	b	717	C
53	b	718	A
53	b	719	C
53	b	720	U
53	b	723	C
53	b	727	A
53	b	730	A
53	b	733	G
53	b	734	A
53	b	738	G
53	b	745	G
53	b	746	U
53	b	747	U
53	b	748	G
53	b	749	A
53	b	750	A
53	b	752	A
53	b	753	A
53	b	757	G
53	b	758	C
53	b	763	G
53	b	764	A
53	b	765	C
53	b	766	U
53	b	770	G
53	b	775	G
53	b	776	G
53	b	777	G
53	b	781	A
53	b	782	A
53	b	783	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	784	G
53	b	785	G
53	b	788	A
53	b	789	A
53	b	790	U
53	b	791	C
53	b	792	A
53	b	794	A
53	b	798	G
53	b	799	G
53	b	800	A
53	b	801	G
53	b	805	G
53	b	812	C
53	b	819	A
53	b	822	G
53	b	827	U
53	b	828	U
53	b	836	G
53	b	844	A
53	b	845	A
53	b	846	U
53	b	847	U
53	b	848	C
53	b	856	G
53	b	858	G
53	b	859	G
53	b	866	A
53	b	867	C
53	b	869	G
53	b	872	U
53	b	873	C
53	b	874	G
53	b	876	C
53	b	877	A
53	b	878	A
53	b	879	G
53	b	880	G
53	b	881	G
53	b	882	G
53	b	883	G
53	b	887	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	888	C
53	b	889	C
53	b	893	C
53	b	895	U
53	b	896	A
53	b	897	C
53	b	899	A
53	b	900	A
53	b	902	C
53	b	910	A
53	b	911	A
53	b	912	C
53	b	914	G
53	b	915	C
53	b	919	U
53	b	931	U
53	b	932	U
53	b	934	U
53	b	938	G
53	b	941	A
53	b	945	A
53	b	946	C
53	b	948	C
53	b	951	C
53	b	957	C
53	b	958	U
53	b	959	A
53	b	961	C
53	b	962	G
53	b	964	C
53	b	965	C
53	b	968	C
53	b	969	G
53	b	972	A
53	b	973	A
53	b	974	G
53	b	975	A
53	b	979	A
53	b	980	A
53	b	981	A
53	b	983	A
53	b	984	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	985	C
53	b	986	C
53	b	995	C
53	b	996	A
53	b	1003	G
53	b	1005	C
53	b	1006	C
53	b	1010	A
53	b	1011	G
53	b	1012	U
53	b	1013	C
53	b	1018	U
53	b	1019	U
53	b	1022	G
53	b	1023	U
53	b	1025	G
53	b	1026	G
53	b	1027	A
53	b	1028	A
53	b	1032	A
53	b	1033	U
53	b	1034	G
53	b	1036	G
53	b	1037	G
53	b	1038	G
53	b	1039	A
53	b	1044	C
53	b	1047	G
53	b	1048	A
53	b	1049	C
53	b	1051	G
53	b	1052	C
53	b	1053	C
53	b	1054	A
53	b	1055	G
53	b	1056	G
53	b	1057	A
53	b	1058	U
53	b	1059	G
53	b	1061	U
53	b	1062	G
53	b	1063	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1064	C
53	b	1065	U
53	b	1067	A
53	b	1068	G
53	b	1069	A
53	b	1070	A
53	b	1071	G
53	b	1072	C
53	b	1073	A
53	b	1074	G
53	b	1078	U
53	b	1079	C
53	b	1080	A
53	b	1081	U
53	b	1084	A
53	b	1085	A
53	b	1086	A
53	b	1087	G
53	b	1088	A
53	b	1089	A
53	b	1090	A
53	b	1091	G
53	b	1092	C
53	b	1093	G
53	b	1095	A
53	b	1096	A
53	b	1097	U
53	b	1098	A
53	b	1099	G
53	b	1100	C
53	b	1102	C
53	b	1103	A
53	b	1104	C
53	b	1105	U
53	b	1106	G
53	b	1107	G
53	b	1109	C
53	b	1110	G
53	b	1111	A
53	b	1112	G
53	b	1115	G
53	b	1116	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1117	C
53	b	1121	C
53	b	1122	G
53	b	1126	A
53	b	1130	U
53	b	1132	U
53	b	1133	A
53	b	1134	A
53	b	1135	C
53	b	1136	G
53	b	1138	G
53	b	1139	G
53	b	1141	U
53	b	1142	A
53	b	1143	A
53	b	1144	A
53	b	1145	C
53	b	1148	U
53	b	1156	A
53	b	1157	G
53	b	1163	G
53	b	1165	A
53	b	1169	A
53	b	1171	G
53	b	1172	C
53	b	1173	U
53	b	1174	U
53	b	1175	A
53	b	1176	U
53	b	1178	C
53	b	1179	G
53	b	1184	U
53	b	1185	G
53	b	1187	G
53	b	1188	U
53	b	1195	G
53	b	1200	C
53	b	1203	U
53	b	1204	A
53	b	1205	A
53	b	1206	G
53	b	1207	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1208	C
53	b	1209	U
53	b	1210	G
53	b	1211	C
53	b	1218	G
53	b	1221	C
53	b	1222	U
53	b	1223	G
53	b	1224	U
53	b	1225	G
53	b	1227	G
53	b	1231	U
53	b	1232	G
53	b	1234	U
53	b	1236	G
53	b	1237	A
53	b	1238	G
53	b	1240	U
53	b	1241	A
53	b	1247	A
53	b	1248	G
53	b	1249	U
53	b	1251	C
53	b	1253	A
53	b	1254	A
53	b	1255	U
53	b	1256	G
53	b	1258	U
53	b	1260	A
53	b	1265	A
53	b	1266	G
53	b	1267	U
53	b	1268	A
53	b	1269	A
53	b	1272	A
53	b	1273	U
53	b	1274	A
53	b	1275	A
53	b	1276	A
53	b	1288	G
53	b	1289	C
53	b	1294	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1296	G
53	b	1300	G
53	b	1301	A
53	b	1302	A
53	b	1306	C
53	b	1307	A
53	b	1311	G
53	b	1312	U
53	b	1314	C
53	b	1316	U
53	b	1318	U
53	b	1319	C
53	b	1320	C
53	b	1322	A
53	b	1323	C
53	b	1326	U
53	b	1327	A
53	b	1329	U
53	b	1330	C
53	b	1332	G
53	b	1337	G
53	b	1338	G
53	b	1341	G
53	b	1342	A
53	b	1343	G
53	b	1344	U
53	b	1347	A
53	b	1348	C
53	b	1349	C
53	b	1352	U
53	b	1355	G
53	b	1358	G
53	b	1365	A
53	b	1368	G
53	b	1369	G
53	b	1373	A
53	b	1374	G
53	b	1378	A
53	b	1379	U
53	b	1382	G
53	b	1383	A
53	b	1384	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1390	U
53	b	1392	A
53	b	1393	A
53	b	1394	U
53	b	1395	A
53	b	1396	U
53	b	1397	U
53	b	1398	C
53	b	1400	U
53	b	1401	G
53	b	1403	A
53	b	1408	G
53	b	1416	G
53	b	1419	A
53	b	1420	A
53	b	1421	G
53	b	1422	G
53	b	1424	G
53	b	1426	G
53	b	1427	A
53	b	1428	C
53	b	1429	G
53	b	1435	G
53	b	1438	U
53	b	1451	C
53	b	1452	G
53	b	1453	A
53	b	1454	C
53	b	1458	U
53	b	1459	G
53	b	1460	U
53	b	1461	C
53	b	1467	U
53	b	1471	G
53	b	1476	U
53	b	1477	A
53	b	1478	G
53	b	1481	U
53	b	1482	G
53	b	1483	G
53	b	1487	U
53	b	1494	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1495	A
53	b	1496	A
53	b	1497	U
53	b	1498	C
53	b	1500	G
53	b	1503	A
53	b	1507	C
53	b	1508	A
53	b	1509	A
53	b	1510	G
53	b	1517	G
53	b	1522	A
53	b	1523	U
53	b	1524	G
53	b	1526	C
53	b	1529	G
53	b	1530	G
53	b	1534	U
53	b	1535	A
53	b	1536	C
53	b	1537	G
53	b	1539	U
53	b	1540	G
53	b	1542	U
53	b	1552	A
53	b	1554	U
53	b	1556	C
53	b	1558	C
53	b	1562	U
53	b	1566	A
53	b	1568	G
53	b	1569	A
53	b	1570	A
53	b	1572	A
53	b	1576	U
53	b	1578	U
53	b	1583	A
53	b	1584	U
53	b	1585	C
53	b	1592	C
53	b	1595	C
53	b	1598	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1600	C
53	b	1602	U
53	b	1603	A
53	b	1606	C
53	b	1607	C
53	b	1608	A
53	b	1609	A
53	b	1610	A
53	b	1612	C
53	b	1615	C
53	b	1616	A
53	b	1617	C
53	b	1618	A
53	b	1624	U
53	b	1631	G
53	b	1632	A
53	b	1633	G
53	b	1634	A
53	b	1635	A
53	b	1643	G
53	b	1644	C
53	b	1646	C
53	b	1647	U
53	b	1648	U
53	b	1649	G
53	b	1653	G
53	b	1654	A
53	b	1656	C
53	b	1658	C
53	b	1660	G
53	b	1663	G
53	b	1667	G
53	b	1668	A
53	b	1669	A
53	b	1674	G
53	b	1681	G
53	b	1682	G
53	b	1683	U
53	b	1687	G
53	b	1693	U
53	b	1694	C
53	b	1695	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1697	G
53	b	1698	A
53	b	1699	G
53	b	1700	A
53	b	1703	G
53	b	1705	A
53	b	1706	C
53	b	1707	G
53	b	1710	G
53	b	1713	A
53	b	1714	U
53	b	1715	G
53	b	1731	G
53	b	1732	C
53	b	1733	G
53	b	1738	G
53	b	1739	A
53	b	1746	A
53	b	1750	G
53	b	1755	A
53	b	1757	A
53	b	1758	U
53	b	1761	C
53	b	1763	G
53	b	1764	C
53	b	1766	G
53	b	1773	A
53	b	1774	C
53	b	1775	U
53	b	1776	G
53	b	1783	A
53	b	1785	A
53	b	1786	A
53	b	1787	A
53	b	1792	G
53	b	1794	A
53	b	1800	C
53	b	1801	A
53	b	1802	A
53	b	1807	G
53	b	1808	A
53	b	1809	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1811	G
53	b	1815	A
53	b	1816	C
53	b	1817	G
53	b	1823	G
53	b	1825	U
53	b	1826	G
53	b	1829	A
53	b	1833	C
53	b	1839	G
53	b	1840	G
53	b	1843	C
53	b	1846	G
53	b	1848	A
53	b	1849	G
53	b	1858	A
53	b	1860	G
53	b	1862	G
53	b	1865	U
53	b	1866	A
53	b	1867	G
53	b	1868	C
53	b	1870	C
53	b	1871	A
53	b	1872	A
53	b	1873	G
53	b	1890	A
53	b	1897	G
53	b	1905	C
53	b	1906	G
53	b	1907	G
53	b	1908	C
53	b	1913	A
53	b	1915	U
53	b	1917	U
53	b	1918	A
53	b	1919	A
53	b	1924	C
53	b	1928	A
53	b	1929	G
53	b	1930	G
53	b	1931	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	1932	A
53	b	1936	A
53	b	1937	A
53	b	1938	A
53	b	1940	U
53	b	1941	C
53	b	1943	U
53	b	1944	U
53	b	1951	U
53	b	1952	A
53	b	1954	G
53	b	1955	U
53	b	1963	U
53	b	1964	G
53	b	1966	A
53	b	1967	C
53	b	1969	A
53	b	1970	A
53	b	1971	U
53	b	1972	G
53	b	1975	G
53	b	1980	G
53	b	1981	A
53	b	1982	U
53	b	1991	U
53	b	1993	U
53	b	1997	C
53	b	1999	C
53	b	2007	U
53	b	2014	A
53	b	2016	U
53	b	2019	A
53	b	2020	A
53	b	2021	C
53	b	2022	U
53	b	2023	C
53	b	2030	A
53	b	2031	A
53	b	2032	G
53	b	2033	A
53	b	2035	G
53	b	2036	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2043	C
53	b	2046	G
53	b	2051	A
53	b	2052	A
53	b	2054	A
53	b	2055	C
53	b	2056	G
53	b	2060	A
53	b	2061	G
53	b	2063	C
53	b	2065	C
53	b	2066	C
53	b	2068	U
53	b	2069	G
53	b	2077	A
53	b	2080	A
53	b	2083	G
53	b	2087	G
53	b	2088	A
53	b	2092	U
53	b	2093	G
53	b	2094	A
53	b	2102	G
53	b	2104	C
53	b	2105	U
53	b	2107	G
53	b	2109	U
53	b	2110	G
53	b	2111	U
53	b	2112	G
53	b	2113	U
53	b	2114	A
53	b	2115	G
53	b	2116	G
53	b	2117	A
53	b	2118	U
53	b	2119	A
53	b	2120	G
53	b	2123	G
53	b	2124	G
53	b	2125	G
53	b	2127	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2128	G
53	b	2129	C
53	b	2130	U
53	b	2131	U
53	b	2132	U
53	b	2133	G
53	b	2135	A
53	b	2138	G
53	b	2144	G
53	b	2145	C
53	b	2146	C
53	b	2147	A
53	b	2149	U
53	b	2150	C
53	b	2153	C
53	b	2156	G
53	b	2158	A
53	b	2159	G
53	b	2160	C
53	b	2161	C
53	b	2162	G
53	b	2163	A
53	b	2164	C
53	b	2165	C
53	b	2166	U
53	b	2168	G
53	b	2169	A
53	b	2170	A
53	b	2171	A
53	b	2172	U
53	b	2173	A
53	b	2174	C
53	b	2175	C
53	b	2176	A
53	b	2177	C
53	b	2178	C
53	b	2179	C
53	b	2182	U
53	b	2185	U
53	b	2193	G
53	b	2198	A
53	b	2199	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2202	U
53	b	2203	U
53	b	2204	G
53	b	2206	C
53	b	2207	C
53	b	2210	U
53	b	2211	A
53	b	2212	A
53	b	2213	U
53	b	2214	C
53	b	2215	C
53	b	2225	A
53	b	2230	G
53	b	2238	G
53	b	2239	G
53	b	2243	U
53	b	2249	U
53	b	2250	G
53	b	2255	G
53	b	2257	U
53	b	2258	C
53	b	2259	U
53	b	2265	U
53	b	2266	A
53	b	2267	A
53	b	2268	A
53	b	2273	A
53	b	2274	A
53	b	2275	C
53	b	2276	G
53	b	2279	G
53	b	2282	G
53	b	2283	C
53	b	2286	G
53	b	2287	A
53	b	2288	A
53	b	2289	G
53	b	2297	A
53	b	2304	G
53	b	2305	U
53	b	2308	G
53	b	2309	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2319	G
53	b	2320	U
53	b	2321	U
53	b	2322	A
53	b	2324	U
53	b	2331	G
53	b	2333	A
53	b	2334	U
53	b	2335	A
53	b	2336	A
53	b	2339	C
53	b	2340	A
53	b	2344	U
53	b	2345	G
53	b	2347	C
53	b	2350	C
53	b	2351	G
53	b	2361	G
53	b	2366	A
53	b	2371	G
53	b	2377	A
53	b	2379	G
53	b	2382	G
53	b	2383	G
53	b	2385	C
53	b	2388	A
53	b	2396	G
53	b	2398	U
53	b	2400	G
53	b	2402	U
53	b	2403	C
53	b	2406	A
53	b	2407	A
53	b	2410	G
53	b	2411	A
53	b	2420	C
53	b	2423	U
53	b	2425	A
53	b	2427	C
53	b	2428	G
53	b	2429	G
53	b	2430	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2434	A
53	b	2439	A
53	b	2440	C
53	b	2441	U
53	b	2445	G
53	b	2448	A
53	b	2449	U
53	b	2450	A
53	b	2453	A
53	b	2458	G
53	b	2459	A
53	b	2460	U
53	b	2465	C
53	b	2472	G
53	b	2475	C
53	b	2476	A
53	b	2478	A
53	b	2481	G
53	b	2484	G
53	b	2490	G
53	b	2491	U
53	b	2492	U
53	b	2498	C
53	b	2502	G
53	b	2505	G
53	b	2509	G
53	b	2510	C
53	b	2513	A
53	b	2517	C
53	b	2518	A
53	b	2519	U
53	b	2525	G
53	b	2527	C
53	b	2529	G
53	b	2530	A
53	b	2534	A
53	b	2535	G
53	b	2536	G
53	b	2542	A
53	b	2544	G
53	b	2547	A
53	b	2554	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2556	C
53	b	2562	U
53	b	2564	A
53	b	2565	A
53	b	2566	A
53	b	2567	G
53	b	2572	A
53	b	2573	C
53	b	2576	G
53	b	2578	G
53	b	2581	G
53	b	2582	G
53	b	2584	U
53	b	2585	U
53	b	2586	U
53	b	2587	A
53	b	2588	G
53	b	2590	A
53	b	2593	U
53	b	2595	G
53	b	2596	U
53	b	2598	A
53	b	2599	G
53	b	2600	A
53	b	2601	C
53	b	2602	A
53	b	2603	G
53	b	2606	C
53	b	2608	G
53	b	2609	U
53	b	2613	U
53	b	2614	A
53	b	2615	U
53	b	2621	G
53	b	2625	G
53	b	2629	U
53	b	2632	A
53	b	2634	A
53	b	2638	G
53	b	2639	A
53	b	2641	G
53	b	2645	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2646	C
53	b	2655	G
53	b	2657	A
53	b	2658	C
53	b	2659	G
53	b	2660	A
53	b	2661	G
53	b	2663	G
53	b	2673	G
53	b	2677	G
53	b	2685	G
53	b	2688	G
53	b	2689	U
53	b	2690	U
53	b	2691	C
53	b	2699	C
53	b	2702	G
53	b	2703	C
53	b	2707	U
53	b	2712	C
53	b	2713	U
53	b	2714	G
53	b	2716	C
53	b	2718	G
53	b	2719	G
53	b	2722	G
53	b	2727	A
53	b	2729	G
53	b	2733	A
53	b	2735	G
53	b	2736	A
53	b	2738	A
53	b	2744	G
53	b	2746	U
53	b	2747	G
53	b	2750	A
53	b	2751	G
53	b	2752	C
53	b	2753	A
53	b	2755	C
53	b	2757	A
53	b	2758	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2761	A
53	b	2765	A
53	b	2766	A
53	b	2773	C
53	b	2776	A
53	b	2778	A
53	b	2779	U
53	b	2781	A
53	b	2782	G
53	b	2790	U
53	b	2791	G
53	b	2792	A
53	b	2793	C
53	b	2795	C
53	b	2797	U
53	b	2798	U
53	b	2799	A
53	b	2800	A
53	b	2807	U
53	b	2808	G
53	b	2812	G
53	b	2818	U
53	b	2820	A
53	b	2821	A
53	b	2823	A
53	b	2824	C
53	b	2826	A
53	b	2833	U
53	b	2837	A
53	b	2847	U
53	b	2849	U
53	b	2858	C
53	b	2859	G
53	b	2861	U
53	b	2866	U
53	b	2867	G
53	b	2868	A
53	b	2872	A
53	b	2873	A
53	b	2874	C
53	b	2876	G
53	b	2880	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	b	2883	A
53	b	2884	U
53	b	2885	G
53	b	2886	A
53	b	2887	A
53	b	2891	U
53	b	2893	A
53	b	2894	G
53	b	2898	U
53	b	2900	A
53	b	2902	C
53	b	2903	U
54	v	5	A
54	v	6	C
54	v	7	G
54	v	9	A
54	v	16	C
54	v	17	C
54	v	18	G
54	v	19	G
54	v	20	U
54	v	21	A
54	v	28	C
54	v	31	C
54	v	34	G
54	v	36	C
54	v	39	G
54	v	40	U
54	v	41	C
54	v	46	G
54	v	47	U
54	v	48	C
54	v	49	G
54	v	50	G
54	v	52	G
54	v	60	U
54	v	64	C
54	v	72	G
54	v	76	A

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	A	5	U
50	A	14	U
50	A	30	U
50	A	51	A
50	A	64	G
50	A	66	A
50	A	94	G
50	A	132	C
50	A	184	G
50	A	243	A
50	A	279	A
50	A	301	G
50	A	372	C
50	A	484	G
50	A	497	G
50	A	695	A
50	A	701	U
50	A	702	A
50	A	703	G
50	A	811	C
50	A	840	C
50	A	997	U
50	A	998	C
50	A	1065	U
50	A	1129	C
50	A	1135	U
50	A	1201	A
50	A	1300	G
50	A	1302	C
50	A	1332	A
50	A	1346	A
50	A	1347	G
50	A	1348	U
50	A	1377	A
50	A	1493	A
50	A	1527	U
51	X	12	G
51	X	14	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	b	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	1087:G	O3'	1088:A	P	1.81
1	b	2055:C	O3'	2056:G	P	1.80

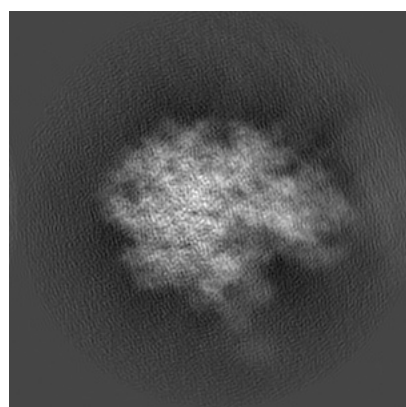
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6483. These allow visual inspection of the internal detail of the map and identification of artifacts.

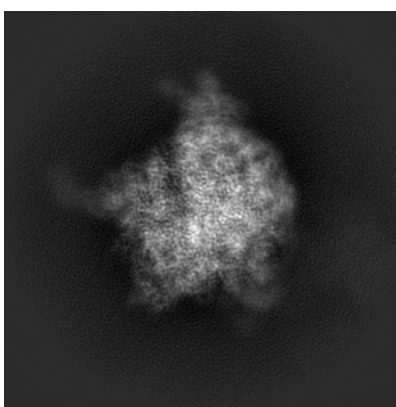
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

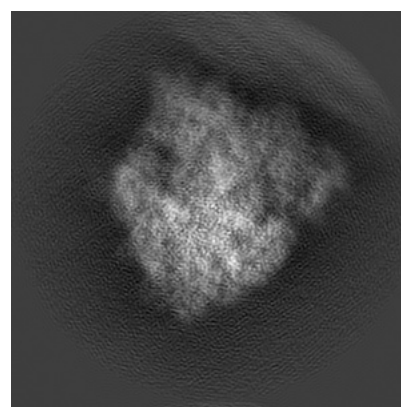
6.1.1 Primary map



X



Y

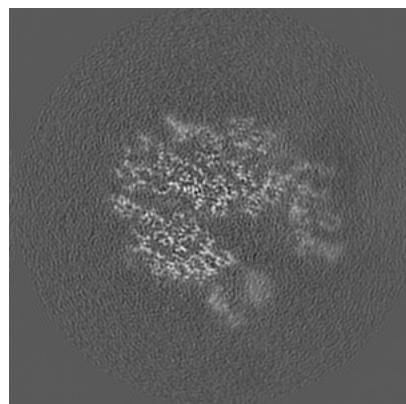


Z

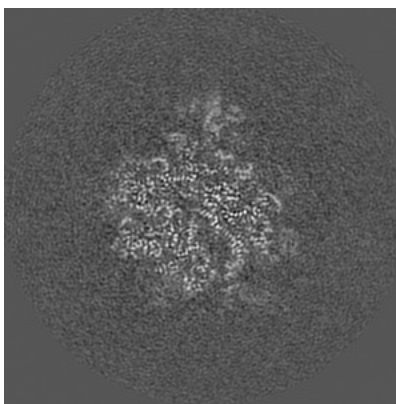
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

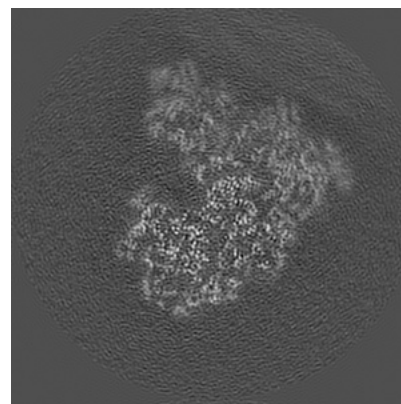
6.2.1 Primary map



X Index: 160



Y Index: 160

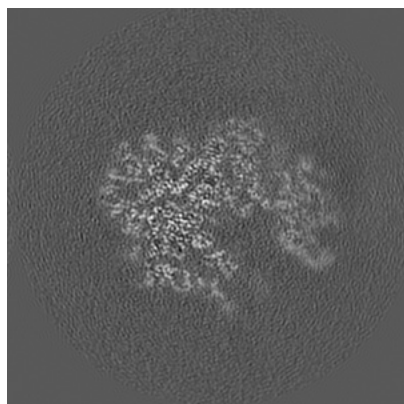


Z Index: 160

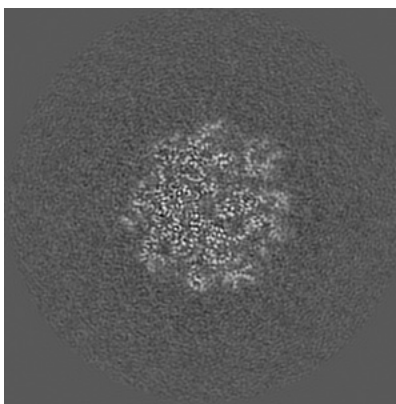
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

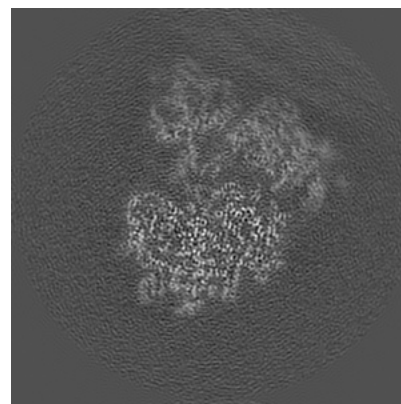
6.3.1 Primary map



X Index: 153



Y Index: 138



Z Index: 153

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

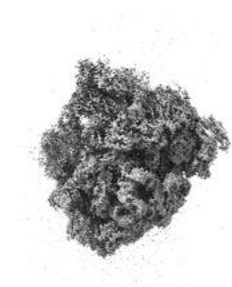
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

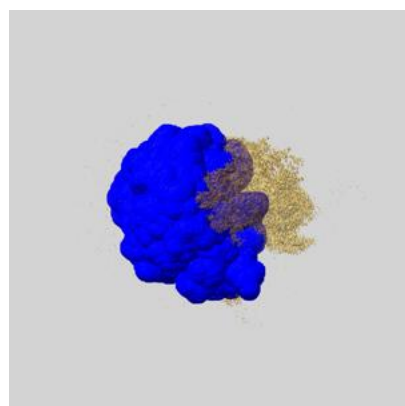
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

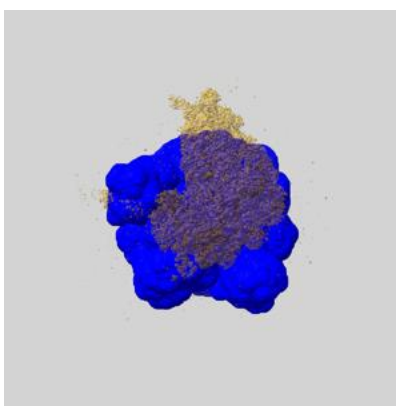
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

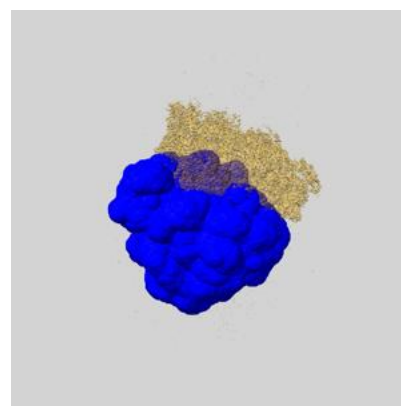
6.5.1 emd_6483_msk.map [i](#)



X



Y

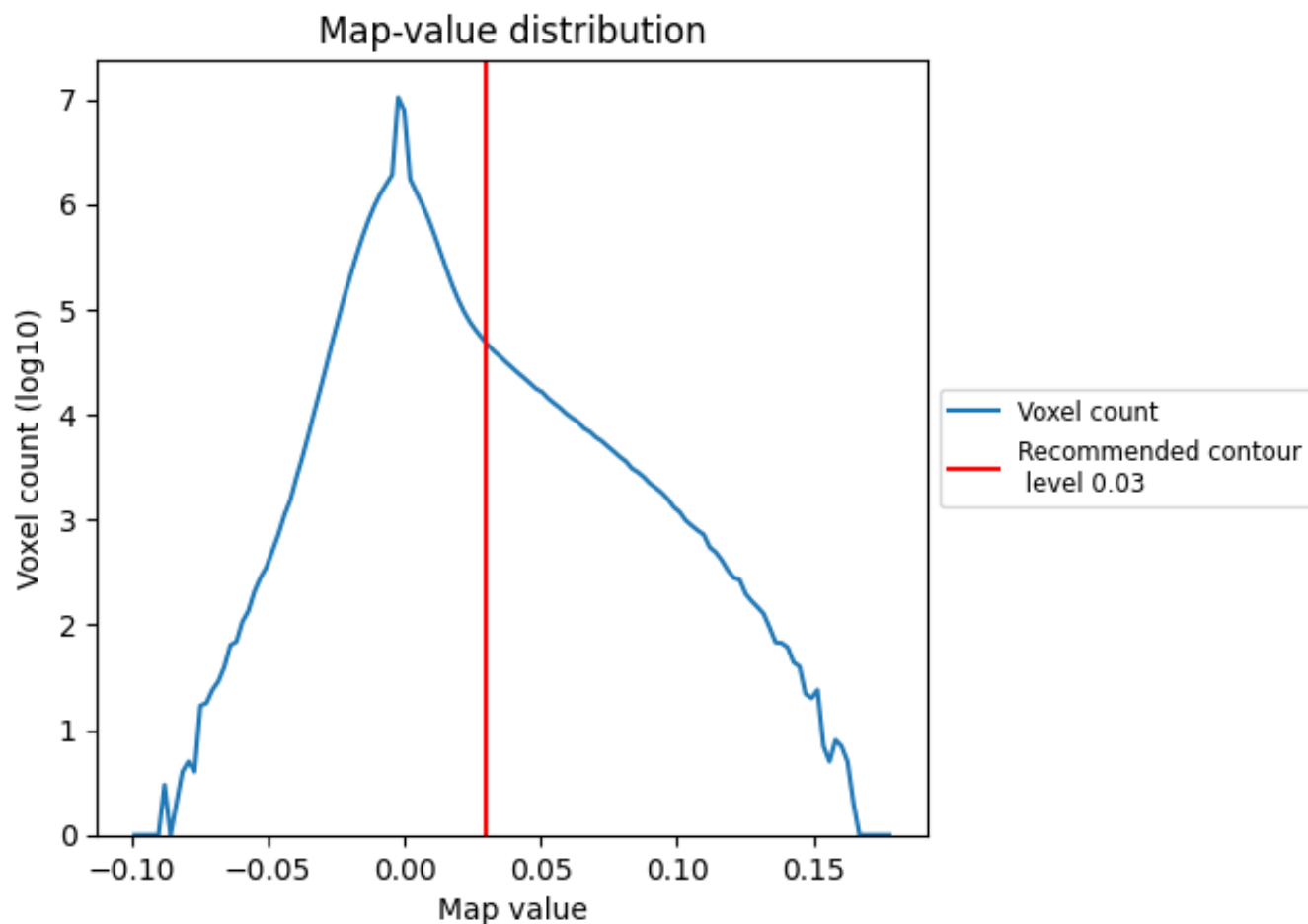


Z

7 Map analysis [i](#)

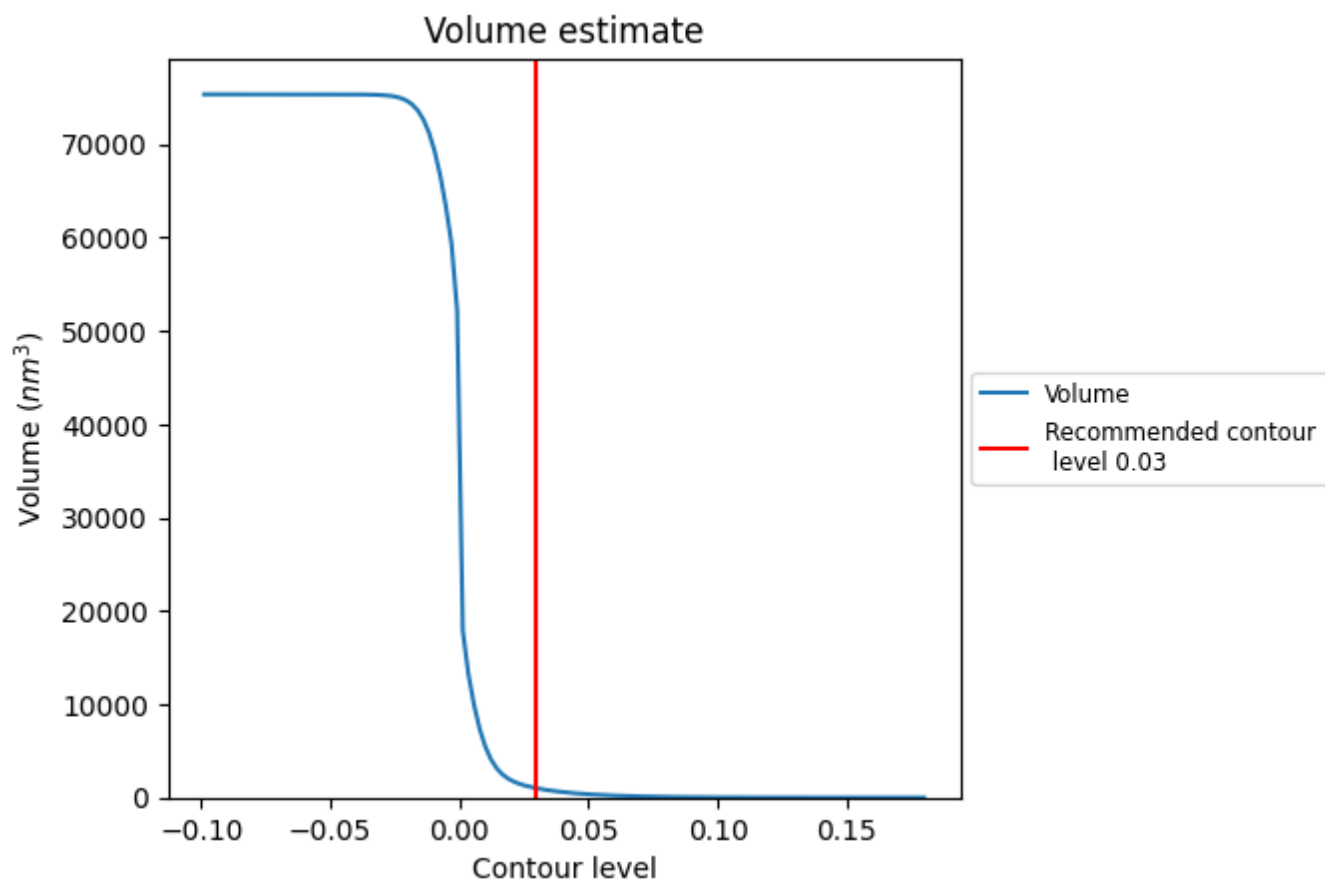
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

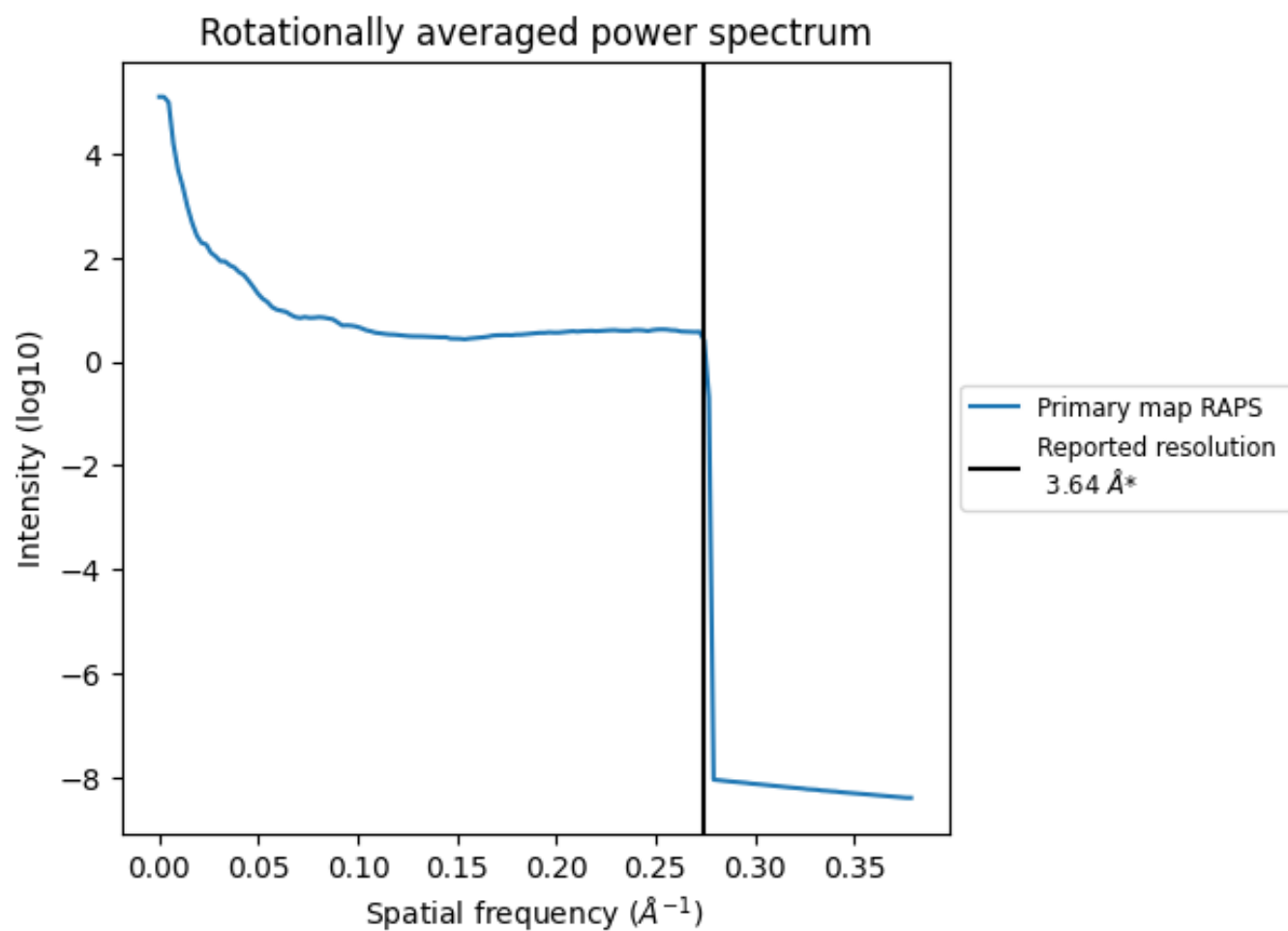
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 995 nm³; this corresponds to an approximate mass of 899 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

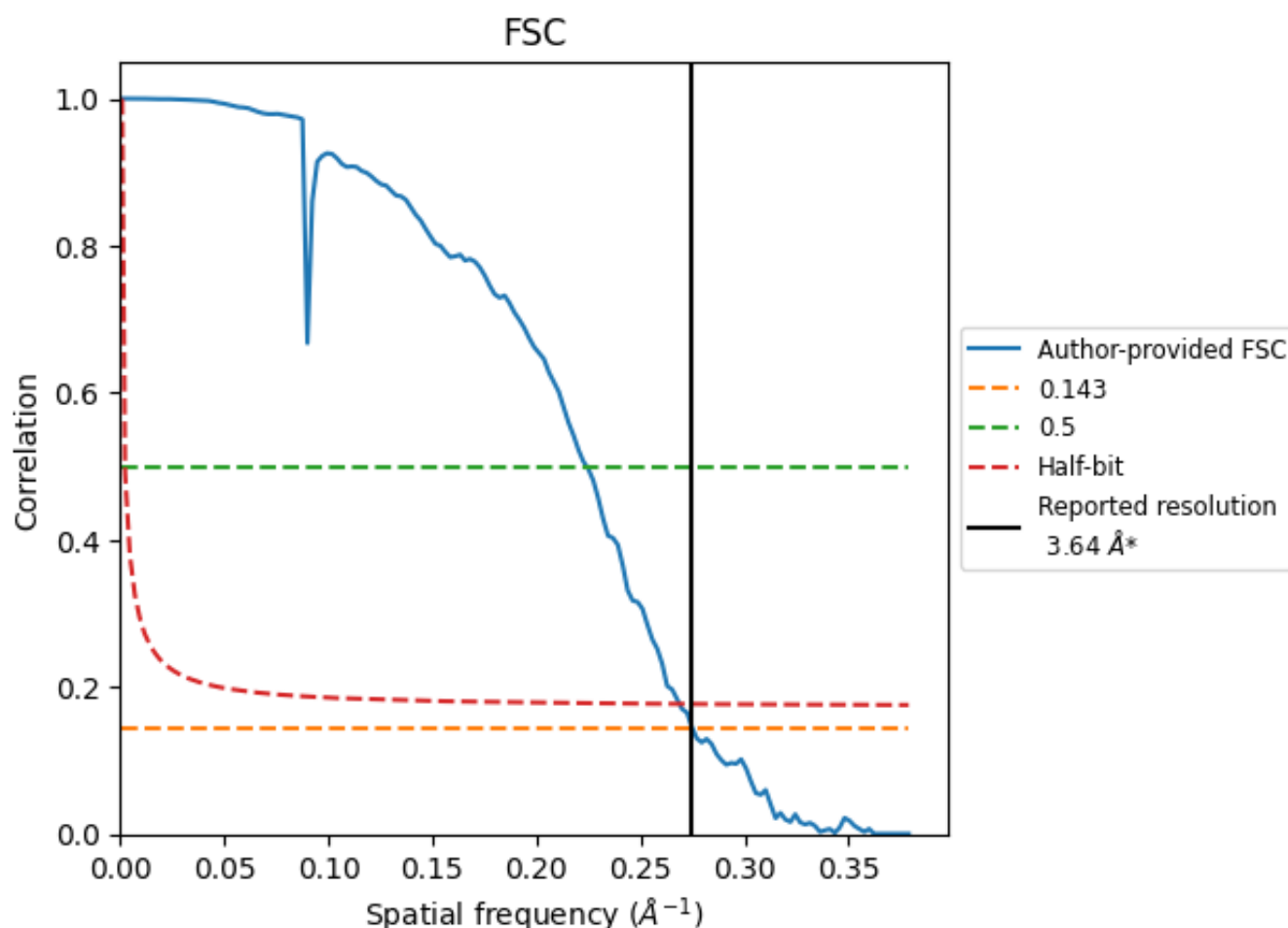


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 \AA^{-1}

8.2 Resolution estimates [i](#)

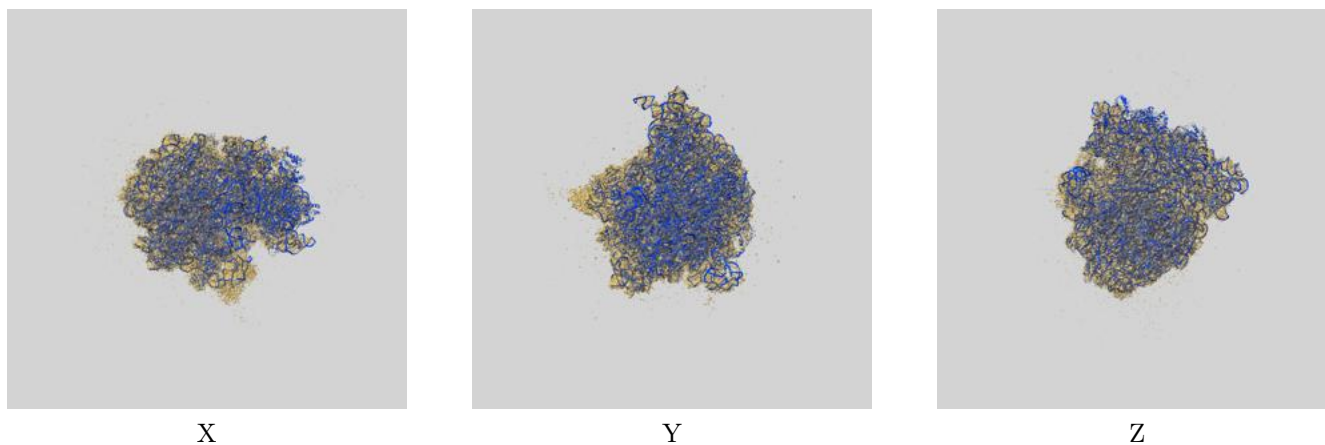
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.64	4.46	3.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

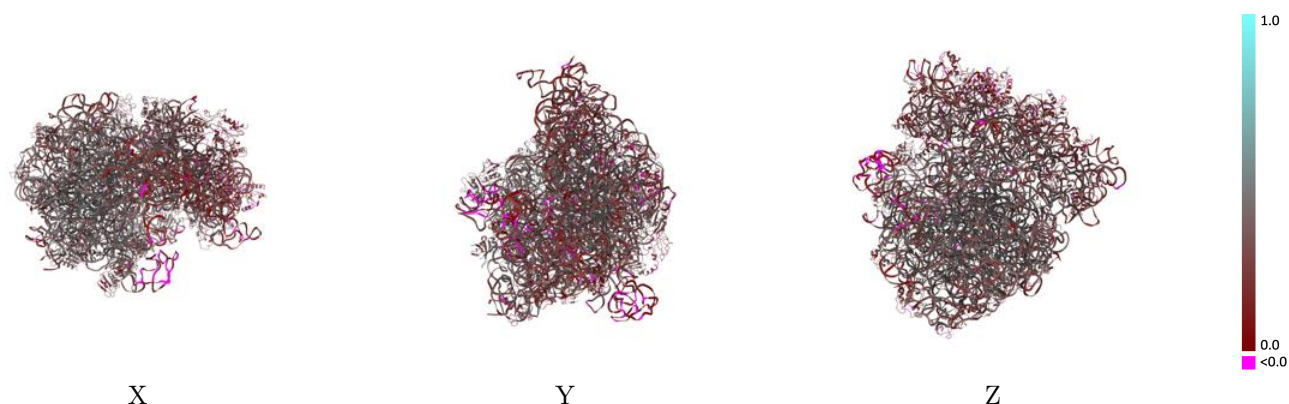
This section contains information regarding the fit between EMDB map EMD-6483 and PDB model 3JBU. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



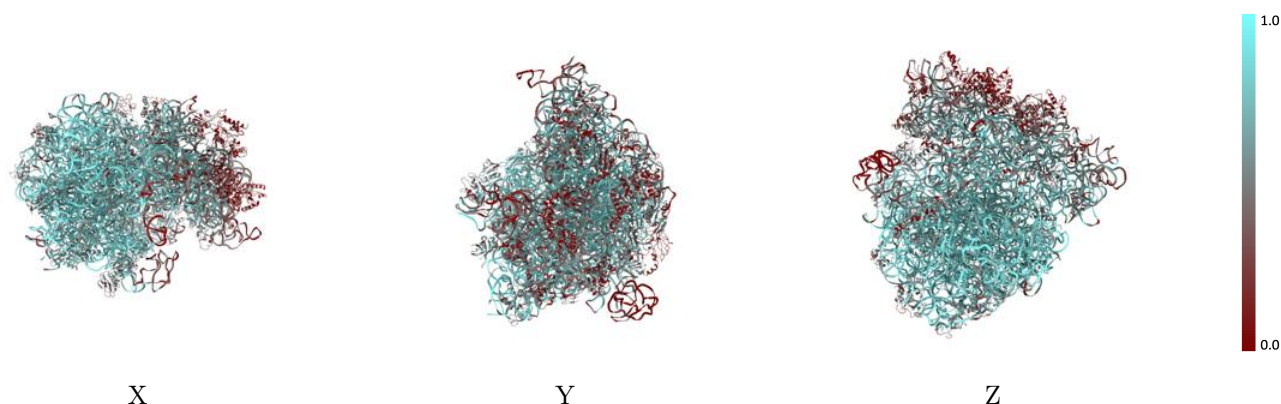
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



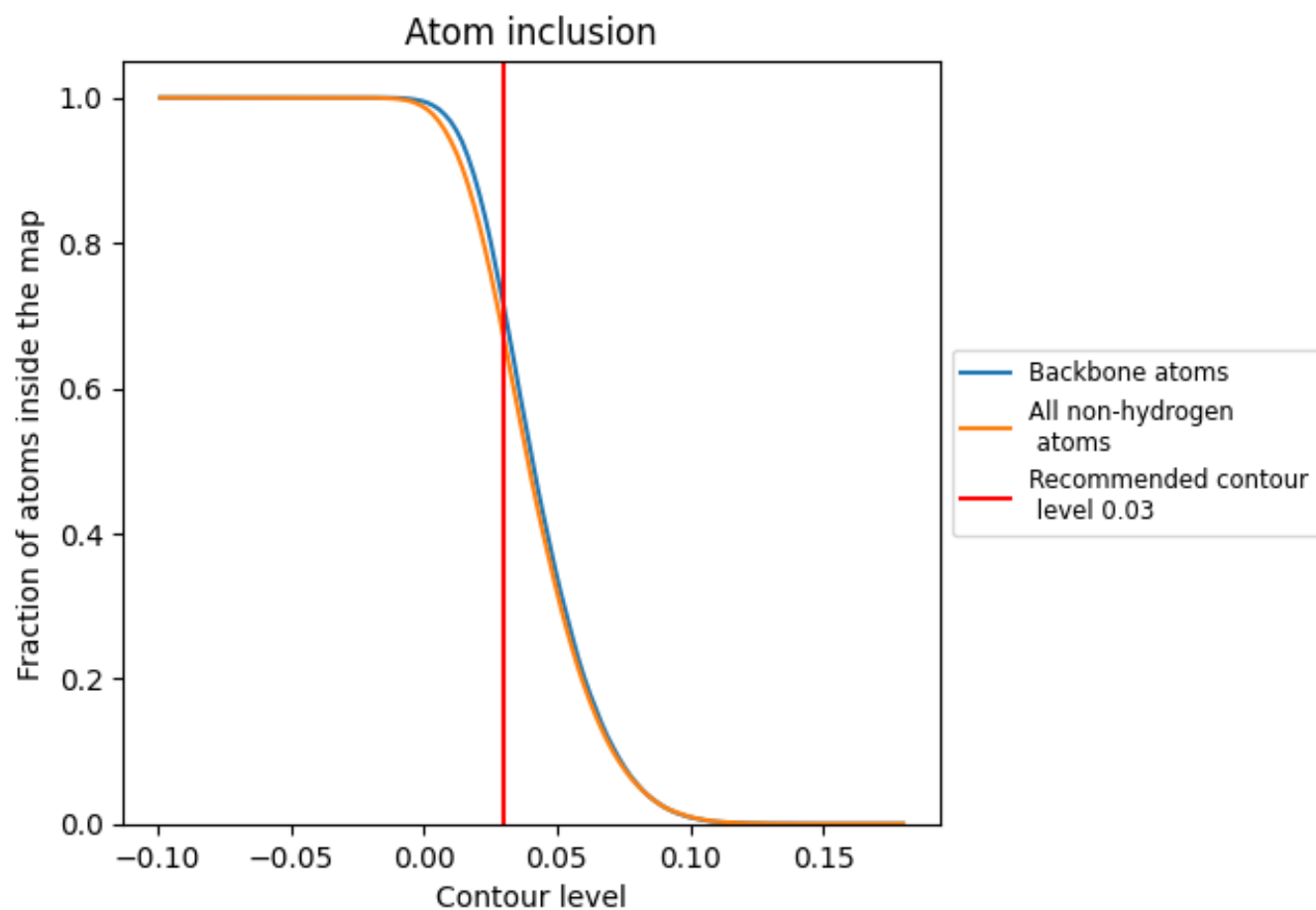
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ









































The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6711	 0.3410
0	 0.6672	 0.3850
1	 0.4724	 0.2700
2	 0.6659	 0.3800
3	 0.6285	 0.3380
4	 0.6234	 0.3720
6	 0.7465	 0.4140
7	 0.7352	 0.4340
8	 0.6884	 0.4020
A	 0.6533	 0.3220
B	 0.1164	 0.2000
C	 0.1565	 0.1960
D	 0.1660	 0.1960
E	 0.2733	 0.2450
F	 0.4636	 0.3230
G	 0.3448	 0.2520
H	 0.2656	 0.2590
I	 0.2176	 0.1810
J	 0.1406	 0.1890
K	 0.4947	 0.3390
L	 0.4647	 0.3250
M	 0.3815	 0.2680
N	 0.2221	 0.2110
O	 0.5203	 0.2980
P	 0.2998	 0.2170
Q	 0.4003	 0.2910
R	 0.4381	 0.3410
S	 0.3237	 0.2680
T	 0.4569	 0.2500
U	 0.3128	 0.2140
X	 0.4483	 0.2590
a	 0.8220	 0.3620
b	 0.8134	 0.3760
c	 0.7113	 0.3900
d	 0.6573	 0.3880



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.5796	 0.3340
f	 0.5288	 0.2630
g	 0.4888	 0.3040
h	 0.2418	 0.1940
j	 0.6864	 0.3860
k	 0.6068	 0.3850
l	 0.6445	 0.3720
m	 0.6621	 0.3920
n	 0.6627	 0.3710
o	 0.5840	 0.2880
p	 0.5890	 0.3400
q	 0.7093	 0.3910
r	 0.6048	 0.3710
s	 0.6591	 0.3890
t	 0.5651	 0.3130
u	 0.5059	 0.2760
v	 0.5576	 0.2800
w	 0.6057	 0.3440
y	 0.7045	 0.4020
z	 0.1850	 0.3150