



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 03:41 PM EST

PDB ID : 6W6L
EMDB ID : EMD-21435
Title : Cryo-EM structure of the human ribosome-TMCO1 translocon
Authors : Keenan, R.J.; McGilvray, P.T.
Deposited on : 2020-03-17
Resolution : 3.84 Å(reported)
Based on initial models : 5A63, 6OM0, 6FTI

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:

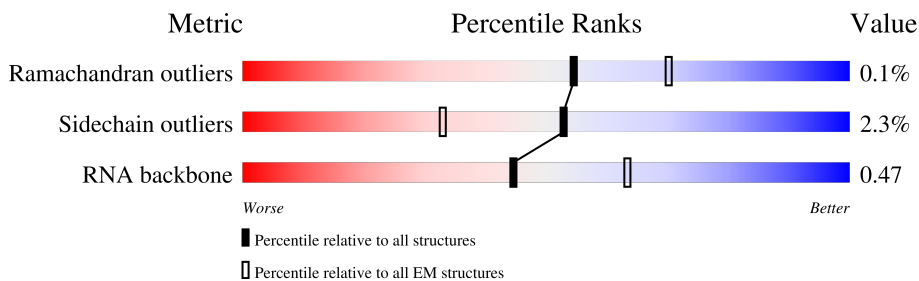
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.84 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	A	257	
2	B	403	
3	C	427	
4	D	157	
5	E	119	
6	F	297	
7	G	288	
8	H	248	

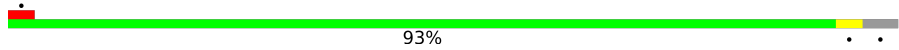
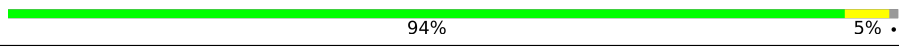
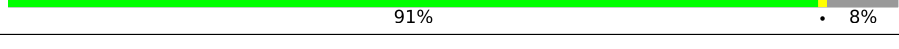
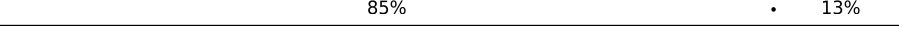
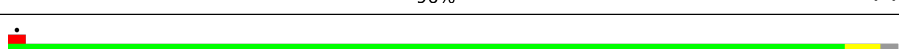
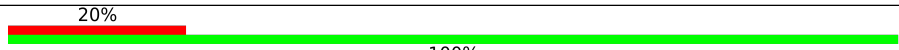

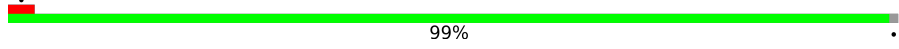

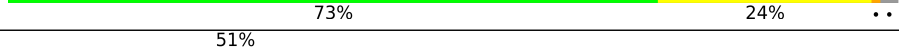
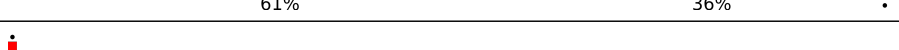


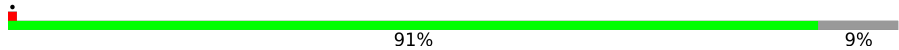

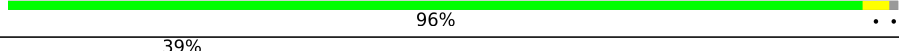





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	266	88% 12%
10	J	192	99%
11	K	214	30% 71% 29%
12	L	178	8% 95% 5%
13	M	211	96%
14	N	215	64% 36%
15	O	204	98%
16	P	203	94%
17	Q	184	82% 17%
18	R	188	98%
19	S	196	79% 20%
20	T	176	98%
21	U	160	98%
22	V	128	14% 76% 23%
23	W	140	92% 8%
24	X	157	39% 61%
25	Y	156	74% 25%
26	Z	145	90% 8%
27	a	136	98%
28	b	148	98%
29	c	159	60% 40%
30	d	115	81% 17%
31	e	125	84% 15%
32	f	135	95%
33	g	110	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	h	117	 93% . .
35	i	123	 94% 5% .
36	j	105	 91% . 8%
37	k	97	 85% . 13%
38	l	70	 96% . .
39	m	51	 94% . .
40	o	25	 20% 100%
41	p	106	 6% 92% . 7%
42	q	92	 99% .
43	r	137	 88% . 11%
44	t	3579	 73% 24% . .
45	u	76	 51% 61% 36% . .
46	v	76	 58% 38% .
47	y	27	 19% 100%
48	1	476	 88% . 11%
49	2	68	 91% 9%
50	3	96	 29% . 70%
51	4	224	 96% . .
52	5	563	 39% 84% 8% 8%
53	7	483	 17% 56% . 40%
54	6	188	 7% 87% 5% 7%

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 259082 atoms, of which 110309 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 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	246	3870	1183	1983	387	311	6	0	0

- Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	396	6535	2036	3338	601	546	14	0	0

- Molecule 3 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	363	5952	1817	3064	577	480	14	0	0

- Molecule 4 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
4	D	157	5029	1489	1692	587	1104	157	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
5	E	119	3825	1132	1284	454	836	119	0	0

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	248	4010	1271	1998	358	370	13	0	0

- Molecule 7 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	220	3689	1138	1917	335	295	4	0	0

- Molecule 8 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	225	3866	1202	1996	358	301	9	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	234	3898	1197	2018	362	317	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	191	3131	960	1605	285	275	6	0	0

- Molecule 11 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	152	2508	789	1270	233	208	8	0	0

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	169	2739	855	1386	252	240	6	0	0

- Molecule 13 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	M	205	3421	1036	1764	344	273	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	N	138	2328	725	1197	217	182	7	0	0

- Molecule 15 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	O	203	3450	1072	1749	359	266	4	0	0

- Molecule 16 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	P	195	3352	1034	1746	315	252	5	0	0

- Molecule 17 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	Q	153	2511	776	1269	241	216	9	0	0

- Molecule 18 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	R	187	3141	944	1628	314	250	5	0	0

- Molecule 19 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	S	156	2750	816	1439	278	209	8	0	0

- Molecule 20 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	T	175	2942	921	1493	283	234	11	0	0

- Molecule 21 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	U	157	2636	815	1352	250	214	5	0	0

- Molecule 22 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	V	99	1639	518	831	141	147	2	0	0

- Molecule 23 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	W	129	2000	613	1031	182	169	5	0	0

- Molecule 24 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	X	61	1032	327	521	100	82	2	0	0

- Molecule 25 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	Y	117	1987	612	1029	180	165	1	0	0

- Molecule 26 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	Z	133	2298	694	1192	224	185	3	0	0

- Molecule 27 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	a	134	2282	712	1179	207	181	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	b	147	2375	736	1213	237	186	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	c	96	1641	489	854	174	121	3	0	0

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	d	95	1512	468	774	131	133	6	0	0

- Molecule 31 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	e	106	1803	555	924	170	152	2	0	0

- Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	f	129	2224	673	1160	220	166	5	0	0

- Molecule 33 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	g	109	1788	555	912	174	144	3	0	0

- Molecule 34 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
34	h	112	1867	555	979	183	144	6	0	0

- Molecule 35 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace	
35	i	122	Total	C	H	N	O	S	0	0
			2163	641	1148	205	168	1		

- Molecule 36 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace	
36	j	97	Total	C	H	N	O	S	0	0
			1664	497	870	168	124	5		

- Molecule 37 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace	
37	k	84	Total	C	H	N	O	S	0	0
			1407	423	718	152	109	5		

- Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace	
38	l	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace	
39	m	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 40 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace	
40	o	25	Total	C	H	N	O	S	0	0
			529	145	289	64	28	3		

- Molecule 41 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
41	p	99	Total	C	H	N	O	S	0	0
			1696	510	882	167	131	6		

- Molecule 42 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	q	91	1464	445	756	136	120	7	0	0

- Molecule 43 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	r	122	2021	607	1041	204	165	4	0	0

- Molecule 44 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
44	t	3510	113261	33507	38018	13757	24469	3510	0	0

- Molecule 45 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
45	u	75	2402	710	809	278	530	75	0	0

- Molecule 46 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
46	v	76	2440	721	822	287	534	76	0	0

- Molecule 47 is a protein called Nascent chain mixture.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
47	y	27	245	81	110	27	27	0	0

- Molecule 48 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	1	426	6775	2189	3452	535	578	21	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	145	SER	ALA	conflict	UNP P61619
1	343	HIS	TYR	conflict	UNP P61619

- Molecule 49 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
49	2	62	1021	326	527	86	79	3	0	0

- Molecule 50 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
50	3	29	474	157	245	36	34	2	0	0

- Molecule 51 is a protein called Transmembrane protein 147.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
51	4	221	3526	1175	1769	272	294	16	0	0

- Molecule 52 is a protein called Nicalin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
52	5	516	8173	2595	4083	722	756	17	0	0

- Molecule 53 is a protein called Coiled-coil domain-containing protein 47.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
53	7	290	4775	1475	2400	435	447	18	0	0

- Molecule 54 is a protein called Calcium load-activated calcium channel.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
54	6	174	2850	887	1463	239	249	12	0	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
55	B	1	Total Mg 1 1	0
55	D	6	Total Mg 6 6	0
55	E	9	Total Mg 9 9	0
55	k	1	Total Mg 1 1	0
55	o	1	Total Mg 1 1	0
55	t	10	Total Mg 10 10	0

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

Mol	Chain	Residues	Atoms	AltConf
56	k	1	Total Zn 1 1	0
56	p	1	Total Zn 1 1	0
56	q	1	Total Zn 1 1	0

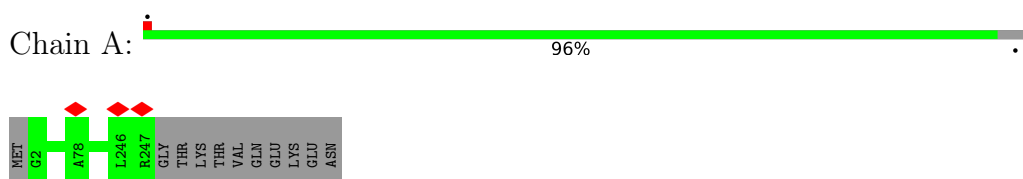
- Molecule 57 is water.

Mol	Chain	Residues	Atoms	AltConf
57	u	1	Total O 1 1	0

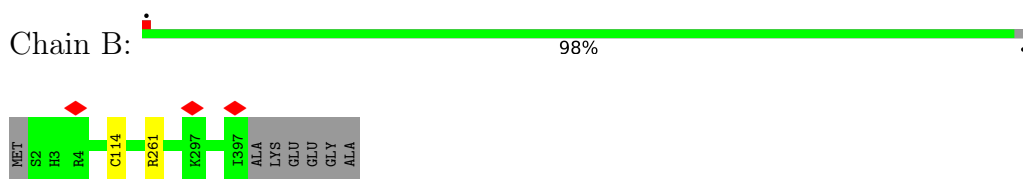
3 Residue-property plots

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.

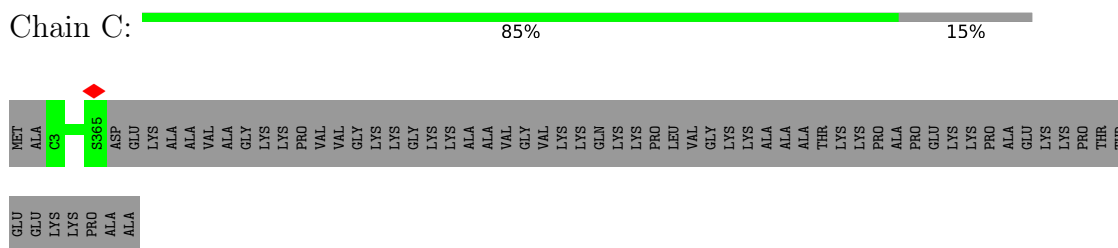
- Molecule 1: 60S ribosomal protein L8



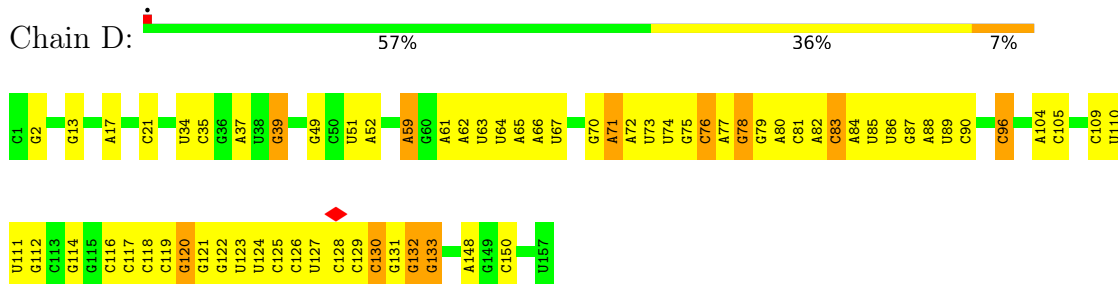
- Molecule 2: 60S ribosomal protein L3



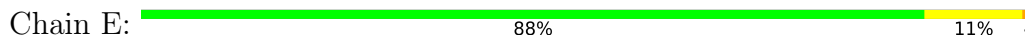
- Molecule 3: 60S ribosomal protein L4



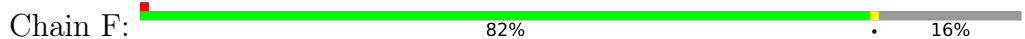
- Molecule 4: 5.8S ribosomal RNA



- Molecule 5: 5S ribosomal RNA

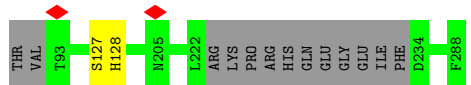
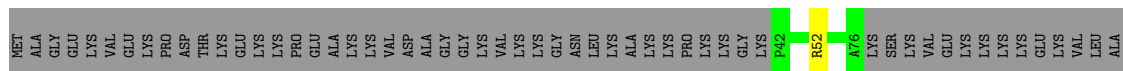


• Molecule 6: 60S ribosomal protein L5

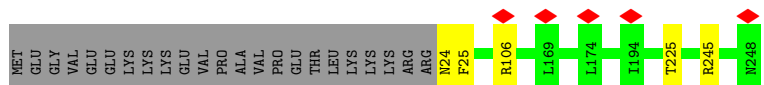
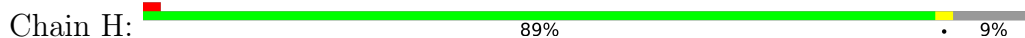


SER

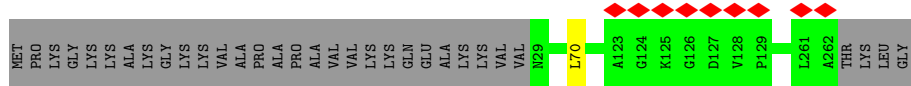
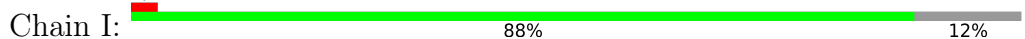
• Molecule 7: 60S ribosomal protein L6



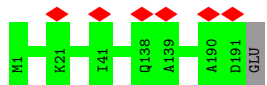
• Molecule 8: 60S ribosomal protein L7



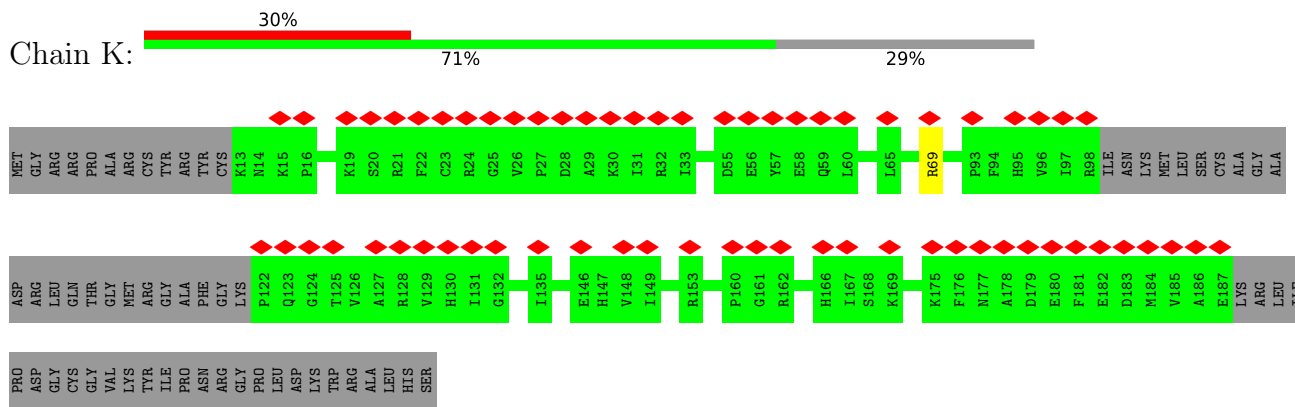
• Molecule 9: 60S ribosomal protein L7a



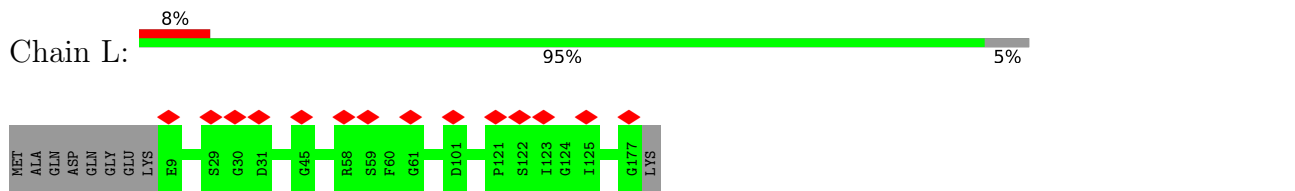
• Molecule 10: 60S ribosomal protein L9



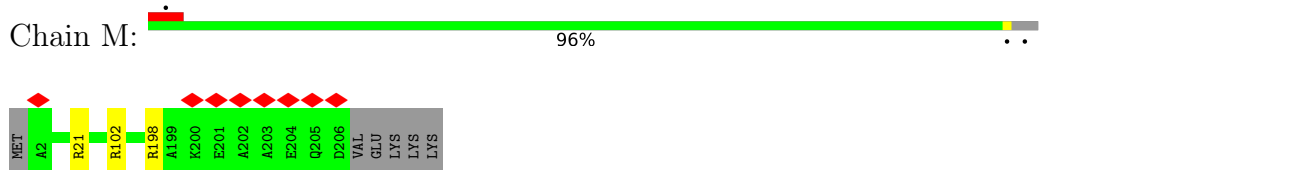
• Molecule 11: 60S ribosomal protein L10



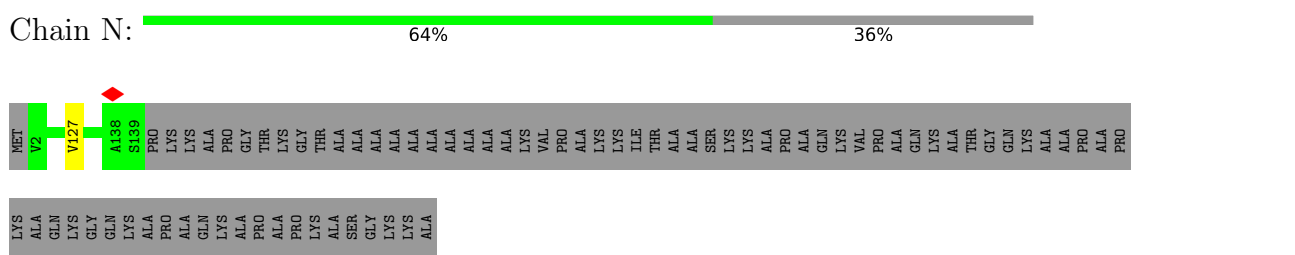
- Molecule 12: 60S ribosomal protein L11



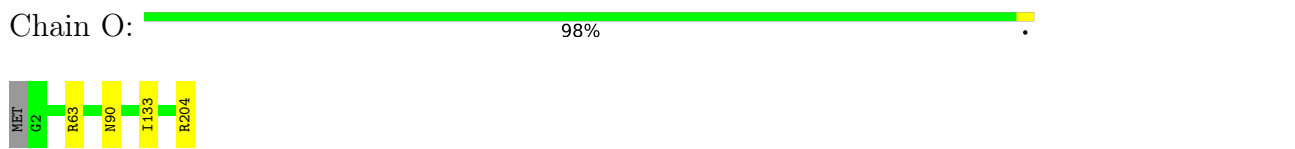
- Molecule 13: 60S ribosomal protein L13



- Molecule 14: 60S ribosomal protein L14



- Molecule 15: 60S ribosomal protein L15

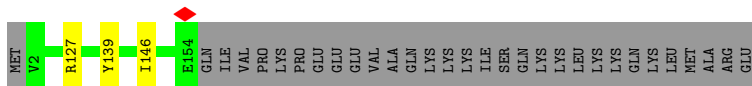
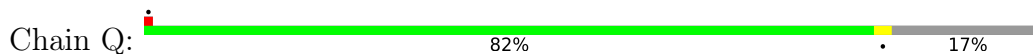


- Molecule 16: 60S ribosomal protein L13a





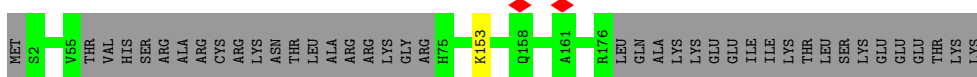
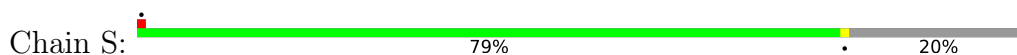
- Molecule 17: 60S ribosomal protein L17



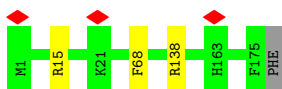
- Molecule 18: 60S ribosomal protein L18



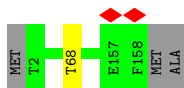
- Molecule 19: 60S ribosomal protein L19



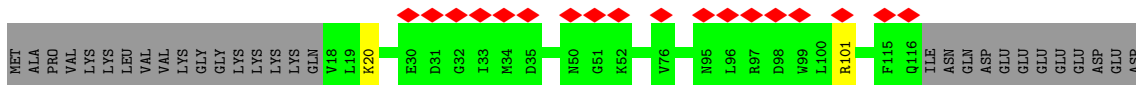
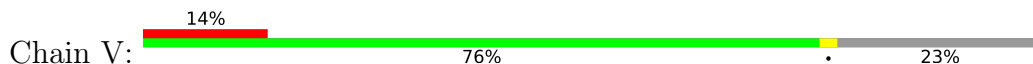
- Molecule 20: 60S ribosomal protein L18a



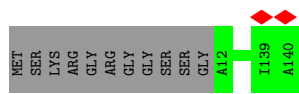
- Molecule 21: 60S ribosomal protein L21



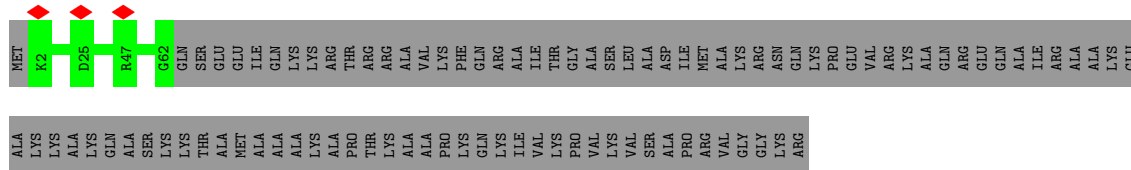
- Molecule 22: 60S ribosomal protein L22



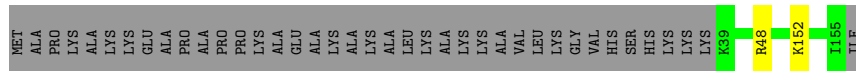
- Molecule 23: 60S ribosomal protein L23



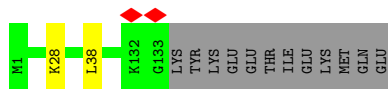
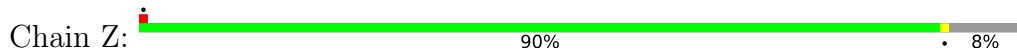
• Molecule 24: 60S ribosomal protein L24



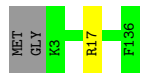
• Molecule 25: 60S ribosomal protein L23a



• Molecule 26: 60S ribosomal protein L26



• Molecule 27: 60S ribosomal protein L27

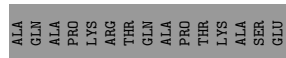


• Molecule 28: 60S ribosomal protein L27a

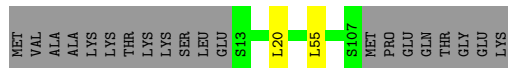


• Molecule 29: 60S ribosomal protein L29

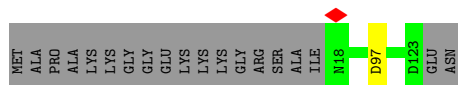
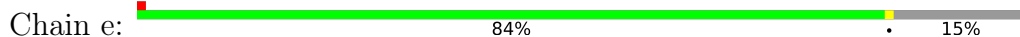




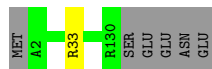
• Molecule 30: 60S ribosomal protein L30



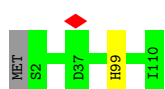
• Molecule 31: 60S ribosomal protein L31



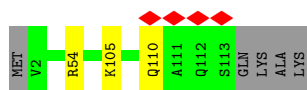
• Molecule 32: 60S ribosomal protein L32



• Molecule 33: 60S ribosomal protein L35a



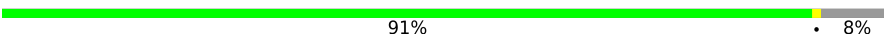
• Molecule 34: 60S ribosomal protein L34



• Molecule 35: 60S ribosomal protein L35




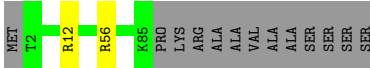
- Molecule 36: 60S ribosomal protein L36

Chain j:  91% 8%



- Molecule 37: 60S ribosomal protein L37

Chain k:  85% 13%



- Molecule 38: 60S ribosomal protein L38

Chain l:  96%



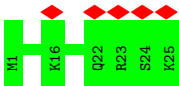
- Molecule 39: 60S ribosomal protein L39

Chain m:  94%

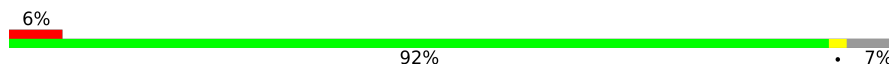


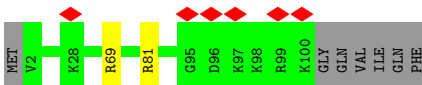
- Molecule 40: 60S ribosomal protein L41

Chain o:  20% 100%



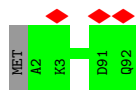
- Molecule 41: 60S ribosomal protein L36a

Chain p:  6% 92% 7%

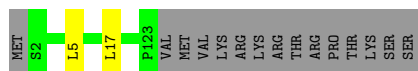
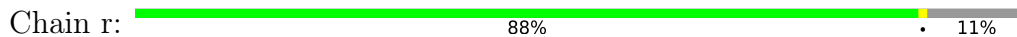


- Molecule 42: 60S ribosomal protein L37a

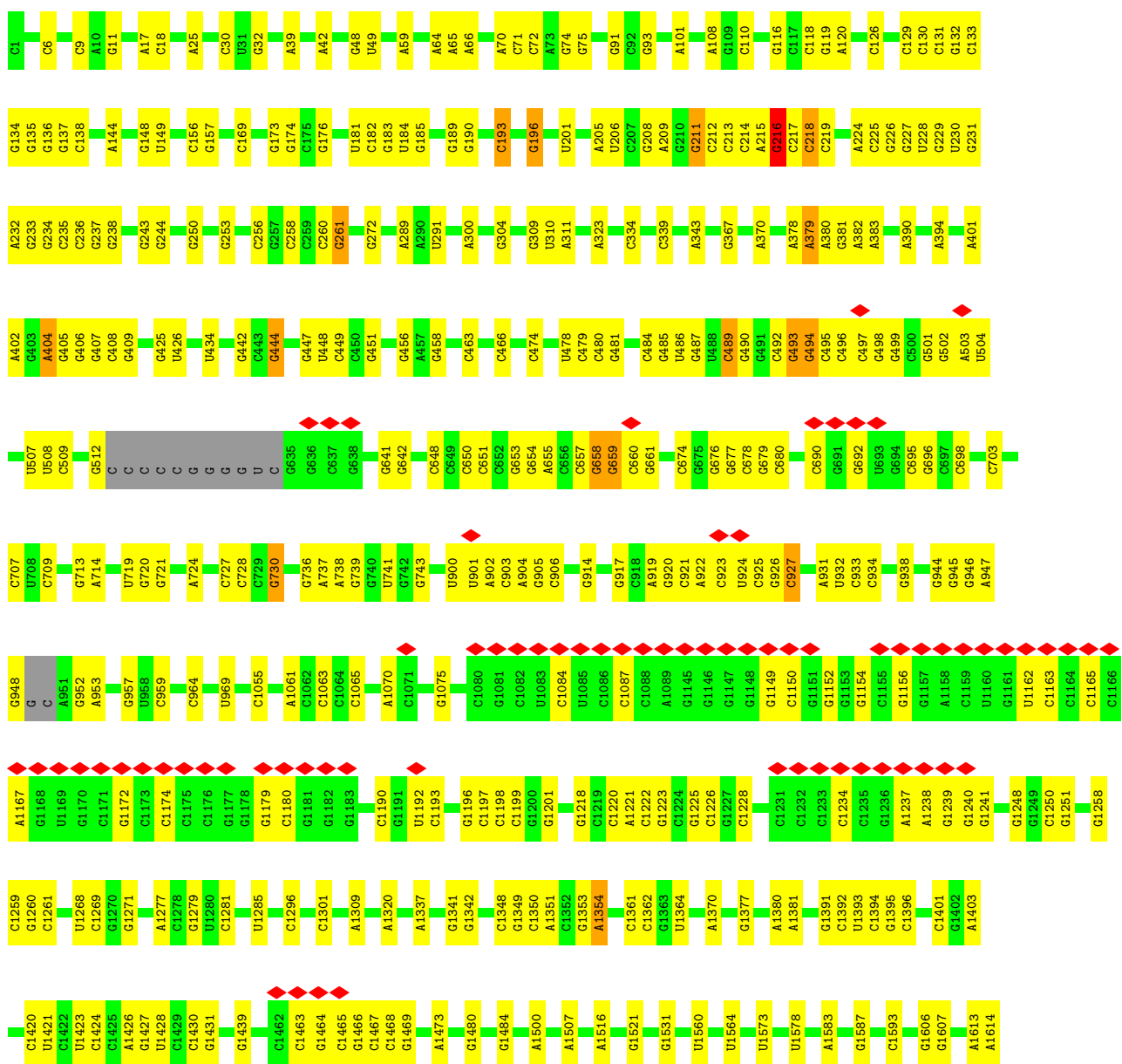
Chain q:  99%

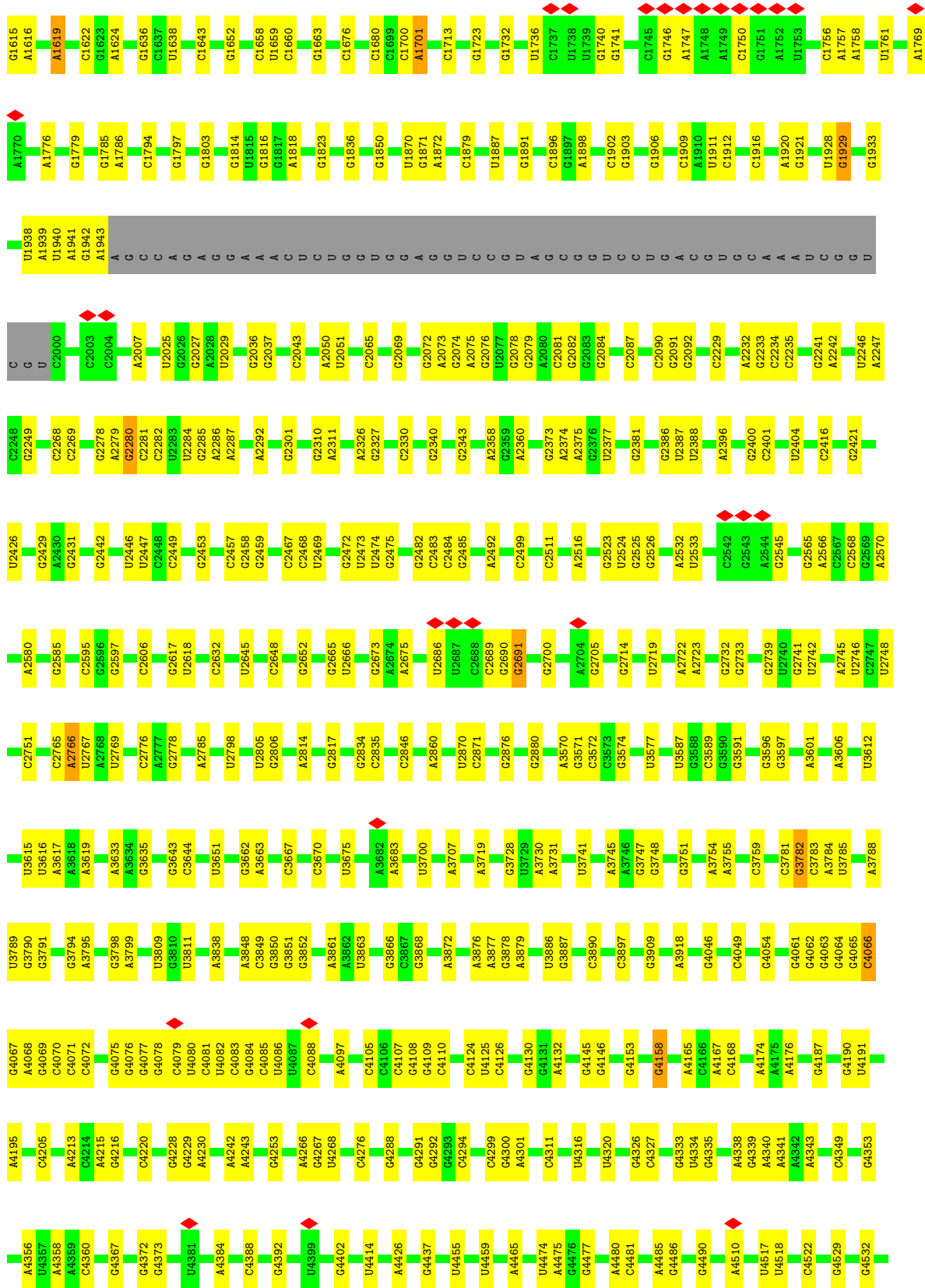


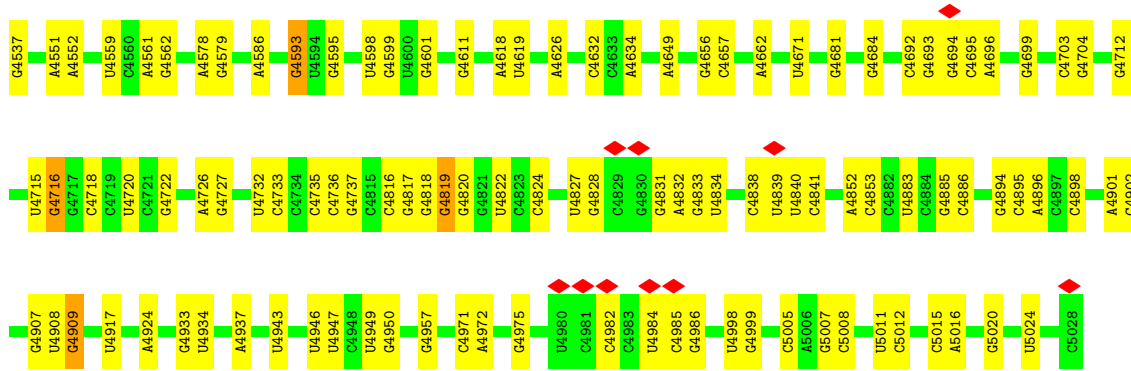
• Molecule 43: 60S ribosomal protein L28



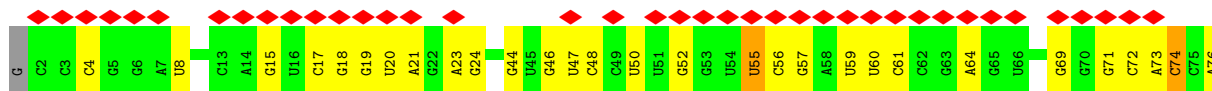
• Molecule 44: 28S ribosomal RNA



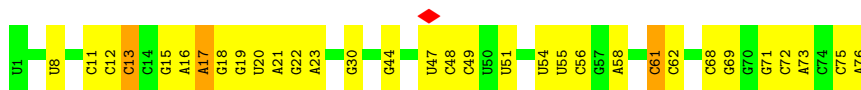




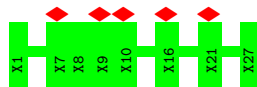
• Molecule 45: tRNA



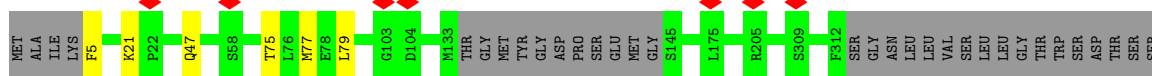
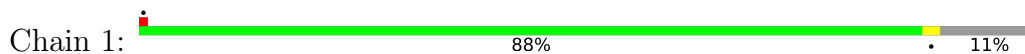
• Molecule 46: tRNA



• Molecule 47: Nascent chain mixture

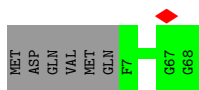


• Molecule 48: Protein transport protein Sec61 subunit alpha isoform 1

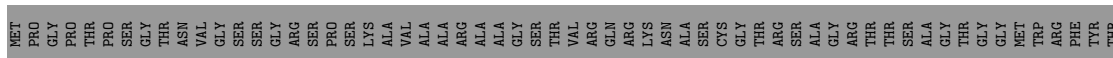


• Molecule 49: Protein transport protein Sec61 subunit gamma





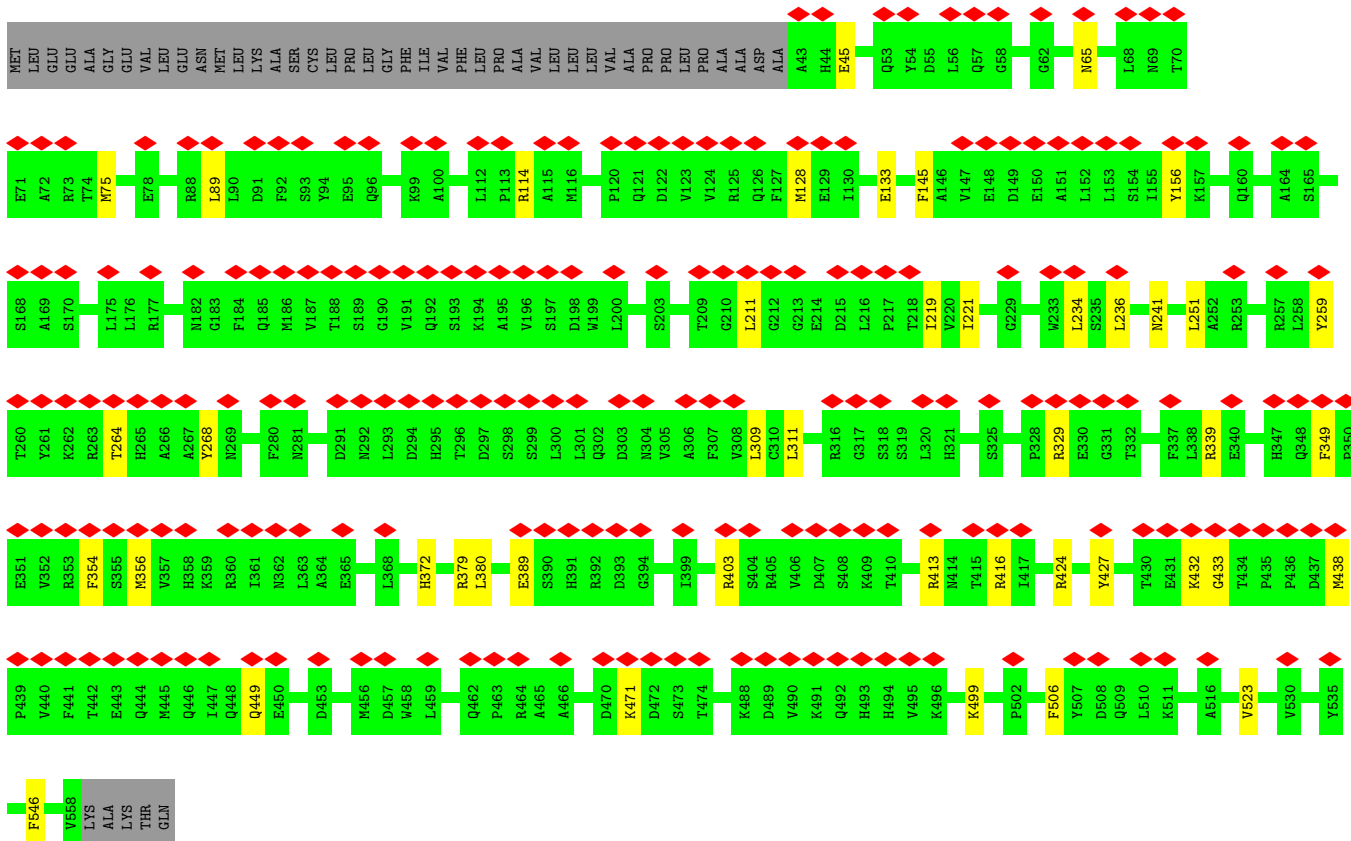
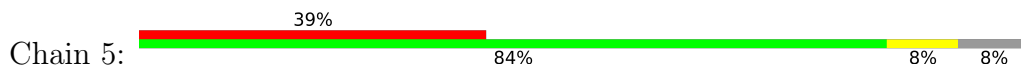
• Molecule 50: Protein transport protein Sec61 subunit beta



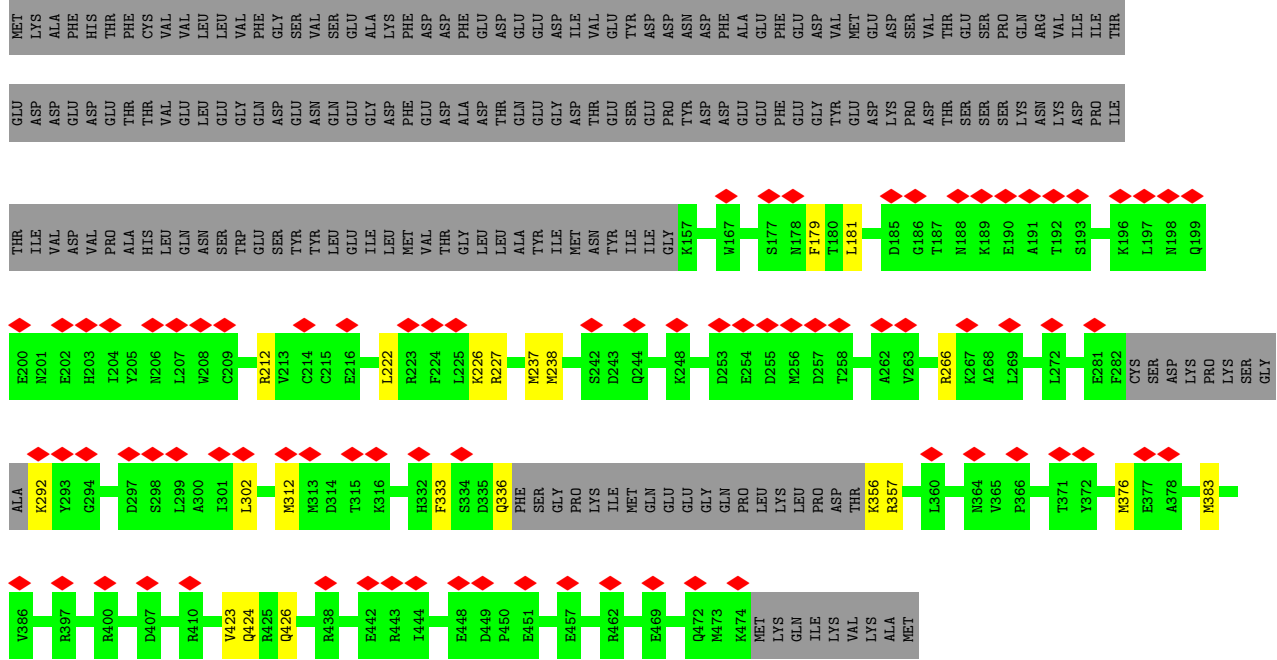
• Molecule 51: Transmembrane protein 147



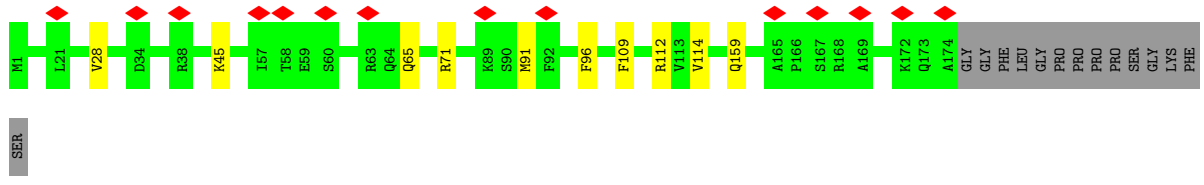
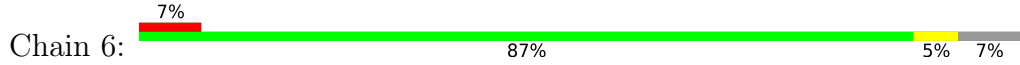
• Molecule 52: Nicalin



Molecule 53: Coiled-coil domain-containing protein 47



Molecule 54: Calcium load-activated calcium channel



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82684	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0073	Depositor
Map size (Å)	680.0, 680.0, 680.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	A	0.42	0/1925	0.52	0/2581
2	B	0.37	0/3265	0.50	0/4370
3	C	0.54	0/2942	0.55	0/3951
4	D	1.50	12/3726 (0.3%)	1.27	17/5804 (0.3%)
5	E	0.49	0/2839	0.90	1/4425 (0.0%)
6	F	0.30	0/2052	0.47	0/2755
7	G	0.32	0/1806	0.48	0/2421
8	H	0.37	0/1905	0.49	0/2539
9	I	0.34	0/1913	0.46	0/2576
10	J	0.30	0/1545	0.48	0/2077
11	K	0.26	0/1265	0.46	0/1688
12	L	0.28	0/1376	0.47	0/1841
13	M	0.39	0/1688	0.52	0/2260
14	N	0.32	0/1153	0.45	0/1542
15	O	0.47	0/1746	0.54	0/2338
16	P	0.37	0/1638	0.49	0/2191
17	Q	0.68	0/1268	0.60	0/1701
18	R	0.40	0/1537	0.53	0/2052
19	S	0.43	0/1325	0.52	0/1750
20	T	0.33	0/1488	0.51	0/1997
21	U	0.32	0/1312	0.45	0/1753
22	V	0.28	0/822	0.45	0/1103
23	W	0.33	0/983	0.47	0/1319
24	X	0.38	0/524	0.45	0/698
25	Y	0.76	0/975	0.58	0/1312
26	Z	0.75	0/1123	0.56	0/1493
27	a	0.36	0/1126	0.48	0/1502
28	b	0.41	0/1191	0.51	0/1591
29	c	0.31	0/799	0.48	0/1053
30	d	0.36	0/748	0.49	0/1004
31	e	0.45	0/894	0.52	0/1204
32	f	0.58	0/1082	0.56	0/1443

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.42	0/895	0.51	0/1198
34	h	0.48	0/898	0.54	0/1197
35	i	0.61	0/1023	0.58	0/1351
36	j	0.32	0/805	0.46	0/1065
37	k	0.75	0/703	0.61	0/929
38	l	0.41	0/575	0.50	0/761
39	m	0.64	0/454	0.59	0/599
40	o	0.28	0/241	0.46	0/305
41	p	0.37	0/827	0.47	0/1090
42	q	0.41	0/718	0.51	0/953
43	r	0.51	0/995	0.56	0/1334
44	t	0.91	40/84165 (0.0%)	1.02	105/131283 (0.1%)
45	u	0.32	0/1777	1.00	5/2767 (0.2%)
46	v	0.48	0/1806	1.28	4/2813 (0.1%)
48	1	0.40	0/3394	0.49	0/4598
49	2	0.42	0/504	0.50	0/673
50	3	0.29	0/236	0.43	0/321
51	4	0.36	0/1808	0.49	0/2459
52	5	0.25	0/4174	0.45	0/5661
53	7	0.30	0/2406	0.48	1/3214 (0.0%)
54	6	0.31	0/1406	0.45	0/1882
All	All	0.76	52/159791 (0.0%)	0.88	133/234787 (0.1%)

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
44	t	0	1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	t	238	G	N9-C4	-7.20	1.32	1.38
4	D	62	A	N9-C4	-6.49	1.33	1.37
44	t	224	A	N9-C4	-6.43	1.33	1.37
44	t	235	C	N1-C2	-6.38	1.33	1.40
44	t	193	C	N3-C4	-6.28	1.29	1.33
44	t	1281	C	C2-O2	-6.22	1.18	1.24
44	t	226	G	N9-C4	-6.17	1.33	1.38
44	t	404	A	N9-C4	-6.15	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	118	C	C2-O2	-6.07	1.19	1.24
44	t	402	A	N3-C4	-5.92	1.31	1.34
44	t	2286	A	N9-C4	-5.86	1.34	1.37
44	t	378	A	N9-C4	-5.72	1.34	1.37
44	t	234	G	N7-C5	-5.66	1.35	1.39
4	D	37	A	N9-C4	-5.66	1.34	1.37
4	D	59	A	N9-C4	-5.64	1.34	1.37
44	t	225	C	N1-C6	-5.64	1.33	1.37
44	t	383	A	N9-C4	-5.60	1.34	1.37
4	D	62	A	N3-C4	-5.56	1.31	1.34
44	t	238	G	N3-C4	-5.50	1.31	1.35
44	t	402	A	N9-C4	-5.46	1.34	1.37
44	t	4716	G	N9-C4	-5.46	1.33	1.38
4	D	21	C	N1-C6	-5.42	1.33	1.37
44	t	2360	A	N9-C4	-5.41	1.34	1.37
44	t	236	C	N3-C4	-5.40	1.30	1.33
44	t	201	U	N1-C2	-5.38	1.33	1.38
44	t	2287	A	N9-C4	-5.37	1.34	1.37
44	t	218	C	N1-C6	-5.33	1.33	1.37
44	t	231	G	N3-C4	-5.31	1.31	1.35
4	D	96	C	N1-C6	-5.26	1.33	1.37
44	t	2766	A	N3-C4	-5.24	1.31	1.34
44	t	394	A	N3-C4	-5.23	1.31	1.34
4	D	76	C	N1-C6	-5.20	1.34	1.37
44	t	494	G	N9-C4	-5.20	1.33	1.38
44	t	401	A	N9-C4	-5.19	1.34	1.37
44	t	1619	A	N9-C4	-5.18	1.34	1.37
44	t	217	C	N1-C6	-5.17	1.34	1.37
4	D	59	A	N3-C4	-5.17	1.31	1.34
44	t	211	G	C6-N1	-5.16	1.35	1.39
44	t	401	A	N3-C4	-5.16	1.31	1.34
44	t	382	A	N9-C4	-5.15	1.34	1.37
44	t	1484	G	N9-C4	-5.15	1.33	1.38
44	t	2281	C	N1-C6	-5.14	1.34	1.37
44	t	380	A	N9-C4	-5.13	1.34	1.37
44	t	379	A	C5-C4	-5.12	1.35	1.38
4	D	17	A	N9-C4	-5.09	1.34	1.37
4	D	90	C	N1-C6	-5.08	1.34	1.37
44	t	2511	C	N1-C6	-5.08	1.34	1.37
44	t	196	G	N9-C4	-5.08	1.33	1.38
44	t	394	A	N9-C4	-5.06	1.34	1.37
44	t	390	A	N9-C4	-5.03	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	t	2280	G	N7-C5	-5.02	1.36	1.39
4	D	71	A	N9-C4	-5.00	1.34	1.37

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	t	494	G	N3-C4-N9	-9.37	120.38	126.00
46	v	61	C	C2-N1-C1'	9.27	129.00	118.80
44	t	4716	G	N3-C4-N9	-9.19	120.49	126.00
44	t	494	G	N3-C4-C5	8.86	133.03	128.60
44	t	444	G	O4'-C1'-N9	8.84	115.27	108.20
44	t	1281	C	C2-N3-C4	-8.68	115.56	119.90
45	u	55	U	N3-C2-O2	-8.67	116.13	122.20
4	D	83	C	C2-N1-C1'	8.62	128.28	118.80
44	t	1484	G	N3-C4-N9	-8.49	120.90	126.00
44	t	4716	G	N3-C4-C5	8.30	132.75	128.60
44	t	1484	G	C4-N9-C1'	-8.24	115.79	126.50
44	t	1281	C	N1-C2-N3	8.13	124.89	119.20
44	t	227	G	C6-C5-N7	-8.01	125.59	130.40
44	t	481	G	N3-C4-N9	-7.88	121.27	126.00
4	D	83	C	C6-N1-C2	-7.70	117.22	120.30
4	D	83	C	N3-C2-O2	-7.67	116.53	121.90
44	t	227	G	N1-C2-N2	-7.61	109.35	116.20
44	t	1484	G	C8-N9-C1'	7.60	136.88	127.00
44	t	227	G	C2-N3-C4	-7.60	108.10	111.90
46	v	61	C	C6-N1-C1'	-7.58	111.70	120.80
44	t	493	G	C4-N9-C1'	7.39	136.11	126.50
44	t	225	C	C2-N3-C4	-7.37	116.22	119.90
4	D	133	G	C2-N3-C4	-7.32	108.24	111.90
4	D	39	G	O4'-C1'-N9	7.12	113.90	108.20
44	t	1484	G	N3-C2-N2	-7.10	114.93	119.90
44	t	1756	C	N1-C2-O2	-7.09	114.65	118.90
4	D	78	G	O4'-C1'-N9	7.00	113.80	108.20
44	t	1281	C	N3-C2-O2	-7.00	117.00	121.90
44	t	493	G	C8-N9-C1'	-6.92	118.00	127.00
4	D	83	C	N1-C2-O2	6.89	123.03	118.90
44	t	2459	G	N3-C4-N9	-6.87	121.88	126.00
44	t	226	G	N3-C4-C5	6.84	132.02	128.60
45	u	55	U	N1-C2-O2	6.83	127.58	122.80
44	t	226	G	C2-N3-C4	-6.71	108.54	111.90
44	t	236	C	C2-N3-C4	-6.64	116.58	119.90
45	u	55	U	C2-N1-C1'	6.61	125.64	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	t	4158	G	C8-N9-C1'	-6.49	118.57	127.00
4	D	133	G	O4'-C1'-N9	-6.44	103.05	108.20
44	t	235	C	C2-N1-C1'	-6.43	111.72	118.80
44	t	238	G	N3-C4-C5	6.43	131.82	128.60
44	t	927	C	C2-N1-C1'	6.35	125.79	118.80
44	t	216	G	C8-N9-C4	-6.35	103.86	106.40
44	t	490	G	O4'-C1'-N9	6.33	113.26	108.20
44	t	234	G	N3-C2-N2	6.28	124.30	119.90
44	t	235	C	N1-C2-O2	-6.28	115.13	118.90
44	t	4158	G	N3-C4-N9	6.25	129.75	126.00
44	t	493	G	N3-C4-N9	6.25	129.75	126.00
44	t	1484	G	N1-C2-N2	6.25	121.82	116.20
44	t	238	G	C2-N3-C4	-6.24	108.78	111.90
44	t	243	G	N3-C4-N9	-6.19	122.28	126.00
44	t	1701	A	C8-N9-C4	-6.19	103.32	105.80
44	t	4158	G	C5-C6-O6	-6.18	124.89	128.60
44	t	4733	C	N3-C2-O2	-6.14	117.61	121.90
44	t	1756	C	C2-N1-C1'	-6.08	112.11	118.80
44	t	1484	G	C6-C5-N7	6.08	134.05	130.40
4	D	130	C	C6-N1-C2	6.00	122.70	120.30
44	t	4158	G	C4-N9-C1'	5.97	134.26	126.50
44	t	1484	G	N3-C4-C5	5.95	131.58	128.60
44	t	481	G	N3-C4-C5	5.89	131.55	128.60
44	t	3791	G	C2-N3-C4	-5.85	108.97	111.90
4	D	96	C	C6-N1-C2	5.80	122.62	120.30
44	t	4909	G	N3-C2-N2	5.78	123.95	119.90
44	t	730	G	N3-C4-N9	-5.77	122.53	126.00
44	t	653	G	N1-C6-O6	-5.77	116.44	119.90
44	t	3782	G	N3-C2-N2	-5.76	115.86	119.90
44	t	227	G	C5-C6-N1	-5.75	108.63	111.50
44	t	227	G	N3-C2-N2	5.73	123.91	119.90
44	t	659	G	C4-N9-C1'	5.73	133.95	126.50
44	t	494	G	C2-N3-C4	-5.69	109.05	111.90
44	t	190	G	N3-C4-N9	-5.66	122.61	126.00
44	t	226	G	N3-C4-N9	-5.65	122.61	126.00
4	D	132	G	C8-N9-C1'	-5.63	119.69	127.00
44	t	227	G	N9-C4-C5	-5.62	103.15	105.40
44	t	232	A	C4-C5-N7	5.55	113.47	110.70
44	t	4909	G	N1-C2-N2	-5.54	111.21	116.20
44	t	653	G	C5-C6-O6	5.53	131.92	128.60
44	t	659	G	C8-N9-C1'	-5.53	119.82	127.00
44	t	1241	G	N3-C4-N9	5.50	129.30	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	t	489	C	C2-N1-C1'	-5.48	112.77	118.80
44	t	1354	A	O4'-C1'-N9	5.48	112.58	108.20
44	t	4158	G	C6-C5-N7	-5.47	127.12	130.40
44	t	442	G	N3-C4-N9	5.44	129.26	126.00
44	t	235	C	C6-N1-C1'	5.42	127.31	120.80
44	t	651	C	N1-C2-O2	5.41	122.15	118.90
44	t	261	G	N3-C4-C5	5.41	131.30	128.60
4	D	62	A	C2-N3-C4	-5.39	107.91	110.60
44	t	236	C	N3-C2-O2	-5.37	118.14	121.90
44	t	189	G	N3-C4-N9	-5.35	122.79	126.00
53	7	356	LYS	N-CA-C	-5.33	96.60	111.00
44	t	261	G	C2-N3-C4	-5.32	109.24	111.90
44	t	225	C	O4'-C1'-N1	5.30	112.44	108.20
44	t	236	C	N3-C4-C5	5.30	124.02	121.90
44	t	4593	G	C4-N9-C1'	5.29	133.38	126.50
44	t	2459	G	C8-N9-C1'	5.29	133.88	127.00
44	t	227	G	C4-C5-C6	5.28	121.97	118.80
4	D	120	G	N9-C4-C5	-5.26	103.30	105.40
44	t	4392	G	N9-C4-C5	-5.25	103.30	105.40
4	D	83	C	C6-N1-C1'	-5.25	114.50	120.80
44	t	235	C	N3-C4-N4	-5.23	114.34	118.00
44	t	2459	G	N3-C4-C5	5.23	131.21	128.60
44	t	707	C	C2-N1-C1'	-5.23	113.05	118.80
45	u	55	U	C6-N1-C2	-5.22	117.87	121.00
45	u	74	C	N1-C2-O2	5.22	122.03	118.90
44	t	481	G	C8-N9-C1'	5.19	133.74	127.00
44	t	485	G	N3-C4-N9	-5.18	122.89	126.00
44	t	2386	G	C4-N9-C1'	5.18	133.24	126.50
44	t	658	G	C4-N9-C1'	-5.18	119.77	126.50
44	t	238	G	N1-C6-O6	5.18	123.00	119.90
44	t	1929	G	N3-C2-N2	-5.17	116.28	119.90
46	v	17	A	P-O3'-C3'	5.17	125.90	119.70
46	v	13	C	C2-N1-C1'	-5.16	113.13	118.80
44	t	4593	G	C8-N9-C1'	-5.16	120.30	127.00
44	t	3794	G	C2-N3-C4	-5.15	109.32	111.90
44	t	4819	G	N3-C4-N9	5.15	129.09	126.00
44	t	658	G	N3-C4-N9	-5.12	122.92	126.00
44	t	244	G	C2-N3-C4	-5.12	109.34	111.90
44	t	2459	G	C4-N9-C1'	-5.12	119.85	126.50
44	t	2765	C	C6-N1-C2	5.11	122.34	120.30
4	D	132	G	C4-N9-C1'	5.10	133.13	126.50
4	D	66	A	N9-C1'-C2'	-5.09	106.40	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	t	232	A	C5-N7-C8	-5.09	101.35	103.90
44	t	2691	G	C8-N9-C1'	-5.08	120.39	127.00
44	t	1761	U	C2-N1-C1'	5.08	123.80	117.70
44	t	493	G	N3-C4-C5	-5.08	126.06	128.60
44	t	261	G	N3-C4-N9	-5.07	122.96	126.00
4	D	120	G	C4-C5-N7	5.07	112.83	110.80
44	t	208	G	C4-N9-C1'	5.07	133.09	126.50
44	t	4066	C	P-O3'-C3'	5.05	125.77	119.70
44	t	707	C	N1-C2-O2	-5.05	115.87	118.90
44	t	493	G	C6-C5-N7	-5.04	127.38	130.40
5	E	64	G	O4'-C1'-N9	-5.01	104.20	108.20
44	t	2373	G	O4'-C1'-N9	5.00	112.20	108.20
44	t	713	G	N3-C4-N9	-5.00	123.00	126.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	t	216	G	Sidechain

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	A	244/257 (95%)	224 (92%)	20 (8%)	0	100	100
2	B	394/403 (98%)	363 (92%)	31 (8%)	0	100	100
3	C	361/427 (84%)	337 (93%)	24 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	246/297 (83%)	235 (96%)	11 (4%)	0	100	100
7	G	214/288 (74%)	186 (87%)	26 (12%)	2 (1%)	17	53
8	H	223/248 (90%)	207 (93%)	16 (7%)	0	100	100
9	I	232/266 (87%)	221 (95%)	11 (5%)	0	100	100
10	J	189/192 (98%)	173 (92%)	16 (8%)	0	100	100
11	K	148/214 (69%)	141 (95%)	7 (5%)	0	100	100
12	L	167/178 (94%)	155 (93%)	12 (7%)	0	100	100
13	M	203/211 (96%)	180 (89%)	23 (11%)	0	100	100
14	N	136/215 (63%)	127 (93%)	9 (7%)	0	100	100
15	O	201/204 (98%)	181 (90%)	19 (10%)	1 (0%)	29	66
16	P	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
17	Q	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
18	R	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
19	S	152/196 (78%)	146 (96%)	6 (4%)	0	100	100
20	T	173/176 (98%)	165 (95%)	8 (5%)	0	100	100
21	U	155/160 (97%)	146 (94%)	9 (6%)	0	100	100
22	V	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
23	W	127/140 (91%)	123 (97%)	4 (3%)	0	100	100
24	X	59/157 (38%)	57 (97%)	2 (3%)	0	100	100
25	Y	115/156 (74%)	107 (93%)	8 (7%)	0	100	100
26	Z	131/145 (90%)	126 (96%)	5 (4%)	0	100	100
27	a	132/136 (97%)	121 (92%)	11 (8%)	0	100	100
28	b	145/148 (98%)	128 (88%)	17 (12%)	0	100	100
29	c	92/159 (58%)	85 (92%)	7 (8%)	0	100	100
30	d	93/115 (81%)	91 (98%)	2 (2%)	0	100	100
31	e	104/125 (83%)	97 (93%)	7 (7%)	0	100	100
32	f	127/135 (94%)	115 (91%)	12 (9%)	0	100	100
33	g	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
34	h	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
35	i	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
36	j	95/105 (90%)	94 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	k	82/97 (84%)	79 (96%)	3 (4%)	0	100	100
38	l	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
39	m	48/51 (94%)	48 (100%)	0	0	100	100
40	o	23/25 (92%)	23 (100%)	0	0	100	100
41	p	97/106 (92%)	94 (97%)	3 (3%)	0	100	100
42	q	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
43	r	120/137 (88%)	106 (88%)	14 (12%)	0	100	100
48	1	420/476 (88%)	403 (96%)	16 (4%)	1 (0%)	47	78
49	2	60/68 (88%)	59 (98%)	1 (2%)	0	100	100
50	3	27/96 (28%)	25 (93%)	2 (7%)	0	100	100
51	4	219/224 (98%)	206 (94%)	13 (6%)	0	100	100
52	5	514/563 (91%)	472 (92%)	39 (8%)	3 (1%)	25	62
53	7	286/483 (59%)	273 (96%)	13 (4%)	0	100	100
54	6	172/188 (92%)	165 (96%)	7 (4%)	0	100	100
All	All	7845/9182 (85%)	7357 (94%)	481 (6%)	7 (0%)	54	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	127	SER
48	1	75	THR
7	G	128	HIS
52	5	432	LYS
15	O	90	ASN
52	5	523	VAL
52	5	433	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/199 (95%)	189 (100%)	0	100	100
2	B	345/349 (99%)	343 (99%)	2 (1%)	86	92
3	C	302/348 (87%)	302 (100%)	0	100	100
6	F	208/250 (83%)	205 (99%)	3 (1%)	67	81
7	G	195/252 (77%)	194 (100%)	1 (0%)	88	94
8	H	194/215 (90%)	189 (97%)	5 (3%)	46	69
9	I	199/223 (89%)	198 (100%)	1 (0%)	88	94
10	J	170/171 (99%)	170 (100%)	0	100	100
11	K	132/181 (73%)	131 (99%)	1 (1%)	81	89
12	L	142/149 (95%)	142 (100%)	0	100	100
13	M	171/177 (97%)	168 (98%)	3 (2%)	59	77
14	N	117/161 (73%)	116 (99%)	1 (1%)	78	88
15	O	171/172 (99%)	168 (98%)	3 (2%)	59	77
16	P	168/174 (97%)	163 (97%)	5 (3%)	41	66
17	Q	134/163 (82%)	131 (98%)	3 (2%)	52	72
18	R	164/165 (99%)	161 (98%)	3 (2%)	59	77
19	S	139/175 (79%)	138 (99%)	1 (1%)	84	91
20	T	156/157 (99%)	153 (98%)	3 (2%)	57	76
21	U	138/140 (99%)	137 (99%)	1 (1%)	84	91
22	V	89/115 (77%)	87 (98%)	2 (2%)	52	72
23	W	100/107 (94%)	100 (100%)	0	100	100
24	X	53/126 (42%)	53 (100%)	0	100	100
25	Y	105/133 (79%)	103 (98%)	2 (2%)	57	76
26	Z	123/135 (91%)	121 (98%)	2 (2%)	62	79
27	a	117/118 (99%)	116 (99%)	1 (1%)	78	88
28	b	120/121 (99%)	118 (98%)	2 (2%)	60	78
29	c	79/126 (63%)	78 (99%)	1 (1%)	69	82
30	d	80/97 (82%)	78 (98%)	2 (2%)	47	70
31	e	97/110 (88%)	96 (99%)	1 (1%)	76	86
32	f	115/121 (95%)	114 (99%)	1 (1%)	78	88
33	g	88/89 (99%)	87 (99%)	1 (1%)	73	85
34	h	96/100 (96%)	93 (97%)	3 (3%)	40	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	i	109/110 (99%)	103 (94%)	6 (6%)	21	53
36	j	83/89 (93%)	82 (99%)	1 (1%)	71	84
37	k	71/80 (89%)	69 (97%)	2 (3%)	43	67
38	l	64/65 (98%)	62 (97%)	2 (3%)	40	65
39	m	47/48 (98%)	45 (96%)	2 (4%)	29	57
40	o	24/24 (100%)	24 (100%)	0	100	100
41	p	88/94 (94%)	86 (98%)	2 (2%)	50	71
42	q	74/75 (99%)	74 (100%)	0	100	100
43	r	106/121 (88%)	104 (98%)	2 (2%)	57	76
48	1	362/399 (91%)	355 (98%)	7 (2%)	57	76
49	2	53/59 (90%)	53 (100%)	0	100	100
50	3	26/74 (35%)	25 (96%)	1 (4%)	33	60
51	4	183/186 (98%)	177 (97%)	6 (3%)	38	64
52	5	438/475 (92%)	397 (91%)	41 (9%)	8	34
53	7	261/436 (60%)	241 (92%)	20 (8%)	13	42
54	6	154/164 (94%)	144 (94%)	10 (6%)	17	48
All	All	6839/7818 (88%)	6683 (98%)	156 (2%)	53	71

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	114	CYS
2	B	261	ARG
6	F	9	ASN
6	F	10	LYS
6	F	196	ARG
7	G	52	ARG
8	H	24	ASN
8	H	25	PHE
8	H	106	ARG
8	H	225	THR
8	H	245	ARG
9	I	70	LEU
11	K	69	ARG
13	M	21	ARG
13	M	102	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	198	ARG
14	N	127	VAL
15	O	63	ARG
15	O	133	ILE
15	O	204	ARG
16	P	94	ARG
16	P	101	ARG
16	P	141	LEU
16	P	169	ARG
16	P	178	ARG
17	Q	127	ARG
17	Q	139	TYR
17	Q	146	ILE
18	R	37	ARG
18	R	91	ARG
18	R	168	ARG
19	S	153	LYS
20	T	15	ARG
20	T	68	PHE
20	T	138	ARG
21	U	68	THR
22	V	20	LYS
22	V	101	ARG
25	Y	48	ARG
25	Y	152	LYS
26	Z	28	LYS
26	Z	38	LEU
27	a	17	ARG
28	b	87	ARG
28	b	105	ARG
29	c	116	LEU
30	d	20	LEU
30	d	55	LEU
31	e	97	ASP
32	f	33	ARG
33	g	99	HIS
34	h	54	ARG
34	h	105	LYS
34	h	110	GLN
35	i	70	ARG
35	i	86	LYS
35	i	93	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	i	97	LYS
35	i	109	ARG
35	i	112	ARG
36	j	66	ASP
37	k	12	ARG
37	k	56	ARG
38	l	9	LYS
38	l	17	ARG
39	m	4	HIS
39	m	21	ARG
41	p	69	ARG
41	p	81	ARG
43	r	5	LEU
43	r	17	LEU
48	1	5	PHE
48	1	21	LYS
48	1	47	GLN
48	1	77	MET
48	1	79	LEU
48	1	436	ASP
48	1	441	ILE
50	3	87	LEU
51	4	6	PHE
51	4	35	CYS
51	4	145	HIS
51	4	154	TRP
51	4	158	ARG
51	4	188	HIS
52	5	45	GLU
52	5	65	ASN
52	5	75	MET
52	5	89	LEU
52	5	114	ARG
52	5	128	MET
52	5	133	GLU
52	5	145	PHE
52	5	156	TYR
52	5	211	LEU
52	5	219	ILE
52	5	221	ILE
52	5	234	LEU
52	5	236	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	5	241	ASN
52	5	251	LEU
52	5	259	TYR
52	5	264	THR
52	5	268	TYR
52	5	309	LEU
52	5	311	LEU
52	5	329	ARG
52	5	339	ARG
52	5	349	PHE
52	5	354	PHE
52	5	356	MET
52	5	372	HIS
52	5	379	ARG
52	5	380	LEU
52	5	389	GLU
52	5	403	ARG
52	5	413	ARG
52	5	416	ARG
52	5	424	ARG
52	5	427	TYR
52	5	438	MET
52	5	449	GLN
52	5	471	LYS
52	5	499	LYS
52	5	506	PHE
52	5	546	PHE
53	7	179	PHE
53	7	181	LEU
53	7	212	ARG
53	7	222	LEU
53	7	226	LYS
53	7	227	ARG
53	7	237	MET
53	7	238	MET
53	7	266	ARG
53	7	292	LYS
53	7	302	LEU
53	7	312	MET
53	7	333	PHE
53	7	336	GLN
53	7	357	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	7	376	MET
53	7	383	MET
53	7	423	VAL
53	7	424	GLN
53	7	426	GLN
54	6	28	VAL
54	6	45	LYS
54	6	65	GLN
54	6	71	ARG
54	6	91	MET
54	6	96	PHE
54	6	109	PHE
54	6	112	ARG
54	6	114	VAL
54	6	159	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
19	S	39	GLN
48	1	456	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	156/157 (99%)	60 (38%)	20 (12%)
44	t	3495/3579 (97%)	849 (24%)	0
45	u	74/76 (97%)	29 (39%)	0
46	v	75/76 (98%)	32 (42%)	0
5	E	118/119 (99%)	14 (11%)	0
All	All	3918/4007 (97%)	984 (25%)	20 (0%)

All (984) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	2	G
4	D	13	G
4	D	34	U
4	D	35	C
4	D	39	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	49	G
4	D	51	U
4	D	52	A
4	D	59	A
4	D	61	A
4	D	63	U
4	D	64	U
4	D	65	A
4	D	67	U
4	D	71	A
4	D	72	A
4	D	73	U
4	D	74	U
4	D	75	G
4	D	76	C
4	D	77	A
4	D	78	G
4	D	79	G
4	D	80	A
4	D	81	C
4	D	82	A
4	D	83	C
4	D	84	A
4	D	85	U
4	D	86	U
4	D	87	G
4	D	88	A
4	D	89	U
4	D	96	C
4	D	104	A
4	D	105	C
4	D	109	C
4	D	110	U
4	D	111	U
4	D	112	G
4	D	114	G
4	D	116	C
4	D	117	C
4	D	119	C
4	D	120	G
4	D	121	G
4	D	122	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	123	U
4	D	124	U
4	D	125	C
4	D	126	C
4	D	127	U
4	D	128	C
4	D	129	C
4	D	130	C
4	D	131	G
4	D	132	G
4	D	133	G
4	D	148	A
4	D	150	C
5	E	7	G
5	E	11	A
5	E	22	A
5	E	23	A
5	E	24	C
5	E	33	U
5	E	35	U
5	E	40	U
5	E	48	G
5	E	49	A
5	E	53	U
5	E	64	G
5	E	96	U
5	E	110	G
44	t	6	C
44	t	9	C
44	t	11	G
44	t	17	A
44	t	18	C
44	t	25	A
44	t	30	C
44	t	32	G
44	t	39	A
44	t	42	A
44	t	48	G
44	t	49	U
44	t	59	A
44	t	64	A
44	t	65	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	66	A
44	t	70	A
44	t	71	C
44	t	72	C
44	t	74	G
44	t	75	G
44	t	91	G
44	t	93	G
44	t	101	A
44	t	108	A
44	t	110	C
44	t	116	G
44	t	118	C
44	t	119	G
44	t	120	A
44	t	126	C
44	t	129	C
44	t	130	C
44	t	131	C
44	t	132	G
44	t	133	C
44	t	134	G
44	t	135	G
44	t	136	G
44	t	137	G
44	t	138	C
44	t	144	A
44	t	148	G
44	t	149	U
44	t	156	C
44	t	157	G
44	t	169	C
44	t	173	G
44	t	174	G
44	t	176	G
44	t	181	U
44	t	182	C
44	t	183	G
44	t	184	U
44	t	185	G
44	t	193	C
44	t	196	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	205	A
44	t	206	U
44	t	209	A
44	t	211	G
44	t	212	C
44	t	213	C
44	t	214	C
44	t	215	A
44	t	216	G
44	t	218	C
44	t	219	C
44	t	228	U
44	t	229	G
44	t	230	U
44	t	233	G
44	t	237	G
44	t	250	G
44	t	253	G
44	t	256	C
44	t	258	C
44	t	260	C
44	t	261	G
44	t	272	G
44	t	289	A
44	t	291	U
44	t	300	A
44	t	304	G
44	t	309	G
44	t	310	U
44	t	311	A
44	t	323	A
44	t	334	C
44	t	339	C
44	t	343	A
44	t	367	G
44	t	370	A
44	t	379	A
44	t	381	G
44	t	404	A
44	t	405	G
44	t	406	G
44	t	407	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	408	C
44	t	409	G
44	t	425	G
44	t	426	U
44	t	434	U
44	t	444	G
44	t	447	G
44	t	448	U
44	t	449	C
44	t	451	G
44	t	456	G
44	t	458	G
44	t	463	C
44	t	466	C
44	t	474	C
44	t	478	U
44	t	479	C
44	t	480	C
44	t	484	C
44	t	486	U
44	t	487	G
44	t	489	C
44	t	492	C
44	t	493	G
44	t	494	G
44	t	495	C
44	t	496	C
44	t	497	C
44	t	498	G
44	t	499	G
44	t	501	G
44	t	502	G
44	t	503	A
44	t	504	U
44	t	507	U
44	t	508	U
44	t	509	C
44	t	512	G
44	t	641	G
44	t	642	G
44	t	648	C
44	t	650	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	654	G
44	t	655	A
44	t	657	C
44	t	658	G
44	t	659	G
44	t	660	C
44	t	661	G
44	t	674	C
44	t	676	G
44	t	677	G
44	t	678	C
44	t	679	G
44	t	680	C
44	t	690	C
44	t	692	G
44	t	695	C
44	t	696	G
44	t	698	C
44	t	703	C
44	t	709	C
44	t	714	A
44	t	719	U
44	t	720	G
44	t	721	G
44	t	724	A
44	t	727	C
44	t	728	C
44	t	730	G
44	t	736	G
44	t	737	A
44	t	738	A
44	t	739	G
44	t	741	U
44	t	743	G
44	t	900	U
44	t	901	U
44	t	902	A
44	t	903	C
44	t	904	A
44	t	905	G
44	t	906	C
44	t	914	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	917	G
44	t	919	A
44	t	920	G
44	t	921	C
44	t	922	A
44	t	923	C
44	t	924	U
44	t	925	C
44	t	926	G
44	t	927	C
44	t	931	A
44	t	932	U
44	t	933	C
44	t	934	C
44	t	938	G
44	t	944	G
44	t	945	G
44	t	946	G
44	t	947	A
44	t	948	G
44	t	952	G
44	t	953	A
44	t	957	G
44	t	959	C
44	t	964	C
44	t	969	U
44	t	1055	C
44	t	1061	A
44	t	1063	C
44	t	1065	C
44	t	1070	A
44	t	1075	G
44	t	1084	C
44	t	1087	C
44	t	1149	G
44	t	1150	C
44	t	1152	G
44	t	1154	G
44	t	1156	G
44	t	1162	U
44	t	1163	C
44	t	1165	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	1167	A
44	t	1172	G
44	t	1174	C
44	t	1179	G
44	t	1180	C
44	t	1190	C
44	t	1192	U
44	t	1193	C
44	t	1196	G
44	t	1197	C
44	t	1198	C
44	t	1199	C
44	t	1201	G
44	t	1218	G
44	t	1220	C
44	t	1221	A
44	t	1222	C
44	t	1223	G
44	t	1225	G
44	t	1226	C
44	t	1228	C
44	t	1234	C
44	t	1237	A
44	t	1238	A
44	t	1239	G
44	t	1240	G
44	t	1248	G
44	t	1250	C
44	t	1251	G
44	t	1258	G
44	t	1259	C
44	t	1260	G
44	t	1261	C
44	t	1268	U
44	t	1269	C
44	t	1271	G
44	t	1277	A
44	t	1279	G
44	t	1285	U
44	t	1296	C
44	t	1301	C
44	t	1309	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	1320	A
44	t	1337	A
44	t	1341	G
44	t	1342	G
44	t	1348	C
44	t	1349	G
44	t	1350	C
44	t	1351	A
44	t	1353	G
44	t	1354	A
44	t	1361	C
44	t	1362	C
44	t	1364	U
44	t	1370	A
44	t	1377	G
44	t	1380	A
44	t	1381	A
44	t	1391	G
44	t	1392	C
44	t	1393	U
44	t	1394	C
44	t	1395	G
44	t	1396	C
44	t	1401	C
44	t	1403	A
44	t	1420	C
44	t	1421	U
44	t	1423	U
44	t	1424	C
44	t	1426	A
44	t	1427	G
44	t	1428	U
44	t	1430	C
44	t	1431	G
44	t	1439	G
44	t	1463	C
44	t	1464	G
44	t	1465	C
44	t	1466	G
44	t	1467	C
44	t	1468	C
44	t	1469	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	1473	A
44	t	1480	G
44	t	1500	A
44	t	1507	A
44	t	1516	A
44	t	1521	G
44	t	1531	G
44	t	1560	U
44	t	1564	U
44	t	1573	U
44	t	1578	U
44	t	1583	A
44	t	1587	G
44	t	1593	C
44	t	1606	G
44	t	1607	G
44	t	1613	A
44	t	1614	A
44	t	1615	G
44	t	1616	A
44	t	1619	A
44	t	1622	C
44	t	1624	A
44	t	1636	G
44	t	1638	U
44	t	1643	C
44	t	1652	G
44	t	1658	C
44	t	1659	U
44	t	1660	C
44	t	1663	G
44	t	1676	C
44	t	1680	C
44	t	1700	C
44	t	1701	A
44	t	1713	C
44	t	1723	G
44	t	1732	G
44	t	1736	U
44	t	1740	G
44	t	1741	G
44	t	1746	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	1747	A
44	t	1750	C
44	t	1757	A
44	t	1758	A
44	t	1769	A
44	t	1776	A
44	t	1779	G
44	t	1785	G
44	t	1786	A
44	t	1794	C
44	t	1797	G
44	t	1803	G
44	t	1814	G
44	t	1816	G
44	t	1818	A
44	t	1823	G
44	t	1836	G
44	t	1850	G
44	t	1870	U
44	t	1871	G
44	t	1872	A
44	t	1879	C
44	t	1887	U
44	t	1891	G
44	t	1896	C
44	t	1898	A
44	t	1902	C
44	t	1903	G
44	t	1906	G
44	t	1909	C
44	t	1911	U
44	t	1912	C
44	t	1916	C
44	t	1920	A
44	t	1921	G
44	t	1928	U
44	t	1929	G
44	t	1933	G
44	t	1938	U
44	t	1939	A
44	t	1940	U
44	t	1941	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	1942	G
44	t	1943	A
44	t	2007	A
44	t	2025	U
44	t	2027	G
44	t	2029	U
44	t	2036	G
44	t	2037	G
44	t	2043	C
44	t	2050	A
44	t	2051	U
44	t	2065	C
44	t	2069	G
44	t	2072	G
44	t	2073	A
44	t	2074	G
44	t	2075	A
44	t	2076	G
44	t	2078	G
44	t	2079	G
44	t	2081	C
44	t	2082	G
44	t	2084	G
44	t	2087	C
44	t	2090	C
44	t	2091	G
44	t	2092	G
44	t	2229	C
44	t	2232	A
44	t	2233	G
44	t	2234	C
44	t	2235	C
44	t	2241	G
44	t	2242	A
44	t	2246	U
44	t	2247	A
44	t	2249	G
44	t	2268	C
44	t	2269	C
44	t	2278	G
44	t	2279	A
44	t	2280	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	2282	C
44	t	2284	U
44	t	2285	G
44	t	2292	A
44	t	2301	G
44	t	2310	G
44	t	2311	A
44	t	2326	A
44	t	2327	G
44	t	2330	C
44	t	2340	G
44	t	2343	G
44	t	2358	A
44	t	2374	A
44	t	2375	A
44	t	2377	U
44	t	2381	G
44	t	2387	U
44	t	2388	U
44	t	2396	A
44	t	2400	G
44	t	2401	C
44	t	2404	U
44	t	2416	C
44	t	2421	G
44	t	2426	U
44	t	2429	G
44	t	2431	G
44	t	2442	G
44	t	2446	U
44	t	2447	U
44	t	2449	C
44	t	2453	G
44	t	2457	C
44	t	2458	G
44	t	2467	C
44	t	2468	C
44	t	2469	U
44	t	2472	G
44	t	2473	U
44	t	2474	U
44	t	2475	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	2482	G
44	t	2483	C
44	t	2484	C
44	t	2485	G
44	t	2492	A
44	t	2499	C
44	t	2516	A
44	t	2523	G
44	t	2524	U
44	t	2525	G
44	t	2526	G
44	t	2532	A
44	t	2533	U
44	t	2545	G
44	t	2565	G
44	t	2566	A
44	t	2568	C
44	t	2570	A
44	t	2580	A
44	t	2585	G
44	t	2595	C
44	t	2597	G
44	t	2606	C
44	t	2617	G
44	t	2618	U
44	t	2632	C
44	t	2645	U
44	t	2648	C
44	t	2652	G
44	t	2665	G
44	t	2666	U
44	t	2673	G
44	t	2675	A
44	t	2686	U
44	t	2689	C
44	t	2690	G
44	t	2691	G
44	t	2700	G
44	t	2705	G
44	t	2714	G
44	t	2719	U
44	t	2722	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	2723	A
44	t	2732	G
44	t	2733	G
44	t	2739	G
44	t	2741	G
44	t	2742	U
44	t	2745	A
44	t	2746	U
44	t	2748	U
44	t	2751	C
44	t	2766	A
44	t	2767	U
44	t	2769	U
44	t	2776	C
44	t	2778	G
44	t	2785	A
44	t	2798	U
44	t	2805	U
44	t	2806	G
44	t	2814	A
44	t	2817	G
44	t	2834	G
44	t	2835	C
44	t	2846	C
44	t	2860	A
44	t	2870	U
44	t	2871	C
44	t	2876	G
44	t	2880	G
44	t	3570	A
44	t	3571	G
44	t	3572	C
44	t	3574	G
44	t	3577	U
44	t	3587	U
44	t	3589	C
44	t	3591	G
44	t	3596	G
44	t	3597	G
44	t	3601	A
44	t	3606	A
44	t	3612	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	3615	U
44	t	3616	U
44	t	3617	A
44	t	3619	A
44	t	3633	A
44	t	3635	G
44	t	3643	G
44	t	3644	C
44	t	3651	U
44	t	3662	G
44	t	3663	A
44	t	3667	C
44	t	3670	C
44	t	3675	U
44	t	3683	A
44	t	3700	U
44	t	3707	A
44	t	3719	A
44	t	3728	G
44	t	3730	A
44	t	3731	A
44	t	3741	U
44	t	3745	A
44	t	3747	G
44	t	3748	G
44	t	3751	G
44	t	3754	A
44	t	3755	A
44	t	3759	C
44	t	3781	C
44	t	3782	G
44	t	3783	C
44	t	3784	A
44	t	3785	U
44	t	3788	A
44	t	3789	U
44	t	3790	G
44	t	3795	A
44	t	3798	G
44	t	3799	A
44	t	3809	U
44	t	3811	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	3838	A
44	t	3848	A
44	t	3849	C
44	t	3850	G
44	t	3851	G
44	t	3852	G
44	t	3861	A
44	t	3863	U
44	t	3866	G
44	t	3868	G
44	t	3872	A
44	t	3876	A
44	t	3877	A
44	t	3878	G
44	t	3879	A
44	t	3886	U
44	t	3887	G
44	t	3890	C
44	t	3897	C
44	t	3909	G
44	t	3918	A
44	t	4046	G
44	t	4049	C
44	t	4054	G
44	t	4061	G
44	t	4062	G
44	t	4063	G
44	t	4064	G
44	t	4065	G
44	t	4066	C
44	t	4067	G
44	t	4068	A
44	t	4069	G
44	t	4070	C
44	t	4071	C
44	t	4072	C
44	t	4075	G
44	t	4076	G
44	t	4077	G
44	t	4078	G
44	t	4079	C
44	t	4080	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	4081	C
44	t	4082	U
44	t	4083	C
44	t	4084	G
44	t	4085	C
44	t	4086	U
44	t	4088	C
44	t	4097	A
44	t	4105	C
44	t	4107	C
44	t	4108	G
44	t	4109	G
44	t	4110	C
44	t	4124	C
44	t	4125	U
44	t	4126	C
44	t	4130	G
44	t	4132	A
44	t	4145	G
44	t	4146	G
44	t	4153	G
44	t	4158	G
44	t	4165	A
44	t	4167	A
44	t	4168	C
44	t	4174	A
44	t	4176	A
44	t	4187	G
44	t	4190	G
44	t	4191	U
44	t	4195	A
44	t	4205	C
44	t	4213	A
44	t	4215	A
44	t	4216	G
44	t	4220	C
44	t	4228	G
44	t	4229	G
44	t	4230	A
44	t	4242	A
44	t	4243	A
44	t	4253	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	4266	A
44	t	4267	G
44	t	4268	U
44	t	4276	C
44	t	4288	G
44	t	4291	G
44	t	4292	G
44	t	4294	C
44	t	4299	C
44	t	4300	G
44	t	4301	A
44	t	4311	C
44	t	4316	U
44	t	4320	U
44	t	4326	G
44	t	4327	C
44	t	4333	G
44	t	4334	U
44	t	4335	G
44	t	4338	A
44	t	4339	G
44	t	4340	A
44	t	4341	A
44	t	4343	A
44	t	4349	C
44	t	4353	G
44	t	4356	A
44	t	4358	A
44	t	4360	C
44	t	4367	G
44	t	4372	G
44	t	4373	G
44	t	4384	A
44	t	4388	C
44	t	4402	G
44	t	4414	U
44	t	4426	A
44	t	4437	G
44	t	4455	U
44	t	4459	U
44	t	4465	A
44	t	4474	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	4475	A
44	t	4477	G
44	t	4480	A
44	t	4481	C
44	t	4485	A
44	t	4486	G
44	t	4490	G
44	t	4510	A
44	t	4517	U
44	t	4518	U
44	t	4522	C
44	t	4529	G
44	t	4532	G
44	t	4537	G
44	t	4551	A
44	t	4552	A
44	t	4559	U
44	t	4561	A
44	t	4562	G
44	t	4578	A
44	t	4579	G
44	t	4586	A
44	t	4593	G
44	t	4595	G
44	t	4598	U
44	t	4599	G
44	t	4601	G
44	t	4611	G
44	t	4618	A
44	t	4619	U
44	t	4626	A
44	t	4632	C
44	t	4634	A
44	t	4649	A
44	t	4656	G
44	t	4657	C
44	t	4662	A
44	t	4671	U
44	t	4681	G
44	t	4684	G
44	t	4692	C
44	t	4693	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	4694	G
44	t	4695	C
44	t	4696	A
44	t	4699	G
44	t	4703	C
44	t	4704	G
44	t	4712	G
44	t	4715	U
44	t	4716	G
44	t	4718	C
44	t	4720	U
44	t	4722	G
44	t	4726	A
44	t	4727	G
44	t	4732	U
44	t	4735	C
44	t	4736	C
44	t	4737	G
44	t	4816	C
44	t	4817	G
44	t	4818	G
44	t	4819	G
44	t	4820	G
44	t	4822	U
44	t	4824	C
44	t	4827	U
44	t	4828	G
44	t	4831	G
44	t	4832	A
44	t	4833	G
44	t	4834	U
44	t	4838	C
44	t	4839	U
44	t	4840	U
44	t	4841	C
44	t	4852	A
44	t	4853	C
44	t	4883	U
44	t	4885	G
44	t	4886	C
44	t	4894	G
44	t	4895	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	t	4896	A
44	t	4898	C
44	t	4901	A
44	t	4902	C
44	t	4907	G
44	t	4908	U
44	t	4909	G
44	t	4917	U
44	t	4924	A
44	t	4933	G
44	t	4934	U
44	t	4937	A
44	t	4943	U
44	t	4946	U
44	t	4947	U
44	t	4949	U
44	t	4950	G
44	t	4957	G
44	t	4971	C
44	t	4972	A
44	t	4975	G
44	t	4982	C
44	t	4984	U
44	t	4985	C
44	t	4986	G
44	t	4998	U
44	t	4999	G
44	t	5005	C
44	t	5007	G
44	t	5008	C
44	t	5011	U
44	t	5012	C
44	t	5015	C
44	t	5016	A
44	t	5020	G
44	t	5024	U
45	u	4	C
45	u	8	U
45	u	15	G
45	u	17	C
45	u	18	G
45	u	19	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	u	20	U
45	u	21	A
45	u	23	A
45	u	24	G
45	u	44	G
45	u	46	G
45	u	47	U
45	u	48	C
45	u	50	U
45	u	52	G
45	u	55	U
45	u	56	C
45	u	57	G
45	u	59	U
45	u	60	U
45	u	61	C
45	u	64	A
45	u	69	G
45	u	71	G
45	u	72	C
45	u	73	A
45	u	74	C
45	u	76	A
46	v	8	U
46	v	11	C
46	v	12	C
46	v	13	C
46	v	15	G
46	v	16	A
46	v	17	A
46	v	18	G
46	v	19	G
46	v	20	U
46	v	21	A
46	v	22	G
46	v	23	A
46	v	30	G
46	v	44	G
46	v	47	U
46	v	48	C
46	v	49	C
46	v	51	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	v	54	U
46	v	55	U
46	v	56	C
46	v	58	A
46	v	61	C
46	v	62	C
46	v	68	C
46	v	69	G
46	v	71	G
46	v	72	C
46	v	73	A
46	v	75	C
46	v	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	70	G
4	D	72	A
4	D	73	U
4	D	75	G
4	D	76	C
4	D	77	A
4	D	78	G
4	D	79	G
4	D	80	A
4	D	81	C
4	D	82	A
4	D	83	C
4	D	84	A
4	D	85	U
4	D	86	U
4	D	87	G
4	D	123	U
4	D	125	C
4	D	126	C
4	D	129	C

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

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](#)

Of 31 ligands modelled in this entry, 31 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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
44	t	11

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	t	750:G	O3'	890:C	P	20.30
1	t	3919:C	O3'	4035:G	P	19.55
1	t	976:U	O3'	1047:G	P	16.16
1	t	1680:C	O3'	1699:C	P	15.85
1	t	1089:A	O3'	1145:G	P	15.56
1	t	2881:G	O3'	3569:C	P	15.47
1	t	2093:C	O3'	2228:C	P	14.21
1	t	1253:A	O3'	1256:G	P	12.99
1	t	4737:G	O3'	4815:C	P	12.48
1	t	4853:C	O3'	4882:C	P	11.15
1	t	1202:G	O3'	1216:G	P	9.86

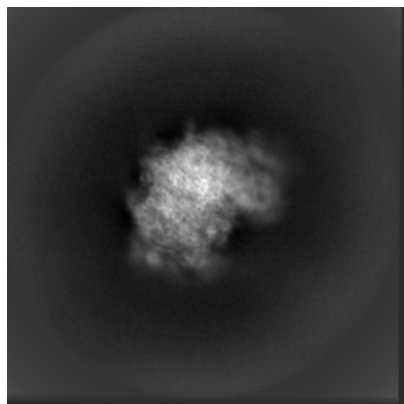
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21435. These allow visual inspection of the internal detail of the map and identification of artifacts.

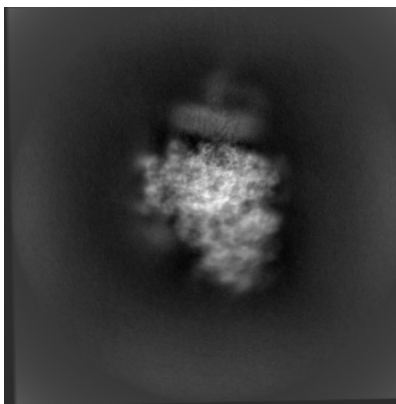
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

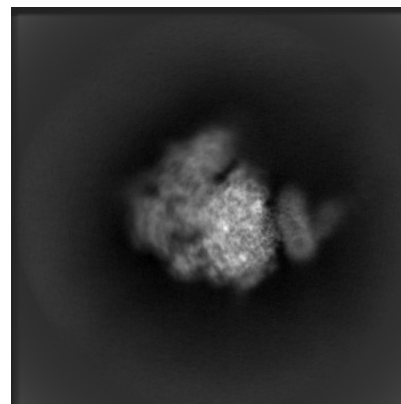
6.1.1 Primary map



X

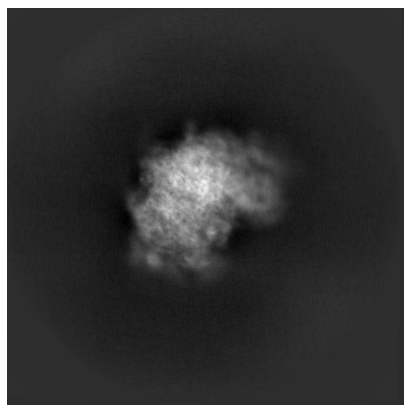


Y

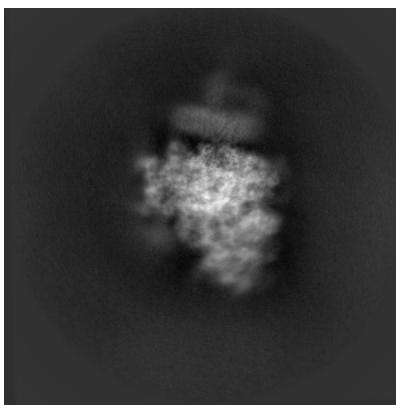


Z

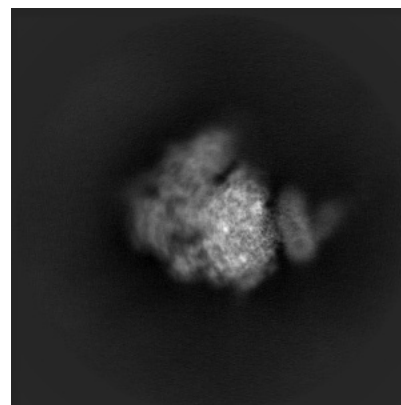
6.1.2 Raw map



X



Y

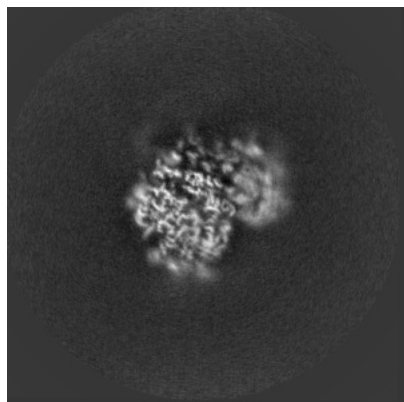


Z

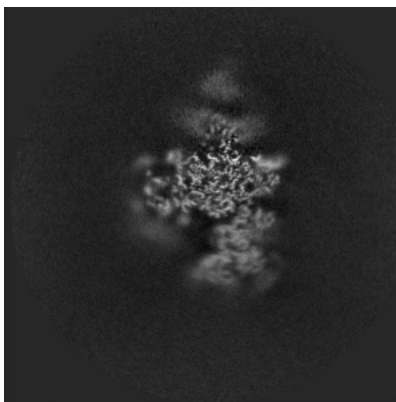
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

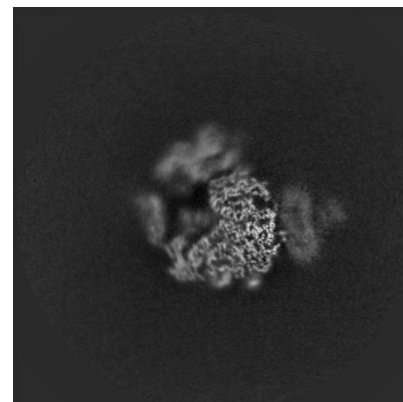
6.2.1 Primary map



X Index: 250

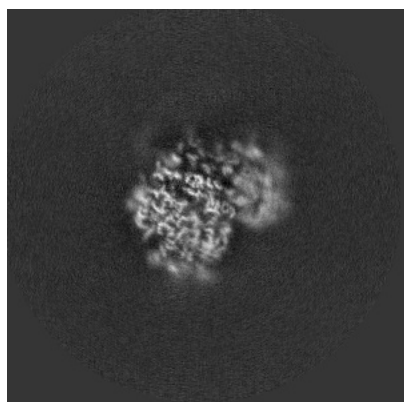


Y Index: 250

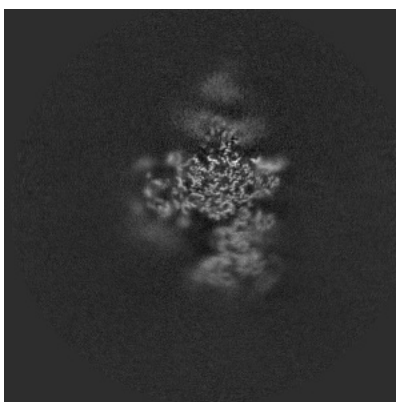


Z Index: 250

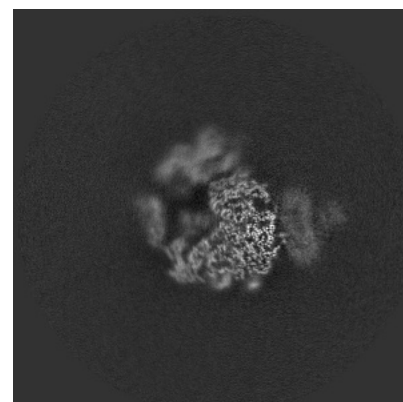
6.2.2 Raw map



X Index: 250



Y Index: 250

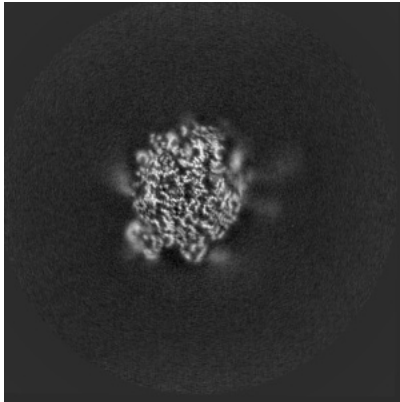


Z Index: 250

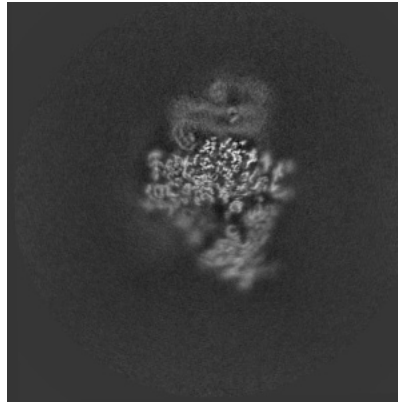
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

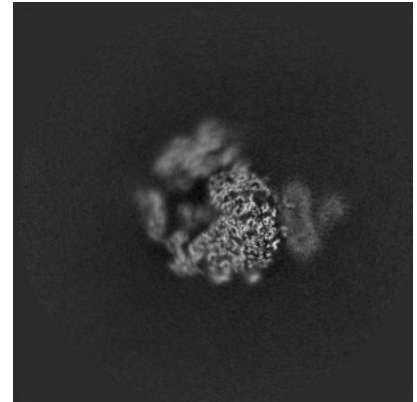
6.3.1 Primary map



X Index: 285

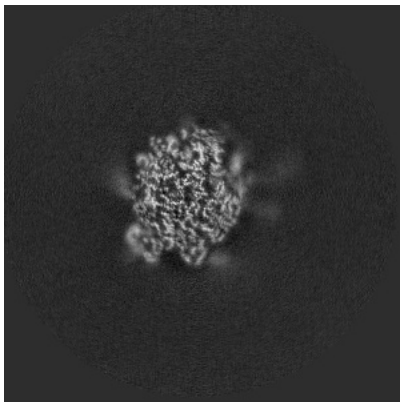


Y Index: 225

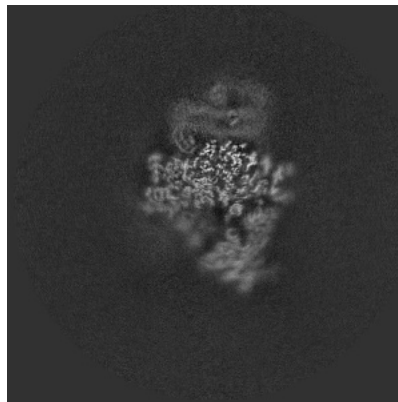


Z Index: 252

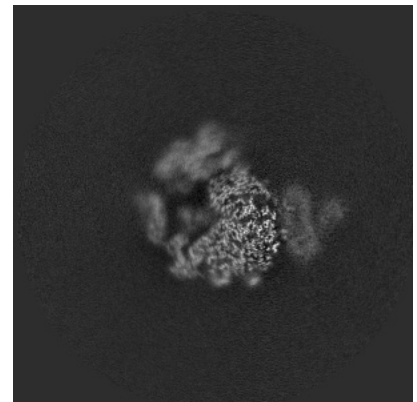
6.3.2 Raw map



X Index: 285



Y Index: 225

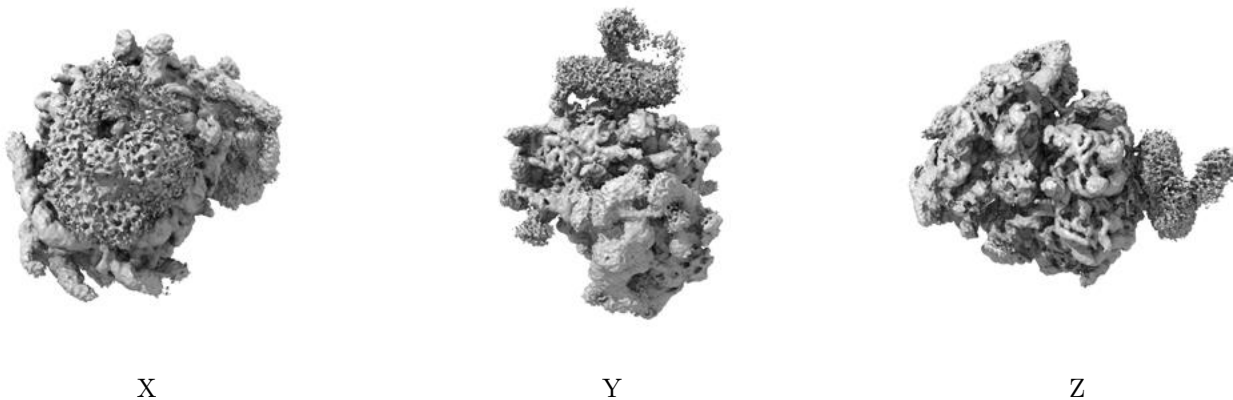


Z Index: 252

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

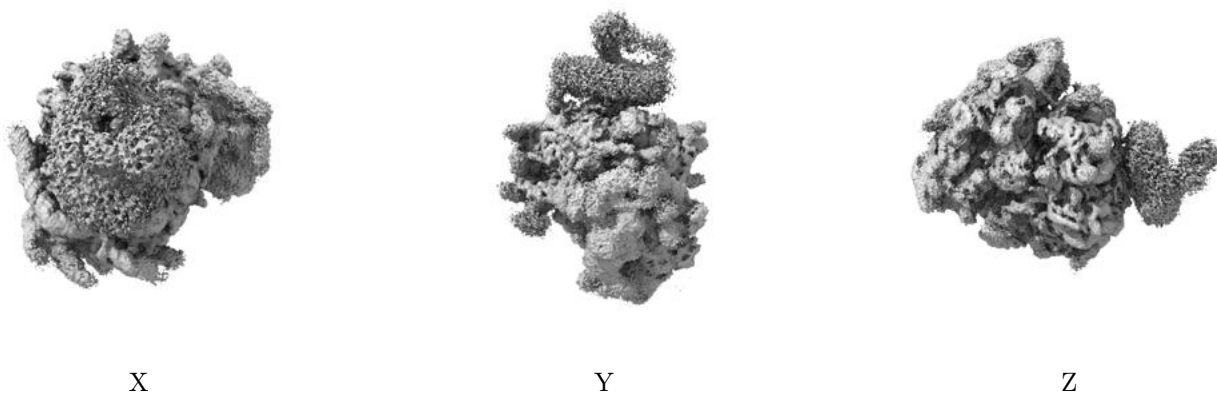
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0073. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

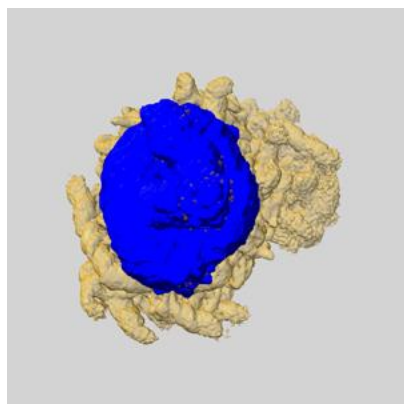
6.5 Mask visualisation [i](#)

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

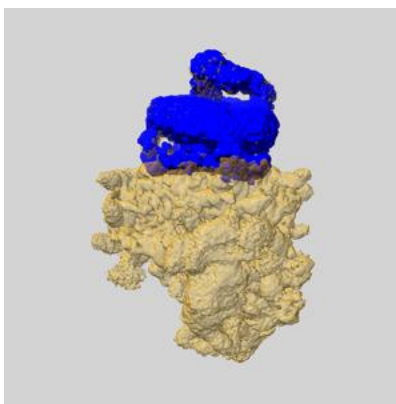
A mask typically either:

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

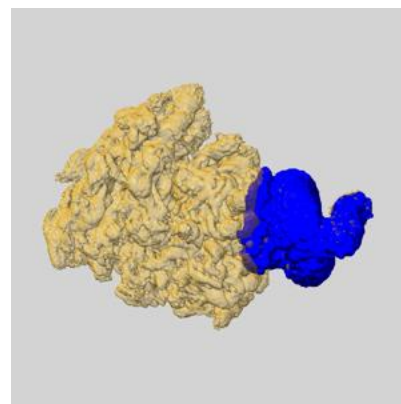
6.5.1 emd_21435_msk_1.map [i](#)



X



Y

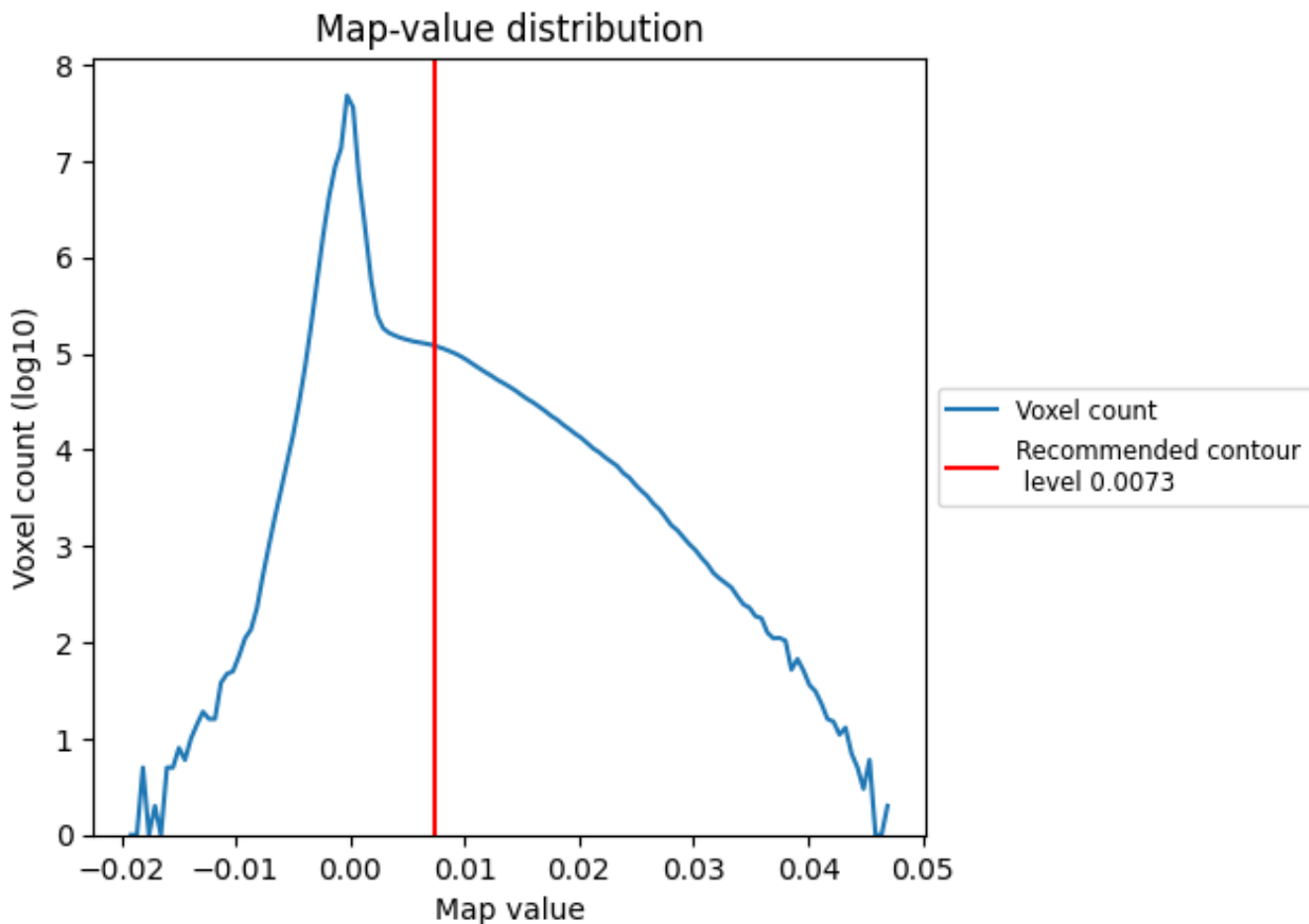


Z

7 Map analysis [i](#)

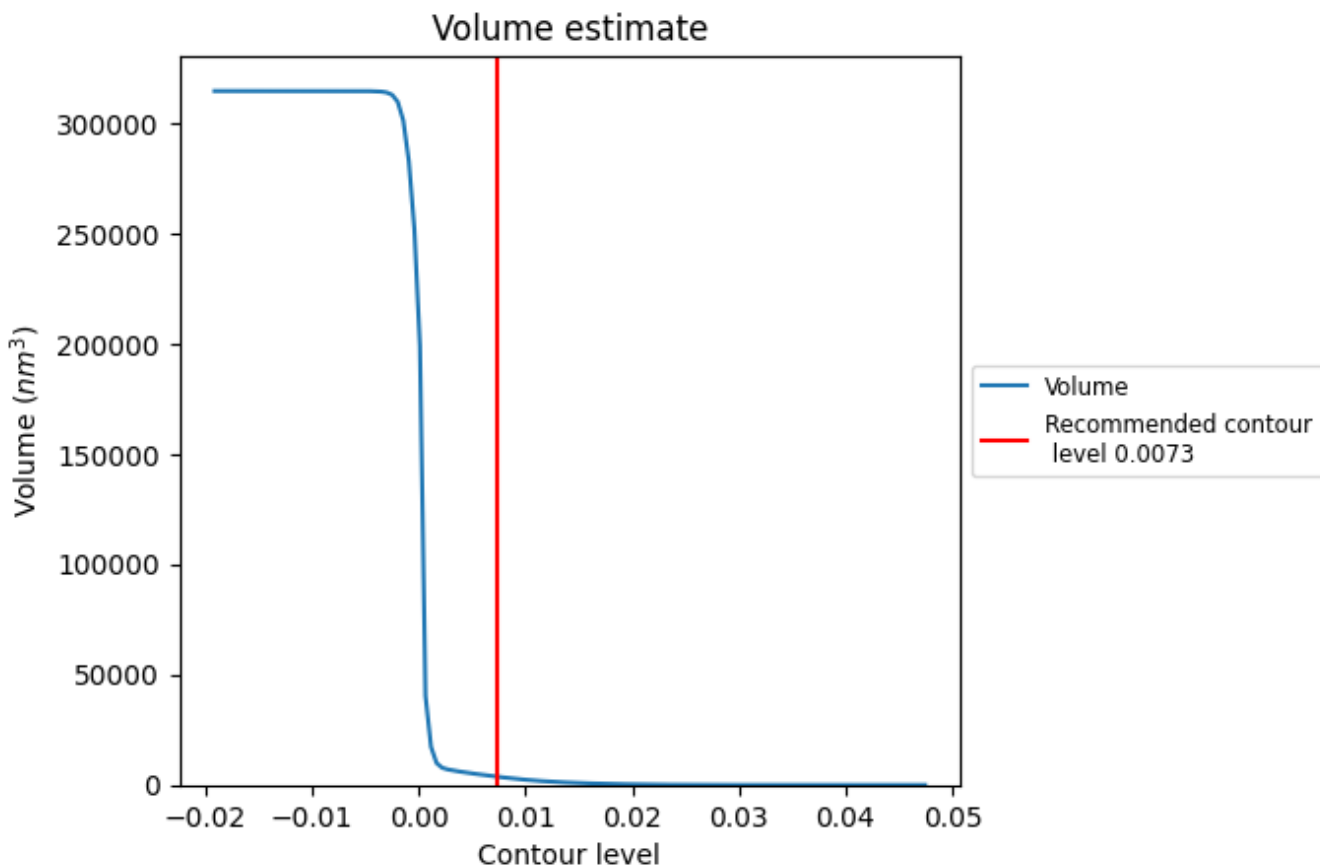
This section contains the results of statistical analysis of the map.

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.

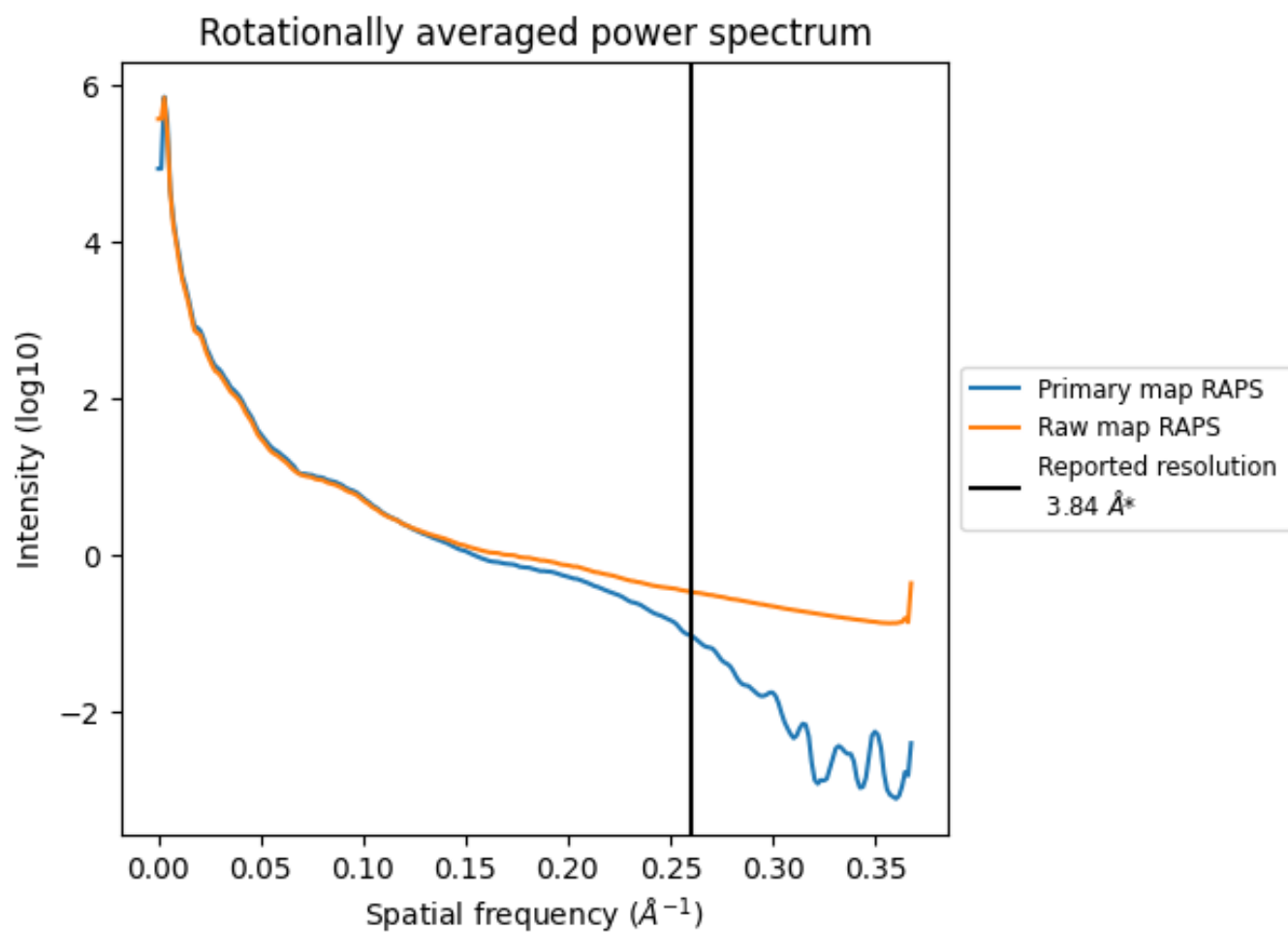
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3776 nm^3 ; this corresponds to an approximate mass of 3411 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 [i](#)

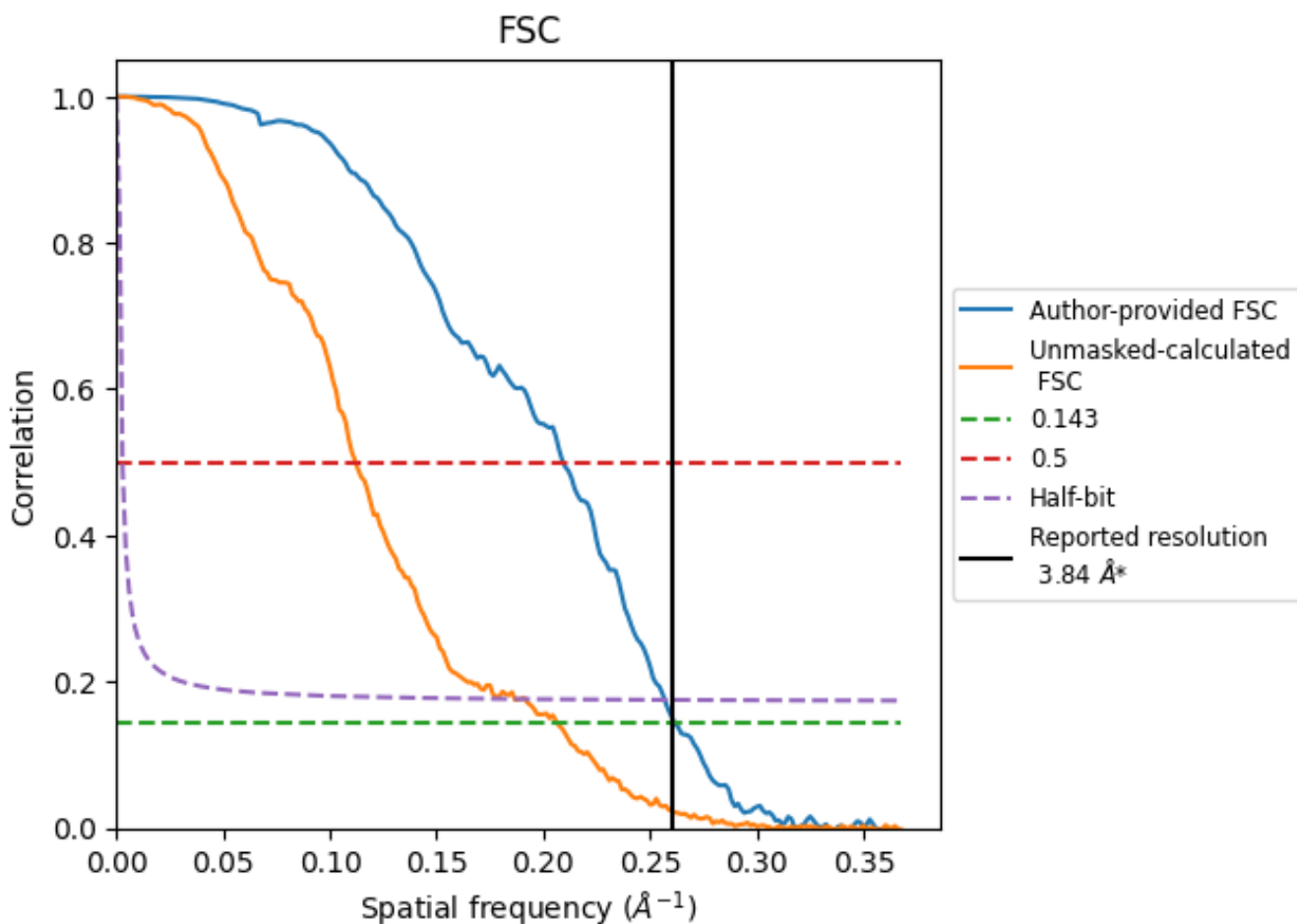


*Reported resolution corresponds to spatial frequency of 0.260 \AA^{-1}

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 0.260 Å⁻¹

8.2 Resolution estimates [i](#)

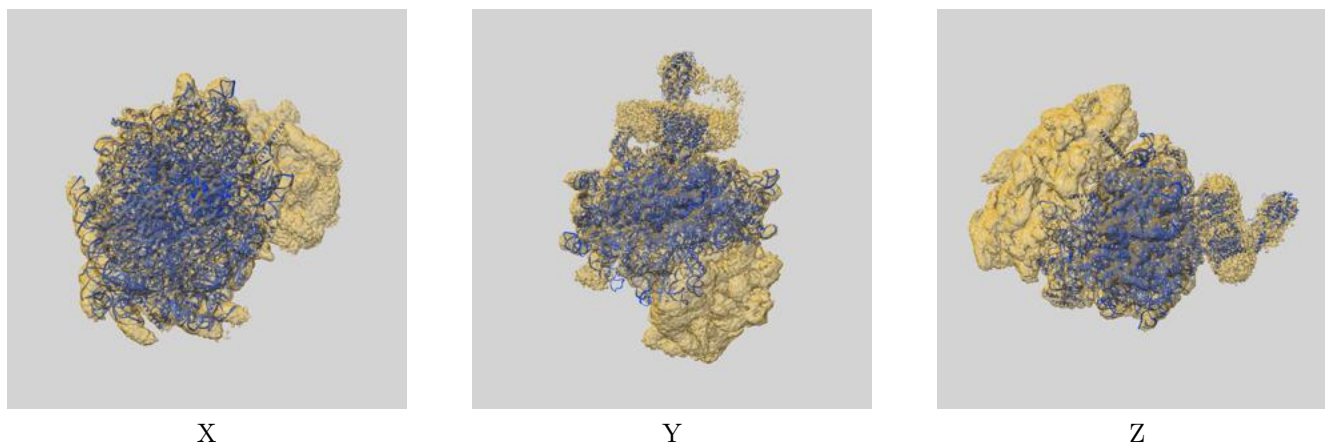
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.82	4.78	3.89
Unmasked-calculated*	4.84	8.93	5.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.84 differs from the reported value 3.84 by more than 10 %

9 Map-model fit [i](#)

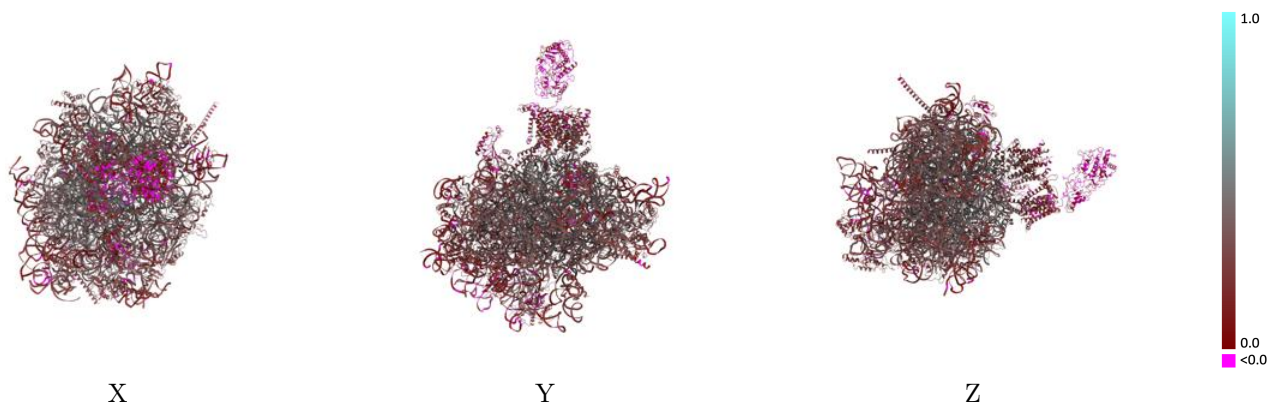
This section contains information regarding the fit between EMDB map EMD-21435 and PDB model 6W6L. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



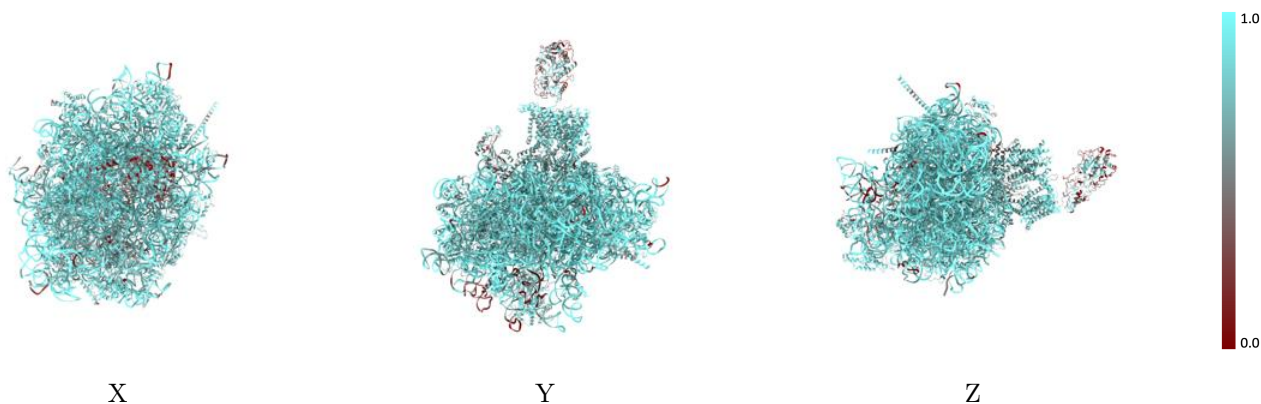
The images above show the 3D surface view of the map at the recommended contour level 0.0073 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



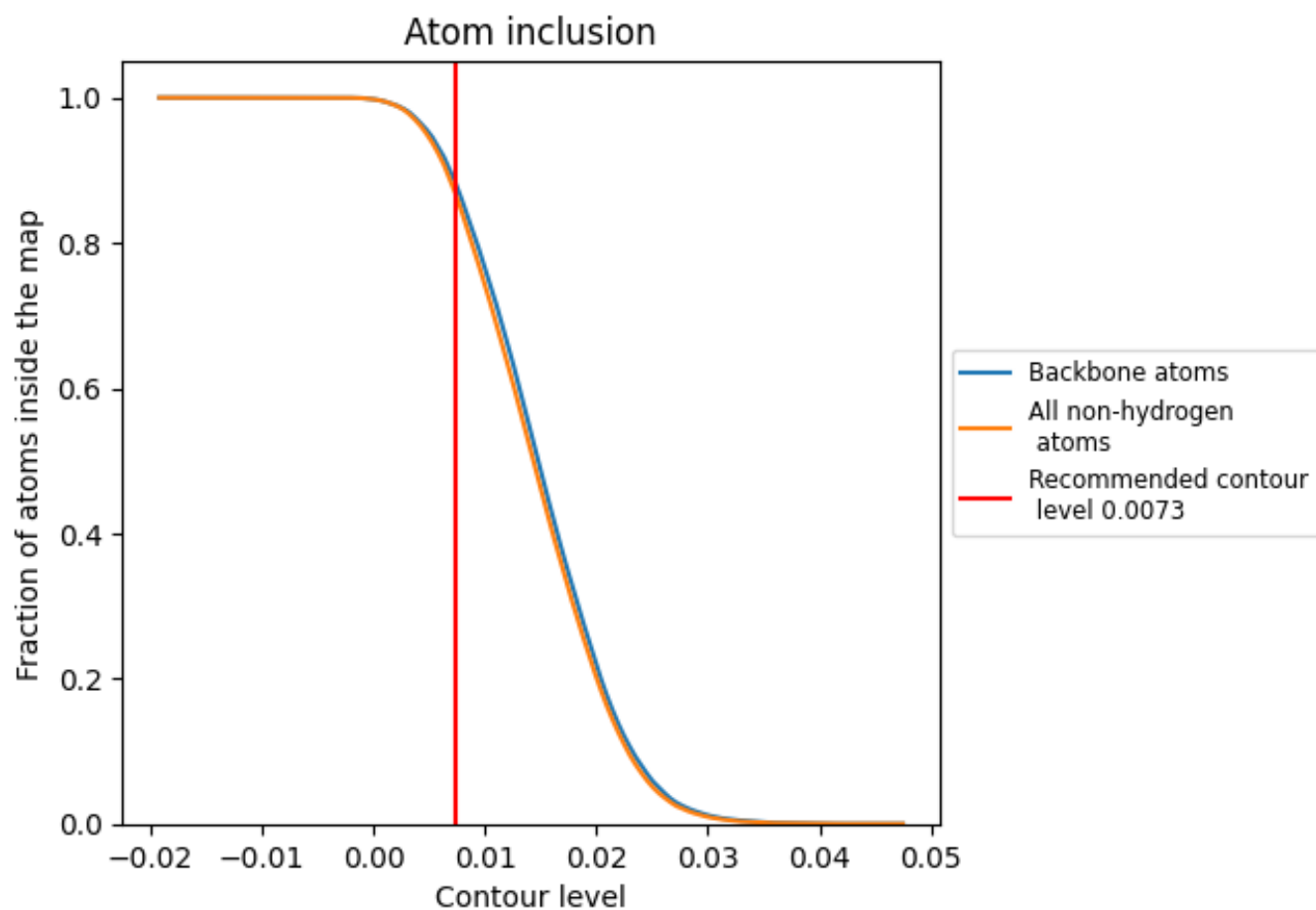
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0073).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.0073) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8714	 0.2910
1	 0.7882	 0.2400
2	 0.7819	 0.2730
3	 0.7556	 0.1440
4	 0.8209	 0.1830
5	 0.4940	 0.0340
6	 0.7636	 0.1550
7	 0.5226	 0.1630
A	 0.8394	 0.3420
B	 0.8623	 0.3090
C	 0.8925	 0.3840
D	 0.9835	 0.3990
E	 0.9937	 0.2630
F	 0.8961	 0.1970
G	 0.8856	 0.2800
H	 0.8218	 0.2760
I	 0.8434	 0.2960
J	 0.8306	 0.2060
K	 0.5281	 0.0810
L	 0.7782	 0.1730
M	 0.8340	 0.3220
N	 0.8818	 0.2330
O	 0.9062	 0.3690
P	 0.8454	 0.2920
Q	 0.8955	 0.4140
R	 0.8867	 0.3530
S	 0.8455	 0.3000
T	 0.8754	 0.2450
U	 0.8423	 0.2700
V	 0.7177	 0.1210
W	 0.7899	 0.3020
X	 0.8333	 0.2910
Y	 0.8679	 0.4090
Z	 0.8634	 0.4170
a	 0.8840	 0.2930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9230	 0.3400
c	 0.8232	 0.2050
d	 0.8710	 0.2620
e	 0.9021	 0.3670
f	 0.8606	 0.4040
g	 0.8634	 0.3580
h	 0.8637	 0.3570
i	 0.8318	 0.3590
j	 0.8609	 0.2760
k	 0.9225	 0.4330
l	 0.8366	 0.3220
m	 0.8913	 0.4240
o	 0.6636	 0.1890
p	 0.7959	 0.2550
q	 0.7997	 0.3020
r	 0.9107	 0.3860
t	 0.9506	 0.3110
u	 0.3949	 0.1160
v	 0.8300	 0.2100
y	 0.7259	 0.3850