



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 05:43 PM EST

PDB ID : 3JAP
EMDB ID : EMD-3048
Title : Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-18
Resolution : 4.90 Å (reported)
Based on initial models : 3CW2, 2D74, 4U1E, 3J81, 4U1C, 4U1D

This is a wwPDB EM Validation Summary 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.31.3

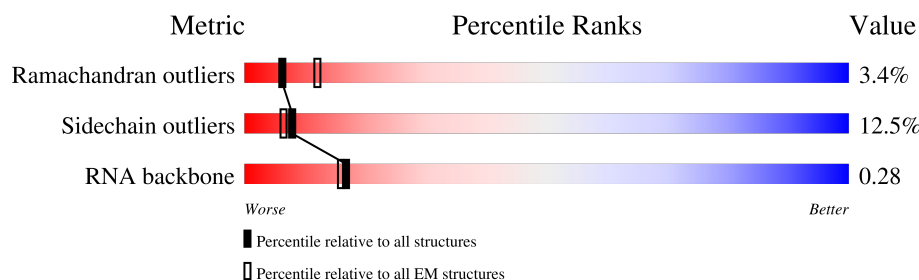
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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	1	75	
2	2	1781	
3	3	25	
4	A	254	
5	B	255	
6	C	259	
7	D	237	
8	E	261	

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Mol	Chain	Length	Quality of chain
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	

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Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	108	
43	o	588	
44	p	652	
45	q	347	
46	r	31	
47	s	52	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 98333 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Met-tRNAi (U31:A39 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1607	716	296	520	75		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	14	Total	C	N	O	P	0	0
			287	129	42	102	14		

- Molecule 4 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 7 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 8 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 11 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	184	Total	C	N	O	S	0	0
			1483	950	270	263			

- Molecule 12 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			885	553	161	171			

- Molecule 17 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 18 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	117	Total	C	N	O	S	0	0
			927	595	166	161	5		

- Molecule 20 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	141	Total	C	N	O	S	0	0
			1105	709	204	192			

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	120	Total	C	N	O	S	0	0
			959	598	178	180	3		

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 23 is a protein called eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 24 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total	C	N	O		
			1061	665	207	189	0	0

- Molecule 29 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	70	Total	C	N	O	S		
			558	355	104	98	1	0	0

- Molecule 30 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S		
			779	480	165	129	5	0	0

- Molecule 31 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S		
			609	379	112	113	5	0	0

- Molecule 32 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	62	Total	C	N	O	S		
			487	301	97	88	1	0	0

- Molecule 33 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S		
			446	280	89	76	1	0	0

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S		
			433	271	88	73	1	0	0

- Molecule 35 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			546	351	101	90	4		

- Molecule 36 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 37 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	111	Total	C	N	O	S	0	0
			884	542	170	167	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	90	Total	C	N	O	S	0	0
			716	452	132	128	4		

- Molecule 43 is a protein called eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	550	Total	C	N	O	S	0	0
			4189	2667	721	794	7		

- Molecule 44 is a protein called eIF3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	634	Total	C	N	O	S	0	0
			4899	3121	826	940	12		

- Molecule 45 is a protein called eIF3i.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	342	Total	C	N	O	S	0	0
			2693	1711	443	530	9		

- Molecule 46 is a protein called eIF3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	31	Total	C	N	O	S	0	0
			277	177	48	50	2		

- Molecule 47 is a protein called eIF3g.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	s	52	Total	C	N	O	0	0
			418	257	82	79		

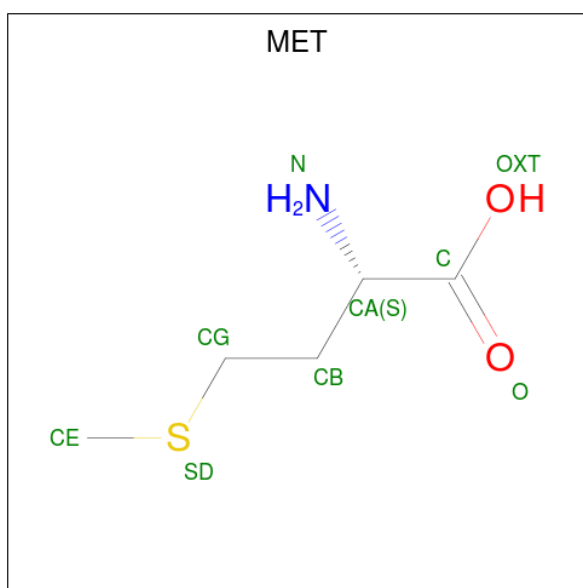
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	80	Total	Mg	0
			80	80	
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

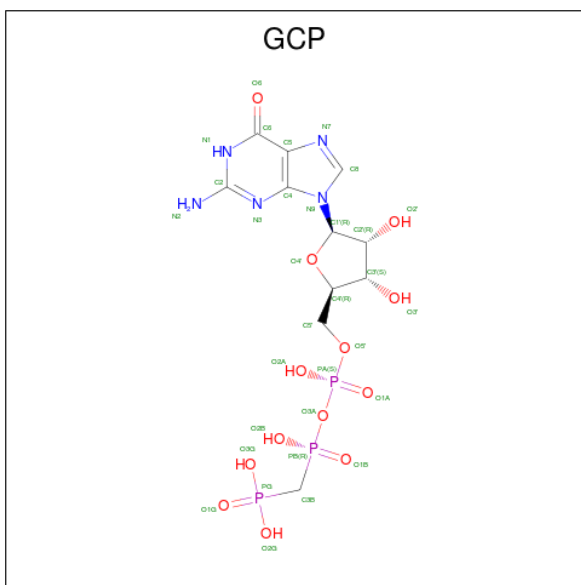
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

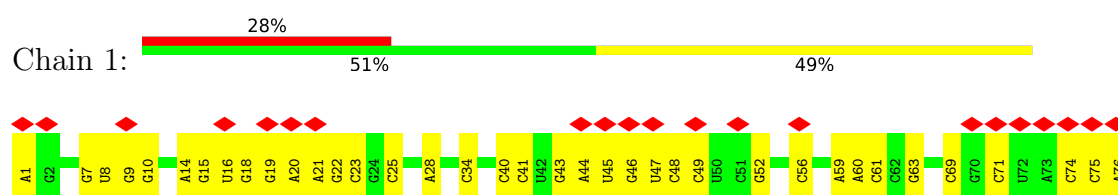


Mol	Chain	Residues	Atoms					AltConf
51	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

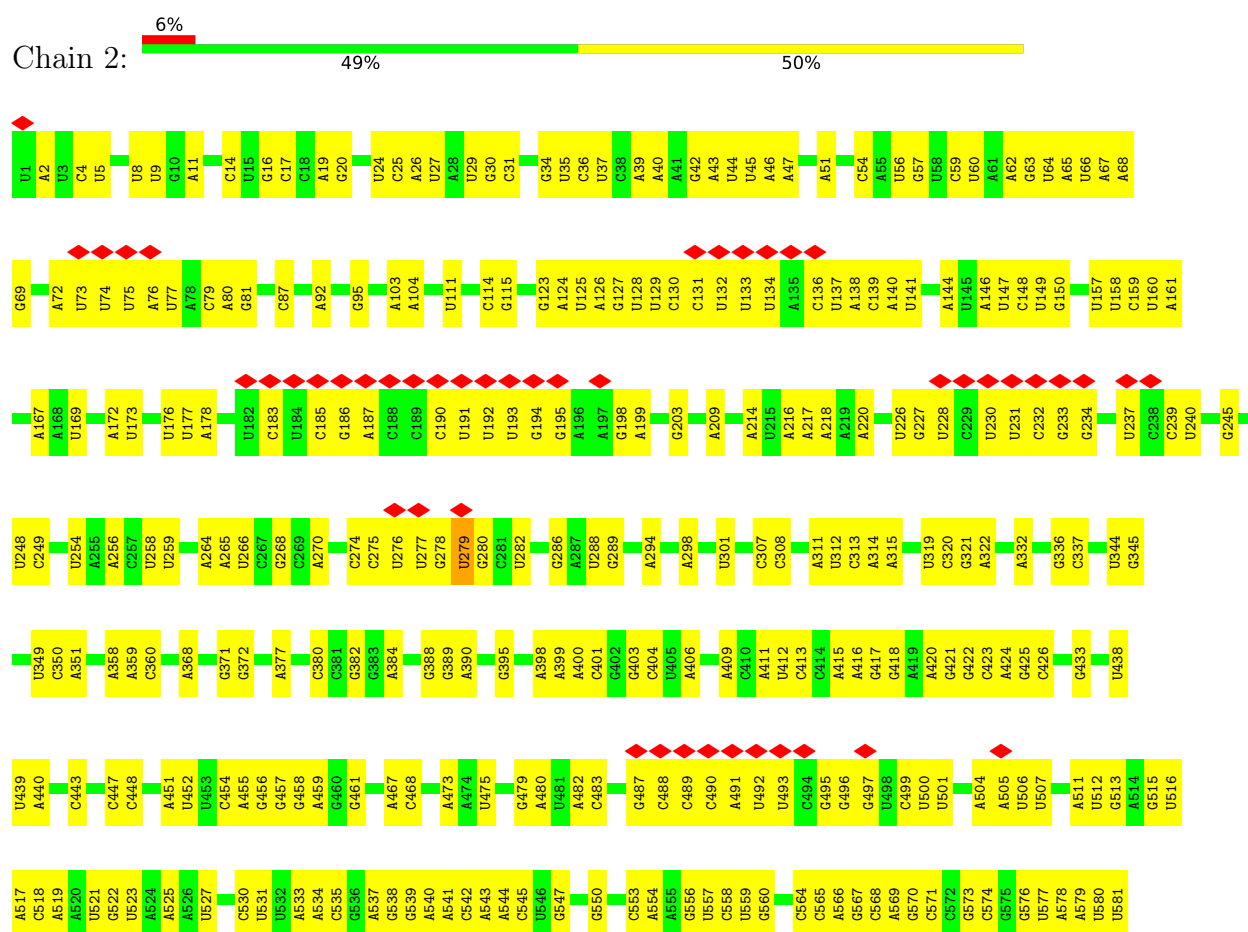
3 Residue-property plots

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: Met-tRNAi (U31:A39 variant)



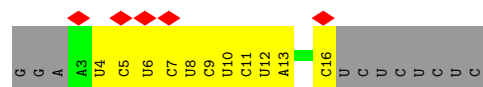
• Molecule 2: 18S rRNA



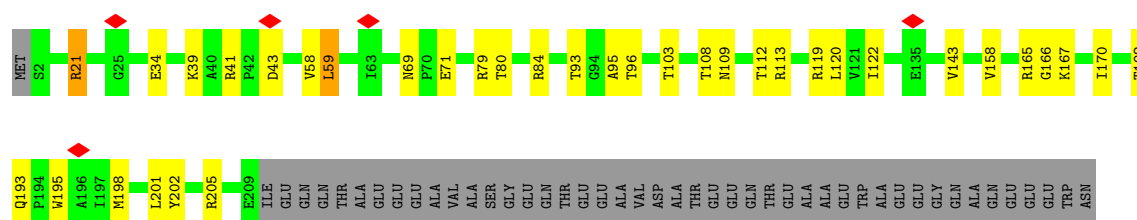


C1794
A1795
U1796
U1797
A1798

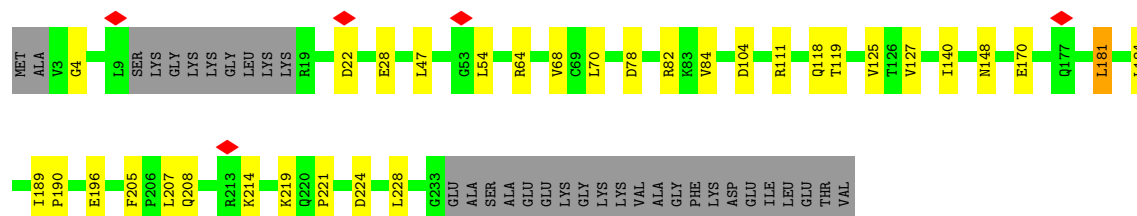
• Molecule 3: mRNA



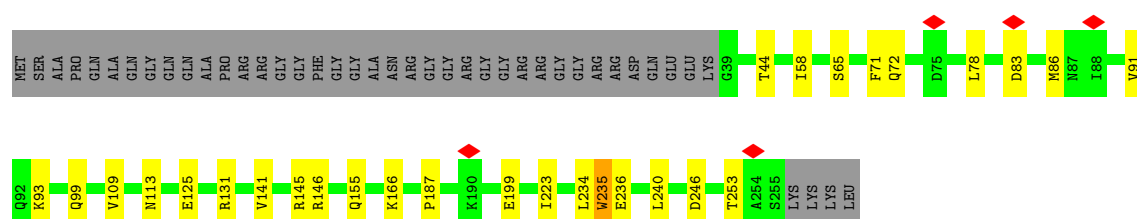
• Molecule 4: uS2



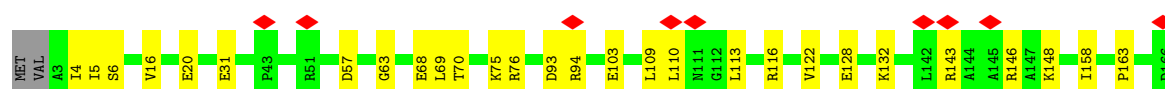
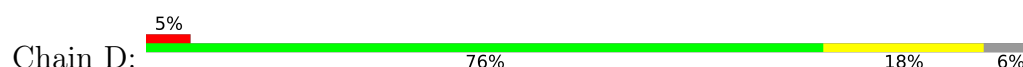
• Molecule 5: eS1



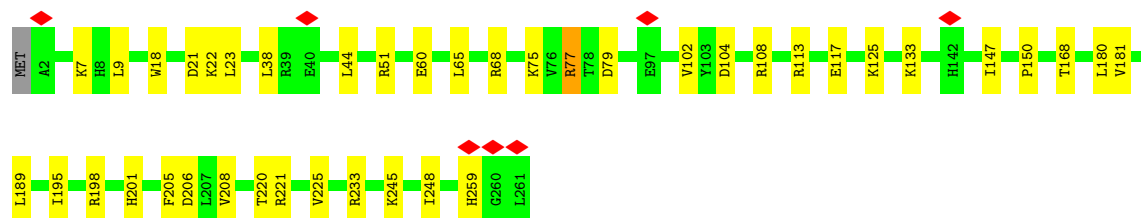
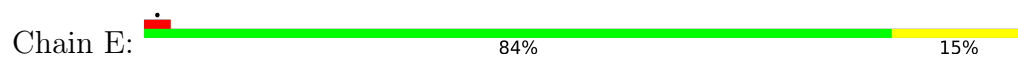
• Molecule 6: uS5



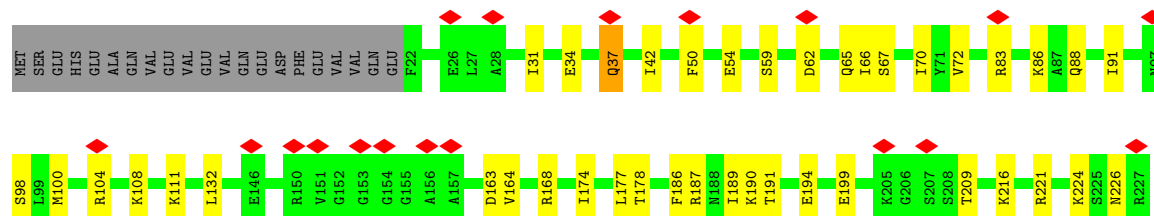
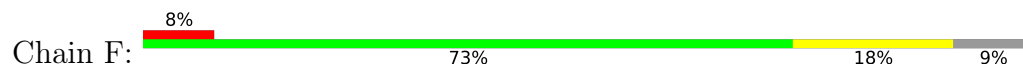
• Molecule 7: uS3



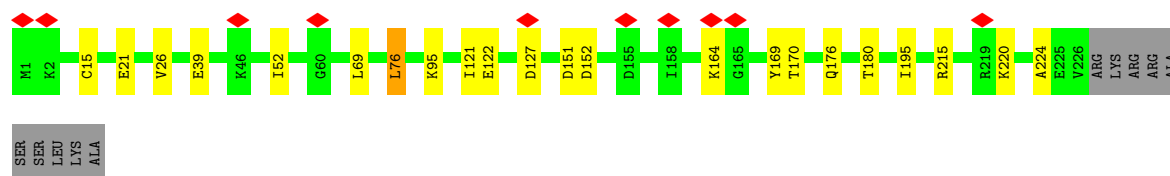
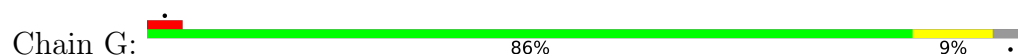
- Molecule 8: eS4



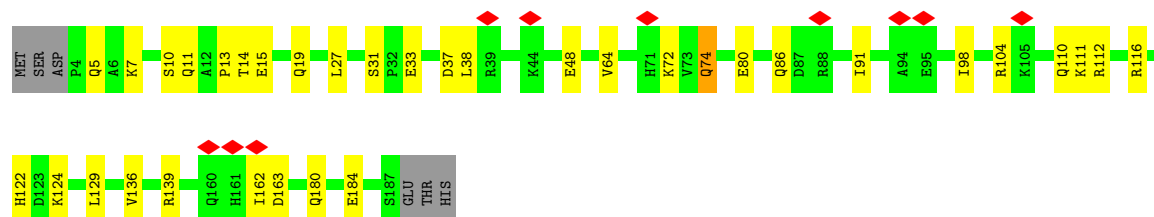
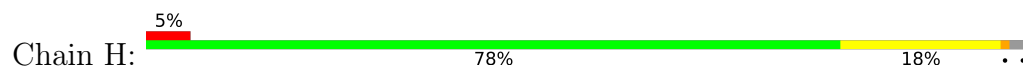
- Molecule 9: uS7



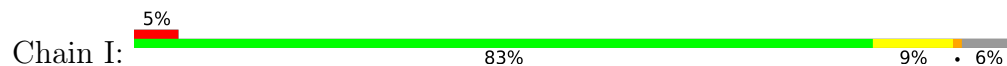
- Molecule 10: eS6

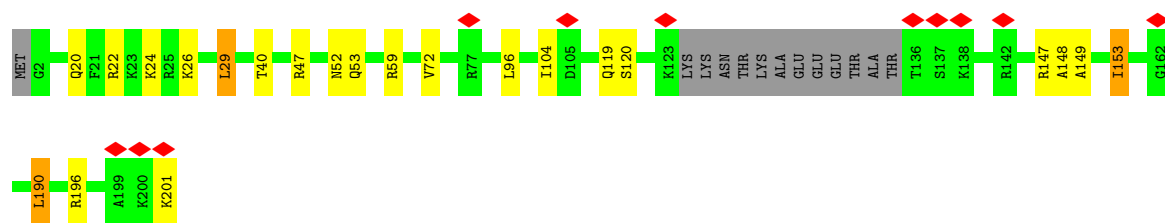


- Molecule 11: eS7

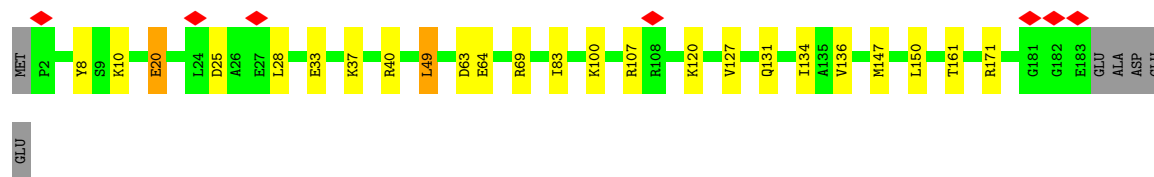
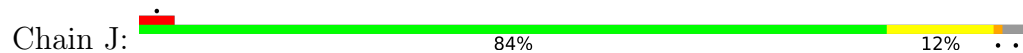


- Molecule 12: eS8

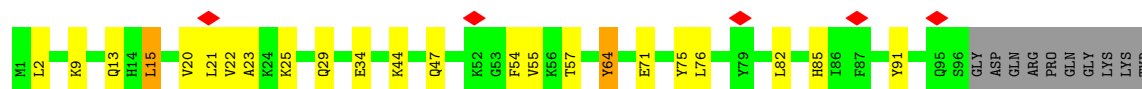




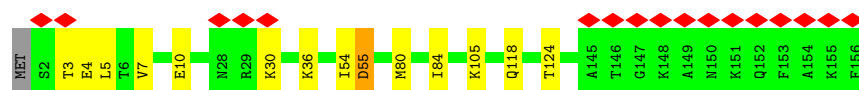
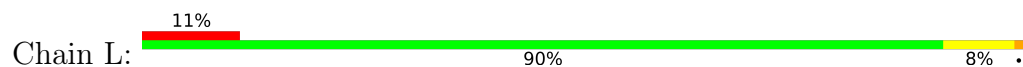
• Molecule 13: uS4



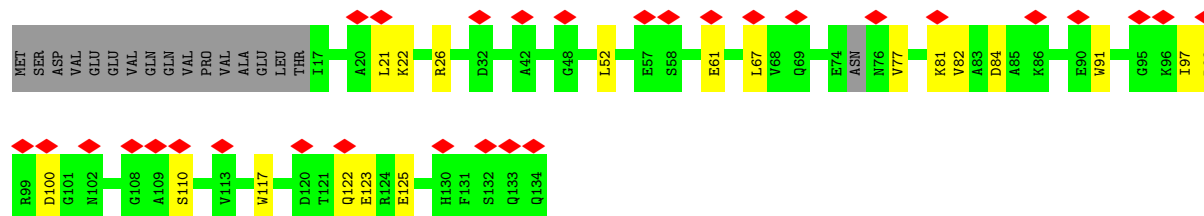
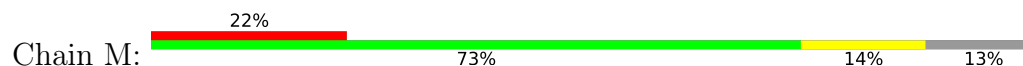
• Molecule 14: eS10



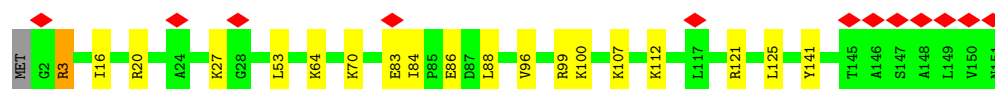
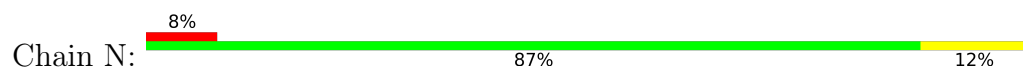
• Molecule 15: uS17




• Molecule 16: eS12



• Molecule 17: uS15



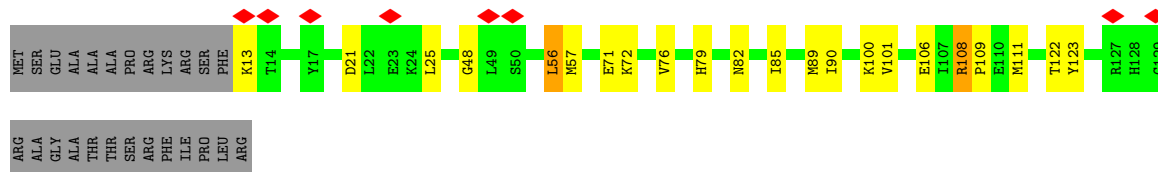
- Molecule 18: uS11

Chain O:  82% 9% 7%




- Molecule 19: uS19

Chain P:  6% 67% 14% 18%




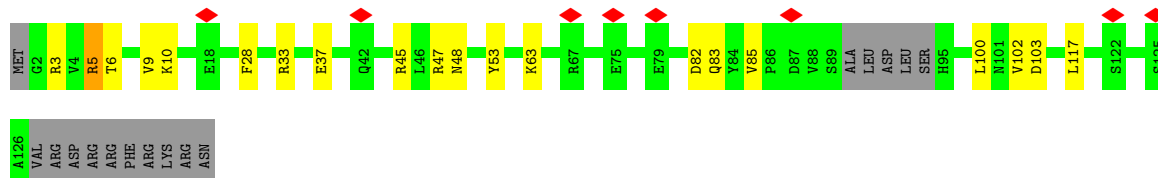
- Molecule 20: uS9

Chain Q:  79% 19% ..




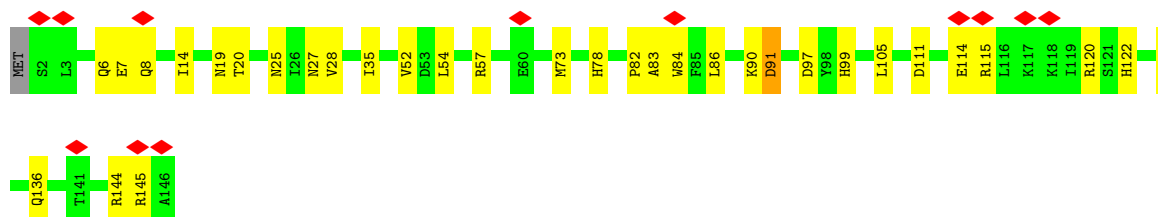
- Molecule 21: eS17

Chain R:  6% 74% 14% 12%




- Molecule 22: uS13

Chain S:  8% 77% 22% ..

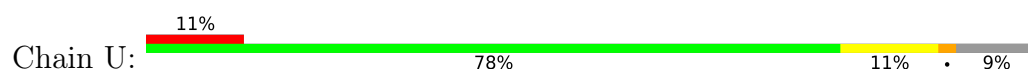


- Molecule 23: eS19

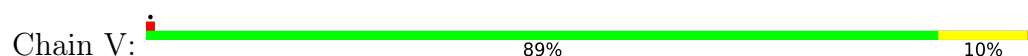
Chain T:  5% 85% 14%



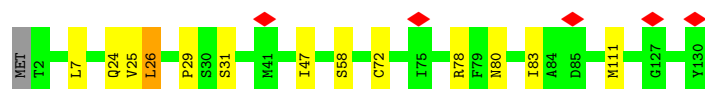
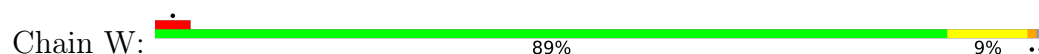
• Molecule 24: uS10



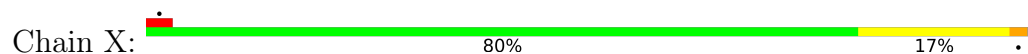
• Molecule 25: eS21



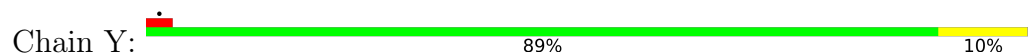
• Molecule 26: uS8



• Molecule 27: uS12



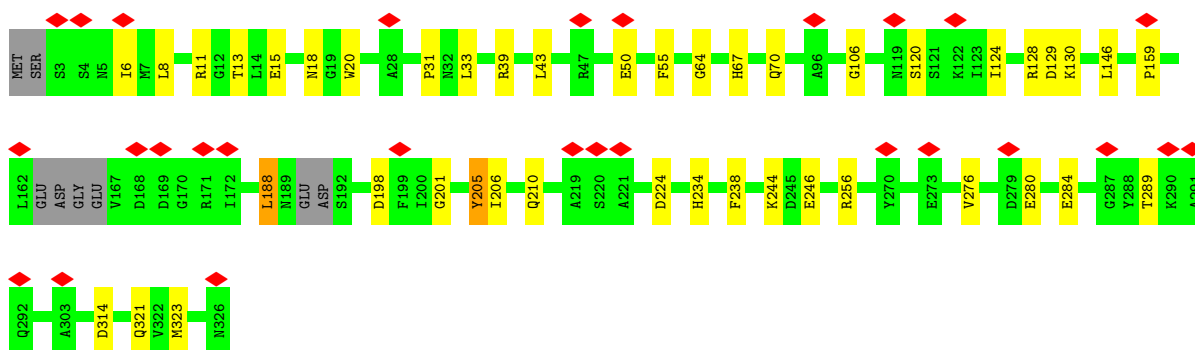
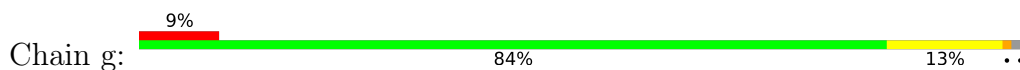
• Molecule 28: eS24



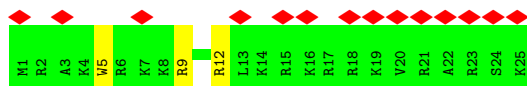
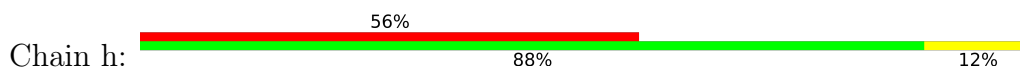
• Molecule 29: eS25



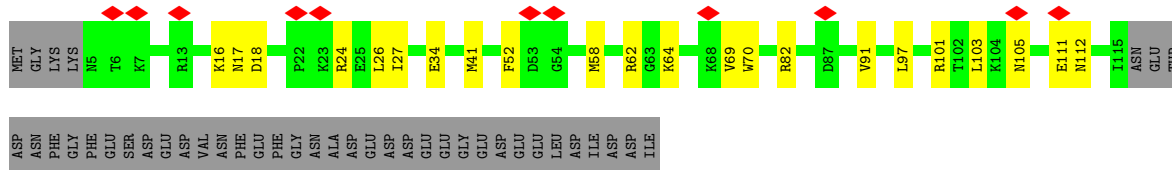
- Molecule 36: RACK1



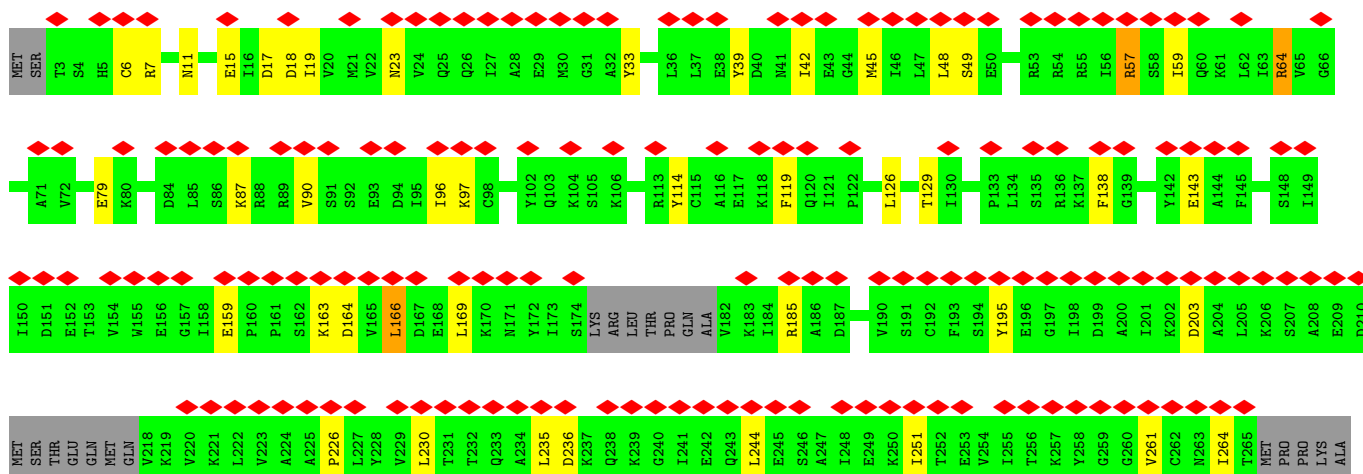
- Molecule 37: eL41



- Molecule 38: eIF1A

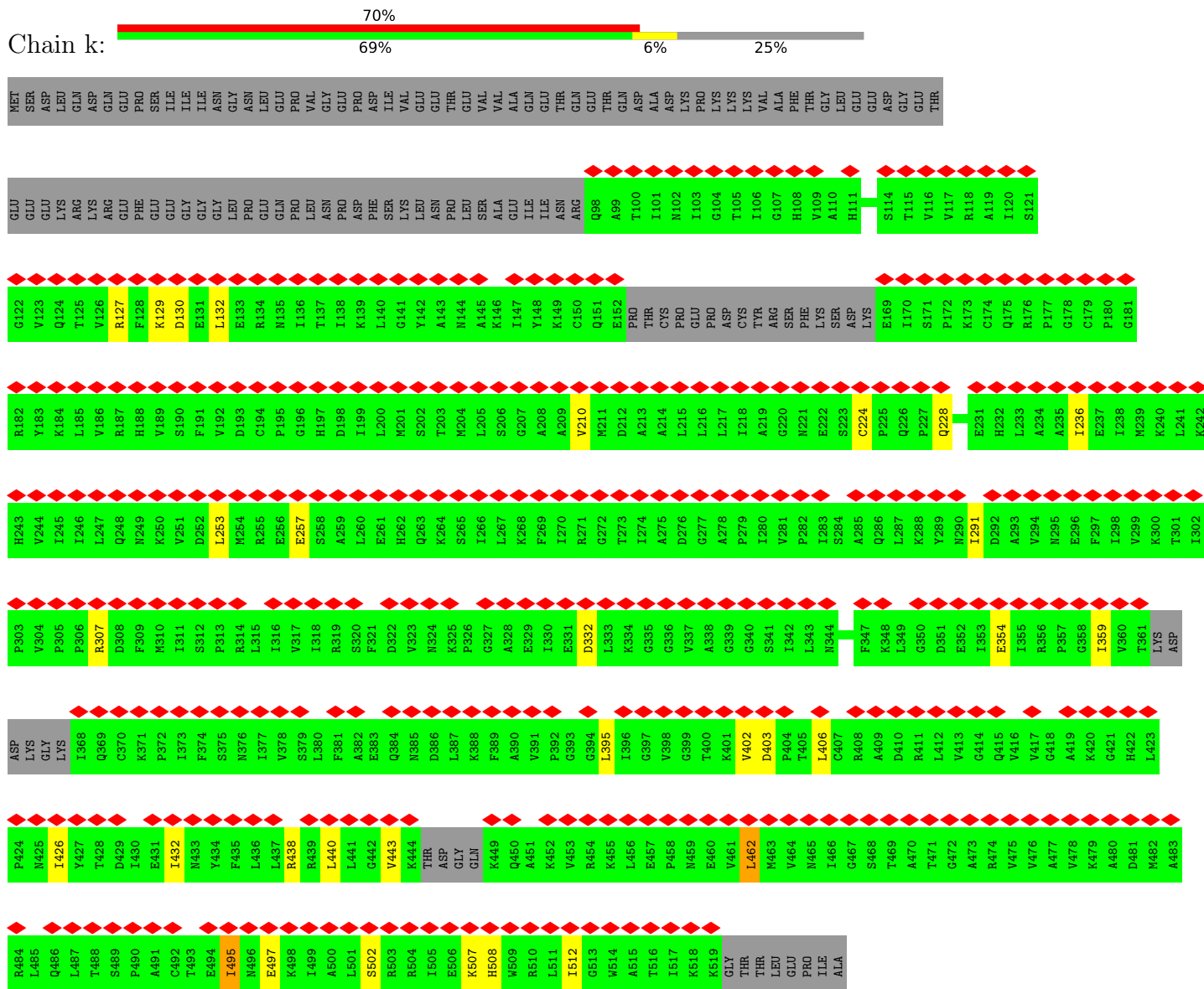


- Molecule 39: eIF2 alpha



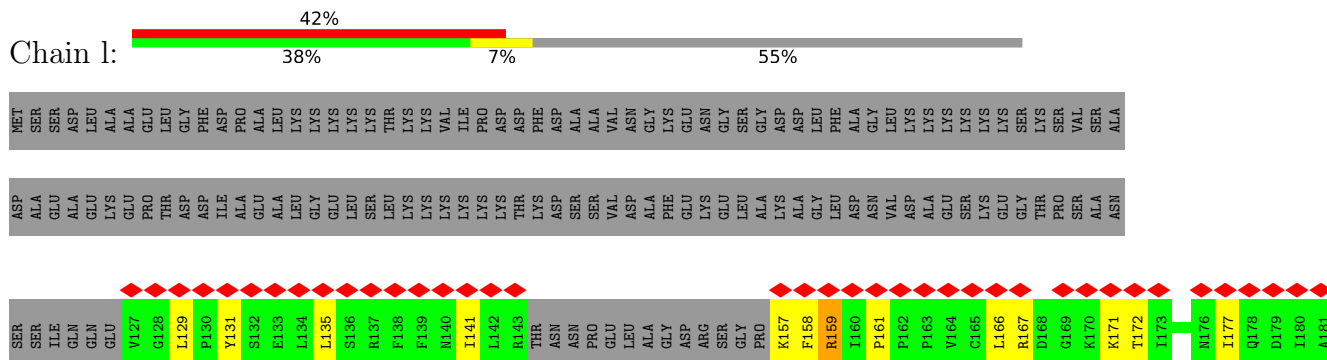
- Molecule 40: eIF2 gamma

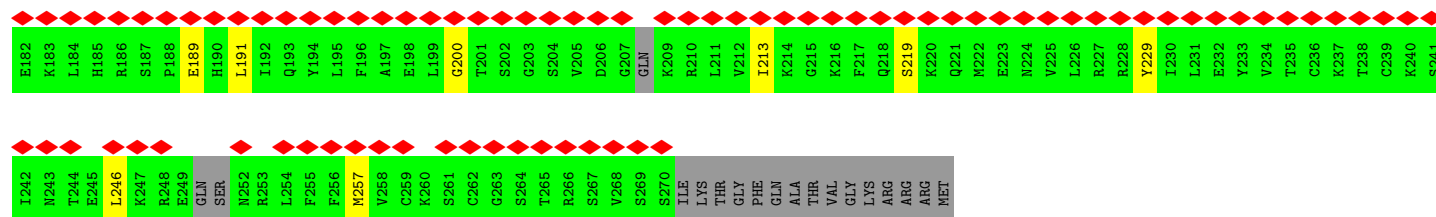
Chain k:



- Molecule 41: eIF2 beta

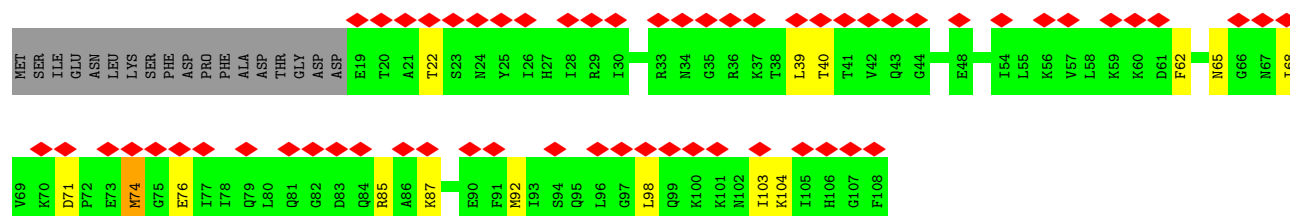
Chain 1:





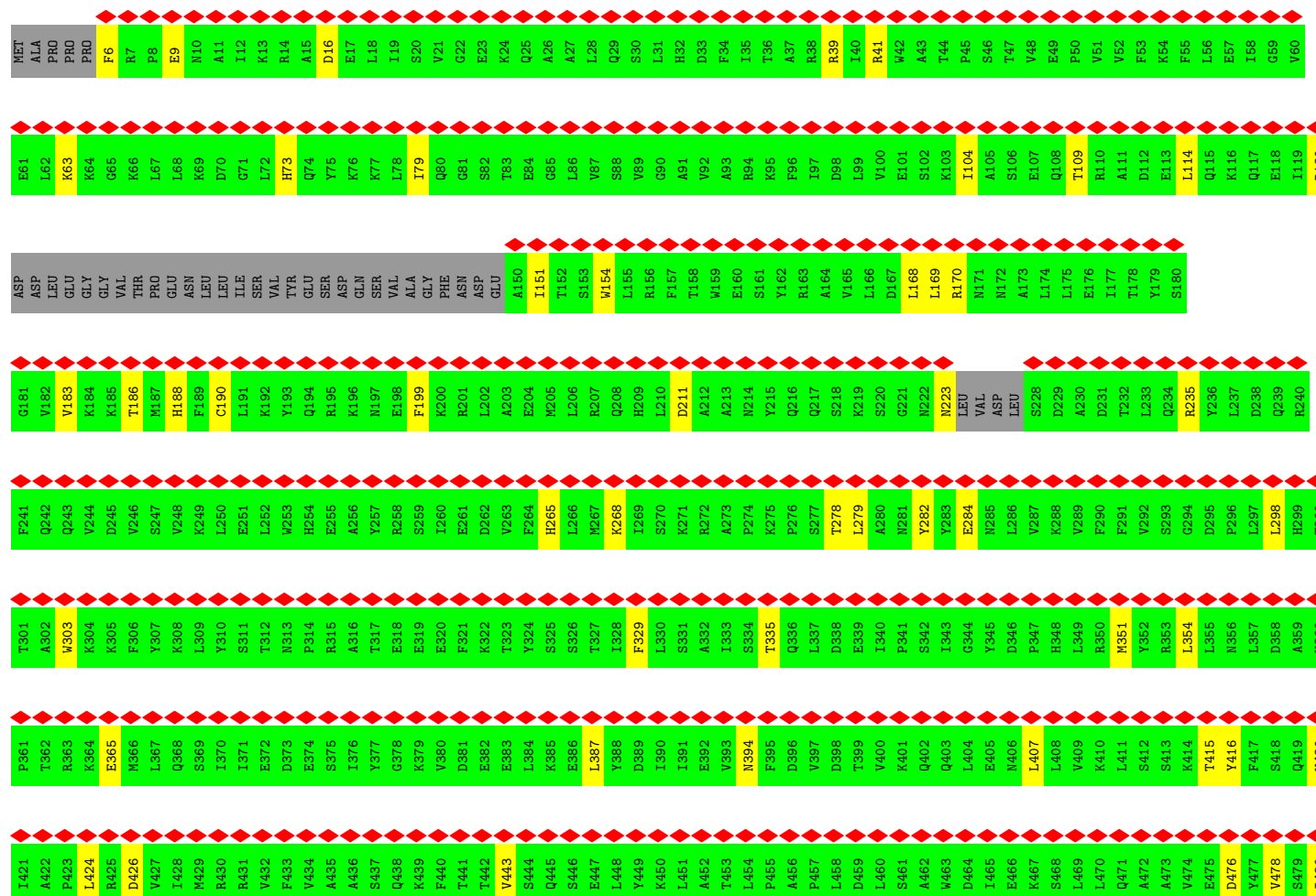
• Molecule 42: eIF1

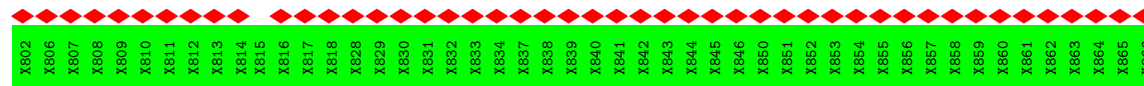
Chain m:



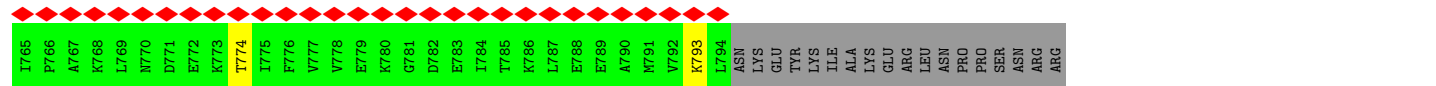
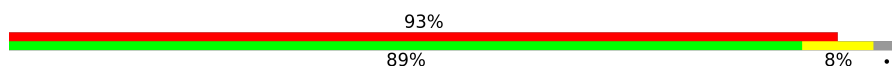
• Molecule 43: eIF3a

Chain o:

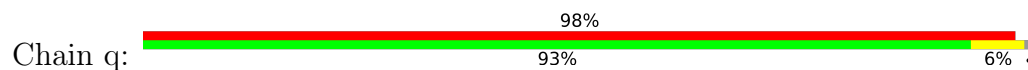




Chain p:

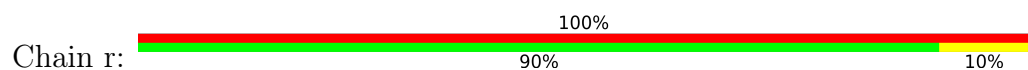


- Molecule 45: eIF3i



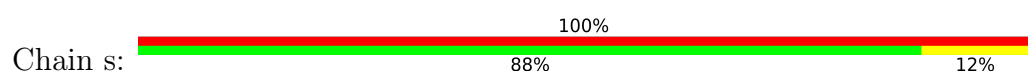
I301	S302	P303	Q304	G305	T306	S307	Y308	A309	S310	G311	G312	E313	D314	G315	F316	I317	R318	L319	H320	H321	F322	E323	K324	S325	Y326	F327	D328	F329	K330	Y331	D332	V333	E334	K335	A336	A337	E338	A339	K340	E341	H342	MET	GLN	GLU	ALA	ASN													
N241	T242	A243	V244	I245	T246	P247	L248	K249	E250	F251	T252	L253	L254	G255	G256	G257	Q258	E259	A260	K261	D262	V263	T264	T265	T266	S267	A268	N269	E270	G271	K272	F273	E274	A275	R276	F277	Y278	H279	K280	I281	F282	E283	E284	E285	L286	G287	R288	V289	Q290	G291	H292	F293	G294	P295	L296	N297	T298	V299	A300
D181	V182	S183	N184	N185	Y186	E187	Y188	V189	D190	S191	I192	D193	L194	H195	E196	K197	S198	I199	S200	D201	M202	Q203	F204	S205	P206	D207	L208	T209	Y210	F211	I212	T213	S214	S215	R216	D217	T218	N219	S220	F221	L222	V223	D224	V225	S226	T227	L228	Q229	V230	L231	K232	K233	Y234	E235	T236	D237	C238	P239	L240
S121	I122	N123	I124	Y125	E126	I127	E128	R129	D130	S131	A132	T133	H134	E135	L136	T137	K138	V139	S140	E141	E142	P143	I144	H145	K146	I147	I148	T149	H150	E151	G152	L153	D154	A155	A156	T157	V158	A159	G160	W161	S162	T163	K164	G165	K166	Y167	I168	I169	A170	G171	H172	K173	D174	G175	K176	I177	S178	K179	Y180
D61	C62	F63	T64	K65	Y66	C67	V68	T69	G70	S71	A72	D73	Y74	S75	I76	K77	L78	W79	D80	V81	S82	N83	G84	Q85	C86	V87	A88	T89	W90	K91	S92	P93	V94	P95	V96	K97	R98	V99	E100	F101	S102	P103	C104	G105	N106	Y107	F108	L109	A110	I111	L112	D113	N114	V115	M116	K117	P118	N119	G120
M1	K2	A3	I4	K5	L6	T7	G8	H9	E10	R11	P12	L13	T14	Q15	V16	K17	Y18	N19	K20	E21	G22	D23	L24	L25	F26	S27	C28	S29	K30	D31	S32	S33	A34	S35	V36	W37	Y38	S39	L40	N41	G42	E43	R44	L45	G46	T47	L48	D49	G50	H51	T52	G53	T54	I55	W56	S57	I58	D59	V60

- Molecule 46: eIF3b



L704	H705	Q706	R707	E708	L709	L710	K711	Q712	W713	T714	E715	Y716	R717	E718	K719	I720	G721	Q722	E723	W724	E725	K726	S727	W728	F730	K731	F732	F733	D734
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- Molecule 47: eIF3g



V45	H46	K47	S48	V49	A50	E51	R52	K53	N54	W55	H56	K57	Y58	G59	S60	E61	K62	G63	S64	P65	A66	G67	P68	S69	A70	V71	T72	A73	L74	L75	G76	E77	E78	V79	E80	L81	R82	L83	S84	R85	N86	W87	K88	Q89	A90	E91	E92	E93	R94	I95	Q96
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21401	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.07	Depositor
Map size (\AA)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.38	1/1797 (0.1%)	0.69	0/2799
2	2	0.27	0/42269	0.69	7/65862 (0.0%)
3	3	0.30	0/317	0.69	0/489
4	A	0.42	0/1666	0.78	2/2279 (0.1%)
5	B	0.40	0/1793	0.72	2/2414 (0.1%)
6	C	0.39	0/1659	0.69	0/2252
7	D	0.42	0/1769	0.72	1/2378 (0.0%)
8	E	0.38	0/2122	0.67	0/2861
9	F	0.41	0/1628	0.75	0/2198
10	G	0.41	0/1835	0.72	1/2451 (0.0%)
11	H	0.42	0/1507	0.71	0/2028
12	I	0.41	0/1515	0.73	2/2029 (0.1%)
13	J	0.40	0/1495	0.75	1/2001 (0.0%)
14	K	0.48	0/831	0.77	1/1123 (0.1%)
15	L	0.41	0/1276	0.63	0/1718
16	M	0.46	0/891	0.80	1/1201 (0.1%)
17	N	0.41	0/1210	0.77	0/1628
18	O	0.38	0/953	0.68	0/1279
19	P	0.42	0/946	0.71	1/1273 (0.1%)
20	Q	0.43	0/1125	0.71	0/1510
21	R	0.43	0/969	0.77	1/1299 (0.1%)
22	S	0.43	0/1212	0.78	0/1629
23	T	0.40	0/1129	0.72	0/1520
24	U	0.40	0/857	0.73	0/1158
25	V	0.36	0/696	0.66	0/938
26	W	0.39	0/1039	0.74	1/1399 (0.1%)
27	X	0.40	0/1137	0.75	2/1516 (0.1%)
28	Y	0.40	0/1075	0.69	0/1433
29	Z	0.44	0/567	0.69	0/762
30	a	0.36	0/791	0.67	0/1059
31	b	0.38	0/619	0.65	0/837
32	c	0.38	0/489	0.71	0/655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.41	0/457	0.62	0/607
34	e	0.40	0/440	0.73	0/586
35	f	0.49	0/559	0.73	1/747 (0.1%)
36	g	0.41	0/2521	0.64	1/3431 (0.0%)
37	h	0.36	0/234	0.75	0/300
38	i	0.39	0/894	0.70	0/1188
39	j	0.47	0/2034	0.77	2/2737 (0.1%)
40	k	0.47	0/3079	0.70	1/4157 (0.0%)
41	l	0.47	0/1051	0.76	1/1402 (0.1%)
42	m	0.41	0/724	0.75	1/968 (0.1%)
43	o	0.49	0/3796	0.80	0/5128
44	p	0.49	0/4602	0.76	2/6226 (0.0%)
45	q	0.50	0/2757	0.67	0/3733
46	r	0.49	0/282	0.74	0/373
47	s	0.47	0/426	0.64	0/571
All	All	0.38	1/103040 (0.0%)	0.71	32/148132 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	F	0	1
27	X	0	1
28	Y	0	1
41	l	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-9.88	1.49	1.61

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	685	A	C2'-C3'-O3'	8.09	127.30	109.50
12	I	29	LEU	CA-CB-CG	7.26	132.00	115.30
39	j	166	LEU	CA-CB-CG	6.66	130.62	115.30
41	l	191	LEU	CA-CB-CG	6.50	130.25	115.30
26	W	26	LEU	CA-CB-CG	6.10	129.33	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	191	THR	Peptide
27	X	63	GLN	Peptide
28	Y	29	HIS	Peptide
41	l	158	PHE	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	
4	A	206/254 (81%)	170 (82%)	27 (13%)	9 (4%)	2	24
5	B	218/255 (86%)	185 (85%)	25 (12%)	8 (4%)	3	27
6	C	215/259 (83%)	186 (86%)	22 (10%)	7 (3%)	4	29
7	D	221/237 (93%)	196 (89%)	16 (7%)	9 (4%)	3	25
8	E	258/261 (99%)	225 (87%)	28 (11%)	5 (2%)	8	40
9	F	204/227 (90%)	169 (83%)	28 (14%)	7 (3%)	3	29
10	G	224/236 (95%)	197 (88%)	23 (10%)	4 (2%)	8	41
11	H	182/190 (96%)	157 (86%)	15 (8%)	10 (6%)	2	21
12	I	184/201 (92%)	160 (87%)	15 (8%)	9 (5%)	2	22
13	J	180/188 (96%)	154 (86%)	19 (11%)	7 (4%)	3	26
14	K	94/106 (89%)	81 (86%)	7 (7%)	6 (6%)	1	18
15	L	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	23
16	M	113/134 (84%)	85 (75%)	21 (19%)	7 (6%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	N	148/151 (98%)	134 (90%)	13 (9%)	1 (1%)	22	62
18	O	125/137 (91%)	102 (82%)	16 (13%)	7 (6%)	2	20
19	P	115/142 (81%)	96 (84%)	13 (11%)	6 (5%)	2	21
20	Q	139/143 (97%)	108 (78%)	20 (14%)	11 (8%)	1	14
21	R	116/136 (85%)	101 (87%)	13 (11%)	2 (2%)	9	43
22	S	143/146 (98%)	111 (78%)	21 (15%)	11 (8%)	1	14
23	T	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
24	U	104/117 (89%)	84 (81%)	16 (15%)	4 (4%)	3	26
25	V	85/87 (98%)	74 (87%)	7 (8%)	4 (5%)	2	23
26	W	127/130 (98%)	112 (88%)	10 (8%)	5 (4%)	3	26
27	X	142/145 (98%)	117 (82%)	14 (10%)	11 (8%)	1	14
28	Y	132/135 (98%)	118 (89%)	7 (5%)	7 (5%)	2	21
29	Z	68/108 (63%)	50 (74%)	17 (25%)	1 (2%)	10	46
30	a	96/119 (81%)	81 (84%)	11 (12%)	4 (4%)	3	24
31	b	79/82 (96%)	61 (77%)	15 (19%)	3 (4%)	3	26
32	c	60/67 (90%)	51 (85%)	6 (10%)	3 (5%)	2	22
33	d	51/56 (91%)	33 (65%)	15 (29%)	3 (6%)	1	19
34	e	52/63 (82%)	45 (86%)	6 (12%)	1 (2%)	8	40
35	f	67/150 (45%)	48 (72%)	9 (13%)	10 (15%)	0	4
36	g	312/326 (96%)	257 (82%)	45 (14%)	10 (3%)	4	30
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	109/153 (71%)	92 (84%)	14 (13%)	3 (3%)	5	32
39	j	243/304 (80%)	205 (84%)	32 (13%)	6 (2%)	5	34
40	k	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	10	46
41	l	120/285 (42%)	100 (83%)	16 (13%)	4 (3%)	4	29
42	m	88/108 (82%)	76 (86%)	10 (11%)	2 (2%)	6	36
43	o	451/588 (77%)	417 (92%)	31 (7%)	3 (1%)	22	62
44	p	554/652 (85%)	497 (90%)	45 (8%)	12 (2%)	6	37
45	q	340/347 (98%)	302 (89%)	33 (10%)	5 (2%)	10	46
46	r	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
47	s	50/52 (96%)	46 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7149/8360 (86%)	6131 (86%)	778 (11%)	240 (3%)	6	29

5 of 240 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	95	ALA
4	A	166	GLY
6	C	141	VAL
6	C	235	TRP
7	D	216	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	
4	A	174/211 (82%)	147 (84%)	27 (16%)	2	15
5	B	198/228 (87%)	174 (88%)	24 (12%)	5	22
6	C	176/203 (87%)	153 (87%)	23 (13%)	4	20
7	D	185/196 (94%)	152 (82%)	33 (18%)	2	11
8	E	223/224 (100%)	186 (83%)	37 (17%)	2	13
9	F	174/194 (90%)	140 (80%)	34 (20%)	1	9
10	G	192/200 (96%)	174 (91%)	18 (9%)	8	30
11	H	164/170 (96%)	138 (84%)	26 (16%)	2	15
12	I	147/159 (92%)	133 (90%)	14 (10%)	8	29
13	J	153/158 (97%)	135 (88%)	18 (12%)	5	22
14	K	88/96 (92%)	70 (80%)	18 (20%)	1	7
15	L	136/137 (99%)	128 (94%)	8 (6%)	19	46
16	M	93/109 (85%)	82 (88%)	11 (12%)	5	22
17	N	127/128 (99%)	108 (85%)	19 (15%)	3	16
18	O	96/104 (92%)	88 (92%)	8 (8%)	11	36
19	P	100/119 (84%)	83 (83%)	17 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Q	117/119 (98%)	99 (85%)	18 (15%)	2	15
21	R	109/124 (88%)	91 (84%)	18 (16%)	2	14
22	S	128/129 (99%)	105 (82%)	23 (18%)	1	11
23	T	117/118 (99%)	97 (83%)	20 (17%)	2	12
24	U	96/107 (90%)	83 (86%)	13 (14%)	4	19
25	V	73/73 (100%)	66 (90%)	7 (10%)	8	29
26	W	110/111 (99%)	102 (93%)	8 (7%)	14	40
27	X	119/120 (99%)	102 (86%)	17 (14%)	3	17
28	Y	108/109 (99%)	102 (94%)	6 (6%)	21	48
29	Z	60/88 (68%)	55 (92%)	5 (8%)	11	36
30	a	83/100 (83%)	71 (86%)	12 (14%)	3	17
31	b	71/72 (99%)	67 (94%)	4 (6%)	21	48
32	c	54/59 (92%)	48 (89%)	6 (11%)	6	24
33	d	46/48 (96%)	39 (85%)	7 (15%)	3	16
34	e	47/55 (86%)	39 (83%)	8 (17%)	2	13
35	f	57/133 (43%)	48 (84%)	9 (16%)	2	15
36	g	265/272 (97%)	231 (87%)	34 (13%)	4	20
37	h	23/23 (100%)	20 (87%)	3 (13%)	4	20
38	i	93/130 (72%)	74 (80%)	19 (20%)	1	7
39	j	224/274 (82%)	185 (83%)	39 (17%)	2	12
40	k	332/449 (74%)	306 (92%)	26 (8%)	12	38
41	l	119/246 (48%)	103 (87%)	16 (13%)	4	19
42	m	77/96 (80%)	64 (83%)	13 (17%)	2	13
43	o	411/444 (93%)	364 (89%)	47 (11%)	5	23
44	p	507/536 (95%)	469 (92%)	38 (8%)	13	39
45	q	297/301 (99%)	280 (94%)	17 (6%)	20	47
46	r	30/30 (100%)	27 (90%)	3 (10%)	7	28
47	s	43/43 (100%)	37 (86%)	6 (14%)	3	18
All	All	6242/7045 (89%)	5465 (88%)	777 (12%)	8	21

5 of 777 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	Y	99	LYS
39	j	7	ARG
30	a	38	ARG
28	Y	84	LYS
36	g	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
36	g	161	ASN
43	o	32	HIS
38	i	44	ASN
40	k	508	HIS
43	o	242	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75 (98%)	32 (43%)	7 (9%)
2	2	1778/1781 (99%)	879 (49%)	146 (8%)
3	3	13/25 (52%)	11 (84%)	1 (7%)
All	All	1865/1881 (99%)	922 (49%)	154 (8%)

5 of 922 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	U
1	1	9	G
1	1	10	G
1	1	14	A
1	1	15	G

5 of 154 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1315	G
2	2	1579	C
2	2	1360	C
2	2	1430	U
2	2	1765	G

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 87 ligands modelled in this entry, 85 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	GCP	k	603	48	27,34,34	1.96	8 (29%)	34,54,54	1.98	8 (23%)
50	MET	k	601	-	6,7,8	0.43	0	2,7,9	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	GCP	k	603	48	-	2/15/38/38	0/3/3/3
50	MET	k	601	-	-	1/5/6/8	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.43	1.61	1.50
51	k	603	GCP	C5-C6	4.82	1.49	1.41
51	k	603	GCP	PB-O3A	3.15	1.61	1.58
51	k	603	GCP	PG-O2G	2.86	1.61	1.54
51	k	603	GCP	C5-C4	2.82	1.48	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C2-N3-C4	5.46	121.60	115.36
51	k	603	GCP	C2-N1-C6	4.11	122.46	115.93
51	k	603	GCP	C5-C6-N1	-3.86	118.16	123.43
51	k	603	GCP	C4-C5-C6	-3.77	117.20	120.80
51	k	603	GCP	N3-C2-N1	-3.63	122.38	127.22

There are no chirality outliers.

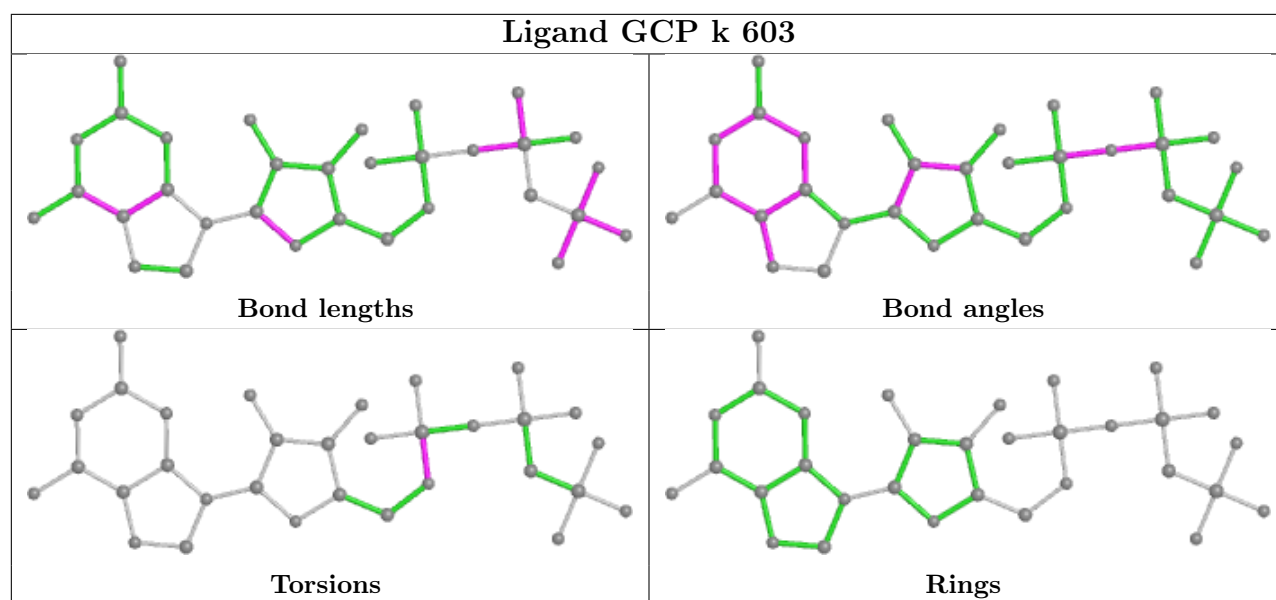
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	k	603	GCP	C5'-O5'-PA-O3A
50	k	601	MET	CA-CB-CG-SD
51	k	603	GCP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
43	o	7
44	p	7

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	495:PRO	C	753:UNK	N	221.30
1	p	218:UNK	C	251:GLN	N	63.04
1	p	32:UNK	C	116:UNK	N	42.95
1	p	185:UNK	C	193:ARG	N	15.92
1	o	818:UNK	C	828:UNK	N	14.63

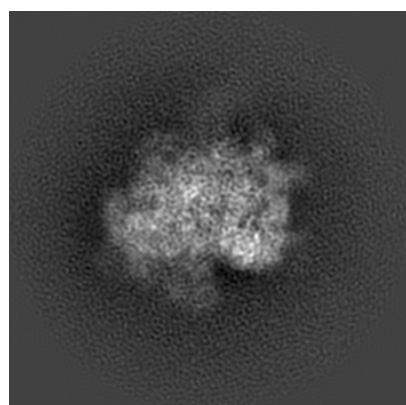
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3048. These allow visual inspection of the internal detail of the map and identification of artifacts.

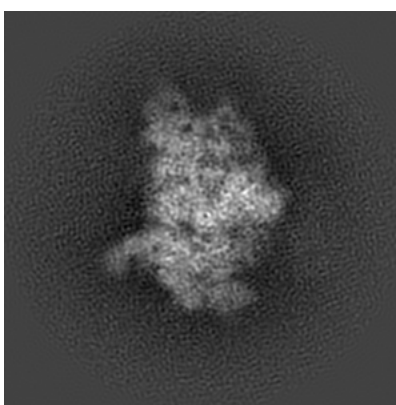
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

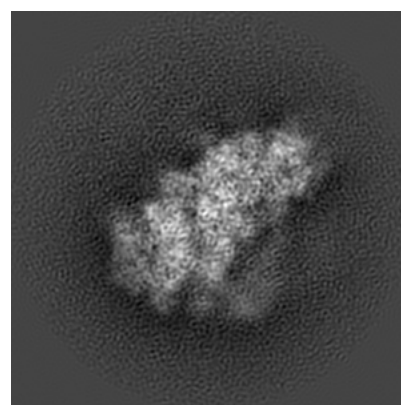
6.1.1 Primary map



X



Y

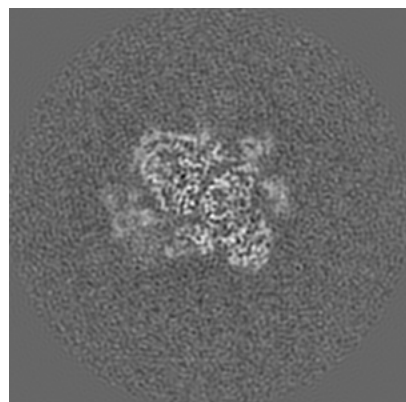


Z

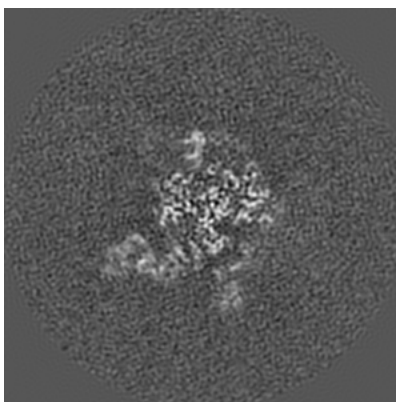
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

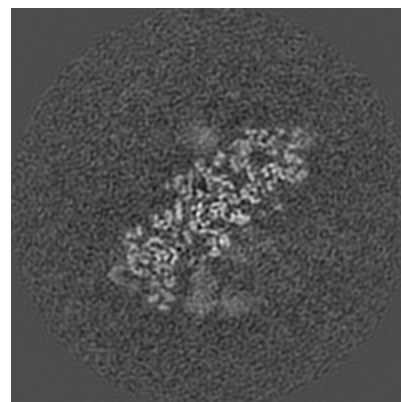
6.2.1 Primary map



X Index: 150



Y Index: 150

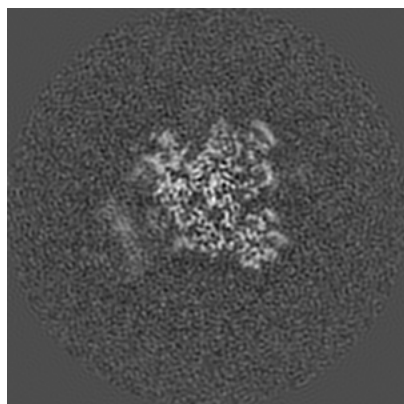


Z Index: 150

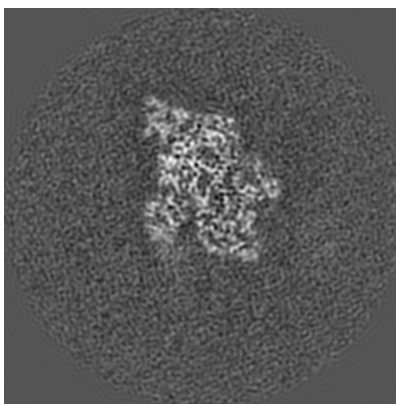
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

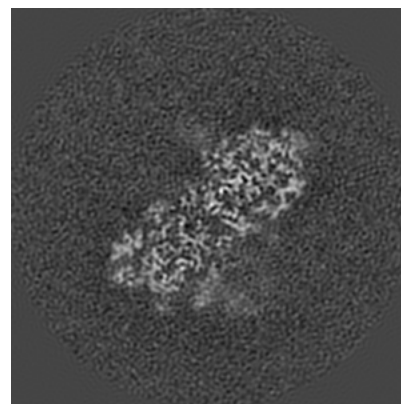
6.3.1 Primary map



X Index: 161



Y Index: 171



Z Index: 143

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

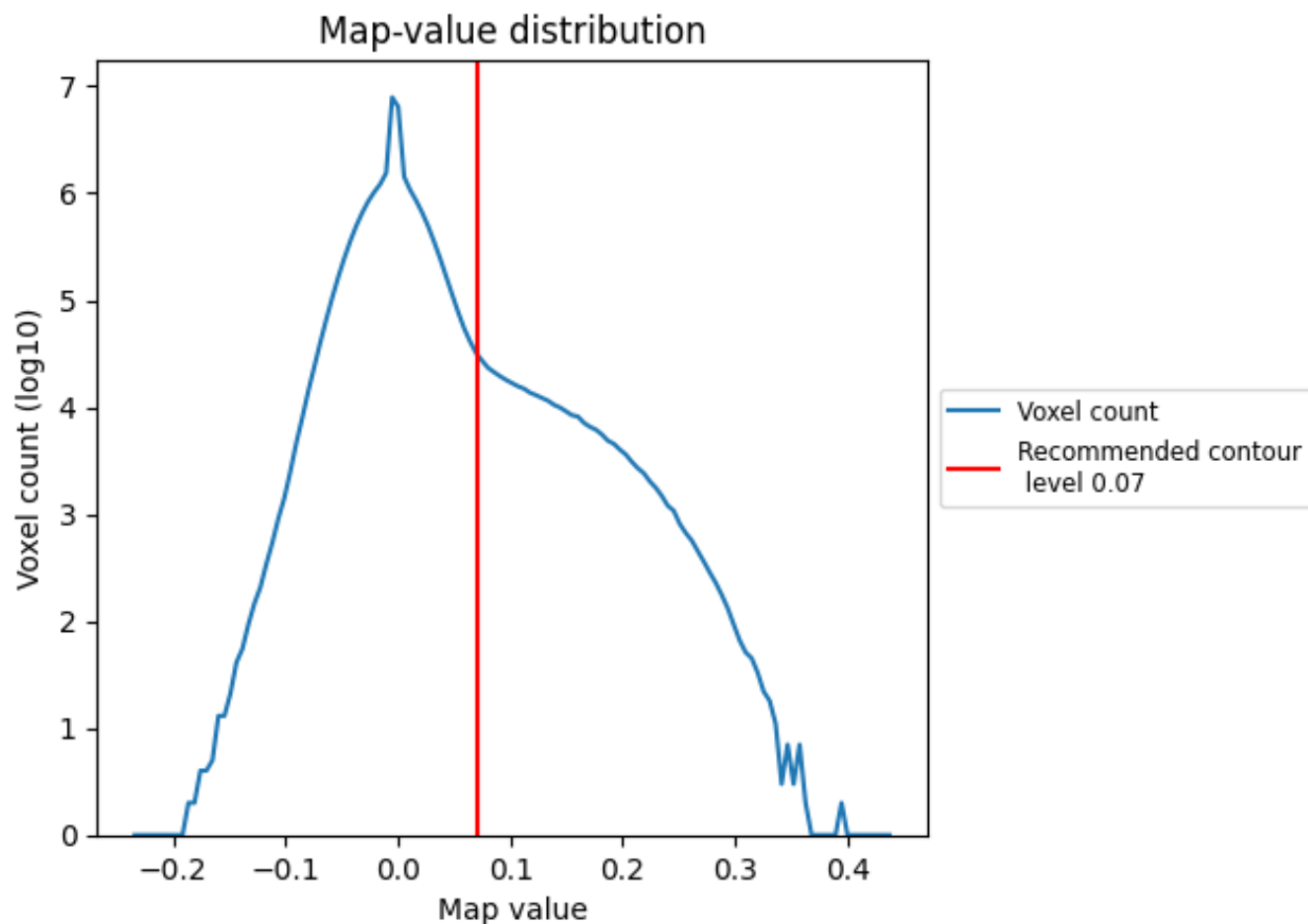
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

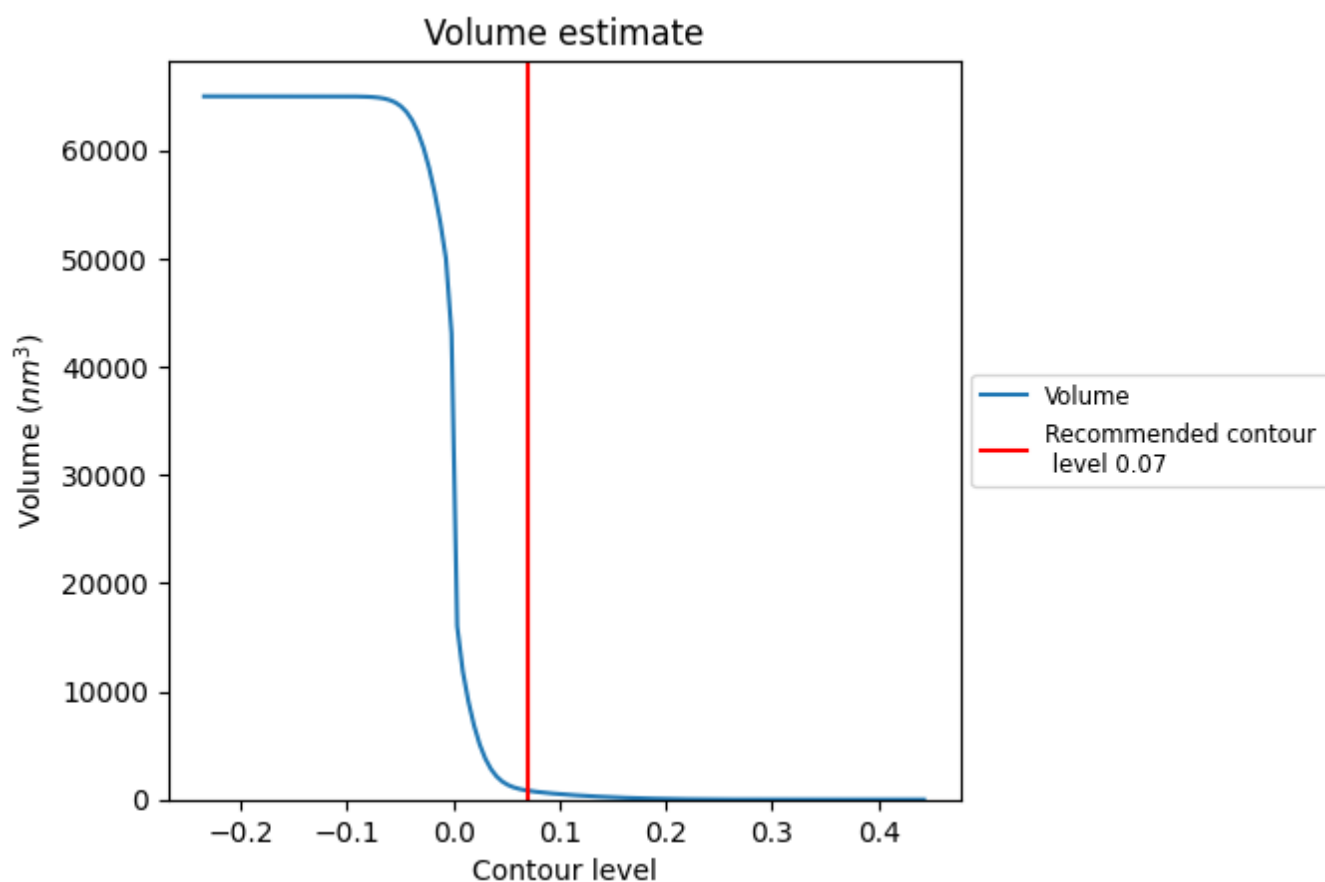
This section contains the results of statistical analysis of the map.

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.

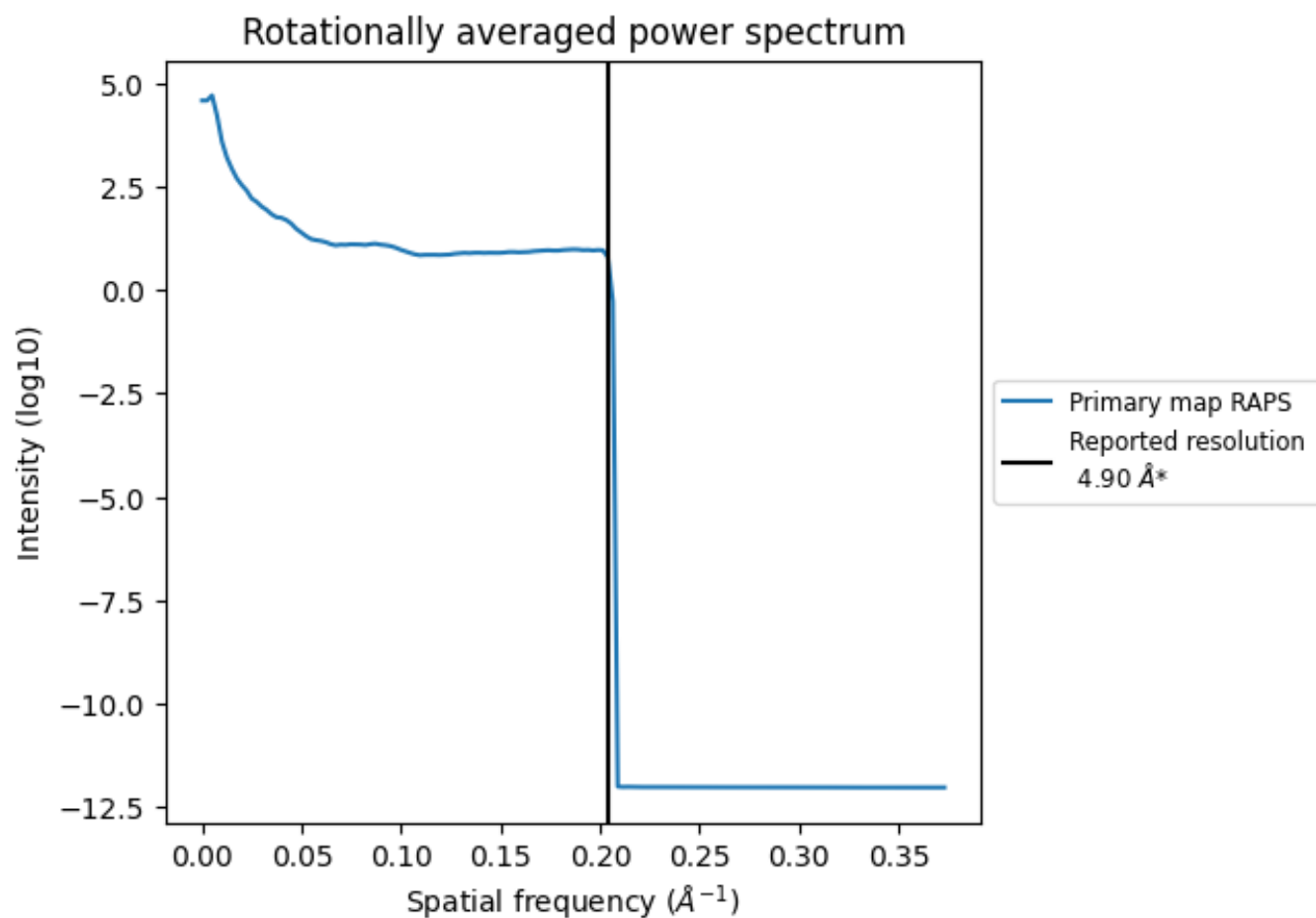
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm³; this corresponds to an approximate mass of 750 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 ⓘ

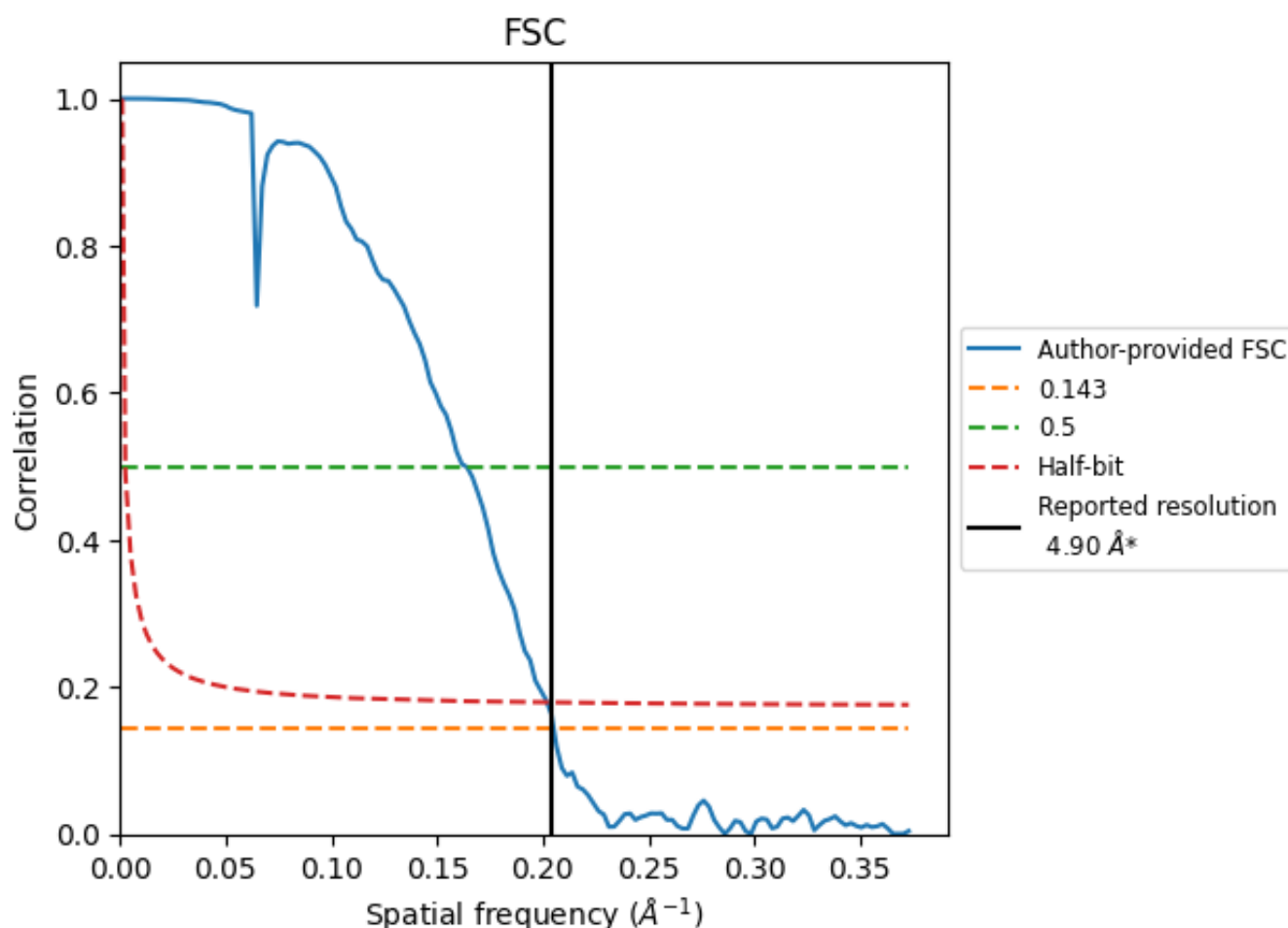


*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

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 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

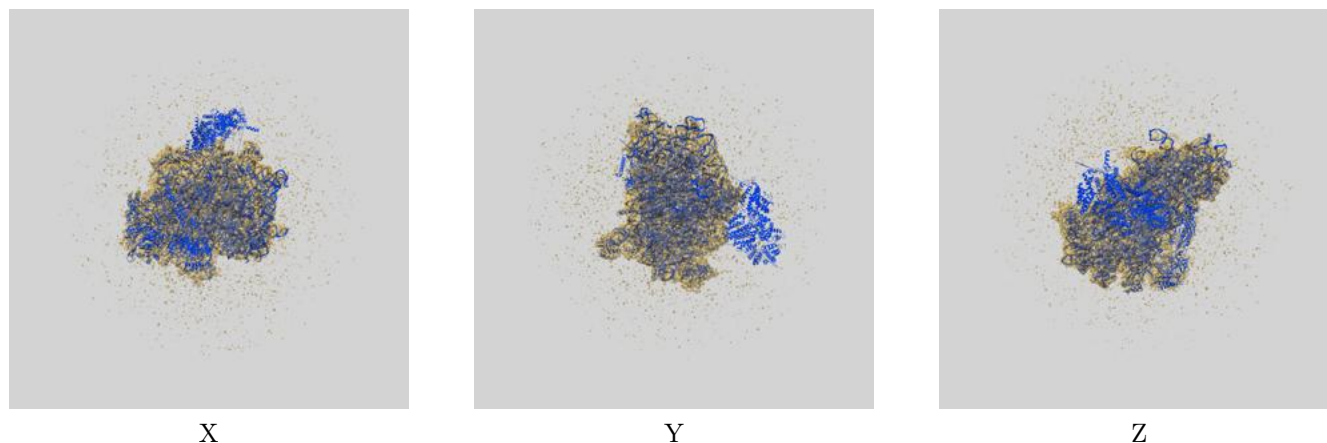
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.88	6.12	4.95
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

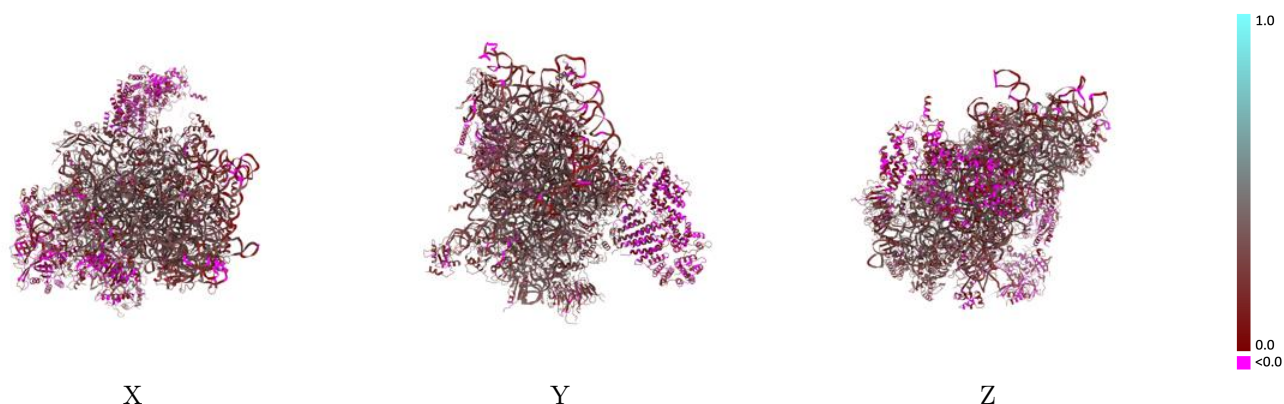
This section contains information regarding the fit between EMDB map EMD-3048 and PDB model 3JAP. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



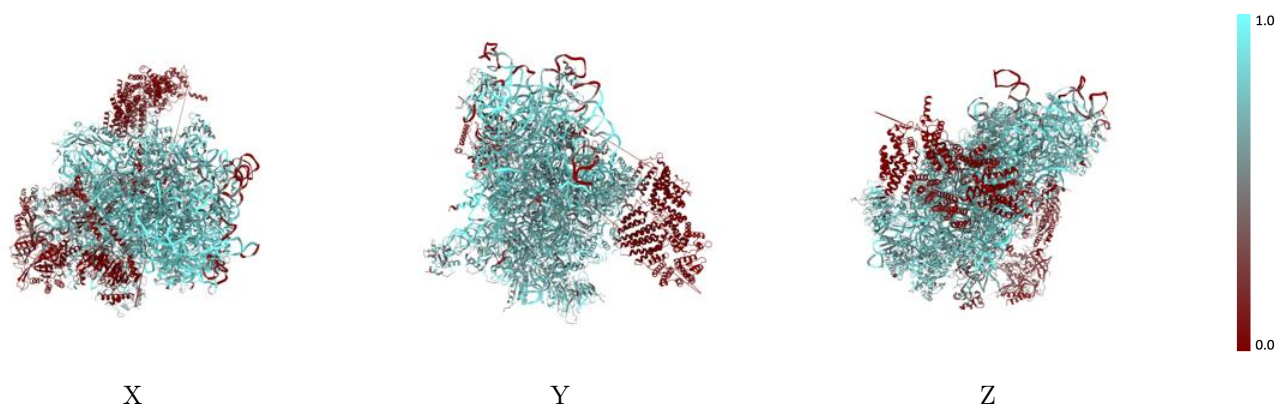
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



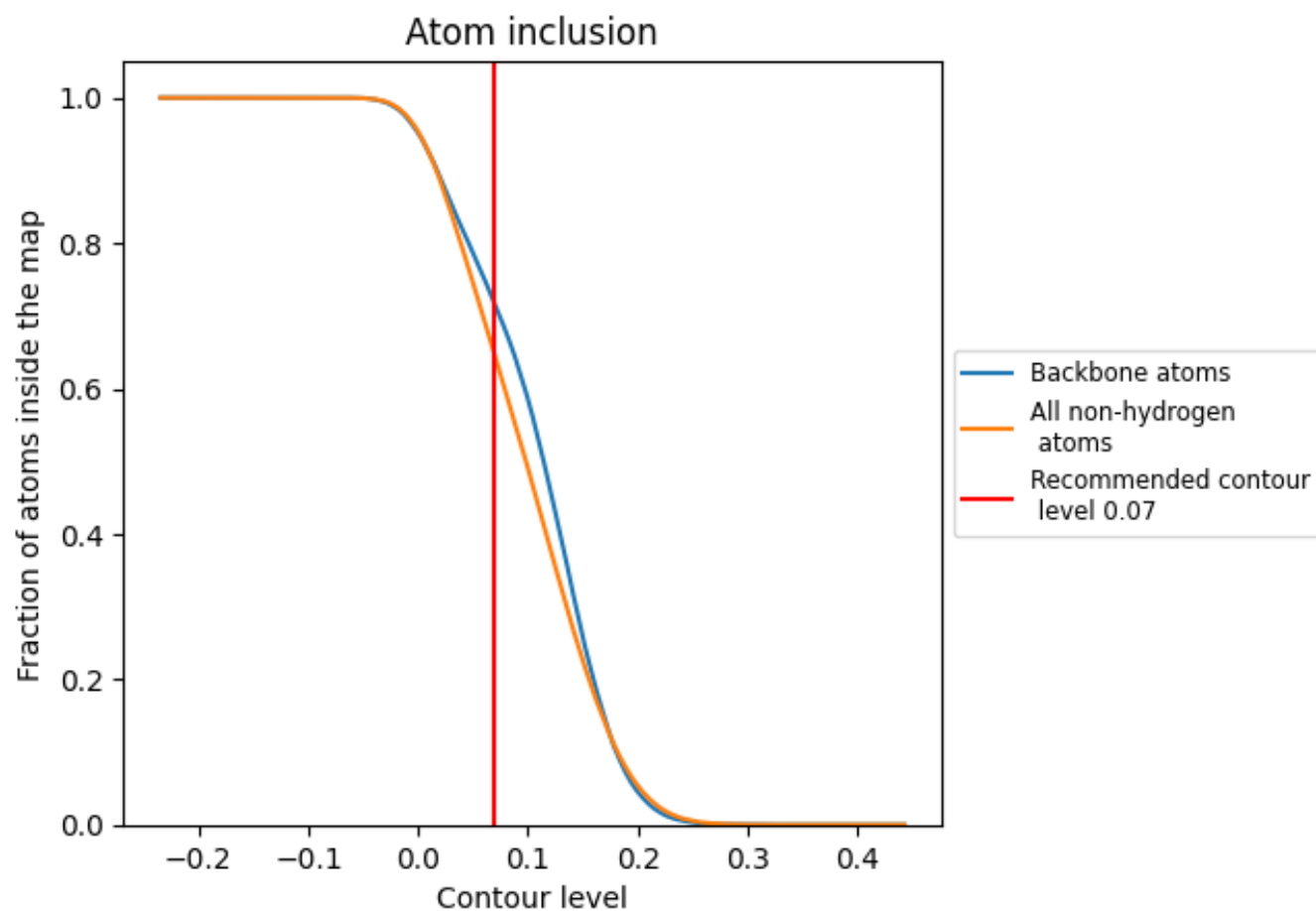
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6445	 0.2440
1	 0.5980	 0.1680
2	 0.8675	 0.2900
3	 0.5505	 0.2110
A	 0.7511	 0.2890
B	 0.7503	 0.2810
C	 0.7189	 0.3090
D	 0.6808	 0.2810
E	 0.7303	 0.2980
F	 0.6794	 0.2580
G	 0.7146	 0.2460
H	 0.6706	 0.2540
I	 0.7155	 0.2620
J	 0.7288	 0.2960
K	 0.7123	 0.2710
L	 0.6856	 0.2970
M	 0.5650	 0.2000
N	 0.7277	 0.2870
O	 0.7508	 0.2800
P	 0.7201	 0.2620
Q	 0.7093	 0.2650
R	 0.7166	 0.2850
S	 0.6782	 0.2640
T	 0.7287	 0.2560
U	 0.6470	 0.2680
V	 0.7316	 0.3010
W	 0.7130	 0.2930
X	 0.7189	 0.3190
Y	 0.7646	 0.2910
Z	 0.6188	 0.2420
a	 0.7426	 0.3170
b	 0.7176	 0.2800
c	 0.6938	 0.2950
d	 0.7588	 0.3010
e	 0.7160	 0.3180



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Chain	Atom inclusion	Q-score
f	 0.6555	 0.2270
g	 0.7093	 0.2410
h	 0.3726	 0.2170
i	 0.6404	 0.2810
j	 0.3060	 0.1650
k	 0.1174	 0.1100
l	 0.1039	 0.1240
m	 0.2756	 0.2020
o	 0.0131	 0.0720
p	 0.0307	 0.0920
q	 0.0264	 0.0530
r	 0.0185	 0.0550
s	 0.0025	 0.0760