



Full wwPDB EM Validation Report ⓘ

Sep 2, 2024 – 05:52 pm BST

PDB ID : 8S8I
EMDB ID : EMD-19806
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation
(model py48S-AUC-eIF1)
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-03-06
Resolution : 4.30 Å(reported)

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.dev112
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

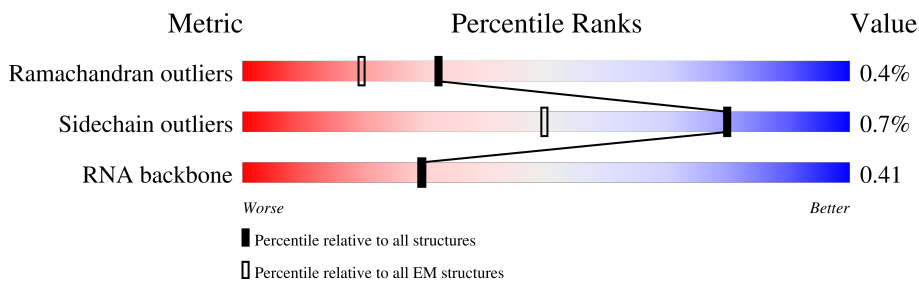
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2	1798	
2	A	254	
3	B	255	
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	

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Mol	Chain	Length	Quality of chain
9	J	188	5% 93%
10	L	156	12% 97%
11	N	151	5% 100%
12	O	137	11% 93% 6%
13	V	87	100%
14	W	130	98%
15	X	145	99%
16	Y	135	98%
17	a	119	6% 85% 14%
18	b	82	6% 98%
19	e	63	24% 95% 5%
20	h	25	100% 100%
21	D	237	10% 95%
22	F	227	17% 89% 9%
23	K	106	12% 91% 9%
24	M	134	73% 84% 13%
25	P	142	13% 82% 18%
26	Q	143	97%
27	R	136	19% 93%
28	S	146	13% 99%
29	T	144	7% 99%
30	U	117	17% 90% 9%
31	Z	108	34% 72% 28%
32	c	67	19% 94%
33	d	56	5% 96%

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Mol	Chain	Length	Quality of chain
34	f	150	
35	g	326	
36	i	153	
37	3	49	
38	1	75	
39	j	304	
40	k	527	
41	l	285	
42	m	108	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 87328 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1789	38003	16989	6694	12531	1789	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	219	1702	1085	299	316	2	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	225	1796	1135	330	328	3	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	220	1648	1053	291	300	4	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	230	1832	1146	352	330	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

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

- Molecule 8 is a protein called 40S ribosomal protein S8.

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

- Molecule 9 is a protein called KLLA0E23673p.

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

- Molecule 10 is a protein called KLLA0A10483p.

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

- Molecule 11 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	151	1195	761	224	207	3	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	129	955	585	191	176	3	0	0

- Molecule 13 is a protein called 40S ribosomal protein S21.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 15 is a protein called KLLA0B11231p.

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

- Molecule 16 is a protein called 40S ribosomal protein S24.

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

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	102	Total	C	N	O	S	0	0
			797	492	168	132	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

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

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 20 is a protein called 40S ribosomal protein L41-A.

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

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 22 is a protein called KLLA0D10659p.

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

- Molecule 23 is a protein called KLLA0B08173p.

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

- Molecule 24 is a protein called 40S ribosomal protein S12.

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

- Molecule 25 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 27 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 28 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	S	145	1189	739	239	209	2	0	0

- Molecule 29 is a protein called KLLA0A07194p.

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Z	78	594	376	111	106	1	0	0

- Molecule 32 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	c	64	499	308	99	91	1	0	0

- Molecule 33 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	d	55	461	289	93	78	1	0	0

- Molecule 34 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	74	584	374	111	95	4	0	0

- Molecule 35 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	95	Total	C	N	O	S	0	0
			764	474	142	143	5		

- Molecule 37 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	26	Total	C	N	O	P	0	0
			536	242	84	184	26		

- Molecule 38 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	267	Total	C	N	O	S	0	0
			2139	1366	355	407	11		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	470	Total	C	N	O	S	0	0
			3596	2279	633	666	18		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	134	Total	C	N	O	S	0	0
			1083	689	194	193	7		

- Molecule 42 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	77	Total	C	N	O	S	0	0
			619	395	109	111	4		

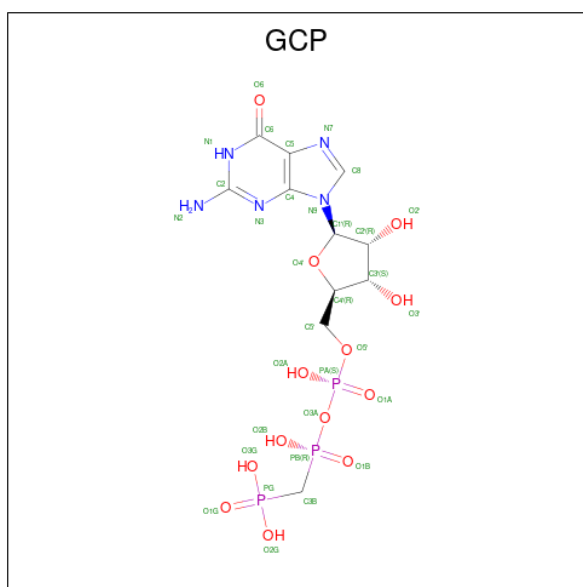
- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
43	2	114	Total	Mg	0
			114	114	
43	S	1	Total	Mg	0
			1	1	
43	i	1	Total	Mg	0
			1	1	
43	k	1	Total	Mg	0
			1	1	

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

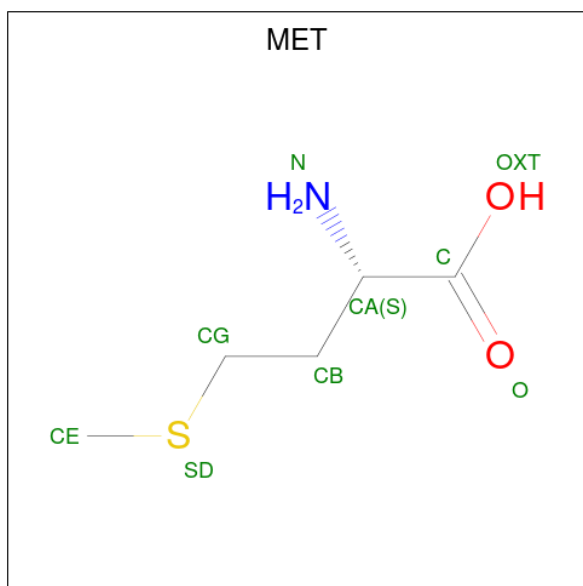
Mol	Chain	Residues	Atoms		AltConf
44	a	1	Total	Zn	0
			1	1	
44	b	1	Total	Zn	0
			1	1	
44	f	1	Total	Zn	0
			1	1	
44	l	1	Total	Zn	0
			1	1	

- Molecule 45 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 46 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



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

- Molecule 47 is water.

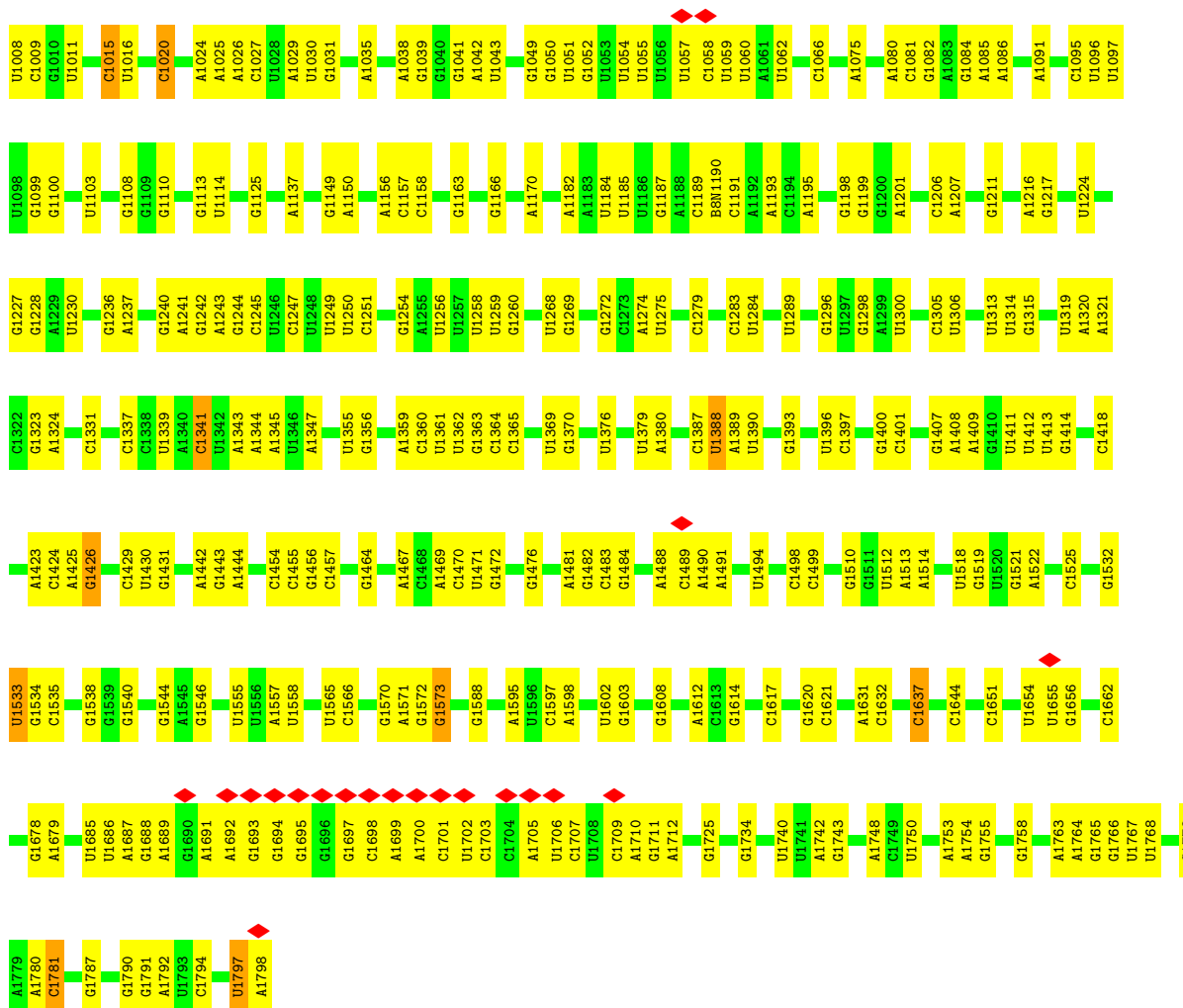
Mol	Chain	Residues	Atoms		AltConf
47	2	3	Total	O	0
			3	3	

3 Residue-property plots

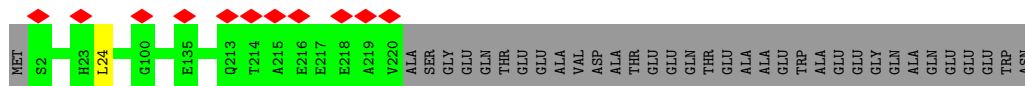
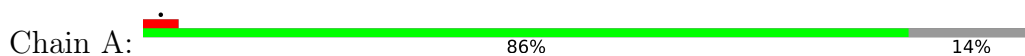
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S ribosomal RNA

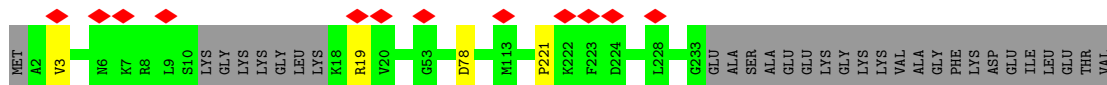
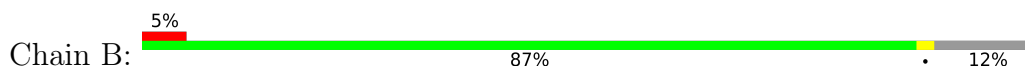




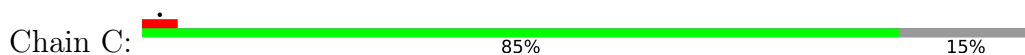
• Molecule 2: Small ribosomal subunit protein uS2

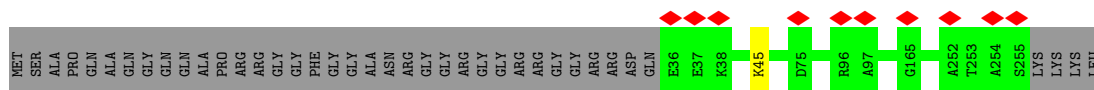


• Molecule 3: Small ribosomal subunit protein eS1

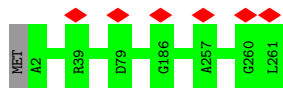


• Molecule 4: Small ribosomal subunit protein uS5

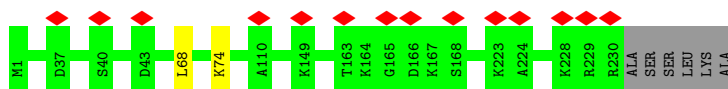




- Molecule 5: 40S ribosomal protein S4



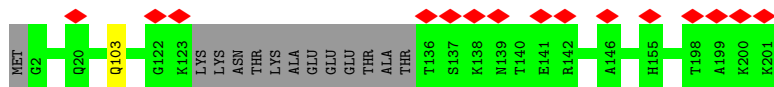
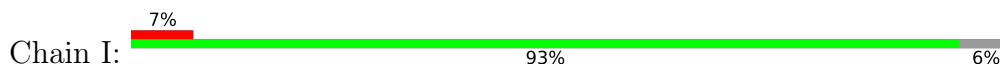
- Molecule 6: Small ribosomal subunit protein eS6



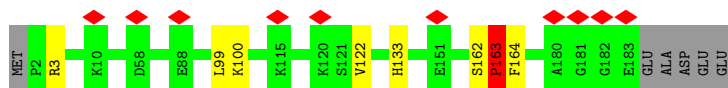
- Molecule 7: 40S ribosomal protein S7



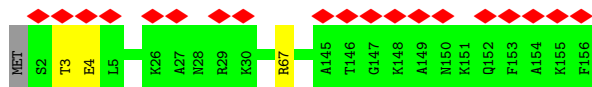
- Molecule 8: 40S ribosomal protein S8



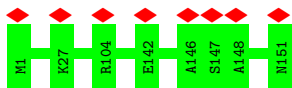
- Molecule 9: KLLA0E23673p



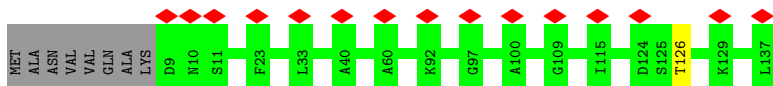
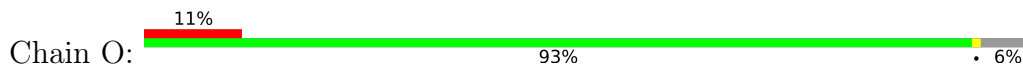
- Molecule 10: KLLA0A10483p



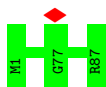
- Molecule 11: KLLA0F18040p



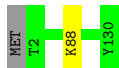
- Molecule 12: Small ribosomal subunit protein uS11



- Molecule 13: 40S ribosomal protein S21



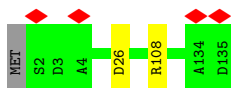
- Molecule 14: Small ribosomal subunit protein uS8



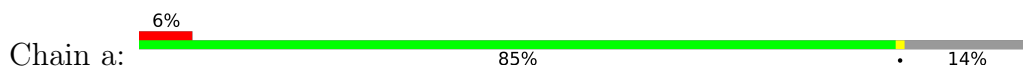
- Molecule 15: KLLA0B11231p



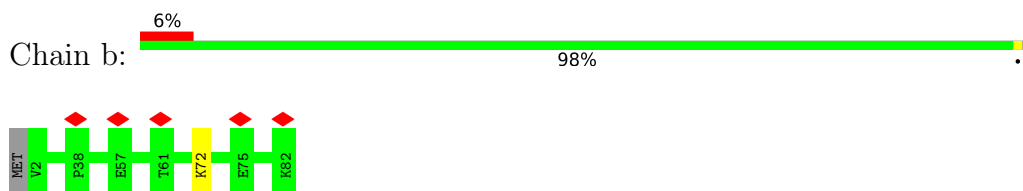
- Molecule 16: 40S ribosomal protein S24



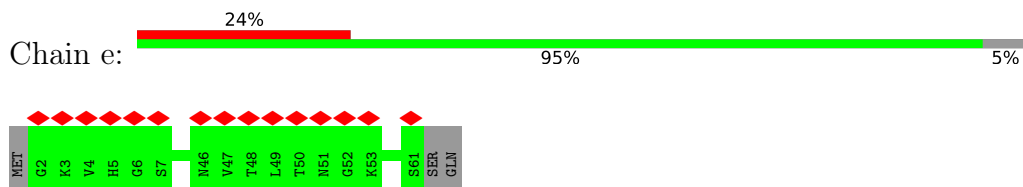
- Molecule 17: 40S ribosomal protein S26



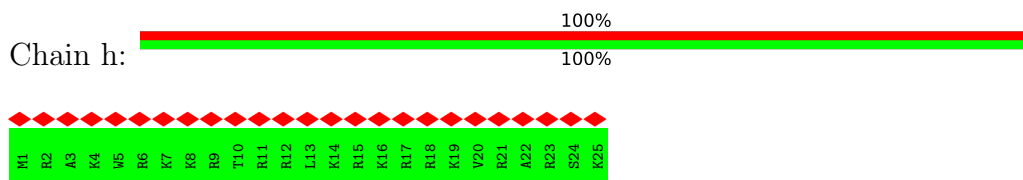
- Molecule 18: 40S ribosomal protein S27



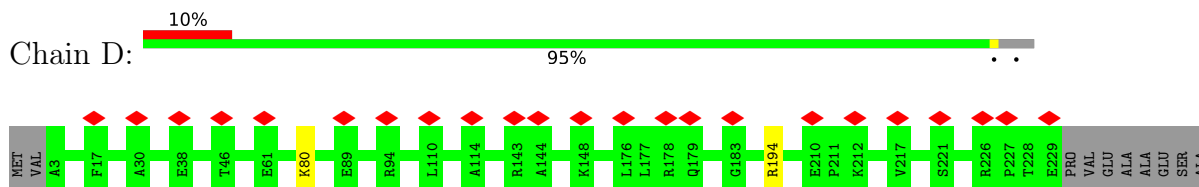
- Molecule 19: 40S ribosomal protein S30



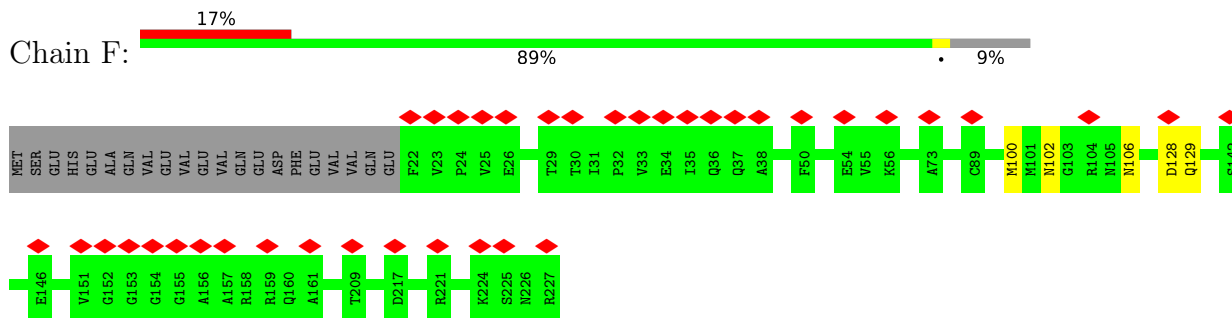
- Molecule 20: 40S ribosomal protein L41-A



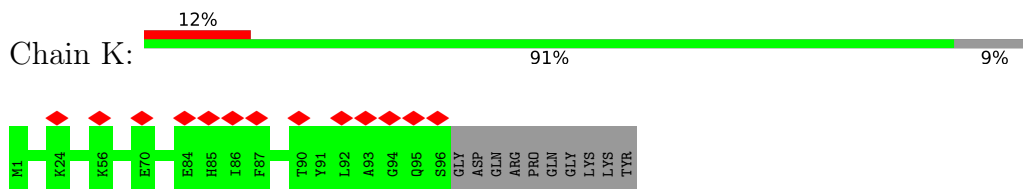
- Molecule 21: 40S ribosomal protein S3



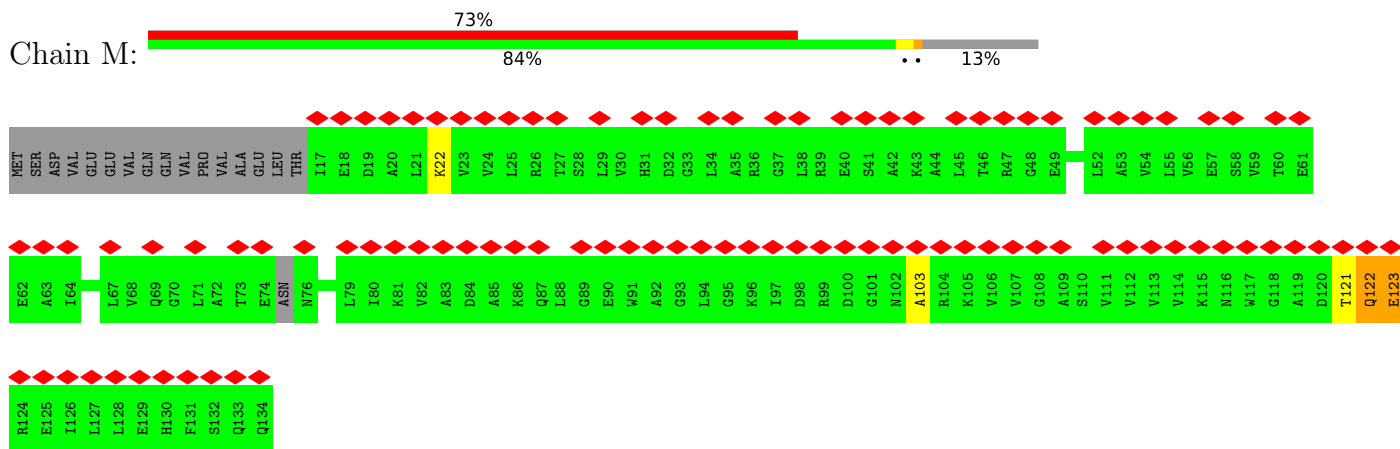
- Molecule 22: KLLA0D10659p



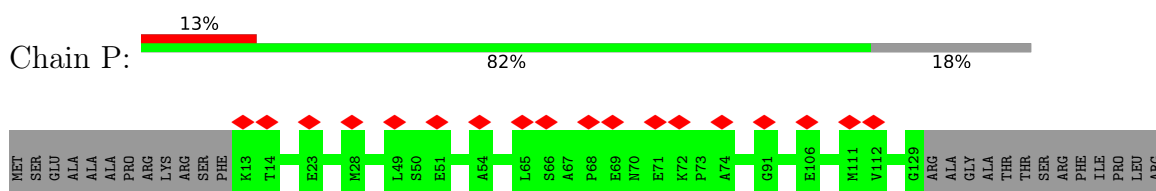
- Molecule 23: KLLA0B08173p



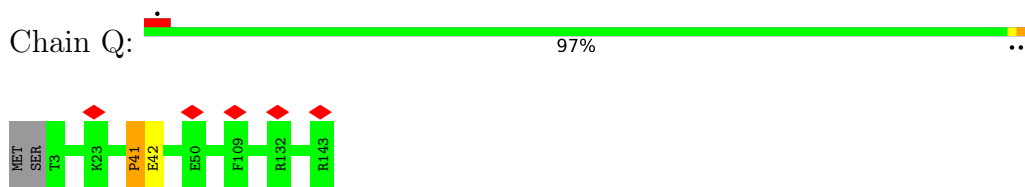
- Molecule 24: 40S ribosomal protein S12



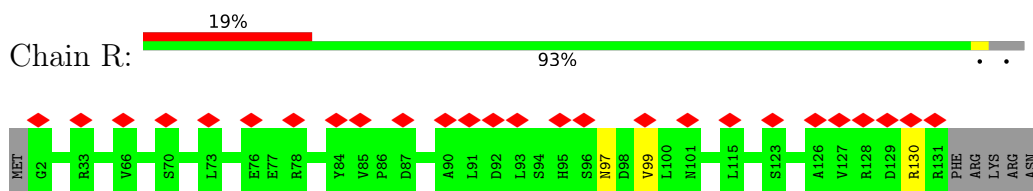
• Molecule 25: KLLA0F07843p



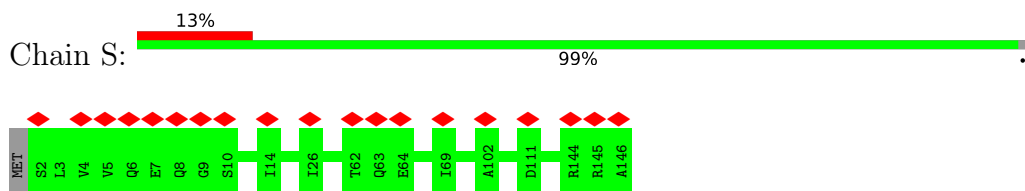
• Molecule 26: Small ribosomal subunit protein uS9



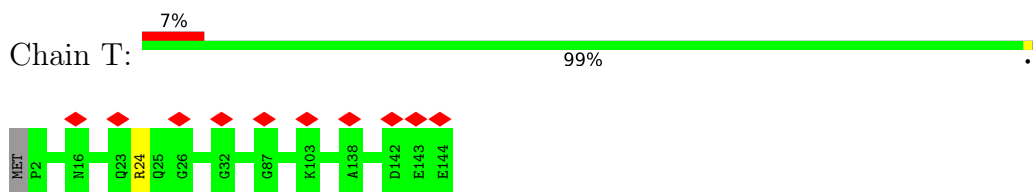
• Molecule 27: KLLA0B01474p



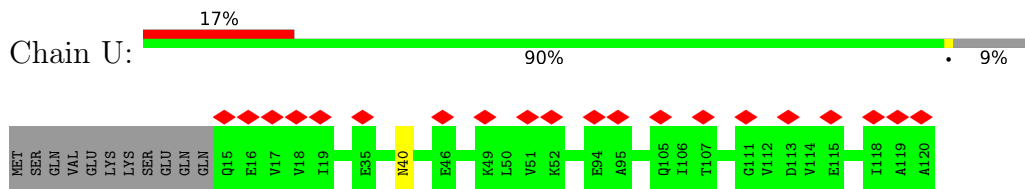
• Molecule 28: KLLA0B01562p



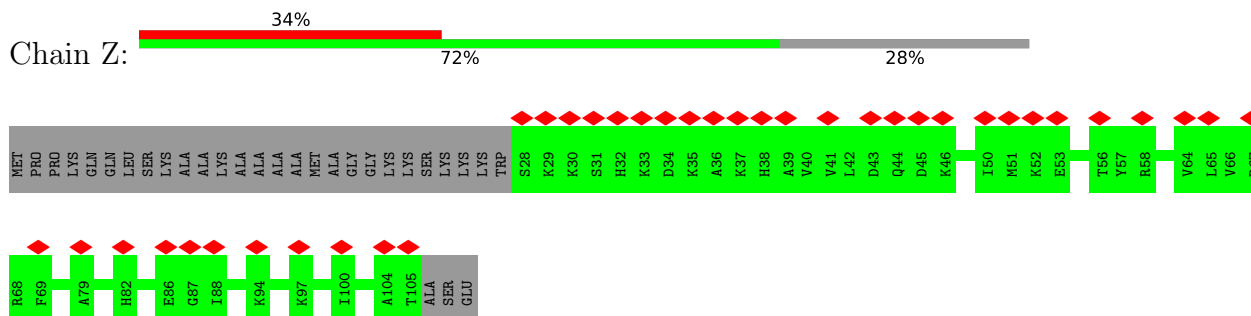
• Molecule 29: KLLA0A07194p



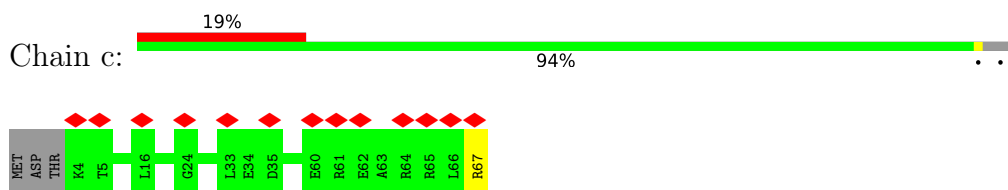
- Molecule 30: Small ribosomal subunit protein uS10



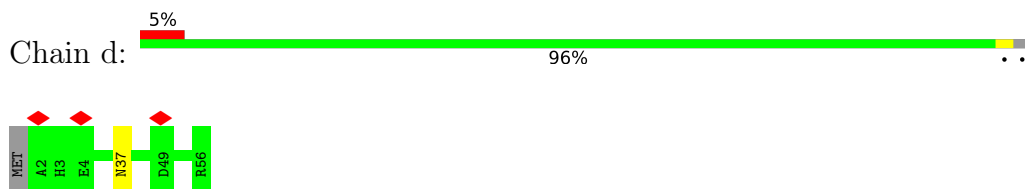
- Molecule 31: 40S ribosomal protein S25



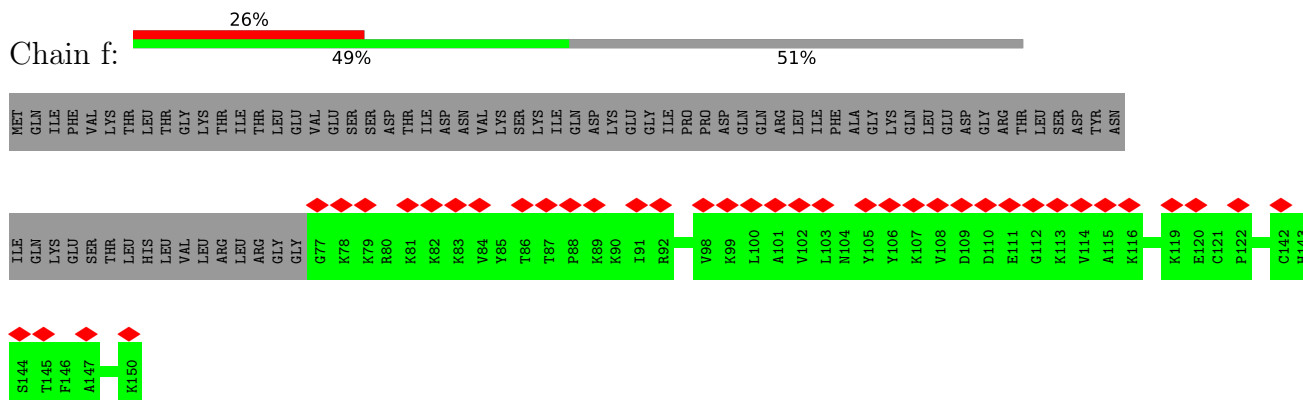
- Molecule 32: Small ribosomal subunit protein eS28



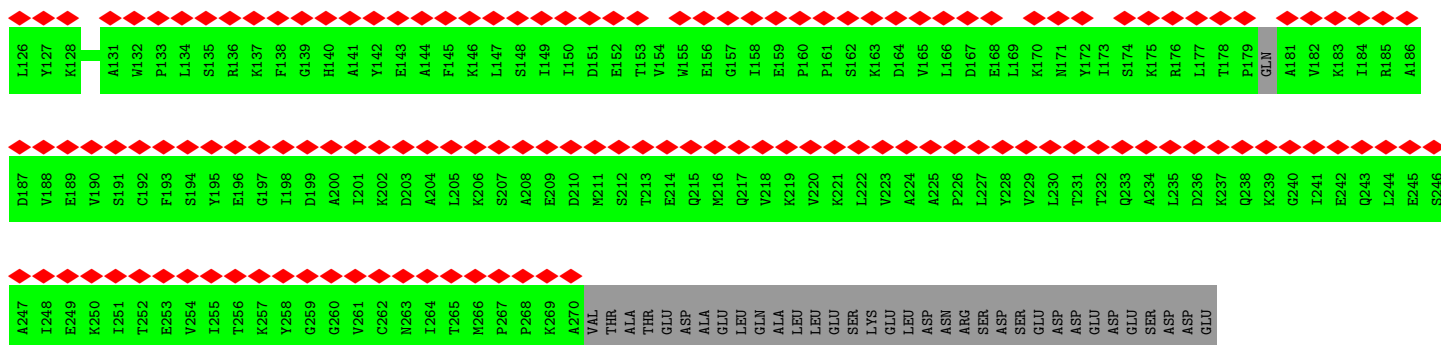
- Molecule 33: Small ribosomal subunit protein uS14



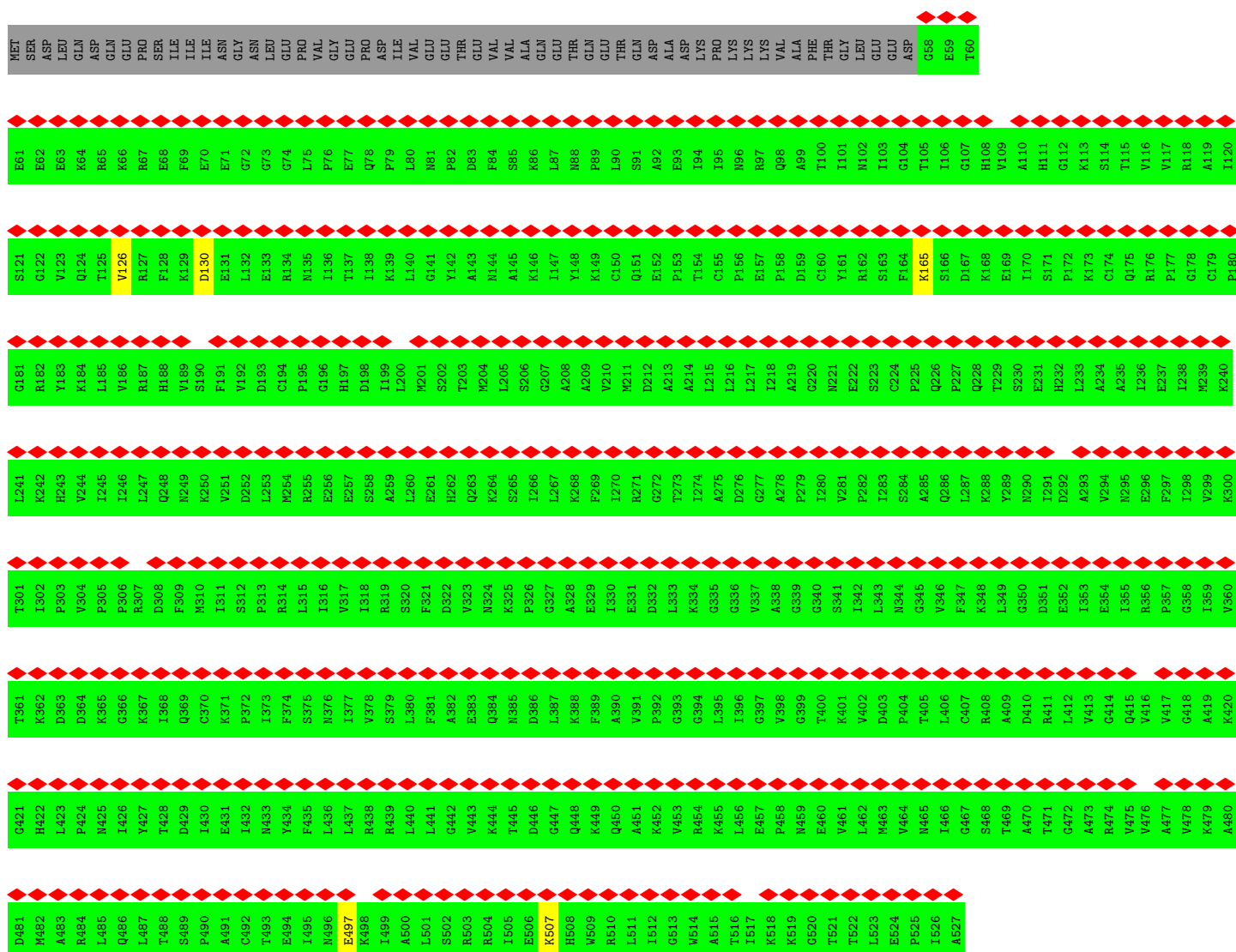
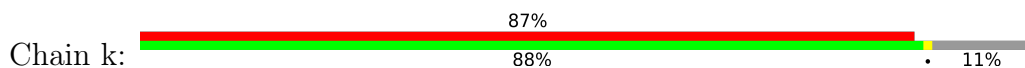
- Molecule 34: Small ribosomal subunit protein eS31



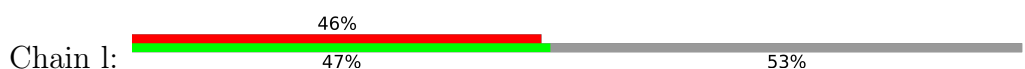
- Molecule 35: KLLA0E12277p



● Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma



● Molecule 41: Eukaryotic translation initiation factor 2 subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26818	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.330	Depositor
Minimum map value	-0.169	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: 5MC, T6A, M2G, 1MG, MG, B8N, PSU, 2MG, RIA, 1MA, ZN, 7MG, H2U, GCP, MA6

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	2	0.44	0/42201	0.89	40/65752 (0.1%)
2	A	0.32	0/1742	0.59	1/2383 (0.0%)
3	B	0.30	0/1820	0.61	1/2448 (0.0%)
4	C	0.33	0/1678	0.56	0/2277
5	E	0.33	0/2122	0.62	0/2861
6	G	0.29	0/1855	0.57	1/2479 (0.0%)
7	H	0.30	0/1507	0.61	0/2028
8	I	0.31	0/1515	0.61	0/2029
9	J	0.34	0/1495	0.68	1/2001 (0.0%)
10	L	0.36	0/1276	0.58	0/1718
11	N	0.29	0/1218	0.54	0/1638
12	O	0.29	0/966	0.64	0/1297
13	V	0.32	0/696	0.59	0/938
14	W	0.35	0/1039	0.61	0/1399
15	X	0.34	0/1137	0.60	0/1516
16	Y	0.31	0/1075	0.62	1/1433 (0.1%)
17	a	0.31	0/810	0.65	0/1087
18	b	0.27	0/619	0.56	0/837
19	e	0.29	0/480	0.56	0/640
20	h	0.25	0/234	0.75	0/300
21	D	0.29	0/1800	0.58	0/2421
22	F	0.31	0/1628	0.58	0/2198
23	K	0.32	0/831	0.53	0/1123
24	M	0.29	0/891	0.63	0/1201
25	P	0.30	0/942	0.59	0/1269
26	Q	0.33	0/1125	0.62	0/1510
27	R	0.34	0/1044	0.64	0/1402
28	S	0.28	0/1208	0.60	0/1624
29	T	0.29	0/1129	0.56	0/1520
30	U	0.30	0/857	0.59	0/1158
31	Z	0.29	0/603	0.59	0/814
32	c	0.31	0/501	0.65	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.32	0/473	0.62	0/629
34	f	0.27	0/597	0.54	0/795
35	g	0.30	0/2523	0.56	0/3434
36	i	0.27	0/773	0.59	0/1031
37	3	0.25	0/595	0.75	0/920
38	1	0.41	1/1529 (0.1%)	0.89	2/2376 (0.1%)
39	j	0.26	0/2171	0.53	0/2924
40	k	0.25	0/3657	0.51	0/4946
41	l	0.25	0/1099	0.52	0/1469
42	m	0.26	0/626	0.54	0/835
All	All	0.38	1/92087 (0.0%)	0.76	47/133333 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	1	A	OP3-P	-10.66	1.48	1.61

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1020	C	N3-C2-O2	-8.03	116.28	121.90
1	2	572	C	N3-C2-O2	-7.90	116.37	121.90
1	2	1020	C	N1-C2-O2	7.22	123.23	118.90
1	2	933	C	N1-C2-O2	7.10	123.16	118.90
1	2	694	U	C2-N1-C1'	7.08	126.19	117.70
1	2	1388	U	C2-N1-C1'	6.86	125.93	117.70
1	2	694	U	N1-C2-O2	6.85	127.59	122.80
16	Y	26	ASP	CB-CG-OD1	6.62	124.25	118.30
1	2	1388	U	N1-C2-O2	6.58	127.40	122.80
1	2	1341	C	N1-C2-O2	6.52	122.81	118.90
1	2	1341	C	C2-N1-C1'	6.51	125.96	118.80
1	2	1279	C	N3-C2-O2	-6.47	117.37	121.90
1	2	1387	C	C2-N1-C1'	6.35	125.78	118.80
9	J	163	PRO	CA-N-CD	-6.11	102.95	111.50
1	2	1388	U	N3-C2-O2	-6.07	117.95	122.20
1	2	694	U	N3-C2-O2	-6.00	118.00	122.20
3	B	78	ASP	CB-CG-OD1	5.99	123.69	118.30
1	2	933	C	N3-C2-O2	-5.91	117.76	121.90
1	2	1279	C	C6-N1-C1'	5.89	127.86	120.80
1	2	113	U	C2-N3-C4	-5.84	123.50	127.00
1	2	1331	C	N1-C2-O2	5.74	122.34	118.90
6	G	68	LEU	CA-CB-CG	5.64	128.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1015	C	C2-N1-C1'	5.56	124.92	118.80
1	2	1525	C	N1-C2-O2	5.54	122.22	118.90
1	2	1781	C	C2-N1-C1'	5.53	124.88	118.80
1	2	1341	C	C6-N1-C1'	-5.47	114.24	120.80
38	1	74	C	P-O3'-C3'	5.33	126.10	119.70
1	2	1454	C	C2-N1-C1'	5.32	124.65	118.80
1	2	275	C	N3-C2-O2	-5.31	118.18	121.90
1	2	1015	C	N1-C2-O2	5.30	122.08	118.90
2	A	24	LEU	CA-CB-CG	5.26	127.39	115.30
1	2	1797	U	OP2-P-O3'	5.22	116.68	105.20
1	2	17	C	C2-N1-C1'	5.22	124.54	118.80
1	2	223	C	C6-N1-C2	-5.16	118.23	120.30
1	2	535	C	C2-N1-C1'	5.16	124.47	118.80
1	2	933	C	C2-N1-C1'	5.13	124.45	118.80
38	1	74	C	OP2-P-O3'	5.13	116.48	105.20
1	2	223	C	OP2-P-O3'	5.12	116.47	105.20
1	2	1279	C	C6-N1-C2	-5.12	118.25	120.30
1	2	277	U	OP2-P-O3'	5.11	116.44	105.20
1	2	277	U	P-O3'-C3'	5.10	125.82	119.70
1	2	412	U	C2-N1-C1'	5.09	123.81	117.70
1	2	989	C	C2-N1-C1'	5.09	124.40	118.80
1	2	412	U	N1-C2-O2	5.08	126.36	122.80
1	2	1331	C	C2-N1-C1'	5.07	124.38	118.80
1	2	1533	U	C2-N1-C1'	5.07	123.78	117.70
1	2	582	C	C2-N1-C1'	5.06	124.36	118.80

There are no chirality outliers.

There are no planarity outliers.

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	
2	A	217/254 (85%)	193 (89%)	24 (11%)	0	100	100
3	B	221/255 (87%)	189 (86%)	31 (14%)	1 (0%)	25	63
4	C	218/259 (84%)	197 (90%)	20 (9%)	1 (0%)	25	63
5	E	258/261 (99%)	224 (87%)	34 (13%)	0	100	100
6	G	228/236 (97%)	211 (92%)	17 (8%)	0	100	100
7	H	182/190 (96%)	157 (86%)	23 (13%)	2 (1%)	12	46
8	I	184/201 (92%)	162 (88%)	22 (12%)	0	100	100
9	J	180/188 (96%)	151 (84%)	24 (13%)	5 (3%)	4	25
10	L	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	10	42
11	N	149/151 (99%)	137 (92%)	12 (8%)	0	100	100
12	O	127/137 (93%)	108 (85%)	19 (15%)	0	100	100
13	V	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
14	W	127/130 (98%)	112 (88%)	15 (12%)	0	100	100
15	X	142/145 (98%)	114 (80%)	28 (20%)	0	100	100
16	Y	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
17	a	100/119 (84%)	81 (81%)	19 (19%)	0	100	100
18	b	79/82 (96%)	66 (84%)	13 (16%)	0	100	100
19	e	58/63 (92%)	50 (86%)	8 (14%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	208 (92%)	17 (8%)	0	100	100
22	F	204/227 (90%)	182 (89%)	21 (10%)	1 (0%)	25	63
23	K	94/106 (89%)	82 (87%)	12 (13%)	0	100	100
24	M	113/134 (84%)	92 (81%)	17 (15%)	4 (4%)	3	21
25	P	115/142 (81%)	97 (84%)	18 (16%)	0	100	100
26	Q	139/143 (97%)	120 (86%)	17 (12%)	2 (1%)	9	40
27	R	128/136 (94%)	106 (83%)	21 (16%)	1 (1%)	16	53
28	S	143/146 (98%)	124 (87%)	19 (13%)	0	100	100
29	T	141/144 (98%)	128 (91%)	13 (9%)	0	100	100
30	U	104/117 (89%)	97 (93%)	7 (7%)	0	100	100
31	Z	76/108 (70%)	68 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	c	62/67 (92%)	57 (92%)	5 (8%)	0	100	100
33	d	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
34	f	72/150 (48%)	52 (72%)	20 (28%)	0	100	100
35	g	314/326 (96%)	280 (89%)	33 (10%)	1 (0%)	37	72
36	i	93/153 (61%)	81 (87%)	12 (13%)	0	100	100
39	j	263/304 (86%)	238 (90%)	25 (10%)	0	100	100
40	k	468/527 (89%)	431 (92%)	33 (7%)	4 (1%)	14	50
41	l	126/285 (44%)	122 (97%)	4 (3%)	0	100	100
42	m	73/108 (68%)	64 (88%)	9 (12%)	0	100	100
All	All	5869/6690 (88%)	5190 (88%)	655 (11%)	24 (0%)	32	67

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	66	SER
9	J	163	PRO
9	J	164	PHE
22	F	106	ASN
24	M	123	GLU
26	Q	41	PRO
26	Q	42	GLU
10	L	3	THR
40	k	130	ASP
40	k	497	GLU
40	k	507	LYS
24	M	103	ALA
24	M	122	GLN
35	g	120	SER
3	B	221	PRO
24	M	121	THR
4	C	45	LYS
10	L	4	GLU
7	H	163	ASP
9	J	133	HIS
27	R	99	VAL
9	J	122	VAL
9	J	162	SER
40	k	126	VAL

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	
2	A	180/211 (85%)	180 (100%)	0	100	100
3	B	202/228 (89%)	200 (99%)	2 (1%)	73	82
4	C	177/203 (87%)	177 (100%)	0	100	100
5	E	223/224 (100%)	223 (100%)	0	100	100
6	G	192/200 (96%)	191 (100%)	1 (0%)	86	90
7	H	164/170 (96%)	164 (100%)	0	100	100
8	I	147/159 (92%)	146 (99%)	1 (1%)	81	87
9	J	153/158 (97%)	149 (97%)	4 (3%)	41	61
10	L	136/137 (99%)	135 (99%)	1 (1%)	81	87
11	N	128/128 (100%)	128 (100%)	0	100	100
12	O	97/104 (93%)	96 (99%)	1 (1%)	73	82
13	V	73/73 (100%)	73 (100%)	0	100	100
14	W	110/111 (99%)	109 (99%)	1 (1%)	75	83
15	X	119/120 (99%)	118 (99%)	1 (1%)	79	85
16	Y	108/109 (99%)	107 (99%)	1 (1%)	75	83
17	a	83/100 (83%)	82 (99%)	1 (1%)	67	79
18	b	71/72 (99%)	70 (99%)	1 (1%)	62	76
19	e	51/55 (93%)	51 (100%)	0	100	100
20	h	23/23 (100%)	23 (100%)	0	100	100
21	D	188/196 (96%)	186 (99%)	2 (1%)	70	80
22	F	174/194 (90%)	170 (98%)	4 (2%)	45	65
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	93/109 (85%)	90 (97%)	3 (3%)	34	55
25	P	99/119 (83%)	99 (100%)	0	100	100
26	Q	117/119 (98%)	116 (99%)	1 (1%)	75	83
27	R	116/124 (94%)	114 (98%)	2 (2%)	56	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	S	127/129 (98%)	127 (100%)	0	100	100
29	T	117/118 (99%)	116 (99%)	1 (1%)	75	83
30	U	96/107 (90%)	95 (99%)	1 (1%)	73	82
31	Z	59/88 (67%)	59 (100%)	0	100	100
32	c	55/59 (93%)	54 (98%)	1 (2%)	54	72
33	d	47/48 (98%)	46 (98%)	1 (2%)	48	67
34	f	60/133 (45%)	60 (100%)	0	100	100
35	g	264/272 (97%)	260 (98%)	4 (2%)	60	75
36	i	80/130 (62%)	80 (100%)	0	100	100
39	j	239/274 (87%)	238 (100%)	1 (0%)	89	91
40	k	393/449 (88%)	392 (100%)	1 (0%)	91	92
41	l	125/246 (51%)	125 (100%)	0	100	100
42	m	69/96 (72%)	69 (100%)	0	100	100
All	All	5043/5691 (89%)	5006 (99%)	37 (1%)	80	87

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	3	VAL
3	B	19	ARG
6	G	74	LYS
8	I	103	GLN
9	J	3	ARG
9	J	99	LEU
9	J	100	LYS
9	J	163	PRO
10	L	67	ARG
12	O	126	THR
14	W	88	LYS
15	X	22	ASN
16	Y	108	ARG
17	a	42	ARG
18	b	72	LYS
21	D	80	LYS
21	D	194	ARG
22	F	100	MET
22	F	102	ASN

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Mol	Chain	Res	Type
22	F	128	ASP
22	F	129	GLN
24	M	22	LYS
24	M	122	GLN
24	M	123	GLU
26	Q	41	PRO
27	R	97	ASN
27	R	130	ARG
29	T	24	ARG
30	U	40	ASN
32	c	67	ARG
33	d	37	ASN
35	g	18	ASN
35	g	119	ASN
35	g	120	SER
35	g	121	SER
39	j	7	ARG
40	k	165	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	46	ASN
3	B	118	GLN
3	B	177	GLN
3	B	211	HIS
4	C	64	HIS
4	C	76	GLN
5	E	57	ASN
6	G	10	ASN
6	G	140	ASN
7	H	150	GLN
8	I	160	GLN
9	J	139	GLN
11	N	49	GLN
14	W	64	GLN
14	W	80	ASN
15	X	48	HIS
16	Y	106	GLN
16	Y	107	GLN
22	F	39	GLN
22	F	102	ASN

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Mol	Chain	Res	Type
22	F	118	HIS
22	F	226	ASN
23	K	17	GLN
23	K	32	HIS
23	K	58	GLN
25	P	103	ASN
26	Q	40	GLN
28	S	78	HIS
30	U	44	ASN
30	U	72	ASN
30	U	87	HIS
34	f	143	HIS
35	g	107	HIS
40	k	111	HIS
42	m	65	ASN
42	m	81	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1785/1798 (99%)	645 (36%)	26 (1%)
37	3	25/49 (51%)	16 (64%)	0
38	1	71/75 (94%)	28 (39%)	3 (4%)
All	All	1881/1922 (97%)	689 (36%)	29 (1%)

All (689) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	9	U
1	2	13	C
1	2	14	C
1	2	16	G
1	2	17	C
1	2	26	A
1	2	27	U
1	2	32	U
1	2	34	G
1	2	42	G

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Mol	Chain	Res	Type
1	2	43	A
1	2	47	A
1	2	50	C
1	2	57	G
1	2	59	C
1	2	64	U
1	2	65	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	78	A
1	2	79	C
1	2	104	A
1	2	111	U
1	2	114	C
1	2	116	U
1	2	121	U
1	2	124	A
1	2	128	U
1	2	129	U
1	2	130	C
1	2	132	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	139	C
1	2	140	A
1	2	145	U
1	2	155	A
1	2	156	A
1	2	158	U
1	2	159	C
1	2	160	U
1	2	161	A
1	2	165	C
1	2	166	U

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Mol	Chain	Res	Type
1	2	167	A
1	2	171	C
1	2	173	U
1	2	176	U
1	2	177	U
1	2	178	A
1	2	183	C
1	2	184	U
1	2	185	C
1	2	187	A
1	2	190	C
1	2	191	U
1	2	192	U
1	2	193	U
1	2	194	G
1	2	209	A
1	2	214	A
1	2	217	A
1	2	218	A
1	2	220	A
1	2	224	A
1	2	225	A
1	2	226	U
1	2	227	G
1	2	228	U
1	2	231	U
1	2	232	C
1	2	234	G
1	2	235	A
1	2	237	U
1	2	239	C
1	2	240	U
1	2	248	U
1	2	249	C
1	2	256	A
1	2	259	U
1	2	260	U
1	2	264	A
1	2	266	U
1	2	267	C
1	2	271	U
1	2	274	C

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Mol	Chain	Res	Type
1	2	275	C
1	2	276	U
1	2	278	G
1	2	280	G
1	2	289	G
1	2	296	U
1	2	298	A
1	2	300	A
1	2	301	U
1	2	307	C
1	2	308	C
1	2	311	A
1	2	313	C
1	2	315	A
1	2	319	U
1	2	321	G
1	2	334	U
1	2	336	G
1	2	337	C
1	2	349	U
1	2	358	A
1	2	359	A
1	2	360	C
1	2	369	A
1	2	382	G
1	2	389	G
1	2	390	A
1	2	399	A
1	2	400	A
1	2	401	C
1	2	403	G
1	2	412	U
1	2	415	A
1	2	416	A
1	2	417	G
1	2	418	G
1	2	421	G
1	2	422	G
1	2	423	C
1	2	424	A
1	2	425	G
1	2	427	A

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Mol	Chain	Res	Type
1	2	433	G
1	2	438	U
1	2	439	U
1	2	440	A
1	2	443	C
1	2	444	A
1	2	445	A
1	2	447	C
1	2	457	G
1	2	459	A
1	2	467	A
1	2	468	C
1	2	469	A
1	2	473	A
1	2	474	A
1	2	476	A
1	2	480	A
1	2	481	U
1	2	482	A
1	2	483	C
1	2	486	G
1	2	488	C
1	2	489	C
1	2	490	C
1	2	491	A
1	2	492	U
1	2	493	U
1	2	494	C
1	2	495	G
1	2	496	G
1	2	499	C
1	2	501	U
1	2	502	G
1	2	504	A
1	2	505	A
1	2	506	U
1	2	507	U
1	2	509	G
1	2	510	A
1	2	516	U
1	2	518	C
1	2	523	U

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Mol	Chain	Res	Type
1	2	526	A
1	2	527	U
1	2	533	A
1	2	534	A
1	2	535	C
1	2	537	A
1	2	539	G
1	2	540	A
1	2	541	A
1	2	542	C
1	2	547	G
1	2	553	C
1	2	554	A
1	2	557	U
1	2	558	C
1	2	560	G
1	2	564	C
1	2	565	C
1	2	567	G
1	2	571	C
1	2	576	G
1	2	577	U
1	2	584	A
1	2	593	A
1	2	594	G
1	2	597	U
1	2	601	U
1	2	605	A
1	2	609	G
1	2	610	U
1	2	614	A
1	2	618	A
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	G
1	2	634	A
1	2	638	U
1	2	641	G
1	2	647	G
1	2	648	U

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Mol	Chain	Res	Type
1	2	650	G
1	2	652	C
1	2	653	C
1	2	657	C
1	2	658	C
1	2	671	C
1	2	675	C
1	2	679	U
1	2	680	U
1	2	681	U
1	2	682	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	688	G
1	2	692	C
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	701	U
1	2	702	G
1	2	704	C
1	2	705	U
1	2	709	C
1	2	710	U
1	2	711	G
1	2	712	U
1	2	713	A
1	2	714	C
1	2	715	U
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	723	G
1	2	724	G
1	2	727	C
1	2	730	G
1	2	731	C

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Mol	Chain	Res	Type
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	737	A
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	745	U
1	2	753	A
1	2	755	A
1	2	763	G
1	2	765	G
1	2	766	PSU
1	2	767	U
1	2	771	A
1	2	774	A
1	2	778	G
1	2	779	A
1	2	780	A
1	2	781	A
1	2	782	G
1	2	783	C
1	2	786	G
1	2	787	A
1	2	788	A
1	2	789	U
1	2	792	A
1	2	793	U
1	2	794	U
1	2	809	G
1	2	811	A
1	2	812	U
1	2	813	A
1	2	814	G
1	2	818	G
1	2	819	U
1	2	820	U
1	2	821	U
1	2	822	G

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Mol	Chain	Res	Type
1	2	823	G
1	2	826	C
1	2	827	U
1	2	828	A
1	2	829	U
1	2	830	U
1	2	832	U
1	2	836	G
1	2	837	G
1	2	839	U
1	2	840	U
1	2	843	A
1	2	845	G
1	2	849	A
1	2	852	G
1	2	862	A
1	2	863	U
1	2	864	A
1	2	869	C
1	2	874	G
1	2	876	G
1	2	884	G
1	2	885	U
1	2	895	U
1	2	896	C
1	2	897	A
1	2	905	A
1	2	911	U
1	2	912	G
1	2	913	G
1	2	915	U
1	2	916	U
1	2	917	U
1	2	919	U
1	2	920	U
1	2	930	C
1	2	931	U
1	2	932	A
1	2	934	U
1	2	941	G
1	2	944	U
1	2	950	A

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Mol	Chain	Res	Type
1	2	958	U
1	2	959	U
1	2	963	U
1	2	965	A
1	2	966	A
1	2	969	A
1	2	970	A
1	2	972	A
1	2	973	A
1	2	982	A
1	2	985	G
1	2	986	G
1	2	987	A
1	2	991	A
1	2	992	A
1	2	995	U
1	2	997	A
1	2	998	PSU
1	2	999	C
1	2	1002	A
1	2	1008	U
1	2	1009	C
1	2	1011	U
1	2	1015	C
1	2	1016	U
1	2	1020	C
1	2	1024	A
1	2	1025	A
1	2	1026	A
1	2	1027	C
1	2	1029	A
1	2	1030	U
1	2	1031	G
1	2	1035	A
1	2	1038	A
1	2	1039	G
1	2	1041	G
1	2	1042	A
1	2	1043	U
1	2	1049	G
1	2	1050	G
1	2	1051	U

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Mol	Chain	Res	Type
1	2	1052	G
1	2	1054	U
1	2	1055	U
1	2	1057	U
1	2	1058	C
1	2	1059	U
1	2	1060	U
1	2	1062	U
1	2	1066	C
1	2	1075	A
1	2	1081	C
1	2	1082	G
1	2	1084	G
1	2	1085	A
1	2	1086	A
1	2	1091	A
1	2	1095	C
1	2	1096	U
1	2	1097	U
1	2	1099	G
1	2	1100	G
1	2	1103	U
1	2	1108	G
1	2	1110	G
1	2	1113	G
1	2	1114	U
1	2	1125	G
1	2	1137	A
1	2	1149	G
1	2	1150	A
1	2	1156	A
1	2	1157	C
1	2	1158	C
1	2	1163	G
1	2	1166	G
1	2	1170	A
1	2	1182	A
1	2	1184	U
1	2	1185	U
1	2	1187	G
1	2	1189	C
1	2	1191	C

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Mol	Chain	Res	Type
1	2	1193	A
1	2	1195	A
1	2	1198	G
1	2	1199	G
1	2	1201	A
1	2	1207	A
1	2	1211	G
1	2	1216	A
1	2	1217	G
1	2	1224	U
1	2	1227	G
1	2	1228	G
1	2	1230	U
1	2	1236	G
1	2	1237	A
1	2	1240	G
1	2	1241	A
1	2	1242	G
1	2	1243	A
1	2	1244	G
1	2	1245	C
1	2	1247	C
1	2	1249	U
1	2	1250	U
1	2	1251	C
1	2	1254	G
1	2	1256	U
1	2	1258	U
1	2	1259	U
1	2	1260	G
1	2	1268	U
1	2	1269	G
1	2	1272	G
1	2	1274	A
1	2	1275	U
1	2	1283	C
1	2	1284	U
1	2	1296	G
1	2	1298	G
1	2	1300	U
1	2	1305	C
1	2	1306	U

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Mol	Chain	Res	Type
1	2	1313	U
1	2	1314	U
1	2	1315	G
1	2	1319	U
1	2	1320	A
1	2	1321	A
1	2	1323	G
1	2	1324	A
1	2	1337	C
1	2	1339	U
1	2	1341	C
1	2	1343	A
1	2	1344	A
1	2	1345	A
1	2	1347	A
1	2	1355	U
1	2	1356	G
1	2	1359	A
1	2	1360	C
1	2	1361	U
1	2	1362	U
1	2	1363	G
1	2	1364	C
1	2	1365	C
1	2	1369	U
1	2	1370	G
1	2	1376	U
1	2	1379	U
1	2	1380	A
1	2	1388	U
1	2	1389	A
1	2	1390	U
1	2	1393	G
1	2	1396	U
1	2	1397	C
1	2	1400	G
1	2	1401	C
1	2	1407	G
1	2	1408	A
1	2	1409	A
1	2	1411	U
1	2	1412	U

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Mol	Chain	Res	Type
1	2	1413	U
1	2	1414	G
1	2	1418	C
1	2	1423	A
1	2	1424	C
1	2	1425	A
1	2	1426	2MG
1	2	1429	C
1	2	1431	G
1	2	1442	A
1	2	1443	G
1	2	1444	A
1	2	1455	C
1	2	1456	G
1	2	1457	C
1	2	1464	G
1	2	1467	A
1	2	1469	A
1	2	1471	U
1	2	1472	G
1	2	1476	G
1	2	1481	A
1	2	1482	G
1	2	1483	C
1	2	1484	G
1	2	1488	A
1	2	1489	C
1	2	1490	A
1	2	1491	A
1	2	1494	U
1	2	1498	C
1	2	1499	C
1	2	1510	G
1	2	1512	U
1	2	1513	A
1	2	1514	A
1	2	1518	U
1	2	1519	G
1	2	1521	G
1	2	1522	A
1	2	1532	G
1	2	1533	U

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Mol	Chain	Res	Type
1	2	1534	G
1	2	1535	C
1	2	1538	G
1	2	1540	G
1	2	1544	G
1	2	1546	G
1	2	1555	U
1	2	1557	A
1	2	1558	U
1	2	1565	U
1	2	1566	C
1	2	1571	A
1	2	1572	G
1	2	1573	7MG
1	2	1588	G
1	2	1595	A
1	2	1597	C
1	2	1598	A
1	2	1602	U
1	2	1603	G
1	2	1608	G
1	2	1612	A
1	2	1614	G
1	2	1617	C
1	2	1620	G
1	2	1621	C
1	2	1631	A
1	2	1632	C
1	2	1637	5MC
1	2	1644	C
1	2	1651	C
1	2	1654	U
1	2	1655	U
1	2	1656	G
1	2	1662	C
1	2	1678	G
1	2	1679	A
1	2	1685	U
1	2	1686	U
1	2	1687	A
1	2	1688	G
1	2	1689	A

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Mol	Chain	Res	Type
1	2	1691	A
1	2	1692	A
1	2	1693	G
1	2	1694	G
1	2	1695	G
1	2	1697	G
1	2	1698	C
1	2	1699	A
1	2	1700	A
1	2	1701	C
1	2	1702	U
1	2	1703	C
1	2	1705	A
1	2	1706	U
1	2	1707	C
1	2	1709	C
1	2	1710	A
1	2	1711	G
1	2	1712	A
1	2	1725	G
1	2	1734	G
1	2	1740	U
1	2	1742	A
1	2	1743	G
1	2	1748	A
1	2	1750	U
1	2	1753	A
1	2	1754	A
1	2	1755	G
1	2	1758	G
1	2	1763	A
1	2	1764	A
1	2	1766	G
1	2	1767	U
1	2	1768	U
1	2	1778	G
1	2	1781	C
1	2	1787	G
1	2	1790	G
1	2	1791	G
1	2	1792	A
1	2	1794	C

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Mol	Chain	Res	Type
1	2	1797	U
1	2	1798	A
37	3	16	U
37	3	17	C
37	3	20	A
37	3	22	U
37	3	23	A
37	3	24	U
37	3	25	A
37	3	26	A
37	3	29	A
37	3	33	C
37	3	34	U
37	3	35	C
37	3	37	U
37	3	38	C
37	3	39	U
37	3	40	C
38	1	4	G
38	1	8	U
38	1	9	1MG
38	1	13	C
38	1	14	A
38	1	15	G
38	1	16	H2U
38	1	19	G
38	1	20	A
38	1	21	A
38	1	22	G
38	1	23	C
38	1	41	C
38	1	44	A
38	1	46	7MG
38	1	47	H2U
38	1	48	5MC
38	1	49	5MC
38	1	50	U
38	1	56	C
38	1	59	A
38	1	60	A
38	1	61	C
38	1	71	C

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Mol	Chain	Res	Type
38	1	73	A
38	1	74	C
38	1	75	C
38	1	76	A

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	72	A
1	2	74	U
1	2	216	A
1	2	217	A
1	2	226	U
1	2	239	C
1	2	277	U
1	2	279	U
1	2	649	U
1	2	670	G
1	2	695	U
1	2	700	C
1	2	781	A
1	2	828	A
1	2	930	C
1	2	998	PSU
1	2	1080	A
1	2	1198	G
1	2	1206	C
1	2	1343	A
1	2	1430	U
1	2	1470	C
1	2	1513	A
1	2	1571	A
1	2	1765	G
1	2	1797	U
38	1	8	U
38	1	48	5MC
38	1	74	C

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

23 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	5MC	1	48	38	18,22,23	3.58	7 (38%)	26,32,35	1.11	1 (3%)
38	7MG	1	46	38	22,26,27	3.87	10 (45%)	29,39,42	2.03	9 (31%)
1	5MC	2	1006	1	18,22,23	3.53	7 (38%)	26,32,35	1.03	3 (11%)
38	2MG	1	10	38	18,26,27	2.50	7 (38%)	16,38,41	1.30	3 (18%)
38	H2U	1	16	38	18,21,22	3.01	4 (22%)	21,30,33	1.93	5 (23%)
38	5MC	1	49	38	18,22,23	3.63	7 (38%)	26,32,35	1.04	1 (3%)
1	7MG	2	1573	1	22,26,27	3.72	10 (45%)	29,39,42	2.03	9 (31%)
1	PSU	2	766	1	18,21,22	4.19	8 (44%)	22,30,33	1.99	6 (27%)
1	PSU	2	120	1	18,21,22	4.28	7 (38%)	22,30,33	1.88	5 (22%)
38	H2U	1	47	38	18,21,22	3.10	4 (22%)	21,30,33	1.88	4 (19%)
38	T6A	1	37	38	27,34,35	2.05	7 (25%)	29,49,52	2.14	8 (27%)
1	5MC	2	1637	1	18,22,23	3.50	7 (38%)	26,32,35	1.15	2 (7%)
38	1MG	1	9	38	18,26,27	2.99	6 (33%)	19,39,42	1.53	3 (15%)
38	M2G	1	26	38	20,27,28	3.81	8 (40%)	22,40,43	1.35	5 (22%)
38	1MA	1	58	38	16,25,26	4.40	4 (25%)	18,37,40	1.70	3 (16%)
1	MA6	2	1780	1	18,26,27	1.04	2 (11%)	19,38,41	3.52	2 (10%)
1	PSU	2	1289	1	18,21,22	4.26	7 (38%)	22,30,33	1.70	3 (13%)
1	2MG	2	1570	1	18,26,27	2.45	7 (38%)	16,38,41	1.49	4 (25%)
1	B8N	2	1190	1	24,29,30	3.03	7 (29%)	29,42,45	1.77	6 (20%)
1	PSU	2	998	1	18,21,22	4.18	8 (44%)	22,30,33	1.86	5 (22%)
1	PSU	2	465	1	18,21,22	4.19	7 (38%)	22,30,33	1.78	5 (22%)
1	2MG	2	1426	43,1	18,26,27	2.48	7 (38%)	16,38,41	1.40	3 (18%)
38	RIA	1	64	38	31,38,39	5.07	12 (38%)	39,57,60	1.99	5 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
38	7MG	1	46	38	-	1/7/37/38	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
38	2MG	1	10	38	-	0/5/27/28	0/3/3/3
38	H2U	1	16	38	-	7/7/38/39	0/2/2/2
38	5MC	1	49	38	-	2/7/25/26	0/2/2/2
1	7MG	2	1573	1	-	2/7/37/38	0/3/3/3
1	PSU	2	766	1	-	2/7/25/26	0/2/2/2
1	PSU	2	120	1	-	0/7/25/26	0/2/2/2
38	H2U	1	47	38	-	5/7/38/39	0/2/2/2
38	T6A	1	37	38	-	2/19/41/42	0/3/3/3
1	5MC	2	1637	1	-	3/7/25/26	0/2/2/2
38	1MG	1	9	38	-	2/3/25/26	0/3/3/3
38	M2G	1	26	38	-	2/7/29/30	0/3/3/3
38	1MA	1	58	38	-	2/3/25/26	0/3/3/3
1	MA6	2	1780	1	-	2/7/29/30	0/3/3/3
1	PSU	2	1289	1	-	0/7/25/26	0/2/2/2
1	2MG	2	1570	1	-	1/5/27/28	0/3/3/3
1	B8N	2	1190	1	-	2/16/34/35	0/2/2/2
1	PSU	2	998	1	-	4/7/25/26	0/2/2/2
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
1	2MG	2	1426	43,1	-	0/5/27/28	0/3/3/3
38	RIA	1	64	38	-	8/13/51/52	0/4/4/4

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C1'-C2'	-16.25	1.32	1.52
38	1	58	1MA	C2-N3	15.88	1.48	1.29
38	1	64	RIA	O4'-C1A	15.56	1.62	1.41
38	1	26	M2G	C2-N3	13.27	1.46	1.30
1	2	1289	PSU	C6-C5	11.05	1.48	1.35
1	2	120	PSU	C6-C5	11.02	1.48	1.35
1	2	465	PSU	C6-C5	10.92	1.48	1.35
38	1	64	RIA	O1'-C1'	10.83	1.61	1.41
1	2	766	PSU	C6-C5	10.72	1.47	1.35
1	2	998	PSU	C6-C5	10.64	1.47	1.35
38	1	46	7MG	C8-N9	9.87	1.51	1.46
38	1	47	H2U	C2-N1	9.68	1.49	1.35
1	2	120	PSU	C2-N1	9.67	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1289	PSU	C2-N1	9.54	1.49	1.36
1	2	1573	7MG	C8-N9	9.53	1.51	1.46
1	2	766	PSU	C2-N1	9.47	1.49	1.36
38	1	16	H2U	C2-N1	9.37	1.49	1.35
1	2	465	PSU	C2-N1	9.35	1.49	1.36
1	2	998	PSU	C2-N1	9.27	1.49	1.36
38	1	48	5MC	C6-C5	9.21	1.49	1.34
38	1	49	5MC	C6-C5	9.16	1.49	1.34
1	2	1637	5MC	C6-C5	8.94	1.49	1.34
1	2	1006	5MC	C6-C5	8.91	1.49	1.34
38	1	9	1MG	C2-N2	8.82	1.50	1.34
1	2	1190	B8N	C6-N1	8.14	1.56	1.36
38	1	46	7MG	C5-N7	7.95	1.44	1.35
1	2	1190	B8N	C4-N3	-7.40	1.26	1.40
1	2	998	PSU	C2-N3	7.30	1.50	1.37
1	2	120	PSU	C2-N3	7.24	1.49	1.37
1	2	766	PSU	C2-N3	7.19	1.49	1.37
1	2	1289	PSU	C2-N3	7.14	1.49	1.37
1	2	1573	7MG	C5-N7	7.07	1.43	1.35
1	2	465	PSU	C2-N3	7.06	1.49	1.37
38	1	49	5MC	C4-N3	6.64	1.45	1.34
38	1	64	RIA	O1'-C4'	-6.54	1.30	1.45
38	1	47	H2U	C2-N3	6.50	1.49	1.38
38	1	48	5MC	C4-N3	6.46	1.45	1.34
1	2	1006	5MC	C4-N3	6.46	1.45	1.34
38	1	64	RIA	O4'-C4A	-6.30	1.30	1.45
38	1	49	5MC	C2-N3	6.27	1.49	1.36
38	1	16	H2U	C2-N3	6.24	1.49	1.38
38	1	26	M2G	C2-N2	6.19	1.47	1.35
1	2	1637	5MC	C4-N3	6.13	1.44	1.34
1	2	1006	5MC	C2-N3	6.11	1.48	1.36
38	1	48	5MC	C2-N3	6.05	1.48	1.36
38	1	37	T6A	C10-N11	6.05	1.48	1.35
1	2	1573	7MG	C2-N3	6.00	1.47	1.33
38	1	46	7MG	C2-N3	5.94	1.47	1.33
1	2	1637	5MC	C2-N3	5.92	1.48	1.36
1	2	1190	B8N	C2-N1	5.62	1.55	1.39
38	1	10	2MG	C2-N2	5.61	1.45	1.33
1	2	1573	7MG	C4-N9	5.58	1.44	1.37
38	1	46	7MG	C4-N3	5.56	1.47	1.34
38	1	9	1MG	C2-N3	5.49	1.44	1.34
1	2	1573	7MG	C4-N3	5.48	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	46	7MG	C4-N9	5.46	1.44	1.37
1	2	120	PSU	C6-N1	5.41	1.45	1.36
38	1	58	1MA	C2-N1	5.37	1.45	1.35
1	2	1289	PSU	C6-N1	5.34	1.45	1.36
1	2	1426	2MG	C2-N2	5.34	1.45	1.33
38	1	37	T6A	C10-N6	5.32	1.48	1.37
1	2	1570	2MG	C2-N2	5.25	1.45	1.33
1	2	465	PSU	C6-N1	5.17	1.44	1.36
38	1	26	M2G	C4-N3	5.12	1.49	1.37
1	2	1190	B8N	C6-C5	5.10	1.42	1.34
1	2	766	PSU	C6-N1	5.07	1.44	1.36
1	2	998	PSU	C6-N1	5.04	1.44	1.36
38	1	47	H2U	C4-N3	5.02	1.46	1.37
38	1	10	2MG	C4-N3	5.01	1.49	1.37
38	1	46	7MG	C2-N2	4.91	1.45	1.34
1	2	1570	2MG	C4-N3	4.86	1.49	1.37
38	1	16	H2U	C4-N3	4.84	1.45	1.37
1	2	1570	2MG	C2-N1	4.79	1.44	1.36
38	1	9	1MG	C4-N3	4.74	1.48	1.37
1	2	1426	2MG	C2-N1	4.74	1.44	1.36
1	2	1426	2MG	C4-N3	4.71	1.48	1.37
38	1	10	2MG	C2-N1	4.70	1.44	1.36
38	1	48	5MC	C6-N1	4.63	1.46	1.38
1	2	1573	7MG	C2-N2	4.63	1.45	1.34
1	2	1190	B8N	C1'-C5	-4.55	1.39	1.50
38	1	49	5MC	C6-N1	4.54	1.45	1.38
38	1	49	5MC	C2-N1	4.49	1.49	1.40
1	2	1637	5MC	C2-N1	4.43	1.49	1.40
38	1	49	5MC	C4-N4	4.40	1.45	1.34
1	2	1006	5MC	C4-N4	4.38	1.45	1.34
1	2	1637	5MC	C6-N1	4.37	1.45	1.38
1	2	1006	5MC	C6-N1	4.35	1.45	1.38
38	1	37	T6A	C6-N6	4.32	1.43	1.36
1	2	1637	5MC	C4-N4	4.26	1.45	1.34
38	1	48	5MC	C4-N4	4.24	1.45	1.34
38	1	48	5MC	C2-N1	4.19	1.49	1.40
38	1	64	RIA	C6-N6	4.19	1.49	1.34
38	1	58	1MA	C4-N3	4.15	1.50	1.37
1	2	1006	5MC	C2-N1	3.99	1.48	1.40
38	1	26	M2G	C6-N1	3.95	1.43	1.37
1	2	998	PSU	C4-N3	3.87	1.46	1.38
38	1	46	7MG	C2-N1	3.81	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1289	PSU	C4-N3	3.74	1.45	1.38
1	2	120	PSU	C4-N3	3.73	1.45	1.38
1	2	465	PSU	C4-N3	3.73	1.45	1.38
38	1	9	1MG	O6-C6	-3.73	1.15	1.22
1	2	1426	2MG	C6-N1	3.63	1.43	1.37
1	2	766	PSU	C4-N3	3.62	1.45	1.38
1	2	1573	7MG	C2-N1	3.62	1.46	1.37
1	2	1570	2MG	C6-N1	3.52	1.43	1.37
38	1	46	7MG	C5-C6	3.52	1.52	1.43
38	1	10	2MG	C6-N1	3.39	1.42	1.37
1	2	1573	7MG	C5-C6	3.39	1.52	1.43
38	1	26	M2G	C2-N1	3.33	1.45	1.36
38	1	46	7MG	C6-N1	3.32	1.45	1.38
38	1	26	M2G	C5-C6	3.26	1.54	1.47
38	1	64	RIA	O3A-C3A	-3.24	1.35	1.43
38	1	64	RIA	O2'-C2'	3.21	1.50	1.43
1	2	1426	2MG	C5-C6	3.09	1.53	1.47
1	2	1006	5MC	O2-C2	-2.96	1.18	1.23
1	2	1573	7MG	C6-N1	2.95	1.44	1.38
38	1	10	2MG	C5-C6	2.94	1.53	1.47
1	2	1570	2MG	C5-C6	2.92	1.53	1.47
38	1	64	RIA	O2A-C2A	2.91	1.51	1.43
1	2	1637	5MC	O2-C2	-2.88	1.18	1.23
38	1	48	5MC	O2-C2	-2.82	1.18	1.23
38	1	64	RIA	C2-N3	2.81	1.36	1.32
1	2	1780	MA6	C5-C4	-2.71	1.33	1.40
38	1	49	5MC	O2-C2	-2.68	1.18	1.23
1	2	766	PSU	O4-C4	-2.67	1.18	1.23
1	2	998	PSU	O4-C4	-2.65	1.18	1.23
1	2	1426	2MG	C5-C4	-2.62	1.36	1.43
1	2	1289	PSU	O4-C4	-2.60	1.18	1.23
1	2	465	PSU	O4-C4	-2.59	1.18	1.23
1	2	1573	7MG	O6-C6	-2.58	1.18	1.23
1	2	120	PSU	O4-C4	-2.57	1.18	1.23
1	2	1570	2MG	C5-C4	-2.54	1.36	1.43
38	1	64	RIA	O3'-C3'	-2.51	1.37	1.43
38	1	46	7MG	O6-C6	-2.50	1.18	1.23
38	1	10	2MG	C5-C4	-2.47	1.36	1.43
38	1	16	H2U	O2-C2	-2.43	1.18	1.23
1	2	1780	MA6	C2-N3	2.41	1.36	1.32
38	1	47	H2U	O2-C2	-2.40	1.18	1.23
1	2	1426	2MG	O6-C6	-2.38	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	26	M2G	C5-C4	-2.38	1.37	1.43
1	2	1190	B8N	O4'-C1'	-2.31	1.40	1.43
1	2	998	PSU	O4'-C1'	-2.28	1.40	1.43
1	2	465	PSU	O2-C2	-2.26	1.18	1.23
1	2	766	PSU	O4'-C1'	-2.26	1.40	1.43
38	1	9	1MG	C5-C6	2.24	1.54	1.47
1	2	1570	2MG	O6-C6	-2.24	1.18	1.23
1	2	1289	PSU	O2-C2	-2.22	1.18	1.23
1	2	120	PSU	O2-C2	-2.21	1.18	1.23
1	2	766	PSU	O2-C2	-2.21	1.18	1.23
38	1	10	2MG	O6-C6	-2.20	1.18	1.23
38	1	37	T6A	C5-C4	-2.19	1.35	1.40
38	1	9	1MG	C5-C4	-2.19	1.37	1.43
1	2	998	PSU	O2-C2	-2.17	1.18	1.23
38	1	64	RIA	P'-O5'	2.16	1.67	1.60
38	1	37	T6A	ODA-C13	2.11	1.28	1.22
38	1	58	1MA	CM1-N1	-2.08	1.42	1.46
38	1	37	T6A	O10-C10	-2.05	1.19	1.23
1	2	1190	B8N	O2-C2	-2.05	1.18	1.22
38	1	37	T6A	C2-N3	2.04	1.35	1.32
38	1	26	M2G	O6-C6	-2.02	1.19	1.23

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-14.08	102.23	117.06
38	1	64	RIA	C5-C6-N6	7.61	131.92	120.35
38	1	16	H2U	C4-N3-C2	-6.56	120.35	125.79
38	1	47	H2U	C4-N3-C2	-6.40	120.48	125.79
38	1	37	T6A	N3-C2-N1	-5.94	119.39	128.68
1	2	1780	MA6	N3-C2-N1	-5.64	119.87	128.68
38	1	37	T6A	C2-N1-C6	5.55	121.35	116.59
38	1	64	RIA	N3-C2-N1	-5.54	120.02	128.68
38	1	64	RIA	N6-C6-N1	-5.35	107.46	118.57
1	2	1190	B8N	C5-C4-N3	5.05	125.53	116.17
38	1	46	7MG	C5-C6-N1	5.02	119.83	110.99
1	2	766	PSU	C4-N3-C2	-4.96	119.20	126.34
1	2	1573	7MG	C5-C6-N1	4.90	119.63	110.99
38	1	58	1MA	N1-C2-N3	-4.90	120.31	126.02
1	2	120	PSU	C4-N3-C2	-4.77	119.47	126.34
1	2	465	PSU	C4-N3-C2	-4.64	119.66	126.34
1	2	1289	PSU	C4-N3-C2	-4.52	119.83	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1	37	T6A	C12-N11-C10	4.50	129.43	121.94
1	2	998	PSU	C4-N3-C2	-4.45	119.92	126.34
1	2	1573	7MG	C5-C4-N3	-4.45	119.66	128.13
1	2	1190	B8N	C4-N3-C2	-4.44	119.85	125.46
1	2	766	PSU	N1-C2-N3	4.38	120.09	115.13
38	1	46	7MG	C2-N3-C4	4.38	120.10	112.30
38	1	48	5MC	C5-C6-N1	-4.33	118.88	123.34
1	2	120	PSU	N1-C2-N3	4.22	119.92	115.13
38	1	9	1MG	C5-C6-N1	4.15	120.15	113.90
1	2	1573	7MG	C2-N3-C4	4.13	119.66	112.30
1	2	465	PSU	N1-C2-N3	4.07	119.74	115.13
38	1	58	1MA	C5-C6-N1	4.06	119.95	113.90
38	1	46	7MG	C5-C4-N3	-4.04	120.43	128.13
1	2	998	PSU	N1-C2-N3	3.87	119.52	115.13
1	2	1289	PSU	N1-C2-N3	3.84	119.48	115.13
1	2	766	PSU	C6-C5-C4	3.72	120.80	118.20
1	2	1426	2MG	C5-C6-N1	3.56	120.23	113.95
38	1	10	2MG	C5-C6-N1	3.36	119.88	113.95
1	2	1570	2MG	C5-C6-N1	3.34	119.85	113.95
38	1	26	M2G	C5-C6-N1	3.28	119.74	113.95
1	2	998	PSU	C6-N1-C2	-3.27	119.34	122.68
1	2	120	PSU	C6-C5-C4	3.24	120.47	118.20
38	1	16	H2U	N3-C2-N1	3.22	120.06	116.65
38	1	9	1MG	C8-N7-C5	3.16	109.01	102.99
1	2	1637	5MC	C5-C6-N1	-3.15	120.09	123.34
1	2	1573	7MG	C2-N1-C6	-3.15	119.36	125.10
38	1	46	7MG	C4-C5-N7	3.14	109.89	105.53
1	2	1573	7MG	C5-C4-N9	3.10	110.37	106.35
38	1	64	RIA	C1 ² -O2A-C2A	-3.09	110.32	117.96
1	2	1573	7MG	C4-C5-N7	3.09	109.82	105.53
38	1	46	7MG	C5-C4-N9	3.08	110.34	106.35
1	2	1573	7MG	N9-C4-N3	3.01	129.97	125.47
38	1	37	T6A	N6-C10-N11	3.01	117.96	113.76
1	2	1190	B8N	N3-C2-N1	3.01	121.01	116.76
1	2	1570	2MG	CM2-N2-C2	-2.90	117.45	123.86
38	1	47	H2U	N3-C2-N1	2.89	119.71	116.65
1	2	1190	B8N	O4-C4-N3	-2.84	115.15	119.98
38	1	46	7MG	O6-C6-C5	-2.83	120.60	127.54
38	1	46	7MG	C2-N1-C6	-2.82	119.96	125.10
38	1	47	H2U	C5-C6-N1	2.77	120.74	111.61
1	2	120	PSU	C6-N1-C2	-2.75	119.87	122.68
38	1	37	T6A	N6-C6-N1	2.74	122.39	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1570	2MG	C8-N7-C5	2.70	108.14	102.99
38	1	58	1MA	C8-N7-C5	2.69	108.12	102.99
38	1	47	H2U	C5-C4-N3	2.67	119.65	116.65
1	2	766	PSU	C6-N1-C2	-2.66	119.97	122.68
38	1	10	2MG	C8-N7-C5	2.64	108.01	102.99
1	2	465	PSU	C6-N1-C2	-2.62	120.01	122.68
1	2	1573	7MG	O6-C6-C5	-2.61	121.14	127.54
38	1	26	M2G	C2-N1-C6	-2.59	119.41	123.71
38	1	26	M2G	C8-N7-C5	2.58	107.91	102.99
1	2	1426	2MG	C8-N7-C5	2.57	107.88	102.99
38	1	16	H2U	C5-C6-N1	2.56	120.04	111.61
38	1	37	T6A	C13-C12-N11	-2.56	104.70	110.28
1	2	1006	5MC	CM5-C5-C6	-2.55	119.45	122.85
1	2	1289	PSU	C6-N1-C2	-2.54	120.09	122.68
1	2	998	PSU	O2-C2-N1	-2.52	120.01	122.79
38	1	46	7MG	N9-C4-N3	2.52	129.23	125.47
38	1	26	M2G	N1-C2-N2	2.51	120.17	118.04
38	1	16	H2U	C5-C4-N3	2.46	119.41	116.65
38	1	16	H2U	O2-C2-N1	-2.45	120.03	123.11
1	2	1637	5MC	O2-C2-N3	-2.41	118.42	122.33
1	2	766	PSU	O2-C2-N1	-2.39	120.16	122.79
38	1	37	T6A	C1'-N9-C4	-2.37	122.48	126.64
1	2	1570	2MG	O6-C6-C5	-2.34	119.81	124.37
38	1	46	7MG	N9-C8-N7	2.31	106.68	103.38
1	2	465	PSU	C6-C5-C4	2.31	119.81	118.20
1	2	1190	B8N	O4'-C1'-C2'	2.30	108.39	105.14
1	2	465	PSU	O2-C2-N1	-2.28	120.28	122.79
1	2	1426	2MG	O6-C6-C5	-2.28	119.93	124.37
38	1	26	M2G	O6-C6-C5	-2.27	119.95	124.37
1	2	1573	7MG	N9-C8-N7	2.26	106.61	103.38
38	1	64	RIA	C1'-C2'-C3'	2.24	105.14	102.30
1	2	998	PSU	O4'-C1'-C2'	2.24	108.31	105.14
38	1	10	2MG	O6-C6-C5	-2.23	120.02	124.37
38	1	49	5MC	C5-C4-N3	-2.22	119.28	121.67
1	2	766	PSU	O4'-C1'-C2'	2.12	108.14	105.14
38	1	9	1MG	O6-C6-C5	-2.11	120.46	124.19
1	2	1006	5MC	C5-C4-N3	-2.07	119.44	121.67
38	1	37	T6A	O10-C10-N6	-2.05	120.16	123.62
1	2	1006	5MC	C5-C6-N1	-2.03	121.25	123.34
1	2	1190	B8N	C31-N3-C2	2.02	120.70	117.67
1	2	120	PSU	O2-C2-N1	-2.02	120.57	122.79

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	766	PSU	C3'-C4'-C5'-O5'
1	2	1190	B8N	O4'-C4'-C5'-O5'
1	2	1190	B8N	C3'-C4'-C5'-O5'
1	2	1637	5MC	O4'-C4'-C5'-O5'
38	1	9	1MG	O4'-C4'-C5'-O5'
38	1	9	1MG	C3'-C4'-C5'-O5'
38	1	16	H2U	C4'-C5'-O5'-P
38	1	16	H2U	C3'-C4'-C5'-O5'
38	1	16	H2U	O4'-C1'-N1-C6
38	1	49	5MC	O4'-C4'-C5'-O5'
38	1	64	RIA	C2'-C1'-O2A-C2A
38	1	64	RIA	C5'-O5'-P'-O1X
1	2	766	PSU	O4'-C4'-C5'-O5'
1	2	1637	5MC	C3'-C4'-C5'-O5'
38	1	47	H2U	O4'-C4'-C5'-O5'
38	1	47	H2U	C3'-C4'-C5'-O5'
38	1	48	5MC	O4'-C4'-C5'-O5'
38	1	48	5MC	C3'-C4'-C5'-O5'
38	1	49	5MC	C3'-C4'-C5'-O5'
38	1	37	T6A	C13-C12-N11-C10
1	2	1573	7MG	C3'-C4'-C5'-O5'
38	1	16	H2U	O4'-C4'-C5'-O5'
38	1	58	1MA	O4'-C4'-C5'-O5'
38	1	58	1MA	C3'-C4'-C5'-O5'
38	1	16	H2U	C2'-C1'-N1-C6
1	2	1573	7MG	O4'-C4'-C5'-O5'
38	1	26	M2G	C3'-C4'-C5'-O5'
38	1	64	RIA	O1'-C1'-O2A-C2A
1	2	998	PSU	O4'-C4'-C5'-O5'
38	1	16	H2U	C2'-C1'-N1-C2
38	1	48	5MC	C4'-C5'-O5'-P
38	1	37	T6A	C14-C12-N11-C10
1	2	1780	MA6	O4'-C4'-C5'-O5'
1	2	998	PSU	C3'-C4'-C5'-O5'
38	1	64	RIA	C3'-C4'-C5'-O5'
38	1	46	7MG	C4'-C5'-O5'-P
38	1	47	H2U	C2'-C1'-N1-C6
38	1	16	H2U	O4'-C1'-N1-C2
38	1	26	M2G	O4'-C4'-C5'-O5'
38	1	64	RIA	C3A-C2A-O2A-C1'
38	1	47	H2U	C4'-C5'-O5'-P
1	2	998	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	1	64	RIA	C5'-O5'-P'-O2X
38	1	64	RIA	C1A-C2A-O2A-C1'
1	2	1637	5MC	C2'-C1'-N1-C2
1	2	1780	MA6	C3'-C4'-C5'-O5'
1	2	998	PSU	O4'-C1'-C5-C6
38	1	64	RIA	O1'-C4'-C5'-O5'
38	1	47	H2U	C2'-C1'-N1-C2
1	2	1570	2MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 123 ligands modelled in this entry, 121 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$
46	MET	k	602	-	6,7,8	0.52	0	2,7,9	0.10	0
45	GCP	k	601	-	27,34,34	1.53	6 (22%)	34,54,54	1.95	8 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	MET	k	602	-	-	1/5/6/8	-
45	GCP	k	601	-	-	0/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	k	601	GCP	C5-C6	4.24	1.48	1.41
45	k	601	GCP	PG-O3G	2.87	1.61	1.54
45	k	601	GCP	PG-O2G	2.83	1.61	1.54
45	k	601	GCP	PB-O3A	2.81	1.61	1.58
45	k	601	GCP	C5-C4	2.49	1.47	1.40
45	k	601	GCP	PB-O2B	2.14	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	k	601	GCP	C2-N3-C4	4.98	121.04	115.36
45	k	601	GCP	C2-N1-C6	4.04	122.35	115.93
45	k	601	GCP	C5-C6-N1	-3.99	117.98	123.43
45	k	601	GCP	PB-O3A-PA	-3.80	120.50	132.56
45	k	601	GCP	C4-C5-C6	-3.70	117.26	120.80
45	k	601	GCP	N3-C2-N1	-3.28	122.84	127.22
45	k	601	GCP	C3'-C2'-C1'	3.17	105.76	100.98
45	k	601	GCP	C4-C5-N7	-2.74	106.55	109.40

There are no chirality outliers.

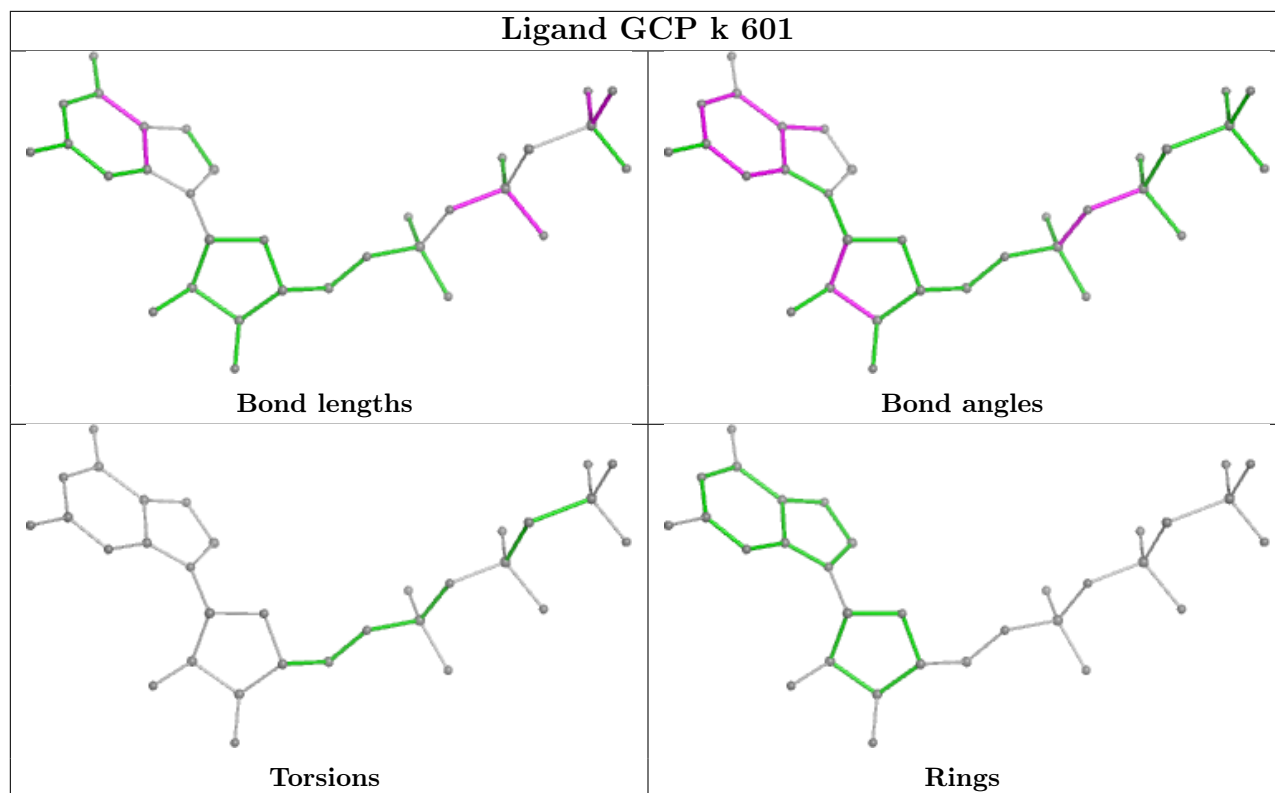
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	k	602	MET	CB-CG-SD-CE

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
38	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	64:RIA	O3'	65:G	P	7.03
1	1	63:G	O3'	64:RIA	P	5.87
1	1	16:H2U	O3'	18:G	P	4.04

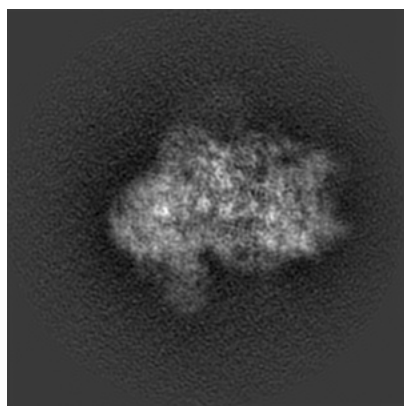
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19806. These allow visual inspection of the internal detail of the map and identification of artifacts.

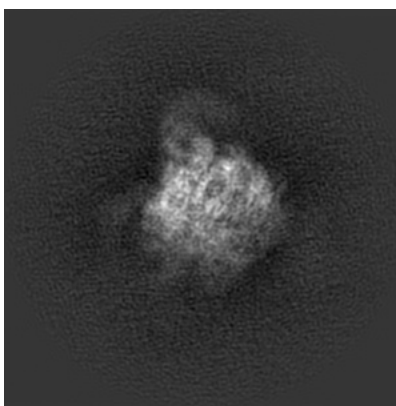
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

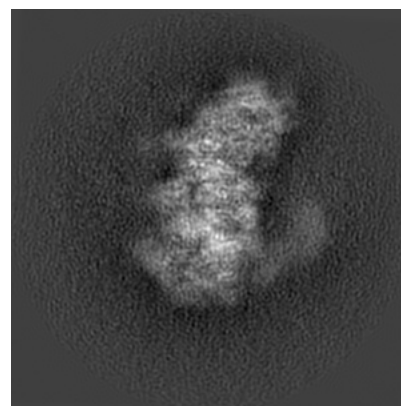
6.1.1 Primary map



X

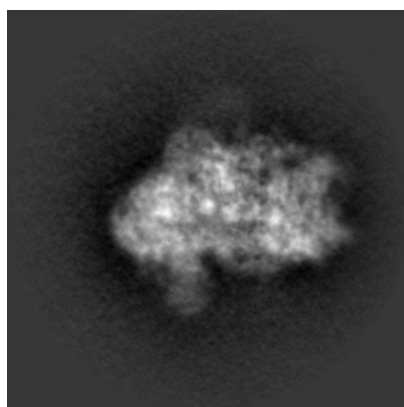


Y

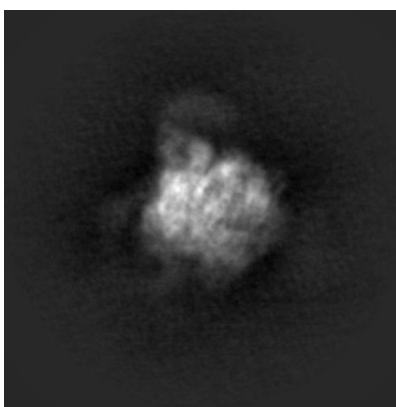


Z

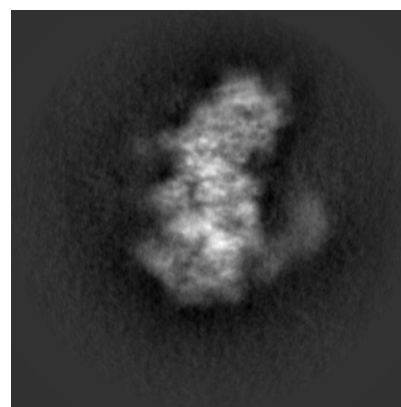
6.1.2 Raw map



X



Y

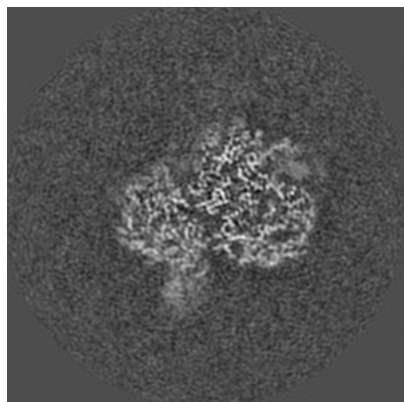


Z

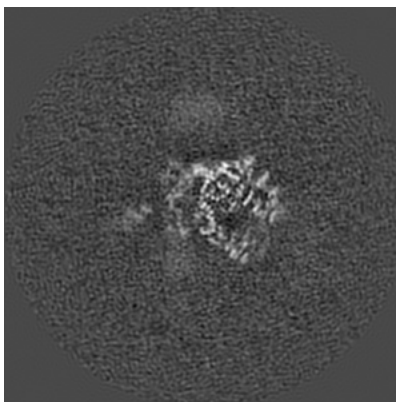
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

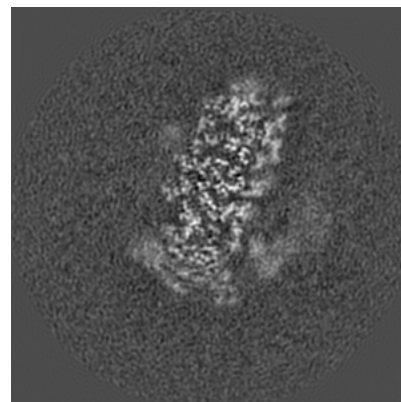
6.2.1 Primary map



X Index: 150

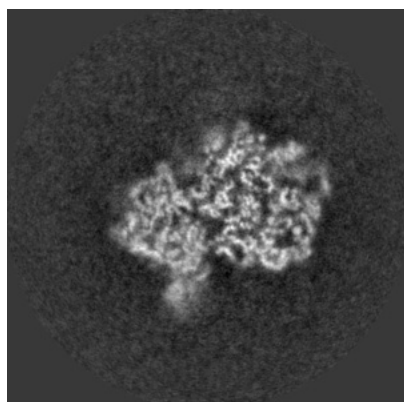


Y Index: 150

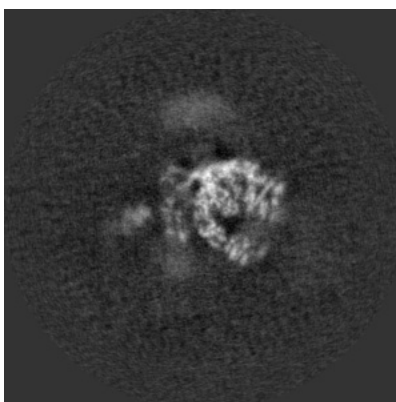


Z Index: 150

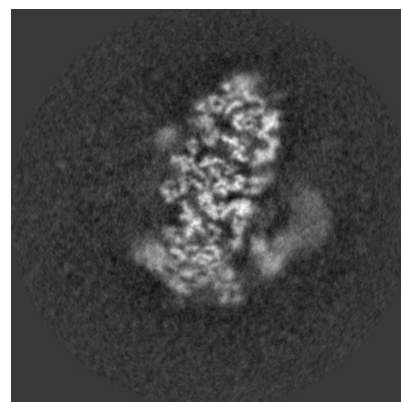
6.2.2 Raw map



X Index: 150



Y Index: 150

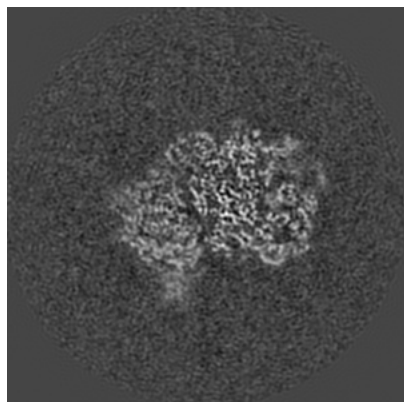


Z Index: 150

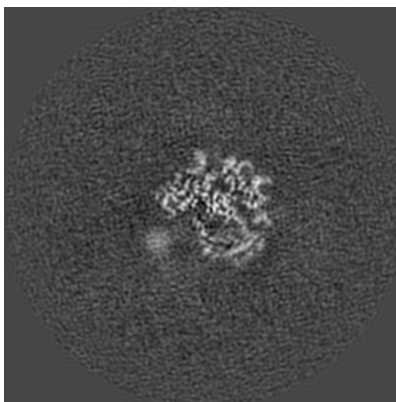
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

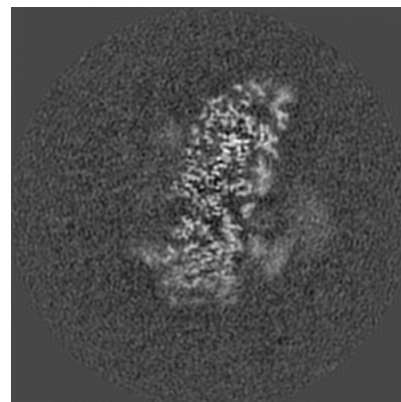
6.3.1 Primary map



X Index: 154

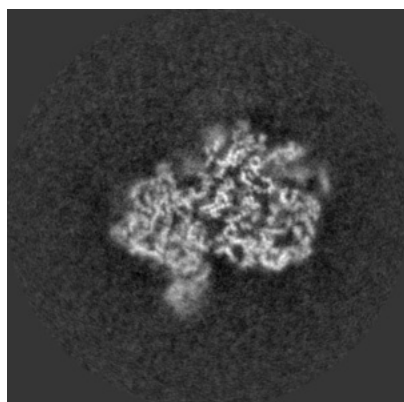


Y Index: 162

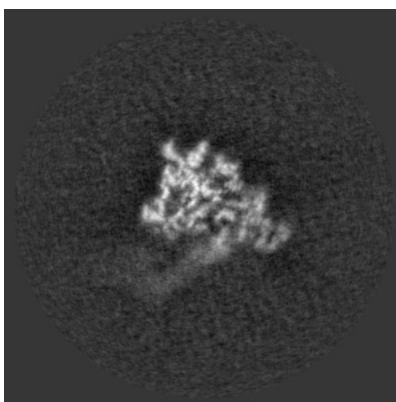


Z Index: 146

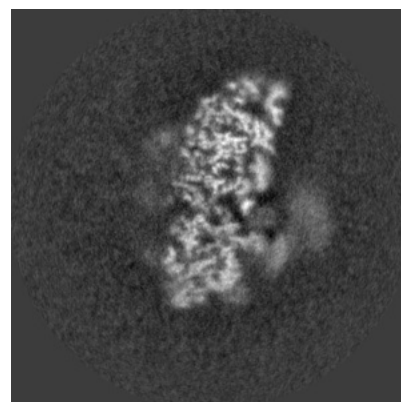
6.3.2 Raw map



X Index: 149



Y Index: 201

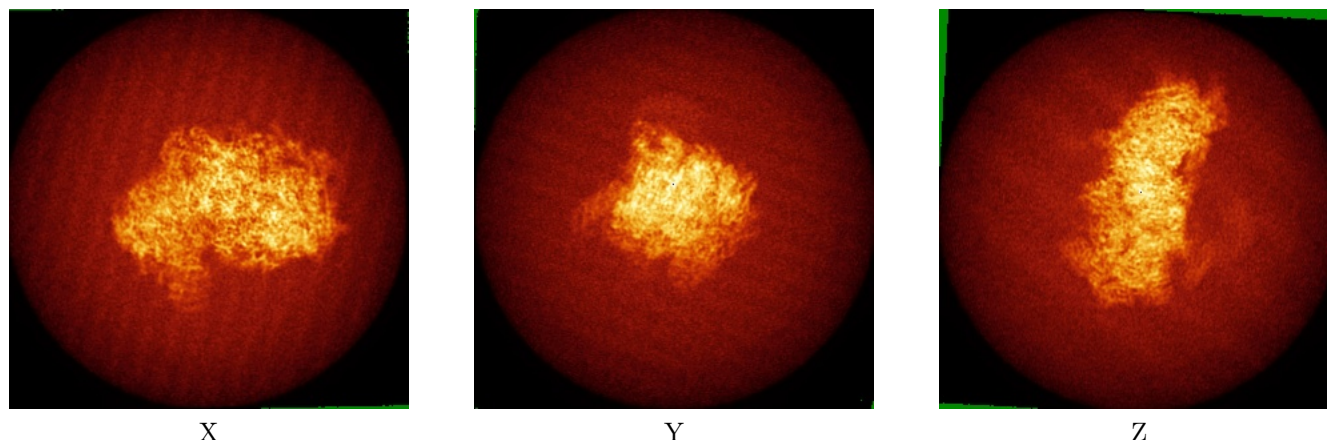


Z Index: 143

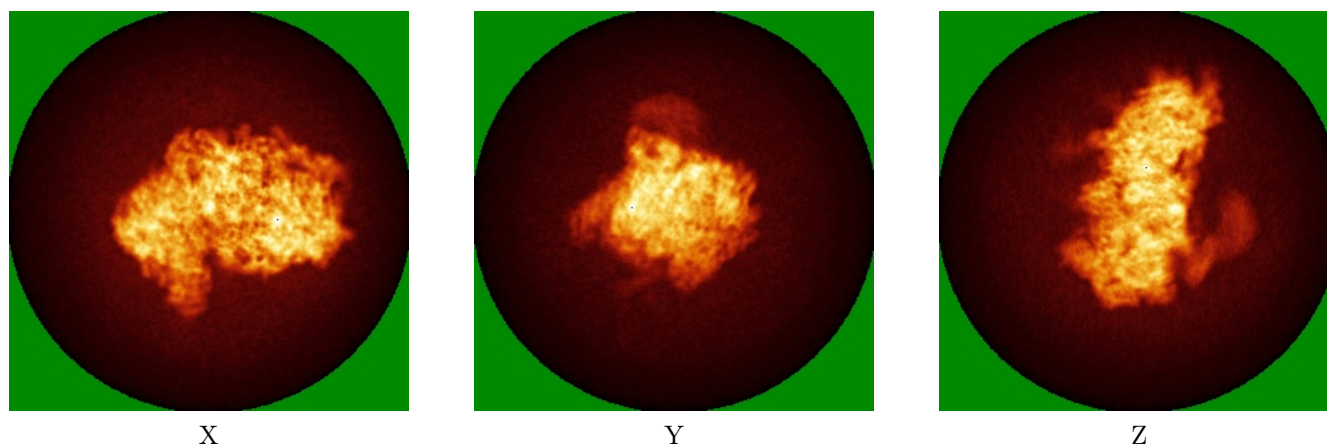
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



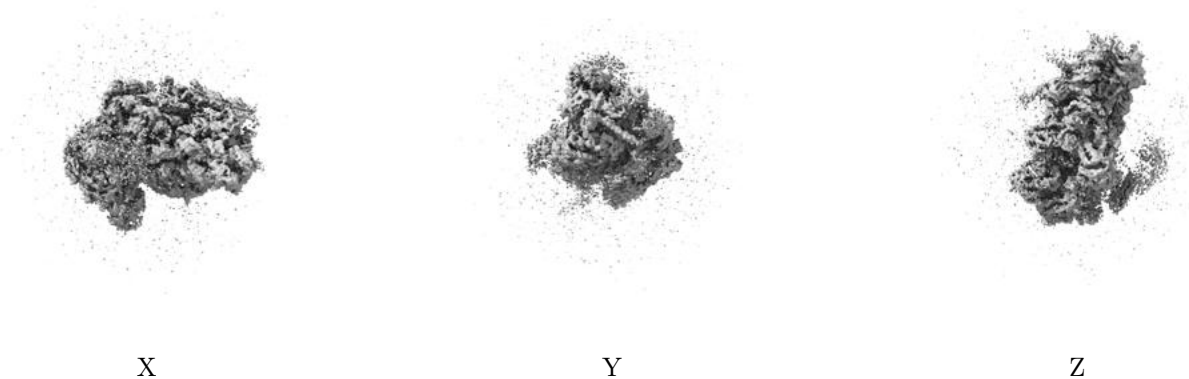
6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

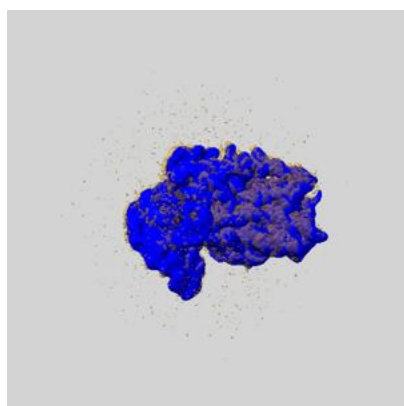
6.6 Mask visualisation [i](#)

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

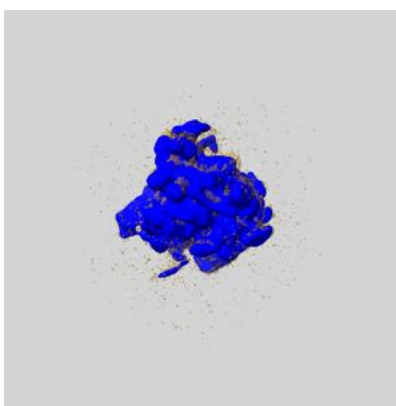
A mask typically either:

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

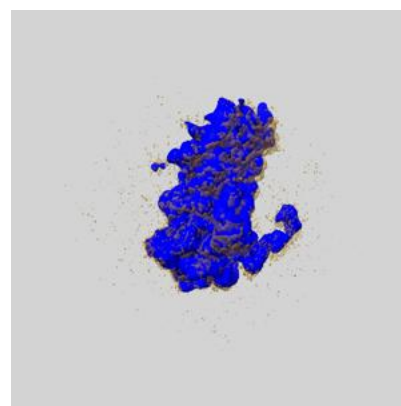
6.6.1 emd_19806_msk_1.map [i](#)



X



Y

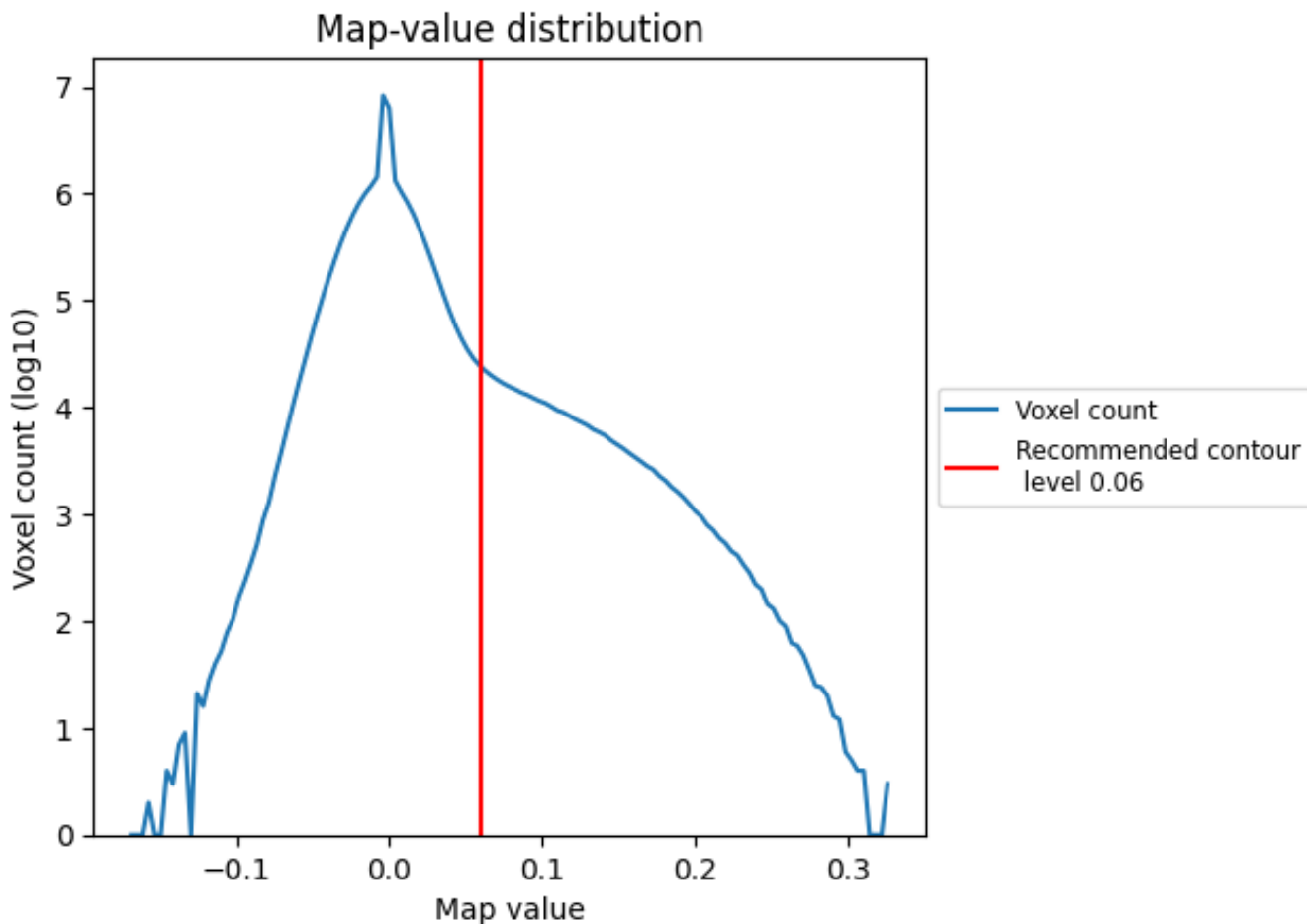


Z

7 Map analysis [i](#)

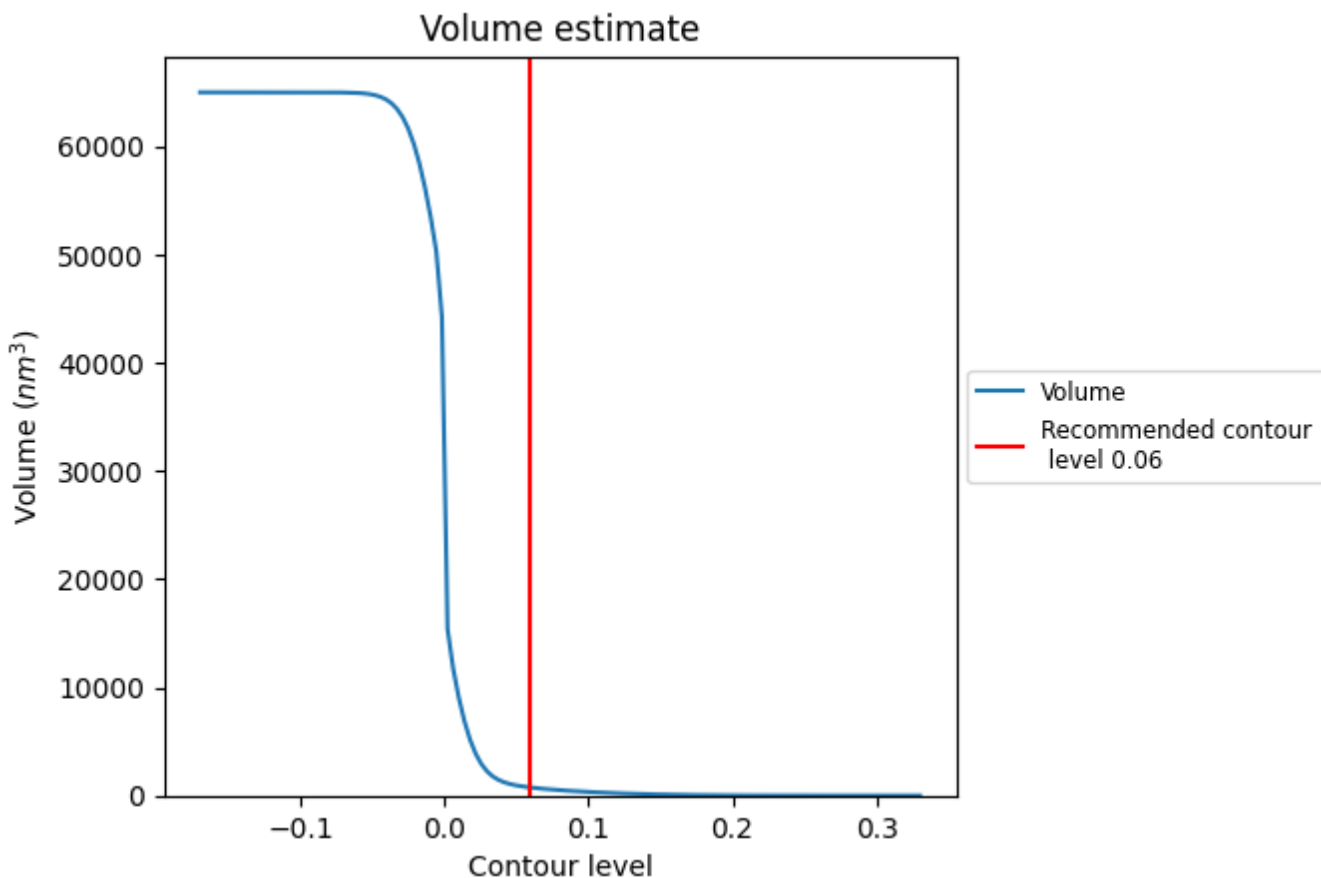
This section contains the results of statistical analysis of the map.

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.

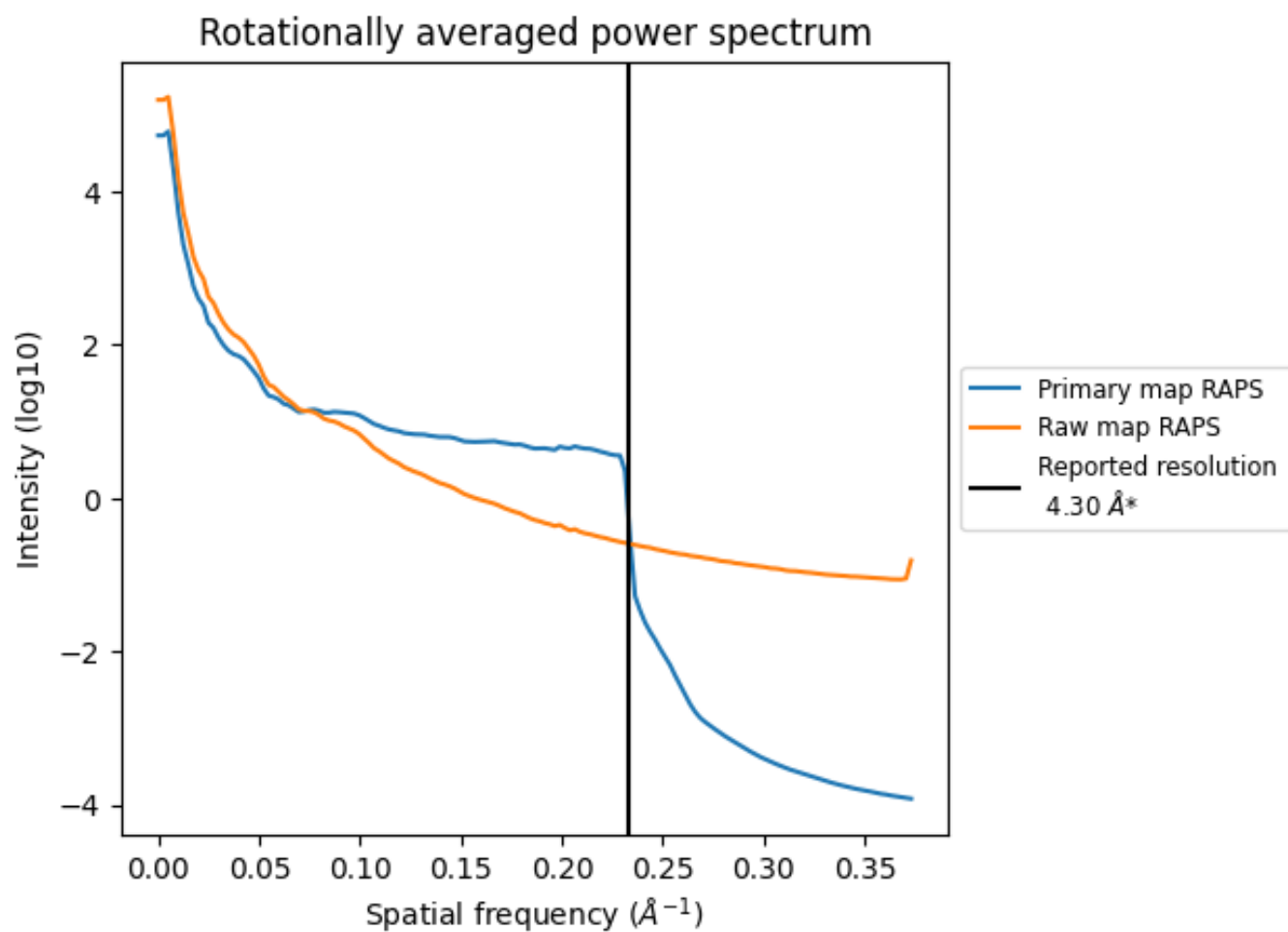
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 744 nm³; this corresponds to an approximate mass of 672 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

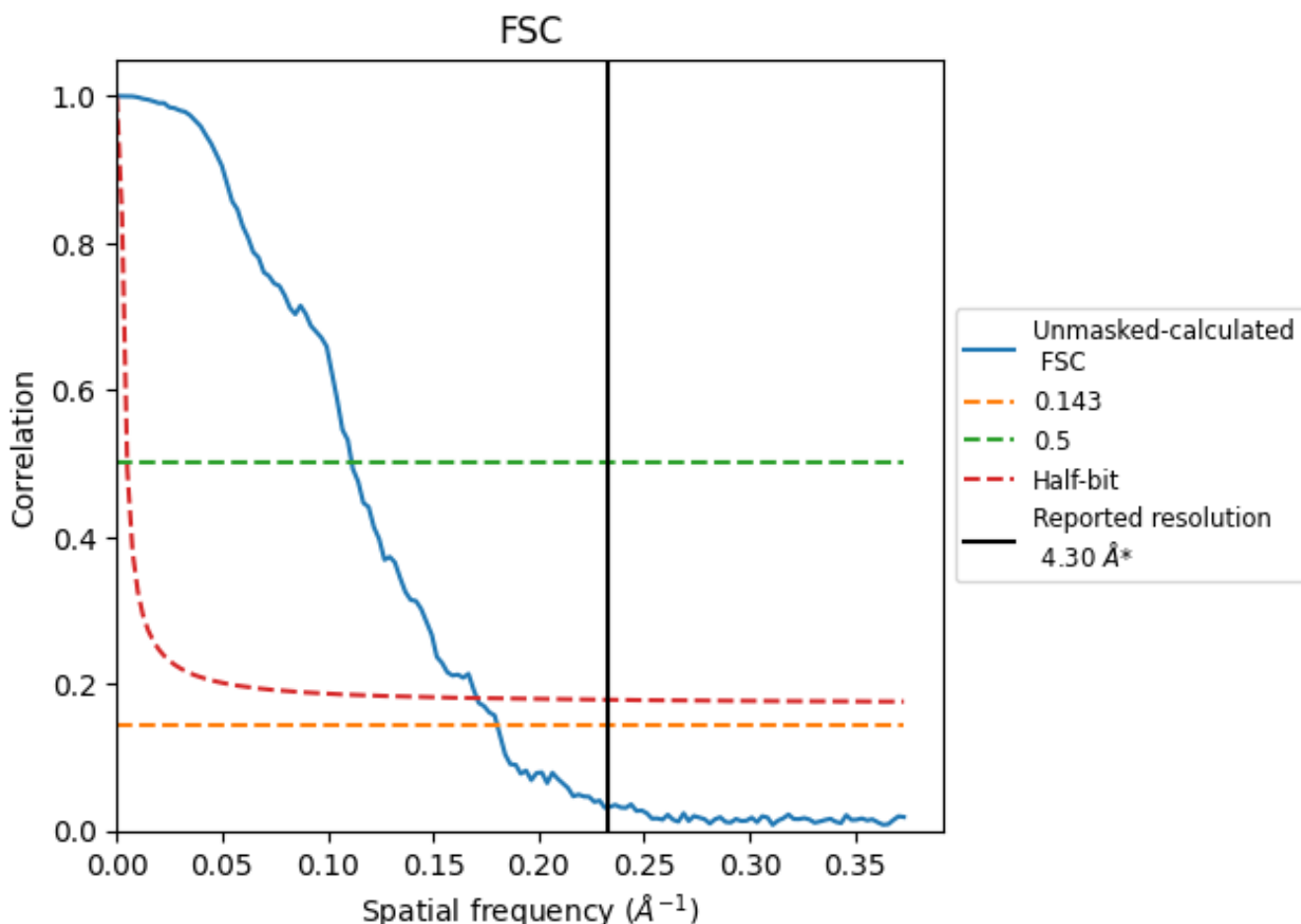


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

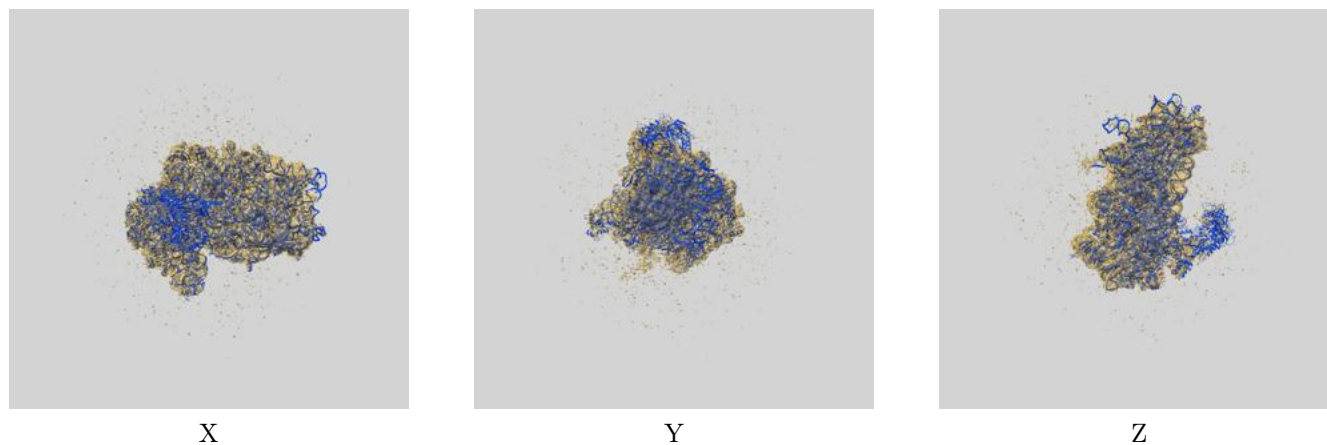
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.54	8.97	5.86

*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 5.54 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

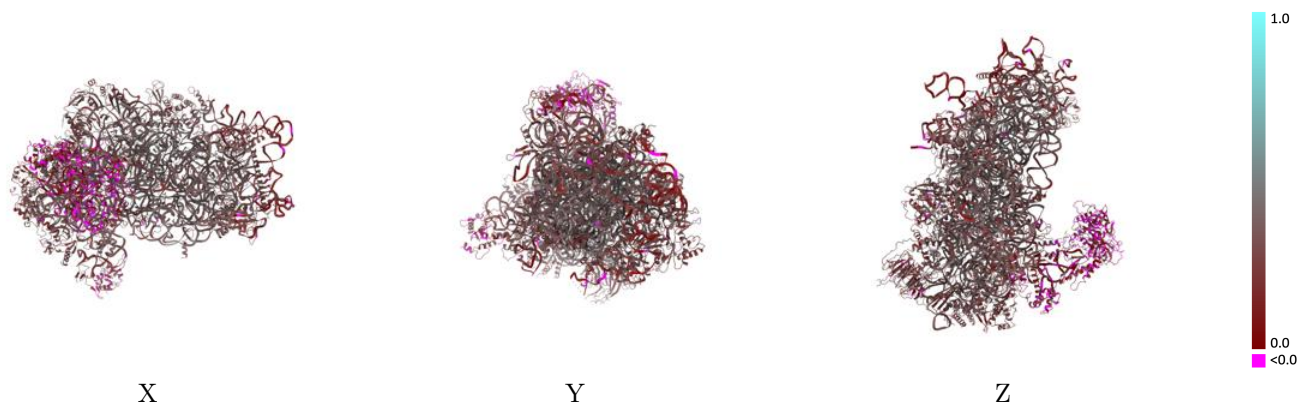
This section contains information regarding the fit between EMDB map EMD-19806 and PDB model 8S8I. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



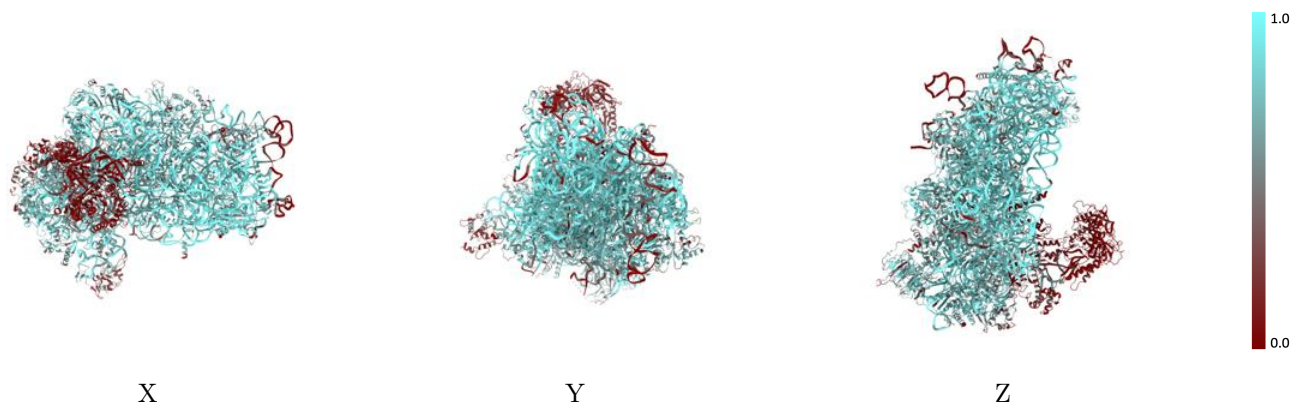
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



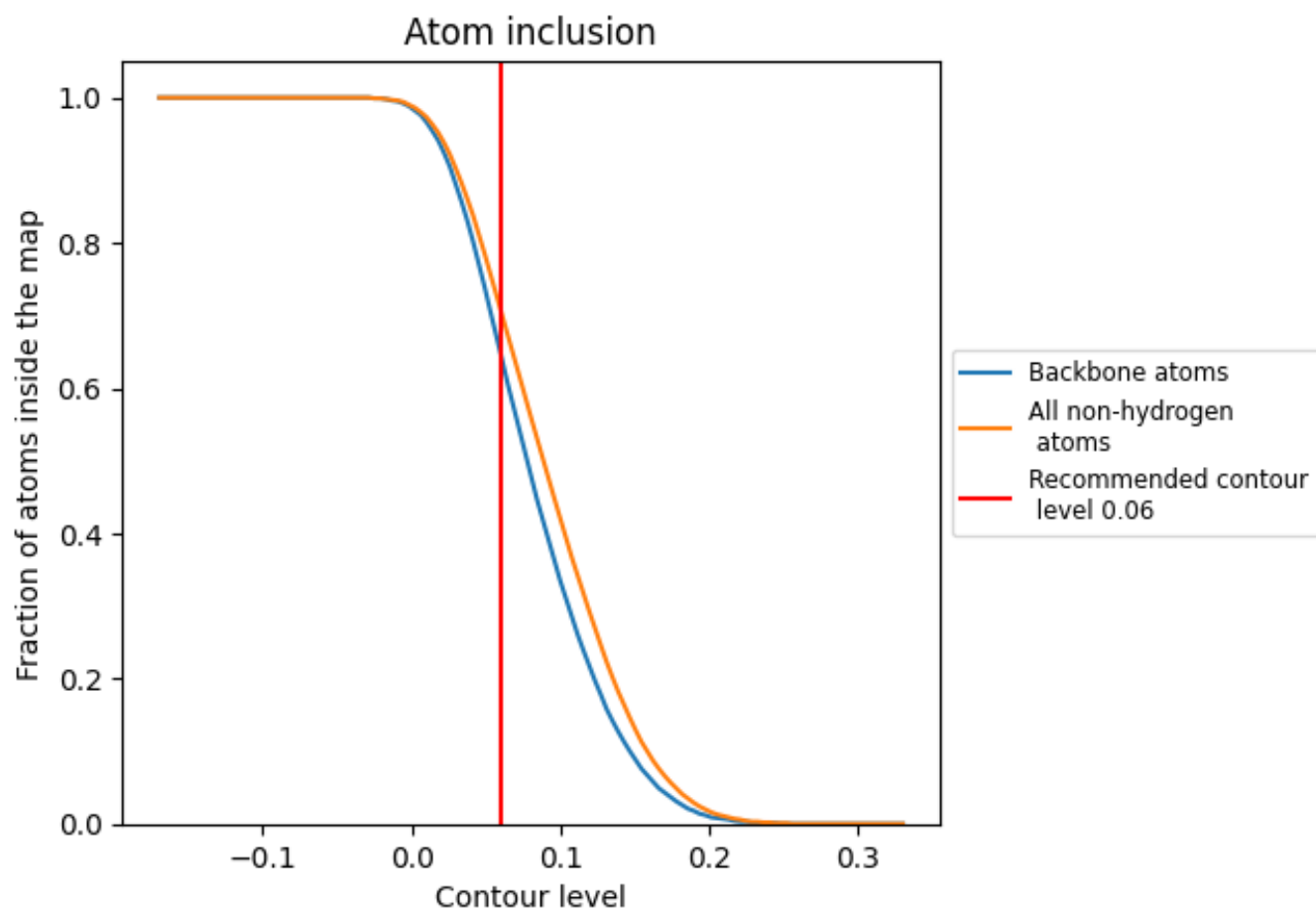
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 71% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7080	 0.3090
1	 0.5620	 0.1870
2	 0.8790	 0.3360
3	 0.2980	 0.3010
A	 0.7530	 0.3390
B	 0.7380	 0.3180
C	 0.7530	 0.3700
D	 0.6640	 0.3330
E	 0.7750	 0.3730
F	 0.6600	 0.3260
G	 0.7680	 0.3060
H	 0.6180	 0.3050
I	 0.7490	 0.3440
J	 0.7440	 0.3490
K	 0.6830	 0.2770
L	 0.7150	 0.3660
M	 0.1900	 0.1540
N	 0.7710	 0.3480
O	 0.7290	 0.3390
P	 0.6820	 0.2860
Q	 0.7520	 0.3260
R	 0.6280	 0.2980
S	 0.6880	 0.2880
T	 0.7740	 0.3000
U	 0.5950	 0.3060
V	 0.8040	 0.3590
W	 0.7760	 0.3790
X	 0.7580	 0.3830
Y	 0.7980	 0.3370
Z	 0.4060	 0.2540
a	 0.7200	 0.3750
b	 0.7390	 0.3590
c	 0.6160	 0.3460
d	 0.7850	 0.3390
e	 0.6550	 0.3690



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Chain	Atom inclusion	Q-score
f	 0.4120	 0.1930
g	 0.6530	 0.2820
h	 0.0660	 0.2370
i	 0.3830	 0.2990
j	 0.1040	 0.1350
k	 0.0370	 0.0900
l	 0.0290	 0.1370
m	 0.0640	 0.2100