Full wwPDB EM Validation Report ⓘ

Jun 2, 2024 – 07:57 AM EDT

PDB ID	:	7UQZ
EMDB ID	:	EMD-26703
Title	:	Nucleoplasmic pre-60S intermediate of the Nog2 containing pre-rotation state from a SPB1 D52A strain
Authors	:	Sekulski, K.; Cruz, V.E.; Weirich, C.S.; Erzberger, J.P.
Deposited on	:	2022-04-20
Resolution	:	2.44 Å(reported)
Based on initial model	:	3JCT

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:

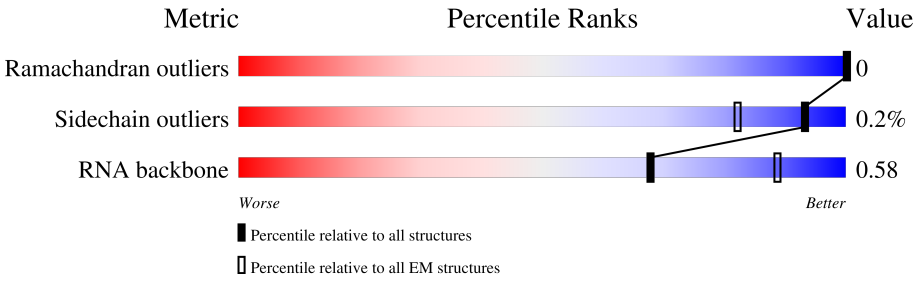
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.44 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	6% 84% 16%
2	1	3396	14% 72% 15% • 12%
3	2	158	5% 81% 19%
4	3	121	73% 79% 20% •
5	5	114	64% 64% 36%
6	6	74	62% 54% 23% • 22%
7	8	165	85% 96% •
8	9	175	22% 67% 33%

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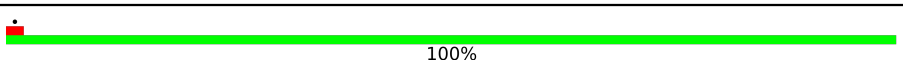
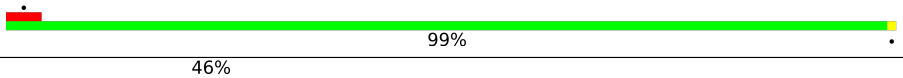
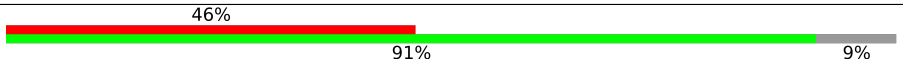
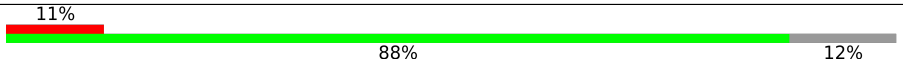
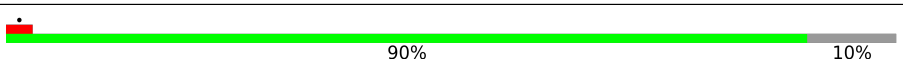
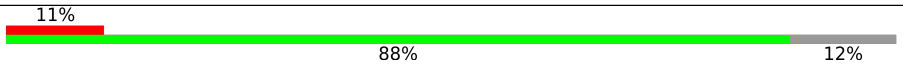
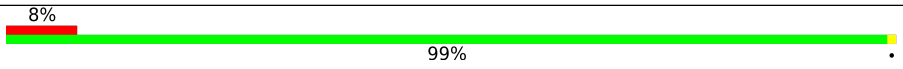
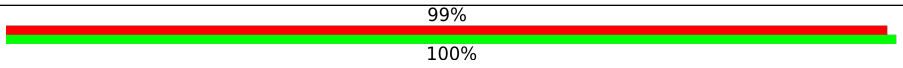
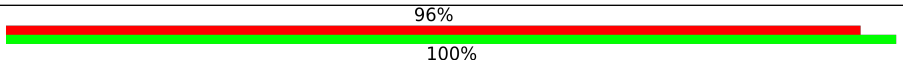
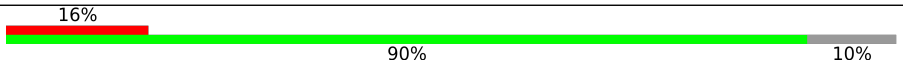
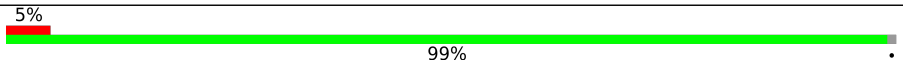
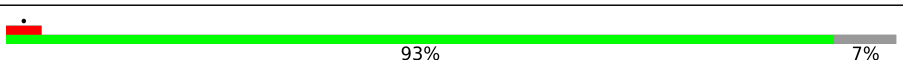
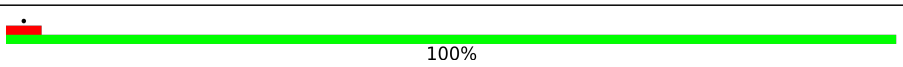
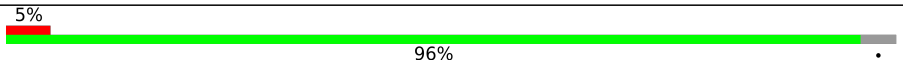
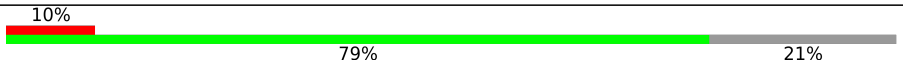
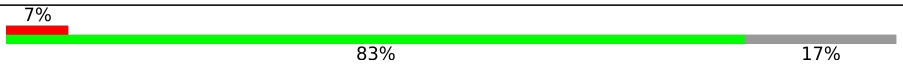
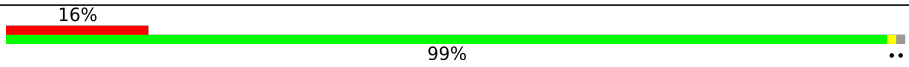
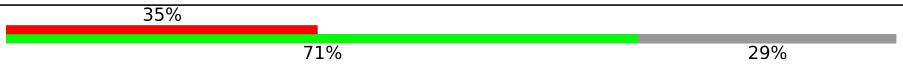
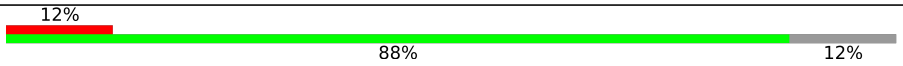
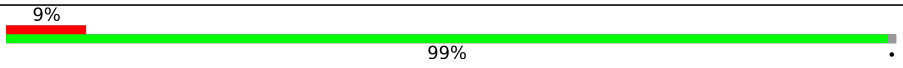
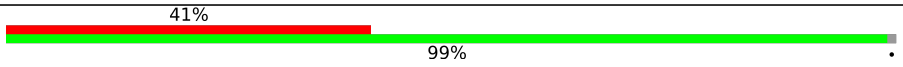
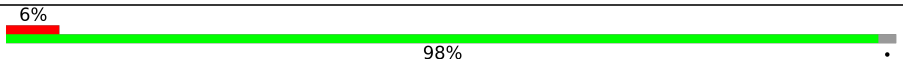
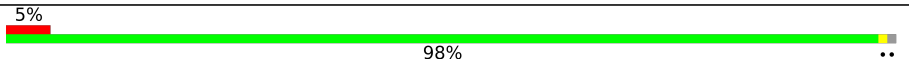
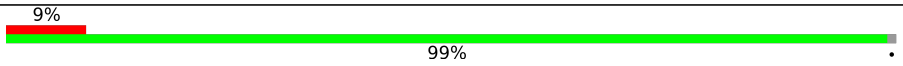
Mol	Chain	Length	Quality of chain
9	B	386	
10	C	362	
11	D	297	
12	E	176	
13	F	244	
14	G	256	
15	H	191	
16	I	131	
17	J	171	
18	K	339	
19	L	199	
20	M	138	
21	N	203	
22	O	197	
23	P	183	
24	Q	186	
25	R	189	
26	S	172	
27	T	160	
28	U	121	
29	V	137	
30	W	236	
31	X	142	
32	Y	127	
33	Z	136	

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Mol	Chain	Length	Quality of chain
34	a	149	12% 62% 38%
35	b	647	20% 99%
36	c	105	20% 92% 8%
37	d	113	10% 95% 5%
38	e	130	5% 98%
39	f	107	99%
40	g	120	9% 93% 7%
41	h	120	99%
42	i	99	25% 100%
43	j	87	97%
44	k	78	26% 99%
45	l	50	100%
46	m	472	21% 99%
47	n	605	32% 61% 39%
48	o	220	42% 60% 40%
49	p	92	7% 98%
50	q	455	26% 34% 66%
51	r	261	7% 88% 12%
52	s	520	7% 14% 86%
53	t	321	73% 89% 11%
54	u	199	5% 75% 25%
55	v	344	45% 85% 15%
56	w	202	46% 96%
57	x	515	37% 98%
58	y	244	9% 100%

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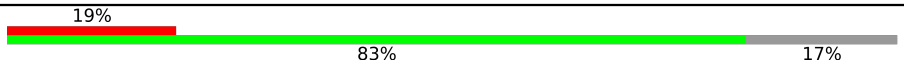
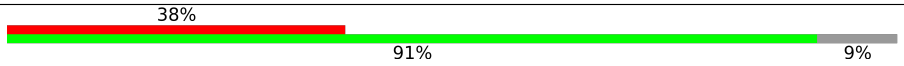
Mol	Chain	Length	Quality of chain
59	z	105	
60	4	592	

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 157839 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	213	1634	1023	326	284	1	0	0

- Molecule 2 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	2986	63938	28571	11549	20832	2986	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	121	2579	1152	461	845	121	0	0

- Molecule 5 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	73	645	395	133	114	3	0	0

- Molecule 6 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	6	58	1227	550	210	409	58	0	0

- Molecule 7 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 8 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	9	118	Total	C	N	O	0	0
			937	590	181	166		

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 10 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 11 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	270	Total	C	N	O	S	0	0
			2180	1379	382	417	2		

- Molecule 12 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	155	Total	C	N	O	S	0	0
			1230	795	221	213	1		

- Molecule 13 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	219	Total	C	N	O	S	0	0
			1761	1138	320	302	1		

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	224	Total	C	N	O	S	0	0
			1753	1122	314	314	3		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 17 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	171	Total	C	N	O	S	0	0
			1368	856	256	252	4		

- Molecule 18 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	268	Total	C	N	O	S	0	0
			2155	1387	355	409	4		

- Molecule 19 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	L	180	Total	C	N	O	0	0
			1438	892	296	250		

- Molecule 20 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 21 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	189	Total	C	N	O	S	0	0
			1620	1016	342	261	1		

- Molecule 22 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 23 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	P	175	Total	C	N	O	0	0
			1388	862	277	249		

- Molecule 24 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	147	Total	C	N	O	S	0	0
			1136	718	219	198	1		

- Molecule 25 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	R	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 26 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 27 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	114	Total	C	N	O	S	0	0
			905	568	175	159	3		

- Molecule 28 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 30 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	234	Total	C	N	O	S	0	0
			1888	1194	323	365	6		

- Molecule 31 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	139	Total	C	N	O	S	0	0
			1088	697	194	195	2		

- Molecule 32 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 33 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 34 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	92	Total	C	N	O	S	0	0
			731	477	129	124	1		

- Molecule 35 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	642	Total	C	N	O	S	0	0
			5185	3251	938	970	26		

- Molecule 36 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 37 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 38 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 40 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 41 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 42 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 43 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 44 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 45 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 46 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	466	Total	C	N	O	S	0	0
			3754	2372	681	691	10		

- Molecule 47 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	369	Total	C	N	O	S	0	0
			3014	1954	521	530	9		

- Molecule 48 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 49 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 50 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	156	Total	C	N	O	S	0	0
			1298	821	233	243	1		

- Molecule 51 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 52 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	72	Total	C	N	O	S	0	0
			602	377	118	104	3		

- Molecule 53 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 54 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 55 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	293	Total	C	N	O	S	0	0
			2366	1512	415	422	17		

- Molecule 56 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	194	Total	C	N	O	S	0	0
			1541	965	277	294	5		

- Molecule 57 is a protein called RSA4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	504	Total	C	N	O	S	0	0
			3927	2468	695	743	21		

- Molecule 58 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 59 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	87	Total	C	N	O	S	0	0
			714	444	142	127	1		

- Molecule 60 is a protein called Probable metalloprotease ARX1.

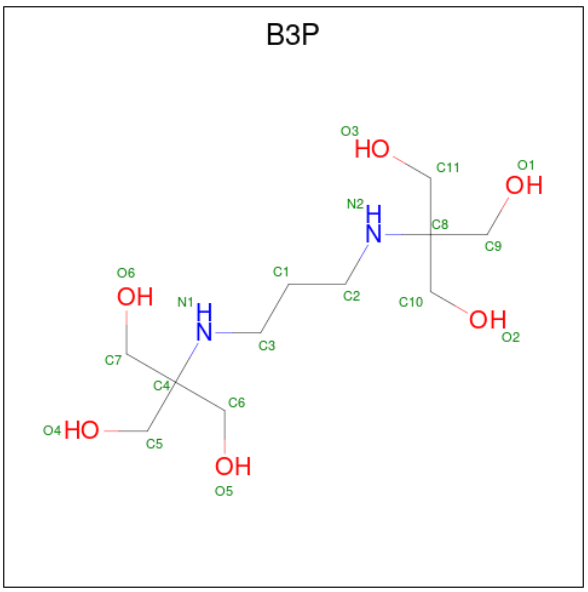
Mol	Chain	Residues	Atoms					AltConf	Trace
60	4	538	Total	C	N	O	S	0	0
			4166	2633	718	800	15		

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
61	1	77	Total	Mg	0
			77	77	
61	R	1	Total	Mg	0
			1	1	
61	V	1	Total	Mg	0
			1	1	
61	b	1	Total	Mg	0
			1	1	
61	m	1	Total	Mg	0
			1	1	

- Molecule 62 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:

$C_{11}H_{26}N_2O_6$).

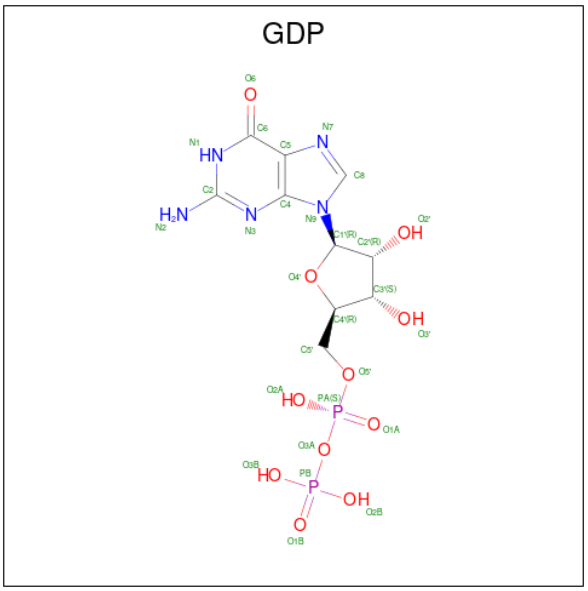


Mol	Chain	Residues	Atoms	AltConf
62	1	1	Total C N O 19 11 2 6	0
62	1	1	Total C N O 19 11 2 6	0
62	1	1	Total C N O 19 11 2 6	0

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
63	I	1	Total Zn 1 1	0
63	g	1	Total Zn 1 1	0
63	j	1	Total Zn 1 1	0
63	p	1	Total Zn 1 1	0
63	u	1	Total Zn 1 1	0

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
64	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	m	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 65 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
65	m	1	Total	K	0
			1	1	

- Molecule 66 is water.

Mol	Chain	Residues	Atoms		AltConf
66	A	2	Total	O	0
			2	2	
66	1	330	Total	O	0
			330	330	
66	2	7	Total	O	0
			7	7	
66	B	1	Total	O	0
			1	1	
66	C	5	Total	O	0
			5	5	
66	E	2	Total	O	0
			2	2	

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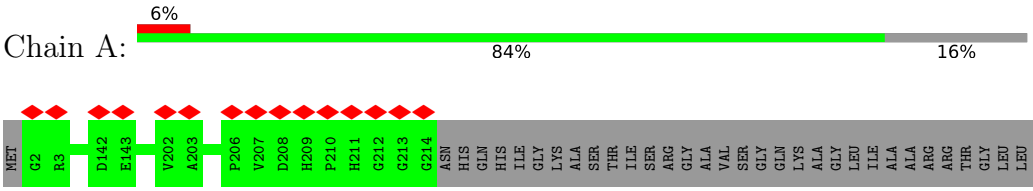
Mol	Chain	Residues	Atoms	AltConf
66	F	3	Total O 3 3	0
66	N	3	Total O 3 3	0
66	O	1	Total O 1 1	0
66	R	1	Total O 1 1	0
66	V	3	Total O 3 3	0
66	X	1	Total O 1 1	0
66	b	3	Total O 3 3	0
66	d	1	Total O 1 1	0
66	j	6	Total O 6 6	0
66	m	4	Total O 4 4	0

3 Residue-property plots (i)

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

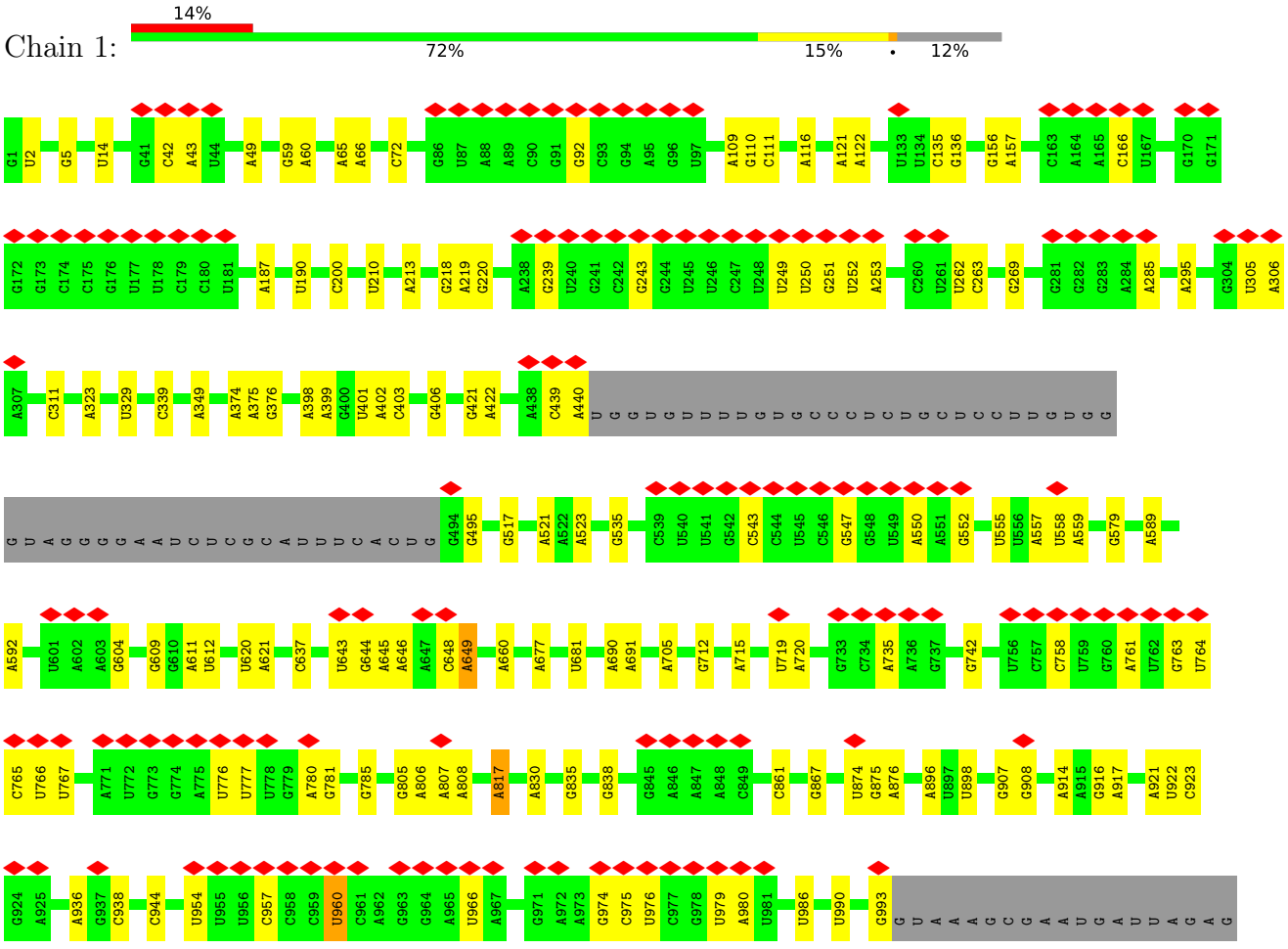
• Molecule 1: 60S ribosomal protein L2-A

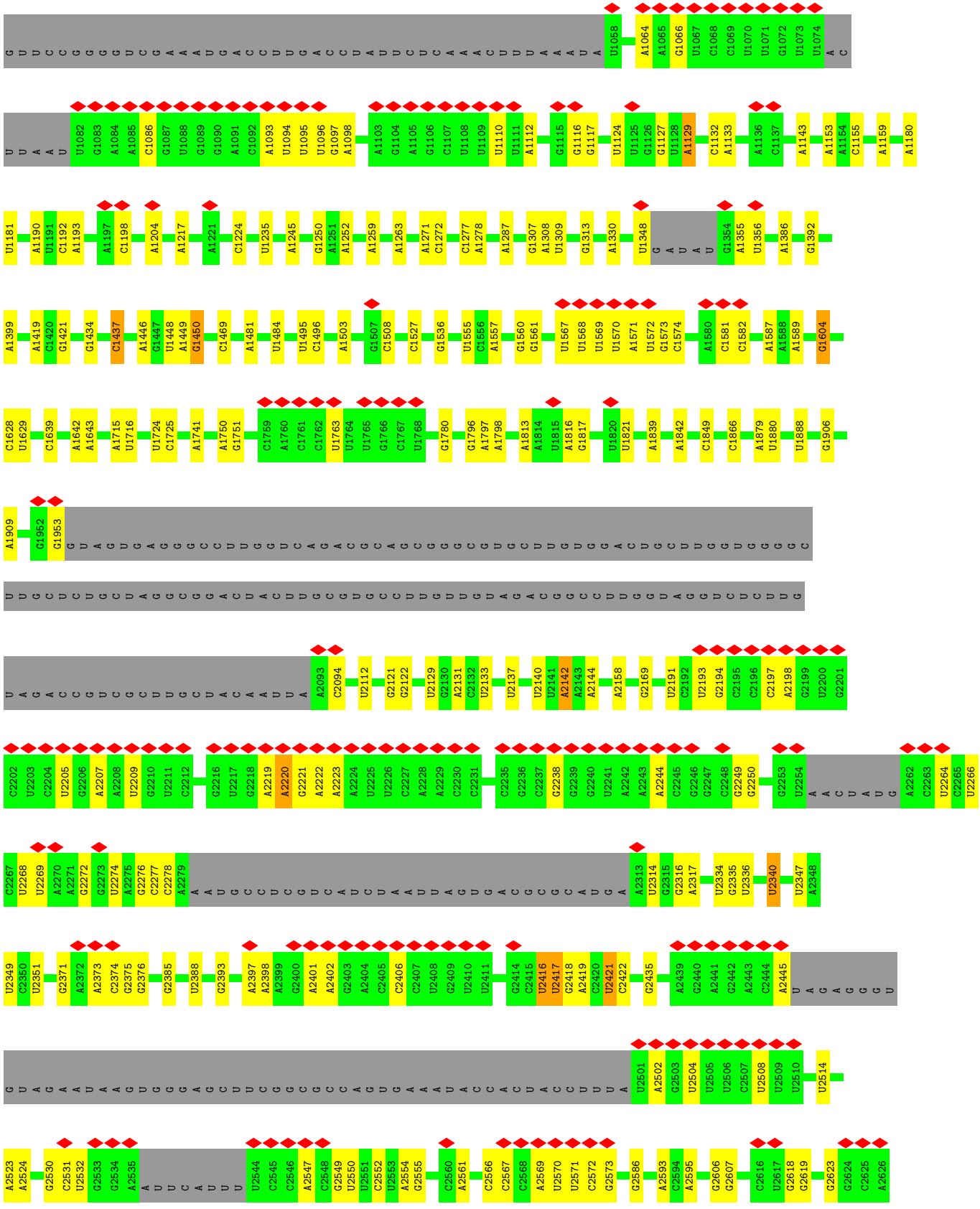
Chain A:

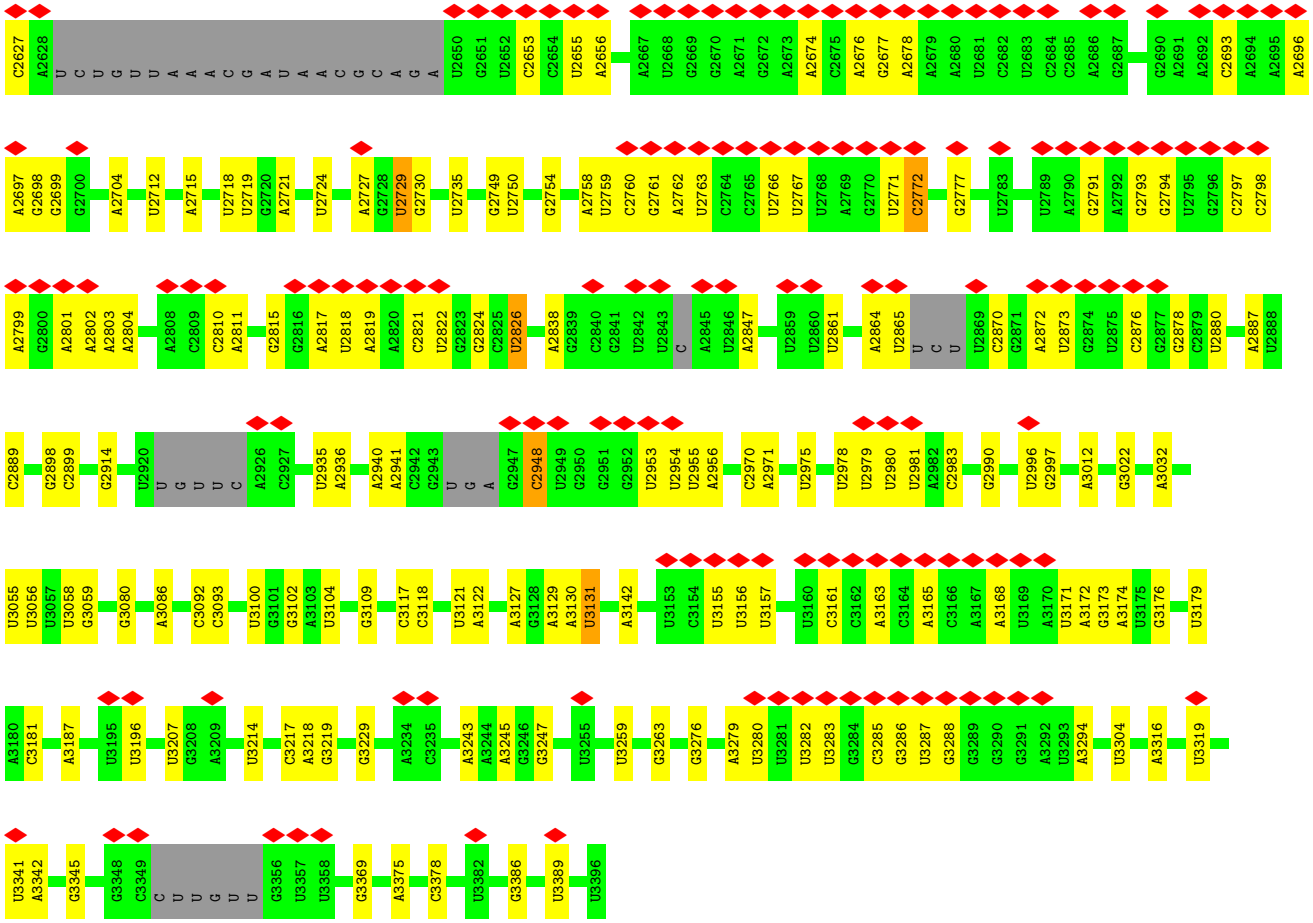


• Molecule 2: 25S rRNA

Chain 1:





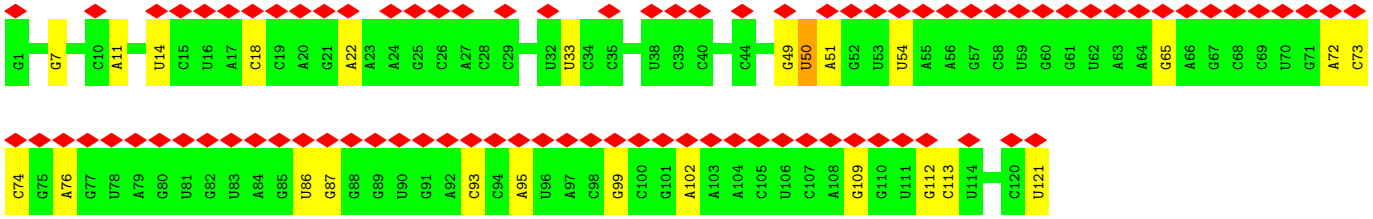


• Molecule 3: 5.8S rRNA

Chain 2:

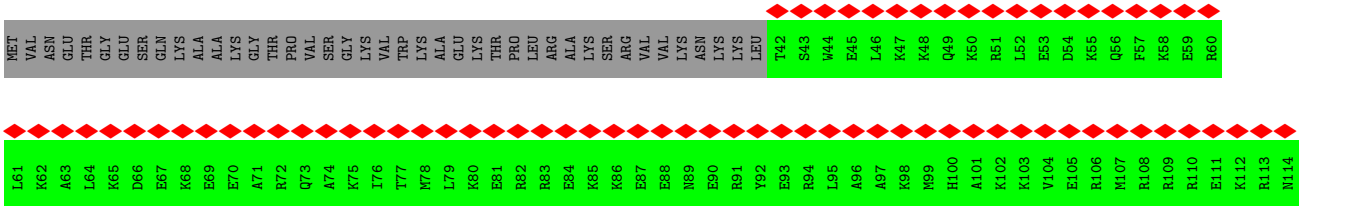
• Molecule 4: 5S rRNA

Chain 3:



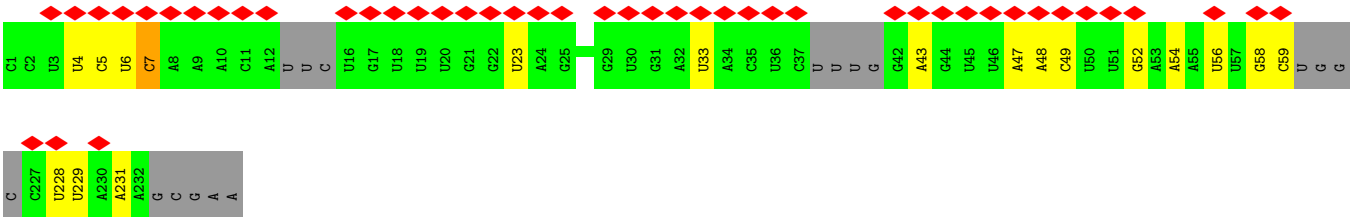
• Molecule 5: rRNA-processing protein

Chain 5:



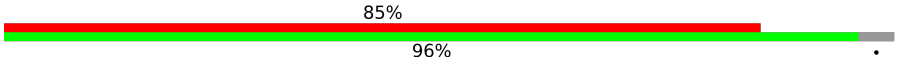
• Molecule 6: ITS2 rRNA

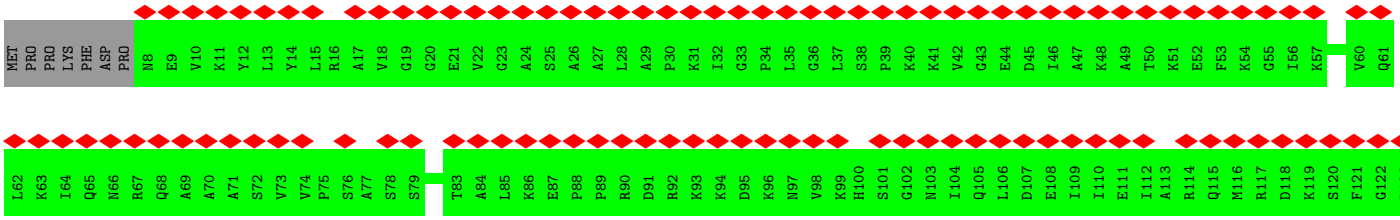
Chain 6:

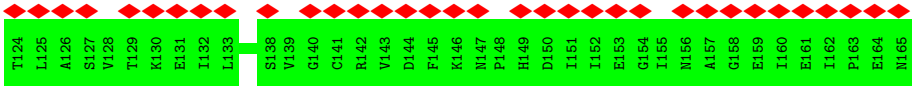


• Molecule 7: 60S ribosomal protein L12-A

Chain 8:

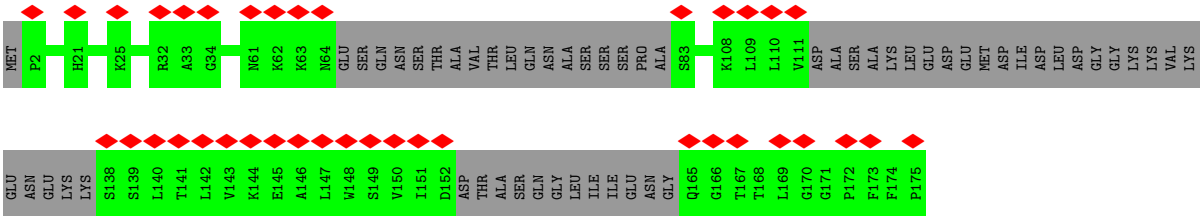






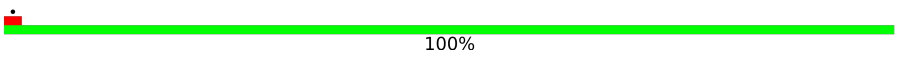
• Molecule 8: Ribosome biogenesis protein ALB1

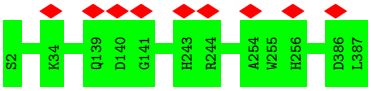
Chain 9:



• Molecule 9: 60S ribosomal protein L3

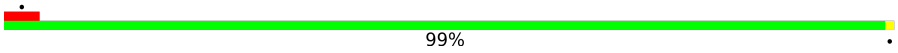
Chain B:

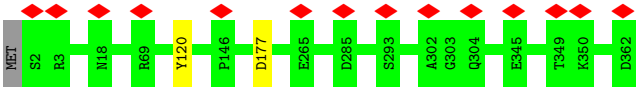




• Molecule 10: 60S ribosomal protein L4-A

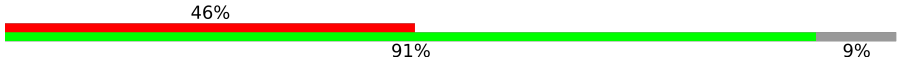
Chain C:

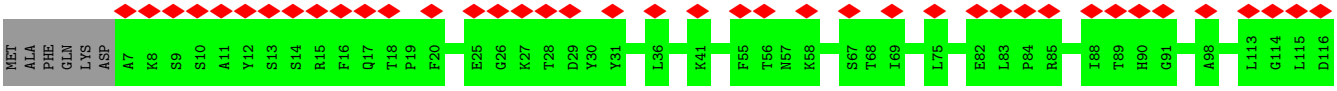


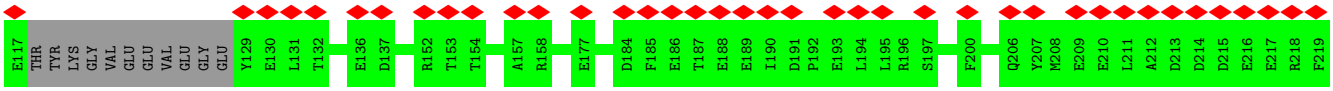


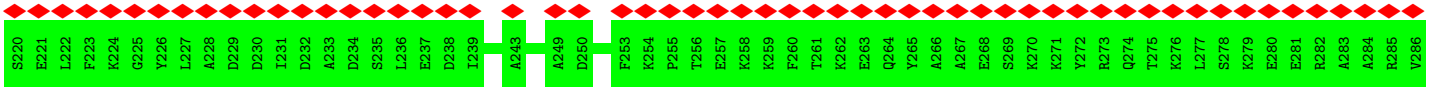
• Molecule 11: 60S ribosomal protein L5

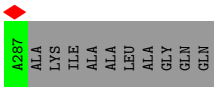
Chain D:





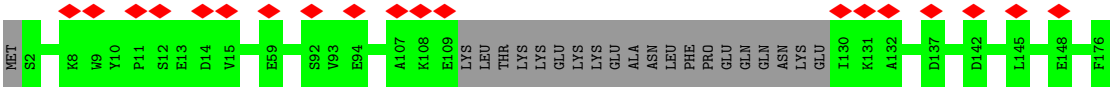






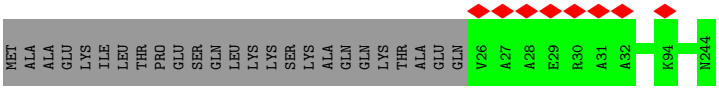
• Molecule 12: 60S ribosomal protein L6-A

Chain E:



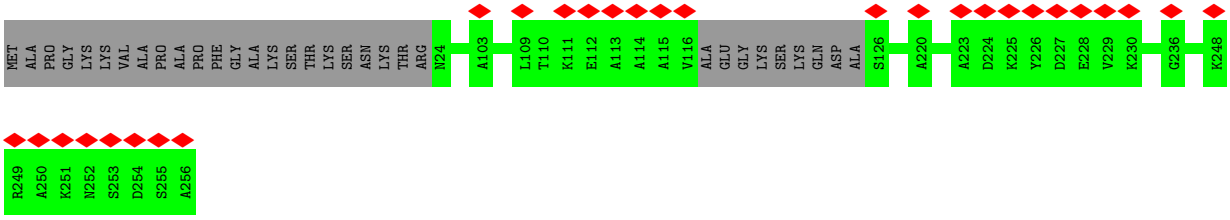
• Molecule 13: 60S ribosomal protein L7-A

Chain F:



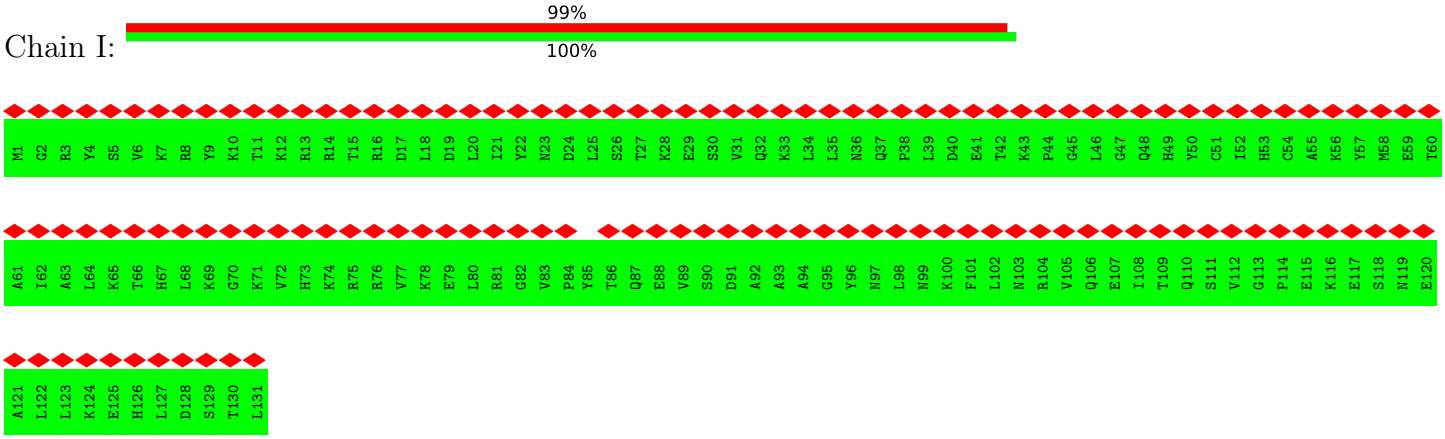
• Molecule 14: 60S ribosomal protein L8-A

Chain G:

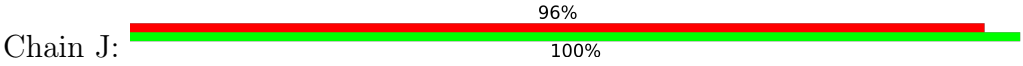


• Molecule 15: 60S ribosomal protein L9-A

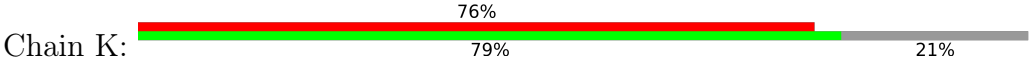
• Molecule 16: Bud site selection protein 20

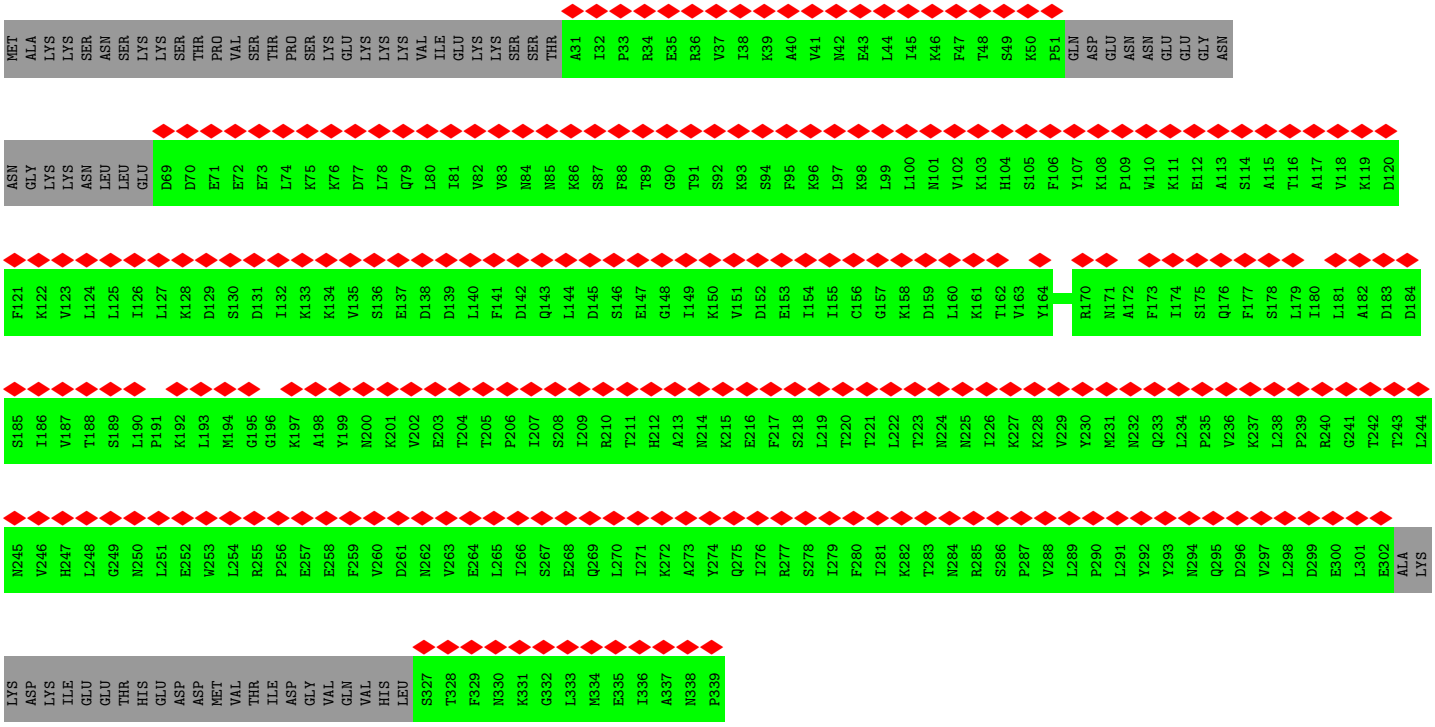


• Molecule 17: 60S ribosomal protein L11-A

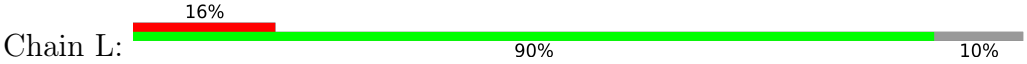


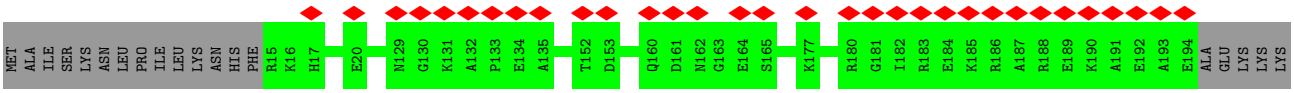
• Molecule 18: Proteasome-interacting protein CIC1



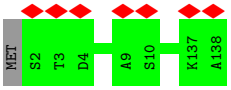


• Molecule 19: 60S ribosomal protein L13-A

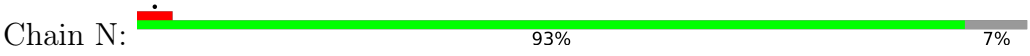


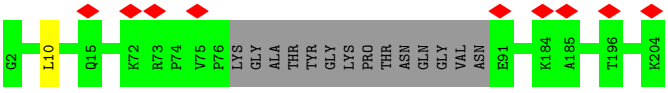


• Molecule 20: 60S ribosomal protein L14-A

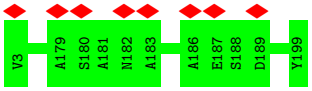


• Molecule 21: 60S ribosomal protein L15-A



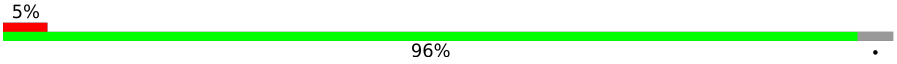


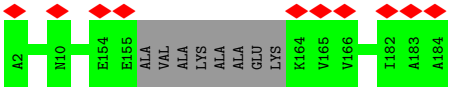
• Molecule 22: 60S ribosomal protein L16-A



• Molecule 23: 60S ribosomal protein L17-A

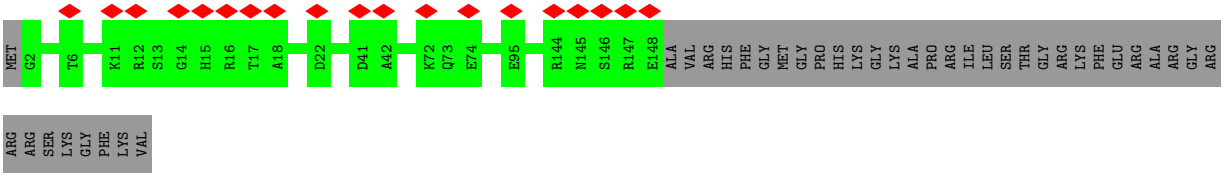
Chain P:





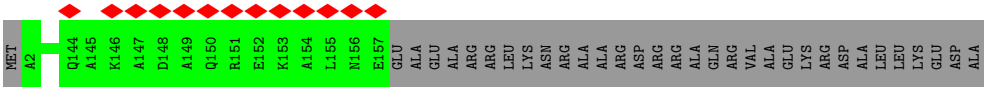
• Molecule 24: 60S ribosomal protein L18-A

Chain Q:



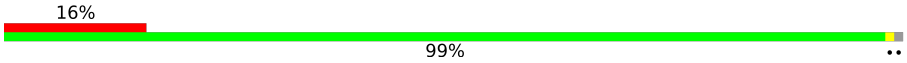
• Molecule 25: 60S ribosomal protein L19-A

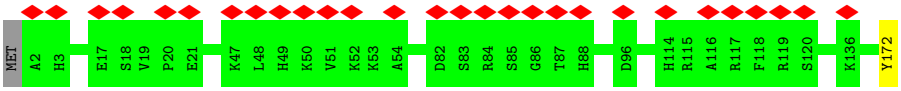
Chain R:



• Molecule 26: 60S ribosomal protein L20-A

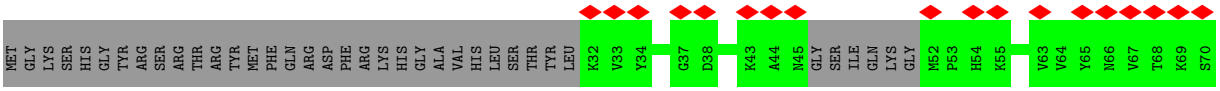
Chain S:

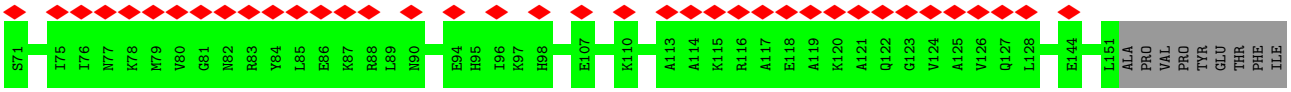




• Molecule 27: 60S ribosomal protein L21-A

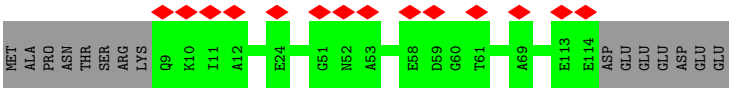
Chain T:





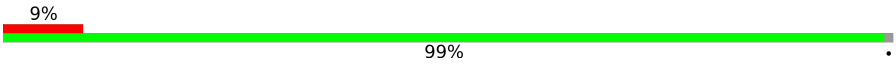
• Molecule 28: 60S ribosomal protein L22-A

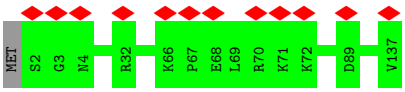
Chain U:



• Molecule 29: 60S ribosomal protein L23-A

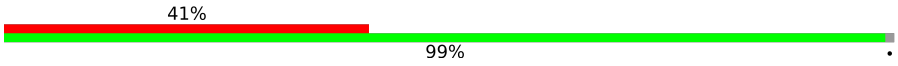
Chain V:

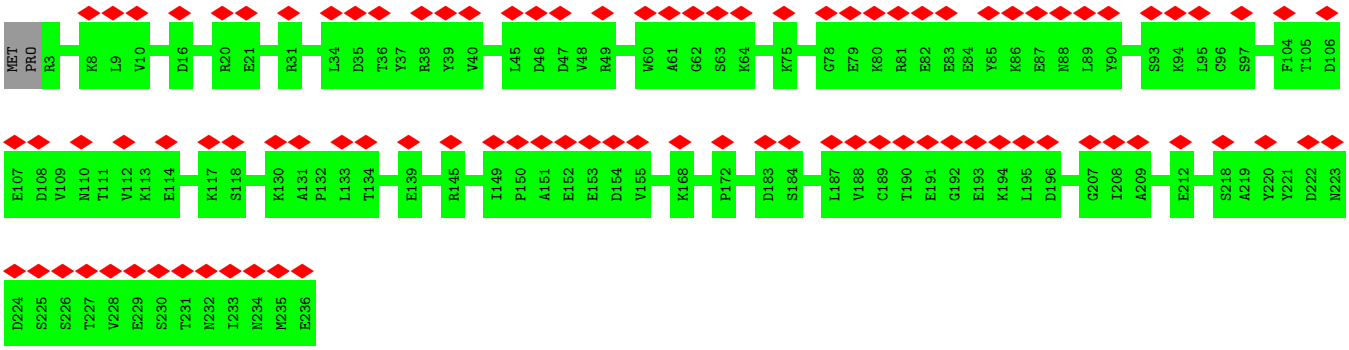




• Molecule 30: Ribosome assembly factor MRT4

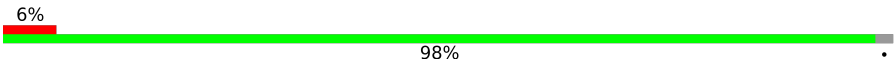
Chain W:

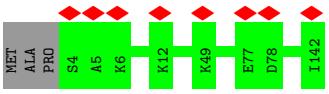




• Molecule 31: 60S ribosomal protein L25

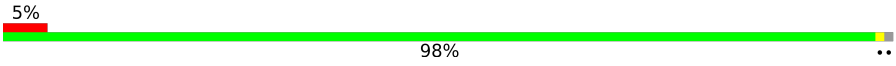
Chain X:

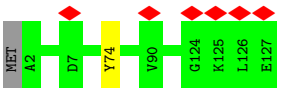




• Molecule 32: 60S ribosomal protein L26-A

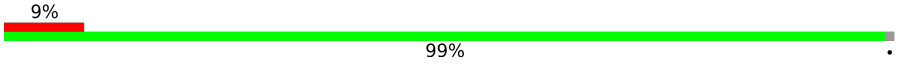
Chain Y:

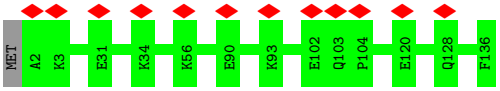




• Molecule 33: 60S ribosomal protein L27-A

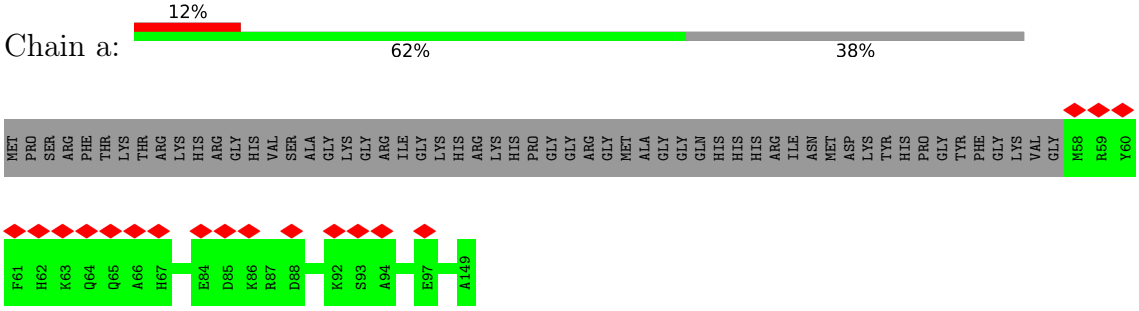
Chain Z:





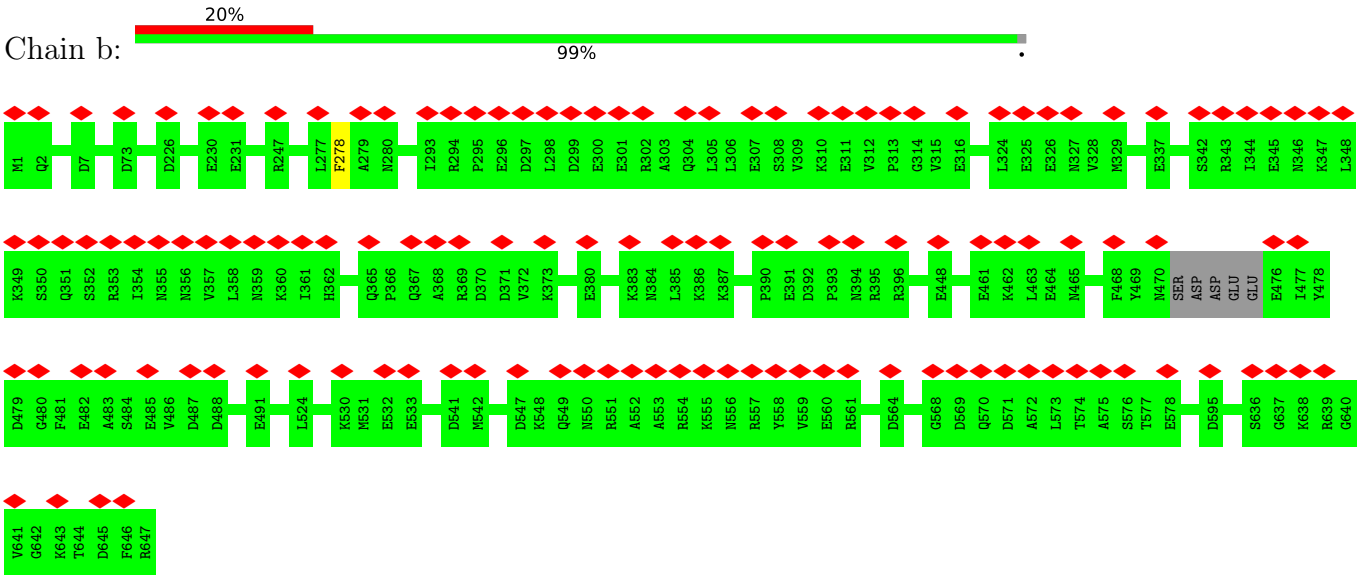
• Molecule 34: 60S ribosomal protein L28

Chain a:



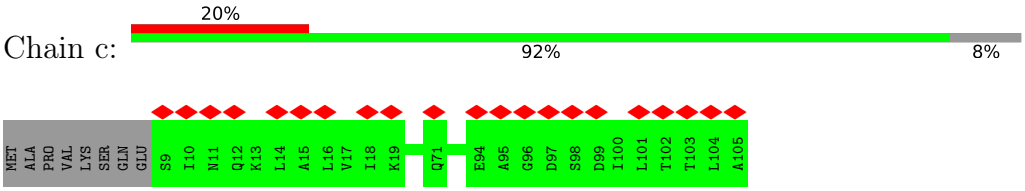
• Molecule 35: Nucleolar GTP-binding protein 1

Chain b:



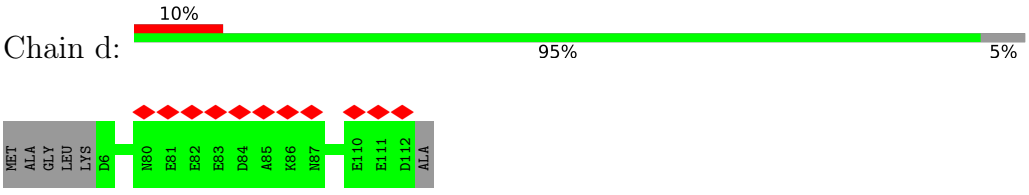
• Molecule 36: 60S ribosomal protein L30

Chain c:



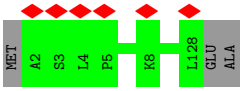
• Molecule 37: 60S ribosomal protein L31-A

Chain d:



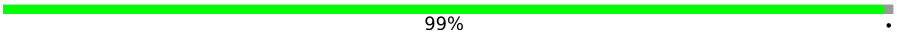
• Molecule 38: 60S ribosomal protein L32

Chain e:



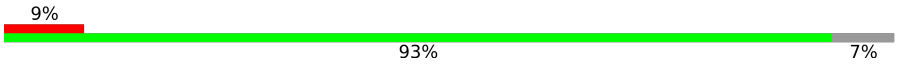
• Molecule 39: 60S ribosomal protein L33-A

Chain f:



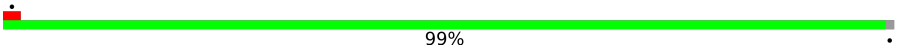
• Molecule 40: 60S ribosomal protein L34-A

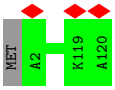
Chain g:



• Molecule 41: 60S ribosomal protein L35-A

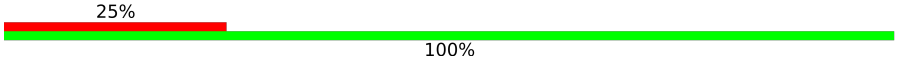
Chain h:

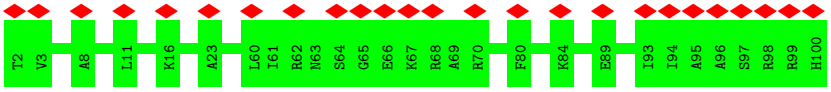




• Molecule 42: 60S ribosomal protein L36-A

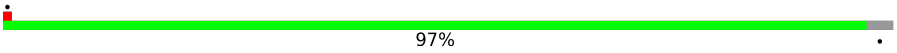
Chain i:

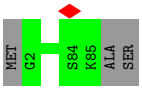




• Molecule 43: 60S ribosomal protein L37-A

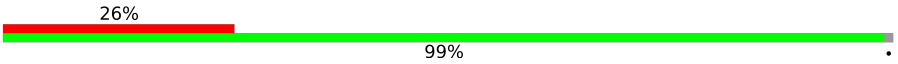
Chain j:

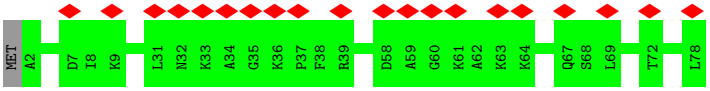




• Molecule 44: 60S ribosomal protein L38

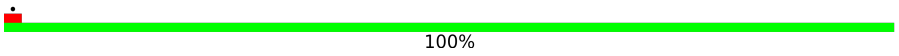
Chain k:





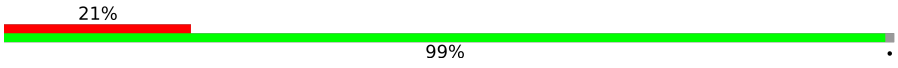
• Molecule 45: 60S ribosomal protein L39

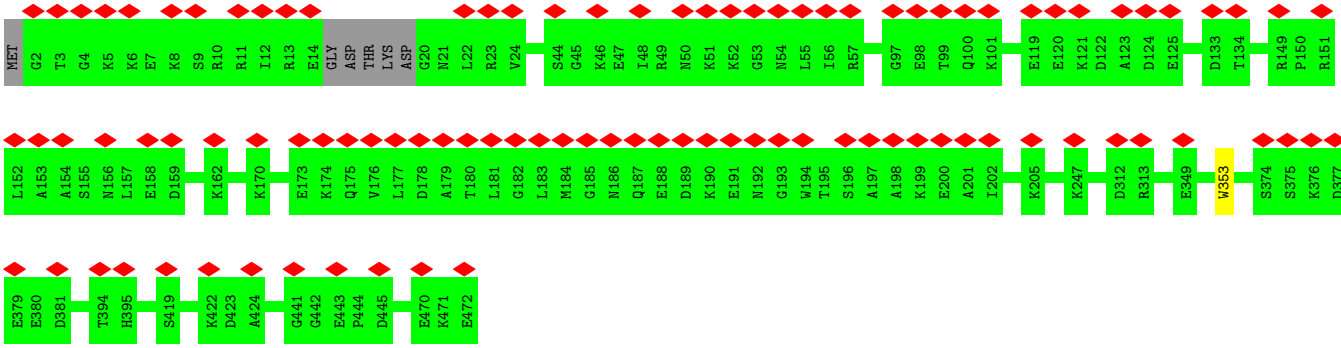
Chain l:



• Molecule 46: Nucleolar GTP-binding protein 2

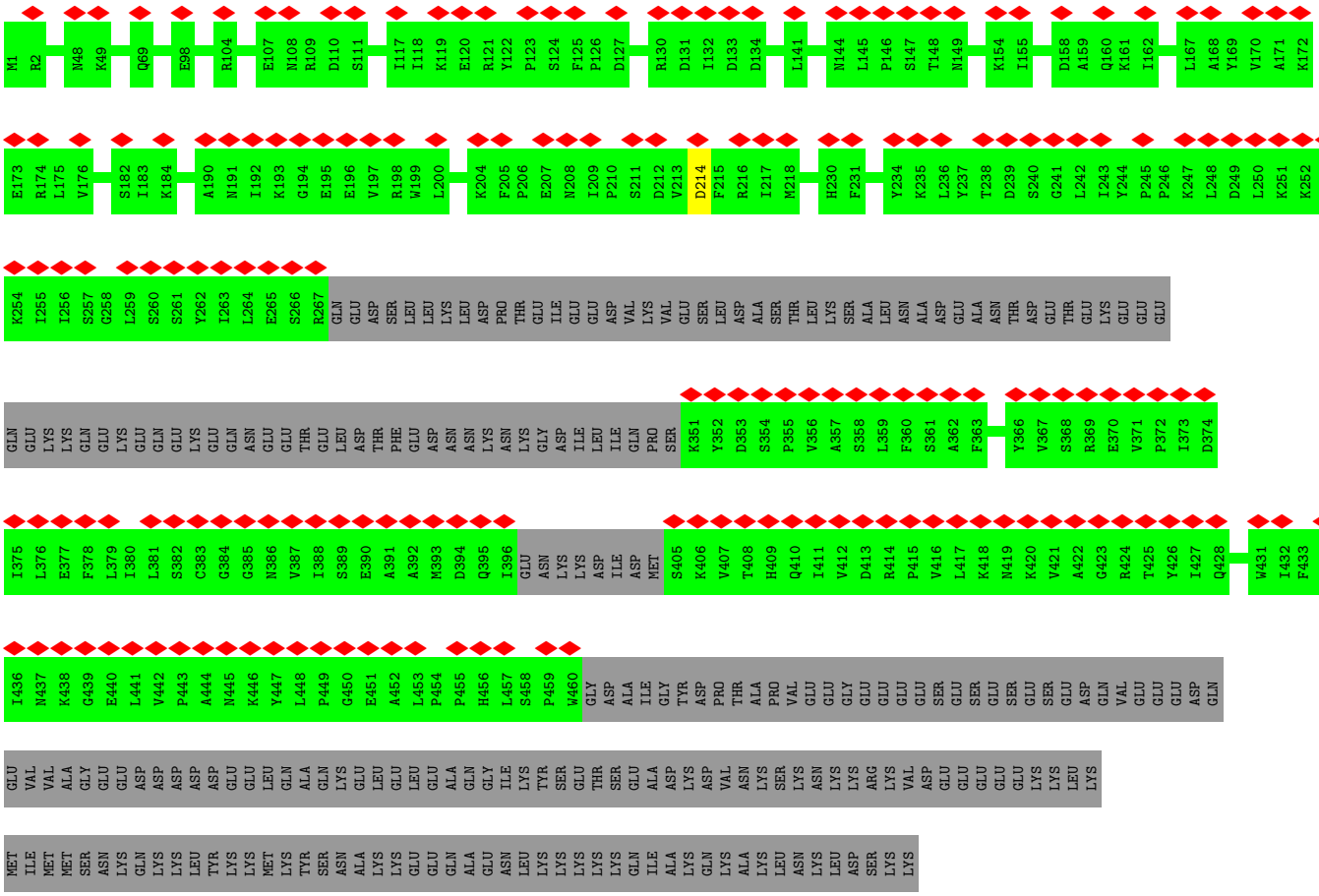
Chain m:





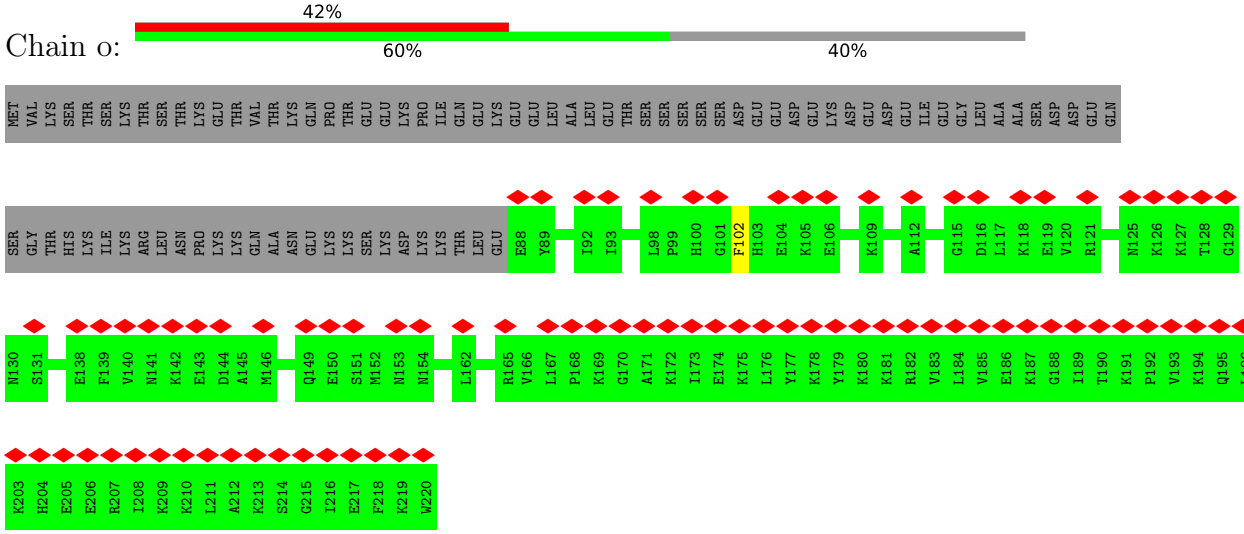
• Molecule 47: Pescadillo homolog

Chain n:



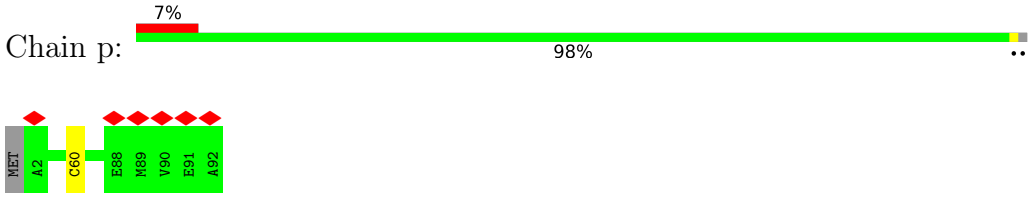
• Molecule 48: Ribosome biogenesis protein 15

Chain o:



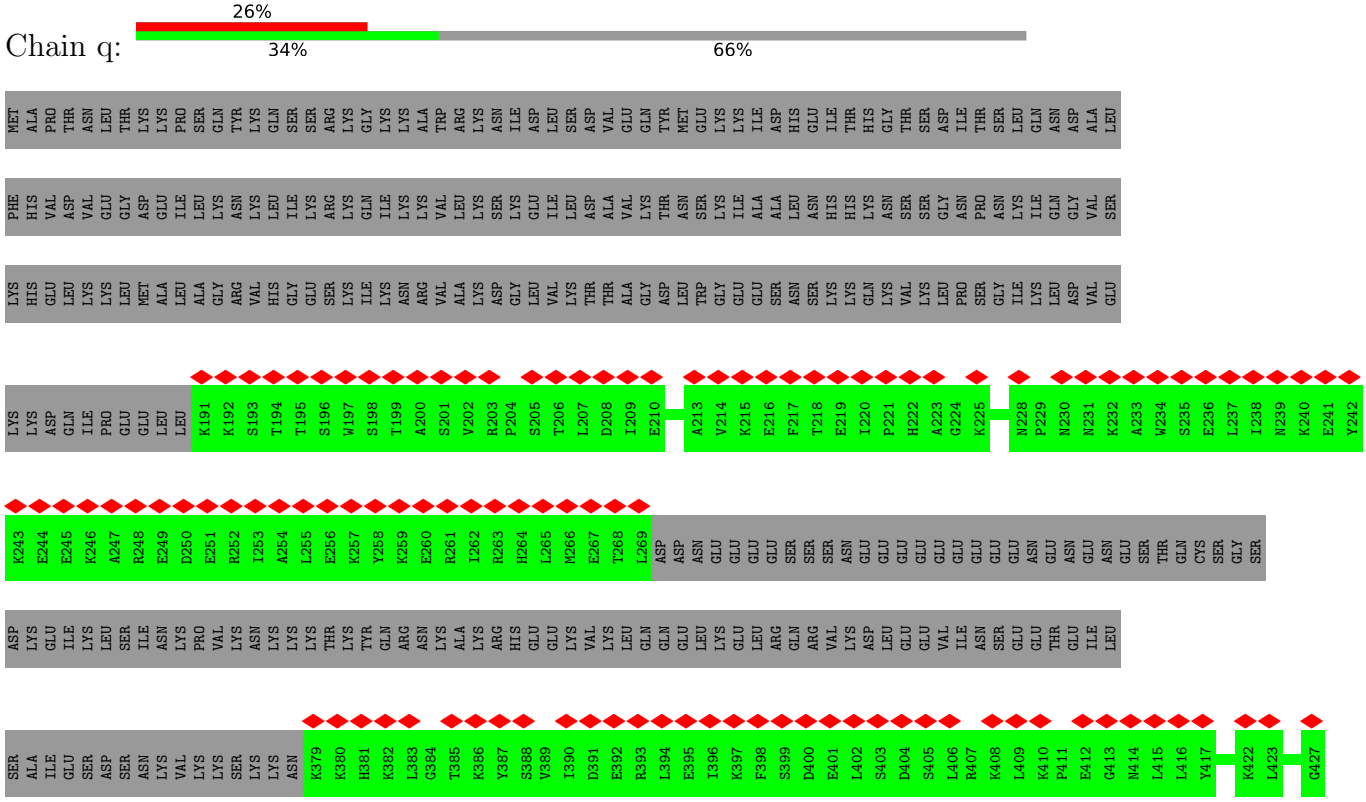
• Molecule 49: 60S ribosomal protein L43-A

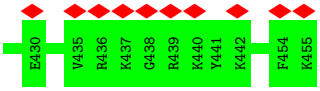
Chain p:



• Molecule 50: Ribosome biogenesis protein NOP53

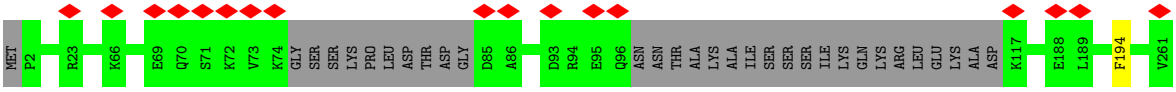
Chain q:





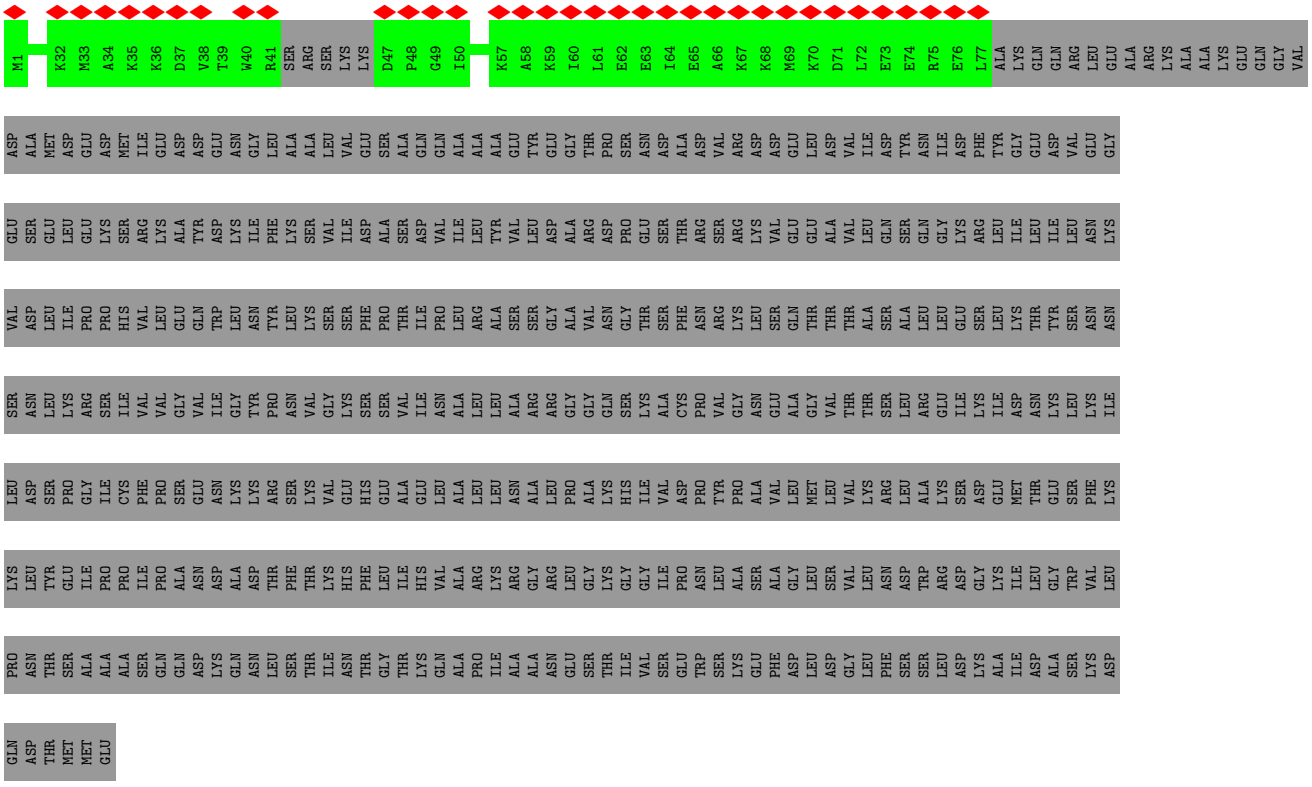
• Molecule 51: Ribosome biogenesis protein NSA2

Chain r:



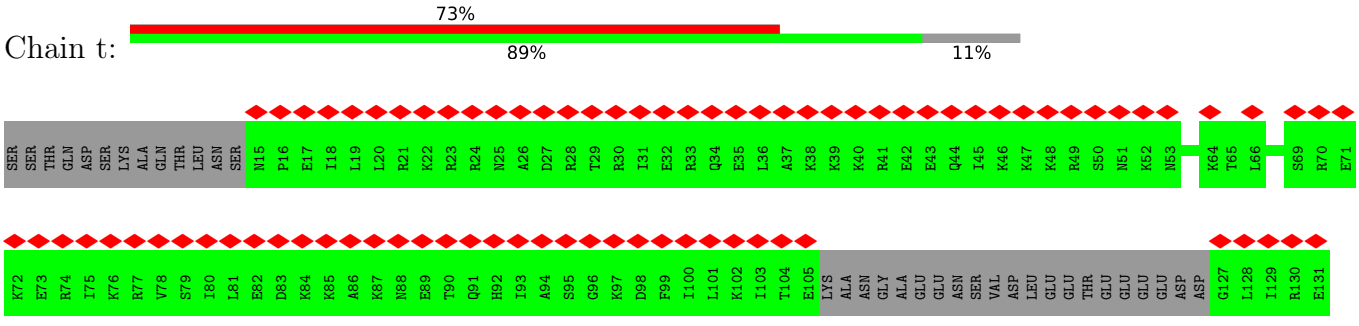
• Molecule 52: Nuclear GTP-binding protein NUG1

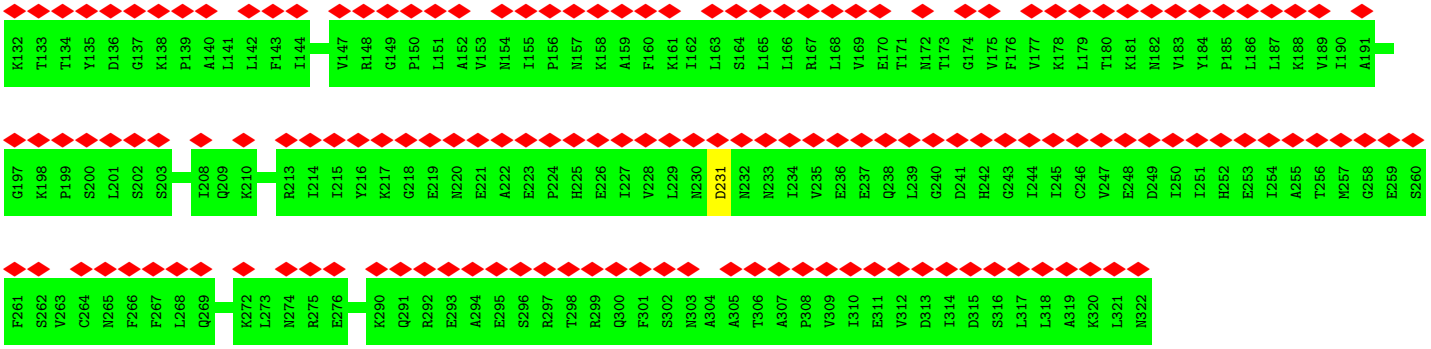
Chain s:



• Molecule 53: Ribosome biogenesis protein RLP7

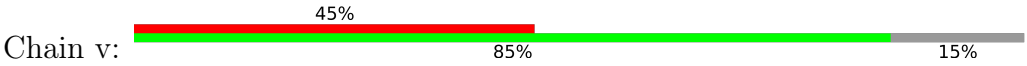
Chain t:

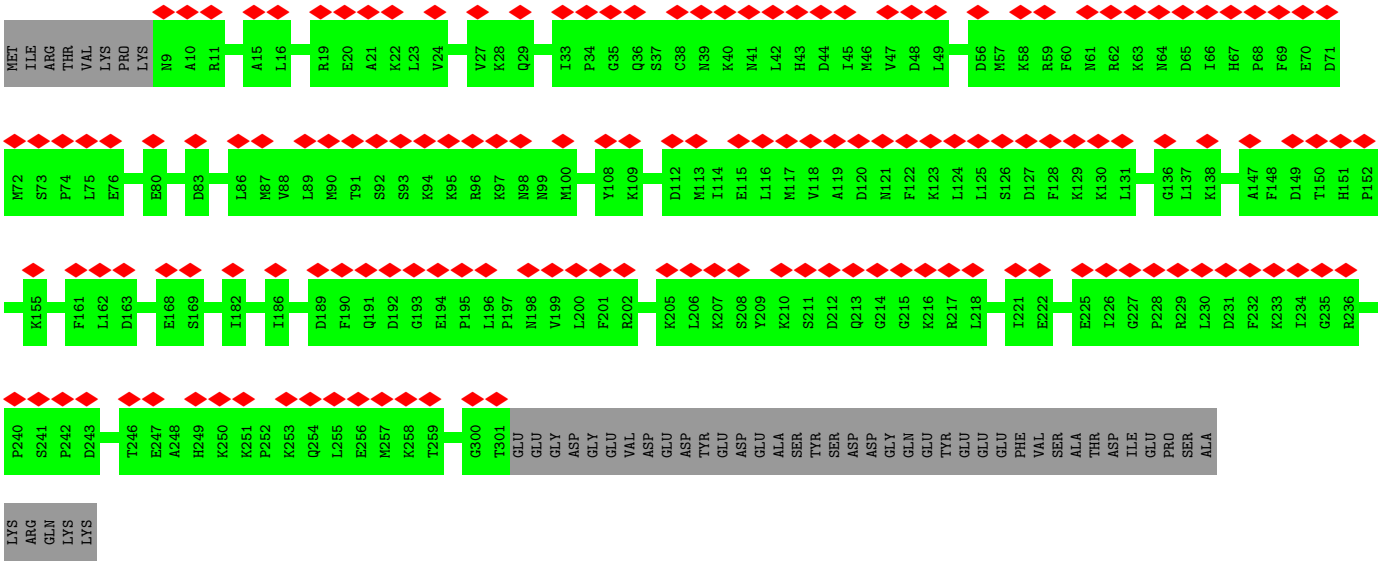




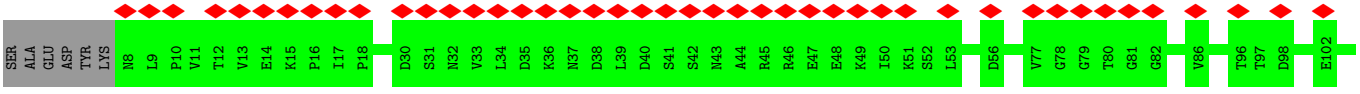
• Molecule 54: Ribosome biogenesis protein RLP24

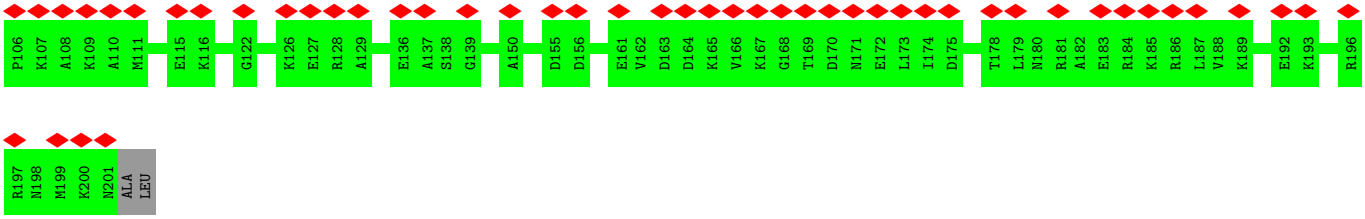
• Molecule 55: Ribosome production factor 2 homolog



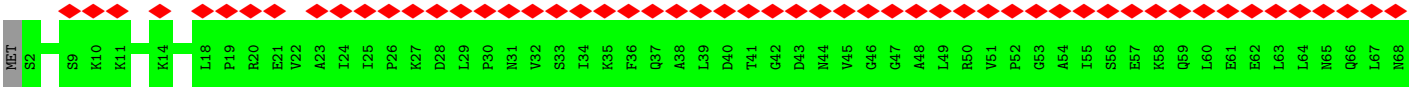


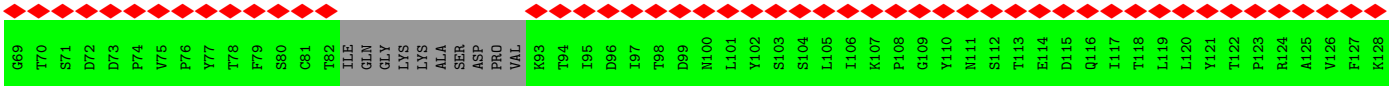
• Molecule 56: Ribosome biogenesis regulatory protein

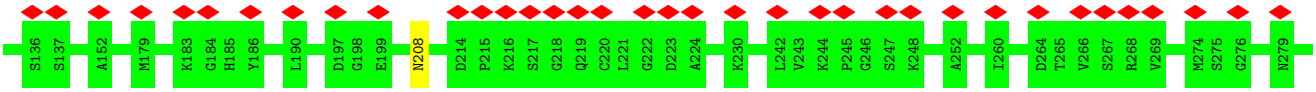


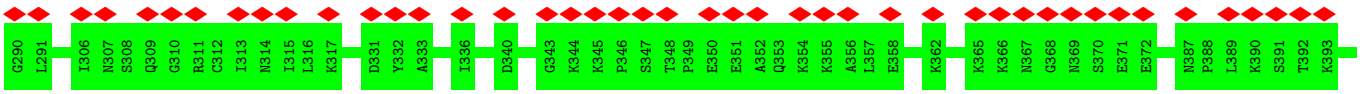


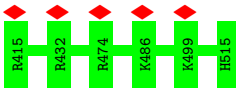
• Molecule 57: RSA4 isoform 1



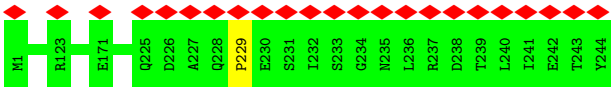




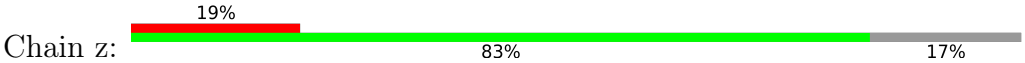


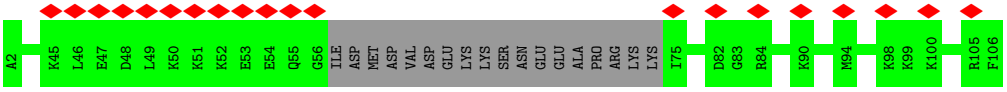


• Molecule 58: Eukaryotic translation initiation factor 6

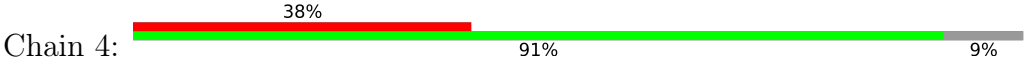


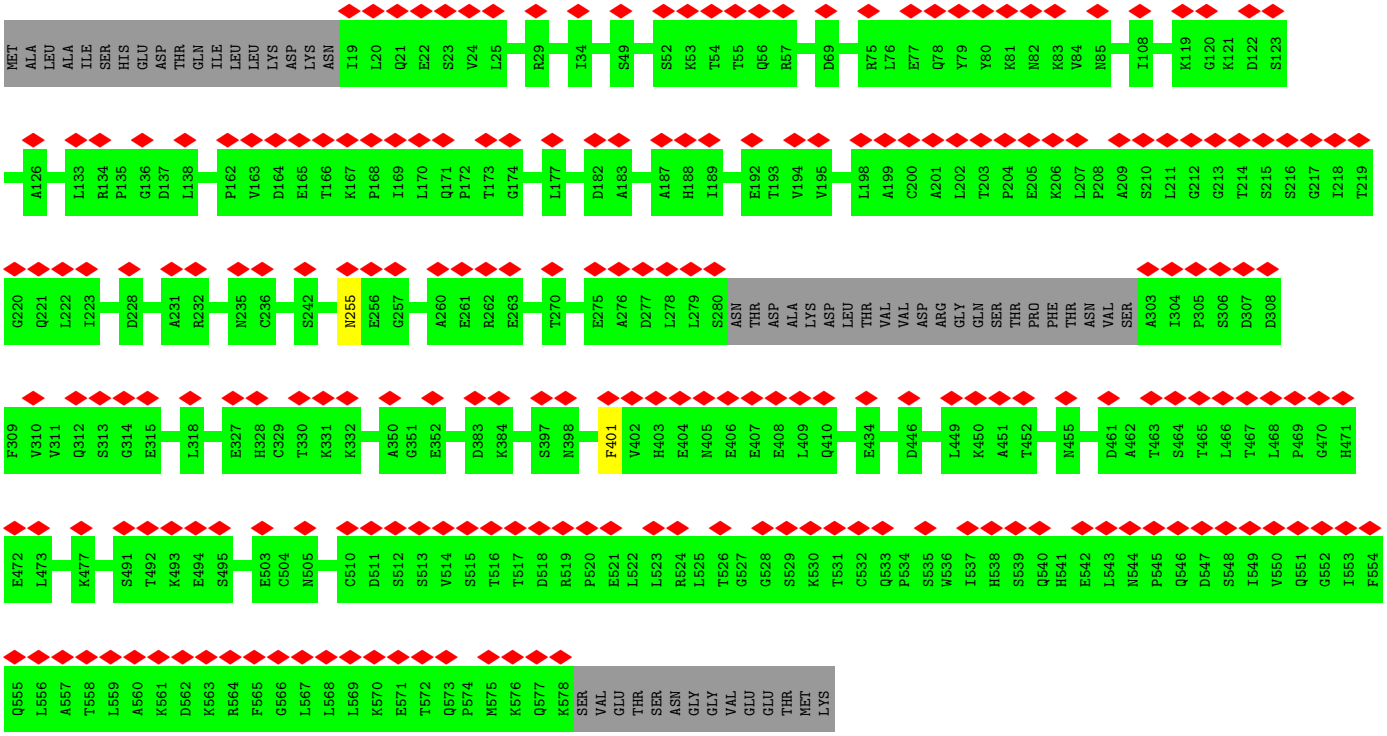
• Molecule 59: UPF0642 protein YBL028C





• Molecule 60: Probable metalloprotease ARX1




MET ALA LEU ALA ILE SER HIS GLU ASP THR GLN ILE LEU LEU LYS ASP LYS ASN I19 L20 Q21 E22 S23 V24 L25 R29 I34 S49 S52 K53 T54 T55 Q56 R57 D69 R75 L76 E77 Q78 Y79 Y80 K81 N82 K83 V84 N85 I108 K119 G120 K121 D122 S123
A126 L133 R134 P135 G136 D137 L138 P162 V163 D164 E165 T166 K167 P168 I169 L170 Q171 P172 T173 G174 L177 D182 A183 A187 H188 I189 E192 T193 V194 V195 L198 A199 C200 A201 L202 T203 P204 E205 K206 L207 P208 A209 S210 L211 G212 G213 T214 S215 S216 G217 I218 T219
G220 Q221 L222 I223 D228 A231 R232 N235 C236 S242 N255 E256 G257 A260 E261 R262 E263 T270 E275 A276 D277 L278 L279 S280 ASN THR ASP ALA LYS ASP LEU THR VAL VAL ASP ARG GLY GLN SER THR PRO PHE THR ASN VAL SER A303 I304 P305 S306 D307 D308
F309 V310 V311 Q312 S313 G314 E315 L318 E327 H328 C329 T330 K331 K332 A350 G351 E352 D383 K384 S397 N398 F401 V402 H403 E404 N405 E406 E407 E408 L409 Q410 E434 D446 L449 K450 A451 T452 N455 D461 A462 T463 S464 T465 L466 T467 L468 P469 G470 H471
E472 L473 K477 S491 T492 K493 E494 S495 E503 C504 N505 C510 D511 S512 S513 V514 S515 T516 T517 D518 R519 P520 E521 L522 L523 R524 L525 T526 G527 G528 S529 K530 T531 C532 Q533 P534 S535 W536 I537 H538 S539 Q540 H541 E542 L543 N544 P545 Q546 D547 S548 I549 V550 Q551 G552 I553 F554
Q555 L556 A557 T558 L559 A560 K561 D562 K563 R564 F565 G566 L567 L568 L569 K570 E571 T572 Q573 P574 M575 K576 Q577 K578 SER VAL GLU THR SER ASN GLY GLY VAL GLU GLU THR MET LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	534641	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.272	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: OMG, 1MA, K, OMC, MG, B3P, ZN, 5MC, OMU, A2M, PSU, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/1666	0.56	0/2241
2	1	0.26	0/70311	0.82	19/109609 (0.0%)
3	2	0.27	0/3724	0.79	1/5798 (0.0%)
4	3	0.18	0/2861	0.77	0/4457
5	5	0.24	0/649	0.50	0/848
6	6	0.22	0/1367	0.87	1/2118 (0.0%)
7	8	0.25	0/1210	0.47	0/1627
8	9	0.24	0/948	0.46	0/1264
9	B	0.25	0/3152	0.54	0/4239
10	C	0.25	0/2801	0.50	0/3792
11	D	0.24	0/2227	0.49	0/3004
12	E	0.25	0/1251	0.49	0/1682
13	F	0.25	0/1798	0.49	0/2420
14	G	0.25	0/1784	0.46	0/2408
15	H	0.25	0/1539	0.51	0/2073
16	I	0.23	0/1075	0.47	0/1443
17	J	0.24	0/1389	0.52	0/1860
18	K	0.24	0/2190	0.46	0/2955
19	L	0.24	0/1460	0.55	0/1960
20	M	0.24	0/1074	0.50	0/1446
21	N	0.24	0/1654	0.58	0/2213
22	O	0.26	0/1585	0.49	0/2128
23	P	0.24	0/1410	0.55	0/1893
24	Q	0.24	0/1153	0.53	0/1555
25	R	0.24	0/1275	0.52	0/1702
26	S	0.25	0/1473	0.50	0/1980
27	T	0.25	0/916	0.49	0/1226
28	U	0.26	0/861	0.48	0/1167
29	V	0.27	0/1018	0.53	0/1369
30	W	0.24	0/1920	0.48	0/2586
31	X	0.25	0/1103	0.49	0/1484
32	Y	0.24	0/1004	0.53	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Z	0.25	0/1118	0.46	0/1497
34	a	0.24	0/747	0.46	0/1008
35	b	0.25	0/5270	0.49	0/7080
36	c	0.25	0/751	0.44	0/1008
37	d	0.24	0/887	0.53	0/1191
38	e	0.23	0/1041	0.51	0/1394
39	f	0.26	0/868	0.55	0/1168
40	g	0.24	0/891	0.55	0/1191
41	h	0.25	0/978	0.49	0/1301
42	i	0.24	0/778	0.53	0/1034
43	j	0.25	0/680	0.57	0/901
44	k	0.25	0/618	0.52	0/826
45	l	0.23	0/443	0.58	0/588
46	m	0.25	0/3828	0.49	0/5154
47	n	0.25	0/3085	0.47	0/4166
48	o	0.24	0/1129	0.47	0/1502
49	p	0.25	0/701	0.56	0/934
50	q	0.24	0/1321	0.48	0/1766
51	r	0.25	0/1892	0.51	0/2528
52	s	0.24	0/608	0.49	0/798
53	t	0.25	0/2333	0.50	0/3128
54	u	0.26	0/1287	0.53	0/1711
55	v	0.25	0/2410	0.48	0/3220
56	w	0.23	0/1565	0.46	0/2108
57	x	0.24	0/4022	0.50	0/5460
58	y	0.39	1/1872 (0.1%)	0.53	0/2548
59	z	0.24	0/721	0.46	0/948
60	4	0.24	0/4242	0.46	0/5758
All	All	0.25	1/165934 (0.0%)	0.68	21/239804 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	y	229	PRO	N-CD	13.17	1.66	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	1495	U	C2-N1-C1'	7.61	126.84	117.70
2	1	1496	C	C2-N1-C1'	7.31	126.84	118.80
2	1	406	G	O4'-C1'-N9	7.26	114.01	108.20
2	1	1495	U	C6-N1-C1'	-7.26	111.04	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	922	U	C2-N1-C1'	6.71	125.75	117.70
2	1	922	U	C6-N1-C1'	-6.48	112.13	121.20
2	1	2772	C	N1-C2-O2	5.97	122.48	118.90
2	1	1604	G	C4-N9-C1'	5.82	134.07	126.50
2	1	2772	C	C2-N1-C1'	5.61	124.97	118.80
2	1	3131	U	C2-N1-C1'	5.47	124.26	117.70
2	1	2238	G	C4-N9-C1'	5.38	133.50	126.50
2	1	2550	U	C2-N1-C1'	5.34	124.11	117.70
2	1	1129	A	O4'-C1'-N9	5.33	112.47	108.20
2	1	1496	C	C6-N1-C1'	-5.33	114.41	120.80
6	6	7	C	C2-N1-C1'	5.30	124.63	118.80
2	1	3058	U	C2-N1-C1'	5.21	123.95	117.70
2	1	2137	U	C2-N1-C1'	5.20	123.94	117.70
2	1	3058	U	C6-N1-C1'	-5.20	113.91	121.20
3	2	100	U	C2-N1-C1'	5.20	123.94	117.70
2	1	835	G	O4'-C1'-N9	5.13	112.30	108.20
2	1	2772	C	N3-C2-O2	-5.00	118.40	121.90

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	
1	A	211/254 (83%)	200 (95%)	11 (5%)	0	100	100
5	5	71/114 (62%)	71 (100%)	0	0	100	100
7	8	156/165 (94%)	153 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	9	110/175 (63%)	109 (99%)	1 (1%)	0	100	100
9	B	384/386 (100%)	379 (99%)	5 (1%)	0	100	100
10	C	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
11	D	266/297 (90%)	259 (97%)	7 (3%)	0	100	100
12	E	151/176 (86%)	144 (95%)	7 (5%)	0	100	100
13	F	217/244 (89%)	213 (98%)	4 (2%)	0	100	100
14	G	220/256 (86%)	217 (99%)	3 (1%)	0	100	100
15	H	189/191 (99%)	183 (97%)	6 (3%)	0	100	100
16	I	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
17	J	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
18	K	262/339 (77%)	259 (99%)	3 (1%)	0	100	100
19	L	178/199 (89%)	175 (98%)	3 (2%)	0	100	100
20	M	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
21	N	185/203 (91%)	178 (96%)	7 (4%)	0	100	100
22	O	195/197 (99%)	193 (99%)	2 (1%)	0	100	100
23	P	171/183 (93%)	164 (96%)	7 (4%)	0	100	100
24	Q	145/186 (78%)	143 (99%)	2 (1%)	0	100	100
25	R	154/189 (82%)	152 (99%)	2 (1%)	0	100	100
26	S	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
27	T	110/160 (69%)	107 (97%)	3 (3%)	0	100	100
28	U	104/121 (86%)	100 (96%)	4 (4%)	0	100	100
29	V	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
30	W	232/236 (98%)	229 (99%)	3 (1%)	0	100	100
31	X	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
32	Y	124/127 (98%)	119 (96%)	5 (4%)	0	100	100
33	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
34	a	90/149 (60%)	87 (97%)	3 (3%)	0	100	100
35	b	638/647 (99%)	619 (97%)	19 (3%)	0	100	100
36	c	95/105 (90%)	95 (100%)	0	0	100	100
37	d	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
38	e	125/130 (96%)	123 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
40	g	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
41	h	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
42	i	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
43	j	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
44	k	75/78 (96%)	75 (100%)	0	0	100	100
45	l	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
46	m	462/472 (98%)	456 (99%)	6 (1%)	0	100	100
47	n	363/605 (60%)	352 (97%)	11 (3%)	0	100	100
48	o	131/220 (60%)	127 (97%)	4 (3%)	0	100	100
49	p	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
50	q	152/455 (33%)	145 (95%)	7 (5%)	0	100	100
51	r	224/261 (86%)	219 (98%)	5 (2%)	0	100	100
52	s	68/520 (13%)	65 (96%)	3 (4%)	0	100	100
53	t	283/321 (88%)	279 (99%)	4 (1%)	0	100	100
54	u	148/199 (74%)	147 (99%)	1 (1%)	0	100	100
55	v	291/344 (85%)	284 (98%)	7 (2%)	0	100	100
56	w	192/202 (95%)	188 (98%)	4 (2%)	0	100	100
57	x	500/515 (97%)	489 (98%)	11 (2%)	0	100	100
58	y	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
59	z	83/105 (79%)	83 (100%)	0	0	100	100
60	4	534/592 (90%)	526 (98%)	8 (2%)	0	100	100
All	All	10648/12739 (84%)	10398 (98%)	250 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/196 (85%)	166 (100%)	0	100	100
5	5	67/101 (66%)	67 (100%)	0	100	100
7	8	129/136 (95%)	129 (100%)	0	100	100
8	9	106/153 (69%)	106 (100%)	0	100	100
9	B	322/322 (100%)	322 (100%)	0	100	100
10	C	288/289 (100%)	286 (99%)	2 (1%)	84	90
11	D	226/245 (92%)	226 (100%)	0	100	100
12	E	133/153 (87%)	133 (100%)	0	100	100
13	F	184/205 (90%)	184 (100%)	0	100	100
14	G	185/208 (89%)	185 (100%)	0	100	100
15	H	171/171 (100%)	170 (99%)	1 (1%)	86	91
16	I	117/117 (100%)	117 (100%)	0	100	100
17	J	148/148 (100%)	148 (100%)	0	100	100
18	K	247/313 (79%)	247 (100%)	0	100	100
19	L	142/159 (89%)	142 (100%)	0	100	100
20	M	108/109 (99%)	108 (100%)	0	100	100
21	N	165/175 (94%)	164 (99%)	1 (1%)	86	91
22	O	160/160 (100%)	160 (100%)	0	100	100
23	P	141/145 (97%)	141 (100%)	0	100	100
24	Q	121/151 (80%)	121 (100%)	0	100	100
25	R	129/154 (84%)	129 (100%)	0	100	100
26	S	155/156 (99%)	154 (99%)	1 (1%)	86	91
27	T	98/137 (72%)	98 (100%)	0	100	100
28	U	93/107 (87%)	93 (100%)	0	100	100
29	V	104/105 (99%)	104 (100%)	0	100	100
30	W	211/213 (99%)	211 (100%)	0	100	100
31	X	116/118 (98%)	116 (100%)	0	100	100
32	Y	109/110 (99%)	108 (99%)	1 (1%)	78	87
33	Z	115/116 (99%)	115 (100%)	0	100	100
34	a	76/119 (64%)	76 (100%)	0	100	100
35	b	568/573 (99%)	567 (100%)	1 (0%)	93	96
36	c	81/88 (92%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	d	94/97 (97%)	94 (100%)	0	100 100
38	e	109/111 (98%)	109 (100%)	0	100 100
39	f	90/91 (99%)	90 (100%)	0	100 100
40	g	95/102 (93%)	95 (100%)	0	100 100
41	h	104/105 (99%)	104 (100%)	0	100 100
42	i	81/81 (100%)	81 (100%)	0	100 100
43	j	69/71 (97%)	69 (100%)	0	100 100
44	k	68/69 (99%)	68 (100%)	0	100 100
45	l	45/45 (100%)	45 (100%)	0	100 100
46	m	411/416 (99%)	410 (100%)	1 (0%)	93 96
47	n	332/548 (61%)	331 (100%)	1 (0%)	92 95
48	o	118/199 (59%)	117 (99%)	1 (1%)	81 88
49	p	71/72 (99%)	70 (99%)	1 (1%)	67 78
50	q	145/420 (34%)	145 (100%)	0	100 100
51	r	203/229 (89%)	202 (100%)	1 (0%)	88 93
52	s	65/445 (15%)	65 (100%)	0	100 100
53	t	256/286 (90%)	255 (100%)	1 (0%)	91 94
54	u	133/180 (74%)	133 (100%)	0	100 100
55	v	264/309 (85%)	264 (100%)	0	100 100
56	w	172/178 (97%)	172 (100%)	0	100 100
57	x	442/451 (98%)	441 (100%)	1 (0%)	93 96
58	y	210/210 (100%)	210 (100%)	0	100 100
59	z	77/94 (82%)	77 (100%)	0	100 100
60	4	471/519 (91%)	469 (100%)	2 (0%)	91 94
All	All	9306/10980 (85%)	9290 (100%)	16 (0%)	93 96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	C	120	TYR
10	C	177	ASP
15	H	157	ASN
21	N	10	LEU
26	S	172	TYR

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Mol	Chain	Res	Type
32	Y	74	TYR
35	b	278	PHE
46	m	353	TRP
47	n	214	ASP
48	o	102	PHE
49	p	60	CYS
51	r	194	PHE
53	t	231	ASP
57	x	208	ASN
60	4	255	ASN
60	4	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
11	D	45	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	2970/3396 (87%)	493 (16%)	4 (0%)
3	2	157/158 (99%)	28 (17%)	0
4	3	120/121 (99%)	25 (20%)	0
6	6	54/74 (72%)	18 (33%)	0
All	All	3301/3749 (88%)	564 (17%)	4 (0%)

All (564) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	2	U
2	1	5	G
2	1	14	U
2	1	42	C
2	1	43	A
2	1	49	A
2	1	59	G
2	1	60	A
2	1	65	A
2	1	66	A
2	1	72	C

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Mol	Chain	Res	Type
2	1	92	G
2	1	109	A
2	1	110	G
2	1	111	C
2	1	116	A
2	1	121	A
2	1	122	A
2	1	135	C
2	1	136	G
2	1	156	G
2	1	157	A
2	1	166	C
2	1	187	A
2	1	190	U
2	1	200	C
2	1	210	U
2	1	213	A
2	1	218	G
2	1	219	A
2	1	220	G
2	1	239	G
2	1	243	G
2	1	249	U
2	1	250	U
2	1	251	G
2	1	252	U
2	1	253	A
2	1	262	U
2	1	263	C
2	1	269	G
2	1	285	A
2	1	295	A
2	1	305	U
2	1	306	A
2	1	311	C
2	1	323	A
2	1	329	U
2	1	339	C
2	1	349	A
2	1	375	A
2	1	376	G
2	1	398	A

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Mol	Chain	Res	Type
2	1	399	A
2	1	401	U
2	1	402	A
2	1	403	C
2	1	421	G
2	1	422	A
2	1	439	C
2	1	440	A
2	1	495	G
2	1	517	G
2	1	521	A
2	1	523	A
2	1	535	G
2	1	543	C
2	1	547	G
2	1	550	A
2	1	552	G
2	1	555	U
2	1	557	A
2	1	558	U
2	1	559	A
2	1	579	G
2	1	589	A
2	1	592	A
2	1	604	G
2	1	609	G
2	1	611	A
2	1	612	U
2	1	620	U
2	1	621	A
2	1	637	C
2	1	643	U
2	1	644	G
2	1	645	A
2	1	646	A
2	1	648	C
2	1	649	A2M
2	1	660	A
2	1	677	A
2	1	681	U
2	1	690	A
2	1	691	A

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Mol	Chain	Res	Type
2	1	705	A
2	1	712	G
2	1	715	A
2	1	719	U
2	1	720	A
2	1	735	A
2	1	742	G
2	1	758	C
2	1	761	A
2	1	763	G
2	1	764	U
2	1	765	C
2	1	766	U
2	1	767	U
2	1	777	U
2	1	780	A
2	1	781	G
2	1	785	G
2	1	806	A
2	1	808	A
2	1	817	A2M
2	1	830	A
2	1	838	G
2	1	861	C
2	1	874	U
2	1	875	G
2	1	896	A
2	1	907	G
2	1	914	A
2	1	916	G
2	1	917	A
2	1	921	A
2	1	923	C
2	1	936	A
2	1	938	C
2	1	944	C
2	1	954	U
2	1	957	C
2	1	960	PSU
2	1	974	G
2	1	975	C
2	1	976	U

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Mol	Chain	Res	Type
2	1	979	U
2	1	980	A
2	1	993	G
2	1	1064	A
2	1	1066	G
2	1	1086	C
2	1	1093	A
2	1	1094	U
2	1	1095	U
2	1	1096	U
2	1	1097	G
2	1	1098	A
2	1	1112	A
2	1	1116	G
2	1	1117	G
2	1	1127	G
2	1	1129	A
2	1	1132	C
2	1	1143	A
2	1	1153	A
2	1	1155	C
2	1	1159	A
2	1	1180	A
2	1	1181	U
2	1	1190	A
2	1	1192	C
2	1	1193	A
2	1	1198	C
2	1	1204	A
2	1	1217	A
2	1	1224	C
2	1	1235	U
2	1	1245	A
2	1	1250	G
2	1	1252	A
2	1	1259	A
2	1	1263	A
2	1	1271	A
2	1	1272	C
2	1	1277	C
2	1	1278	A
2	1	1287	A

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Mol	Chain	Res	Type
2	1	1307	G
2	1	1308	A
2	1	1309	U
2	1	1313	G
2	1	1330	A
2	1	1348	U
2	1	1356	U
2	1	1386	A
2	1	1392	G
2	1	1399	A
2	1	1419	A
2	1	1421	G
2	1	1434	G
2	1	1437	OMC
2	1	1446	A
2	1	1448	U
2	1	1450	OMG
2	1	1469	C
2	1	1481	A
2	1	1484	U
2	1	1503	A
2	1	1508	C
2	1	1527	C
2	1	1536	G
2	1	1555	U
2	1	1557	A
2	1	1560	G
2	1	1561	G
2	1	1567	U
2	1	1568	U
2	1	1569	U
2	1	1570	U
2	1	1571	A
2	1	1572	U
2	1	1573	G
2	1	1574	C
2	1	1581	C
2	1	1582	C
2	1	1587	A
2	1	1589	A
2	1	1604	G
2	1	1628	C

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Mol	Chain	Res	Type
2	1	1629	U
2	1	1639	C
2	1	1642	A
2	1	1643	A
2	1	1715	A
2	1	1716	U
2	1	1724	U
2	1	1725	C
2	1	1741	A
2	1	1750	A
2	1	1751	G
2	1	1763	U
2	1	1780	G
2	1	1796	G
2	1	1797	A
2	1	1798	A
2	1	1813	A
2	1	1816	A
2	1	1817	G
2	1	1821	U
2	1	1839	A
2	1	1842	A
2	1	1849	C
2	1	1866	C
2	1	1879	A
2	1	1880	U
2	1	1906	G
2	1	1909	A
2	1	1953	G
2	1	2094	C
2	1	2112	U
2	1	2121	G
2	1	2122	G
2	1	2131	A
2	1	2140	U
2	1	2142	1MA
2	1	2144	A
2	1	2158	A
2	1	2169	G
2	1	2193	U
2	1	2194	G
2	1	2197	OMC

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Mol	Chain	Res	Type
2	1	2198	A
2	1	2205	U
2	1	2207	A
2	1	2209	U
2	1	2219	A
2	1	2220	A2M
2	1	2221	G
2	1	2222	A
2	1	2223	A
2	1	2244	A
2	1	2249	G
2	1	2250	G
2	1	2268	U
2	1	2269	U
2	1	2272	G
2	1	2274	U
2	1	2276	G
2	1	2277	C
2	1	2316	G
2	1	2317	A
2	1	2334	U
2	1	2335	G
2	1	2336	U
2	1	2340	PSU
2	1	2371	G
2	1	2373	A
2	1	2374	C
2	1	2375	G
2	1	2376	G
2	1	2385	G
2	1	2388	U
2	1	2393	G
2	1	2397	A
2	1	2398	A
2	1	2401	A
2	1	2402	A
2	1	2406	C
2	1	2416	PSU
2	1	2417	OMU
2	1	2418	G
2	1	2419	A
2	1	2421	OMU

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Mol	Chain	Res	Type
2	1	2422	C
2	1	2435	G
2	1	2445	A
2	1	2502	A
2	1	2504	U
2	1	2508	U
2	1	2514	U
2	1	2523	A
2	1	2524	A
2	1	2530	G
2	1	2531	C
2	1	2532	U
2	1	2547	A
2	1	2549	G
2	1	2552	C
2	1	2554	A
2	1	2555	G
2	1	2561	A
2	1	2566	C
2	1	2567	C
2	1	2569	A
2	1	2570	U
2	1	2571	U
2	1	2572	C
2	1	2573	G
2	1	2586	G
2	1	2593	A
2	1	2595	A
2	1	2606	G
2	1	2607	G
2	1	2618	G
2	1	2619	G
2	1	2623	G
2	1	2627	C
2	1	2653	C
2	1	2655	U
2	1	2656	A
2	1	2674	A
2	1	2676	A
2	1	2677	G
2	1	2678	A
2	1	2693	C

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Mol	Chain	Res	Type
2	1	2696	A
2	1	2697	A
2	1	2698	G
2	1	2699	G
2	1	2704	A
2	1	2712	U
2	1	2715	A
2	1	2718	U
2	1	2719	U
2	1	2721	A
2	1	2727	A
2	1	2729	OMU
2	1	2730	G
2	1	2749	G
2	1	2750	U
2	1	2754	G
2	1	2758	A
2	1	2759	U
2	1	2760	C
2	1	2761	G
2	1	2762	A
2	1	2763	U
2	1	2766	U
2	1	2767	U
2	1	2771	U
2	1	2772	C
2	1	2777	G
2	1	2794	G
2	1	2797	C
2	1	2798	C
2	1	2799	A
2	1	2801	A
2	1	2802	A
2	1	2803	A
2	1	2804	A
2	1	2810	C
2	1	2811	A
2	1	2817	A
2	1	2818	U
2	1	2819	A
2	1	2821	C
2	1	2822	U

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Mol	Chain	Res	Type
2	1	2824	G
2	1	2826	PSU
2	1	2838	A
2	1	2847	A
2	1	2861	U
2	1	2864	A
2	1	2872	A
2	1	2873	U
2	1	2876	C
2	1	2878	G
2	1	2887	A
2	1	2889	C
2	1	2898	G
2	1	2899	C
2	1	2914	G
2	1	2935	U
2	1	2936	A
2	1	2940	A
2	1	2941	A
2	1	2948	OMC
2	1	2953	U
2	1	2954	U
2	1	2955	U
2	1	2956	A
2	1	2970	C
2	1	2971	A
2	1	2978	U
2	1	2979	U
2	1	2980	U
2	1	2981	U
2	1	2983	C
2	1	2990	G
2	1	2996	U
2	1	2997	G
2	1	3012	A
2	1	3022	G
2	1	3032	A
2	1	3055	U
2	1	3056	U
2	1	3059	G
2	1	3080	G
2	1	3086	A

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Mol	Chain	Res	Type
2	1	3092	C
2	1	3093	C
2	1	3100	U
2	1	3102	G
2	1	3104	U
2	1	3109	G
2	1	3117	C
2	1	3118	C
2	1	3122	A
2	1	3127	A
2	1	3129	A
2	1	3130	A
2	1	3131	U
2	1	3142	A
2	1	3155	U
2	1	3156	U
2	1	3157	U
2	1	3161	C
2	1	3163	A
2	1	3165	A
2	1	3168	A
2	1	3171	U
2	1	3172	A
2	1	3173	G
2	1	3174	A
2	1	3176	G
2	1	3179	U
2	1	3181	C
2	1	3187	A
2	1	3196	U
2	1	3207	U
2	1	3214	U
2	1	3217	C
2	1	3218	A
2	1	3219	G
2	1	3229	G
2	1	3243	A
2	1	3245	A
2	1	3247	G
2	1	3259	U
2	1	3263	G
2	1	3276	G

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Mol	Chain	Res	Type
2	1	3279	A
2	1	3280	U
2	1	3282	U
2	1	3283	U
2	1	3285	C
2	1	3286	G
2	1	3287	U
2	1	3288	G
2	1	3294	A
2	1	3304	U
2	1	3316	A
2	1	3319	U
2	1	3341	U
2	1	3342	A
2	1	3345	G
2	1	3369	G
2	1	3375	A
2	1	3378	C
2	1	3386	G
2	1	3389	U
3	2	23	U
3	2	34	U
3	2	35	C
3	2	38	U
3	2	51	G
3	2	52	A
3	2	59	A
3	2	62	C
3	2	63	G
3	2	75	G
3	2	80	A
3	2	82	U
3	2	83	C
3	2	84	C
3	2	85	G
3	2	86	U
3	2	87	G
3	2	88	A
3	2	90	U
3	2	95	G
3	2	104	A
3	2	105	A

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Mol	Chain	Res	Type
3	2	106	C
3	2	111	A
3	2	113	U
3	2	125	U
3	2	126	A
3	2	151	C
4	3	7	G
4	3	11	A
4	3	14	U
4	3	18	C
4	3	22	A
4	3	33	U
4	3	49	G
4	3	50	PSU
4	3	51	A
4	3	54	U
4	3	65	G
4	3	72	A
4	3	73	C
4	3	74	C
4	3	76	A
4	3	86	U
4	3	87	G
4	3	93	C
4	3	95	A
4	3	99	G
4	3	102	A
4	3	109	G
4	3	112	G
4	3	113	C
4	3	121	U
6	6	4	U
6	6	5	C
6	6	6	U
6	6	7	C
6	6	23	U
6	6	33	U
6	6	43	A
6	6	47	A
6	6	48	A
6	6	49	C
6	6	52	G

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Mol	Chain	Res	Type
6	6	54	A
6	6	56	U
6	6	58	G
6	6	59	C
6	6	228	U
6	6	229	U
6	6	231	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	374	A
2	1	1355	A
2	1	1568	U
2	1	3121	U

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

55 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	$\#\|Z\| > 2$
2	PSU	1	1124	2	18,21,22	1.19	2 (11%)	22,30,33	1.46	4 (18%)
2	PSU	1	2340	2	18,21,22	1.11	1 (5%)	22,30,33	1.47	4 (18%)
2	OMG	1	1450	2	18,26,27	1.37	3 (16%)	19,38,41	1.36	2 (10%)
2	A2M	1	649	2	18,25,26	1.51	1 (5%)	18,36,39	0.93	1 (5%)
2	PSU	1	966	2	18,21,22	1.19	3 (16%)	22,30,33	1.42	4 (18%)
2	A2M	1	1133	2	18,25,26	1.51	1 (5%)	18,36,39	0.93	0
2	PSU	1	2735	2	18,21,22	1.14	1 (5%)	22,30,33	1.51	4 (18%)
2	OMG	1	2815	2	18,26,27	1.38	2 (11%)	19,38,41	1.48	2 (10%)
2	OMU	1	2347	2	19,22,23	0.83	1 (5%)	26,31,34	0.81	1 (3%)
2	1MA	1	2142	2	16,25,26	0.97	2 (12%)	18,37,40	1.08	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PSU	1	2129	2	18,21,22	1.14	2 (11%)	22,30,33	1.43	4 (18%)
2	PSU	1	2351	2	18,21,22	1.12	1 (5%)	22,30,33	1.48	4 (18%)
2	PSU	1	2416	2	18,21,22	1.13	1 (5%)	22,30,33	1.47	5 (22%)
2	PSU	1	2191	2	18,21,22	1.13	1 (5%)	22,30,33	1.44	5 (22%)
2	A2M	1	1449	61,2	18,25,26	1.45	1 (5%)	18,36,39	1.00	1 (5%)
2	OMU	1	2421	2	19,22,23	0.81	1 (5%)	26,31,34	0.87	2 (7%)
2	OMC	1	663	2	19,22,23	0.55	0	26,31,34	0.70	0
3	PSU	2	73	3	18,21,22	1.09	1 (5%)	22,30,33	1.44	4 (18%)
2	PSU	1	1110	2	18,21,22	1.16	1 (5%)	22,30,33	1.46	4 (18%)
2	OMC	1	650	2	19,22,23	0.54	0	26,31,34	0.64	0
2	OMG	1	908	2	18,26,27	1.39	3 (16%)	19,38,41	1.49	2 (10%)
2	5MC	1	2870	2	18,22,23	0.93	2 (11%)	26,32,35	1.19	2 (7%)
2	PSU	1	2865	2	18,21,22	1.20	3 (16%)	22,30,33	1.43	4 (18%)
2	PSU	1	2826	61,2	18,21,22	1.12	1 (5%)	22,30,33	1.52	4 (18%)
2	OMU	1	1888	2	19,22,23	1.16	1 (5%)	26,31,34	1.32	4 (15%)
2	OMC	1	2959	2	19,22,23	0.59	0	26,31,34	0.76	0
2	A2M	1	2220	2	18,25,26	1.52	1 (5%)	18,36,39	1.11	2 (11%)
2	OMG	1	867	2	18,26,27	1.32	3 (16%)	19,38,41	1.49	2 (10%)
2	A2M	1	876	2	18,25,26	1.50	1 (5%)	18,36,39	0.95	0
2	PSU	1	2264	2	18,21,22	1.19	3 (16%)	22,30,33	1.44	4 (18%)
2	PSU	1	986	2	18,21,22	1.10	2 (11%)	22,30,33	1.38	4 (18%)
2	PSU	1	2880	2	18,21,22	1.14	1 (5%)	22,30,33	1.44	4 (18%)
2	PSU	1	776	2	18,21,22	1.22	2 (11%)	22,30,33	1.47	5 (22%)
2	PSU	1	2133	2	18,21,22	1.05	1 (5%)	22,30,33	1.53	4 (18%)
2	PSU	1	2349	61,2	18,21,22	1.10	1 (5%)	22,30,33	1.39	5 (22%)
2	A2M	1	807	2	18,25,26	1.45	1 (5%)	18,36,39	1.08	1 (5%)
2	OMC	1	1437	61,2	19,22,23	0.58	0	26,31,34	1.07	2 (7%)
2	OMU	1	2729	2	19,22,23	0.77	1 (5%)	26,31,34	0.89	2 (7%)
2	OMG	1	2791	2	18,26,27	1.42	2 (11%)	19,38,41	1.49	2 (10%)
2	OMC	1	2337	2	19,22,23	0.52	0	26,31,34	0.67	0
2	OMU	1	2724	2	19,22,23	0.80	1 (5%)	26,31,34	0.85	1 (3%)
4	PSU	3	50	4	18,21,22	1.19	2 (11%)	22,30,33	1.49	4 (18%)
2	OMU	1	898	2	19,22,23	0.78	1 (5%)	26,31,34	0.88	2 (7%)
2	PSU	1	990	2	18,21,22	1.15	2 (11%)	22,30,33	1.47	4 (18%)
2	PSU	1	2266	2	18,21,22	1.18	2 (11%)	22,30,33	1.44	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OMG	1	805	2	18,26,27	1.34	3 (16%)	19,38,41	1.47	2 (10%)
2	PSU	1	2314	2	18,21,22	1.16	1 (5%)	22,30,33	1.47	4 (18%)
2	OMG	1	2793	2	18,26,27	1.39	3 (16%)	19,38,41	1.46	2 (10%)
2	OMC	1	2948	2	19,22,23	0.56	0	26,31,34	0.83	1 (3%)
2	PSU	1	2975	2	18,21,22	1.12	1 (5%)	22,30,33	1.52	4 (18%)
2	OMU	1	2417	2	19,22,23	0.79	1 (5%)	26,31,34	0.93	2 (7%)
2	5MC	1	2278	2	18,22,23	0.96	2 (11%)	26,32,35	1.12	3 (11%)
2	PSU	1	960	2	18,21,22	1.13	1 (5%)	22,30,33	1.41	5 (22%)
2	A2M	1	817	61,2	18,25,26	1.41	1 (5%)	18,36,39	1.09	1 (5%)
2	OMC	1	2197	2	19,22,23	0.46	0	26,31,34	0.67	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
2	PSU	1	1124	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2340	2	-	3/7/25/26	0/2/2/2
2	OMG	1	1450	2	-	3/5/27/28	0/3/3/3
2	A2M	1	649	2	-	3/5/27/28	0/3/3/3
2	PSU	1	966	2	-	0/7/25/26	0/2/2/2
2	A2M	1	1133	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2735	2	-	0/7/25/26	0/2/2/2
2	OMG	1	2815	2	-	0/5/27/28	0/3/3/3
2	OMU	1	2347	2	-	2/9/27/28	0/2/2/2
2	1MA	1	2142	2	-	2/3/25/26	0/3/3/3
2	PSU	1	2129	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2351	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2416	2	-	3/7/25/26	0/2/2/2
2	PSU	1	2191	2	-	0/7/25/26	0/2/2/2
2	A2M	1	1449	61,2	-	0/5/27/28	0/3/3/3
2	OMU	1	2421	2	-	2/9/27/28	0/2/2/2
2	OMC	1	663	2	-	0/9/27/28	0/2/2/2
3	PSU	2	73	3	-	0/7/25/26	0/2/2/2
2	PSU	1	1110	2	-	0/7/25/26	0/2/2/2
2	OMC	1	650	2	-	0/9/27/28	0/2/2/2
2	OMG	1	908	2	-	1/5/27/28	0/3/3/3
2	5MC	1	2870	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	1	2865	2	-	2/7/25/26	0/2/2/2
2	PSU	1	2826	61,2	-	2/7/25/26	0/2/2/2
2	OMU	1	1888	2	-	2/9/27/28	0/2/2/2
2	OMC	1	2959	2	-	0/9/27/28	0/2/2/2
2	A2M	1	2220	2	-	3/5/27/28	0/3/3/3
2	OMG	1	867	2	-	0/5/27/28	0/3/3/3
2	A2M	1	876	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2264	2	-	0/7/25/26	0/2/2/2
2	PSU	1	986	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2880	2	-	0/7/25/26	0/2/2/2
2	PSU	1	776	2	-	3/7/25/26	0/2/2/2
2	PSU	1	2133	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2349	61,2	-	0/7/25/26	0/2/2/2
2	A2M	1	807	2	-	0/5/27/28	0/3/3/3
2	OMC	1	1437	61,2	-	3/9/27/28	0/2/2/2
2	OMU	1	2729	2	-	2/9/27/28	0/2/2/2
2	OMG	1	2791	2	-	0/5/27/28	0/3/3/3
2	OMC	1	2337	2	-	0/9/27/28	0/2/2/2
2	OMU	1	2724	2	-	0/9/27/28	0/2/2/2
4	PSU	3	50	4	-	2/7/25/26	0/2/2/2
2	OMU	1	898	2	-	0/9/27/28	0/2/2/2
2	PSU	1	990	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2266	2	-	0/7/25/26	0/2/2/2
2	OMG	1	805	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2314	2	-	0/7/25/26	0/2/2/2
2	OMG	1	2793	2	-	0/5/27/28	0/3/3/3
2	OMC	1	2948	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2975	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2417	2	-	2/9/27/28	0/2/2/2
2	5MC	1	2278	2	-	0/7/25/26	0/2/2/2
2	PSU	1	960	2	-	2/7/25/26	0/2/2/2
2	A2M	1	817	61,2	-	2/5/27/28	0/3/3/3
2	OMC	1	2197	2	-	2/9/27/28	0/2/2/2

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2220	A2M	O5'-C5'	-4.80	1.33	1.44
2	1	876	A2M	O5'-C5'	-4.69	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	1449	A2M	O5'-C5'	-4.62	1.33	1.44
2	1	1133	A2M	O5'-C5'	-4.55	1.33	1.44
2	1	2791	OMG	C6-N1	4.53	1.44	1.37
2	1	1888	OMU	C2-N1	4.49	1.45	1.38
2	1	649	A2M	O5'-C5'	-4.47	1.33	1.44
2	1	817	A2M	O5'-C5'	-4.39	1.34	1.44
2	1	908	OMG	C6-N1	4.37	1.44	1.37
2	1	2815	OMG	C6-N1	4.35	1.44	1.37
2	1	2793	OMG	C6-N1	4.32	1.44	1.37
2	1	1450	OMG	C6-N1	4.29	1.44	1.37
2	1	807	A2M	O5'-C5'	-4.29	1.34	1.44
2	1	805	OMG	C6-N1	4.16	1.44	1.37
2	1	867	OMG	C6-N1	4.11	1.44	1.37
2	1	2865	PSU	C2-N1	3.10	1.40	1.36
4	3	50	PSU	C2-N1	3.07	1.40	1.36
2	1	1124	PSU	C2-N1	3.05	1.40	1.36
2	1	1110	PSU	C2-N1	3.03	1.40	1.36
2	1	2826	PSU	C2-N1	3.03	1.40	1.36
2	1	2351	PSU	C2-N1	3.01	1.40	1.36
2	1	966	PSU	C2-N1	2.99	1.40	1.36
2	1	2975	PSU	C2-N1	2.98	1.40	1.36
2	1	2266	PSU	C2-N1	2.98	1.40	1.36
2	1	2314	PSU	C2-N1	2.97	1.40	1.36
2	1	2264	PSU	C2-N1	2.96	1.40	1.36
2	1	2735	PSU	C2-N1	2.95	1.40	1.36
2	1	2340	PSU	C2-N1	2.93	1.40	1.36
2	1	990	PSU	C2-N1	2.90	1.40	1.36
2	1	2191	PSU	C2-N1	2.88	1.40	1.36
2	1	2133	PSU	C2-N1	2.84	1.40	1.36
2	1	776	PSU	C2-N1	2.82	1.40	1.36
2	1	2129	PSU	C2-N1	2.80	1.40	1.36
2	1	2416	PSU	C2-N1	2.80	1.40	1.36
2	1	960	PSU	C2-N1	2.79	1.40	1.36
2	1	2278	5MC	C6-C5	2.77	1.39	1.34
2	1	2880	PSU	C2-N1	2.72	1.40	1.36
2	1	2142	1MA	C8-N7	-2.70	1.30	1.35
3	2	73	PSU	C2-N1	2.69	1.40	1.36
2	1	986	PSU	C2-N1	2.64	1.40	1.36
2	1	2347	OMU	C2-N1	2.64	1.42	1.38
2	1	2815	OMG	C2-N2	2.61	1.40	1.34
2	1	908	OMG	C2-N2	2.60	1.40	1.34
2	1	2791	OMG	C2-N2	2.59	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2349	PSU	C2-N1	2.57	1.40	1.36
2	1	2793	OMG	C2-N2	2.54	1.40	1.34
2	1	1450	OMG	C2-N2	2.50	1.40	1.34
2	1	2870	5MC	C6-C5	2.47	1.38	1.34
2	1	867	OMG	C2-N2	2.47	1.40	1.34
2	1	805	OMG	C2-N2	2.46	1.40	1.34
2	1	2870	5MC	C6-N1	-2.44	1.33	1.38
2	1	2724	OMU	C2-N1	2.29	1.42	1.38
2	1	898	OMU	C2-N1	2.27	1.42	1.38
2	1	2278	5MC	C6-N1	-2.23	1.34	1.38
2	1	1450	OMG	C5-C6	-2.22	1.42	1.47
2	1	2417	OMU	C2-N1	2.20	1.42	1.38
2	1	2142	1MA	C5-C4	-2.17	1.37	1.43
2	1	2421	OMU	C2-N1	2.16	1.41	1.38
2	1	2793	OMG	C5-C6	-2.12	1.43	1.47
4	3	50	PSU	C6-N1	2.11	1.39	1.36
2	1	966	PSU	C4-N3	2.10	1.42	1.38
2	1	2865	PSU	C6-N1	2.10	1.39	1.36
2	1	2266	PSU	C4-N3	2.08	1.42	1.38
2	1	776	PSU	C4-N3	2.07	1.42	1.38
2	1	990	PSU	C6-N1	2.06	1.39	1.36
2	1	1124	PSU	C6-N1	2.06	1.39	1.36
2	1	805	OMG	C5-C6	-2.06	1.43	1.47
2	1	2264	PSU	C4-N3	2.05	1.42	1.38
2	1	2865	PSU	C4-N3	2.04	1.42	1.38
2	1	867	OMG	C5-C6	-2.03	1.43	1.47
2	1	2129	PSU	C4-N3	2.02	1.42	1.38
2	1	2729	OMU	C2-N1	2.02	1.41	1.38
2	1	966	PSU	C6-N1	2.01	1.39	1.36
2	1	2264	PSU	C6-N1	2.01	1.39	1.36
2	1	908	OMG	C5-C6	-2.00	1.43	1.47
2	1	986	PSU	C4-N3	2.00	1.42	1.38

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2826	PSU	C6-C5-C4	4.31	121.21	118.20
2	1	2865	PSU	C6-C5-C4	4.31	121.21	118.20
2	1	2735	PSU	C6-C5-C4	4.27	121.19	118.20
2	1	2975	PSU	C6-C5-C4	4.26	121.17	118.20
4	3	50	PSU	C6-C5-C4	4.23	121.16	118.20
2	1	2314	PSU	C6-C5-C4	4.12	121.08	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	990	PSU	C6-C5-C4	4.09	121.06	118.20
2	1	2351	PSU	C6-C5-C4	4.07	121.04	118.20
2	1	2416	PSU	C6-C5-C4	4.03	121.02	118.20
2	1	1110	PSU	C6-C5-C4	4.02	121.01	118.20
2	1	2264	PSU	C6-C5-C4	3.98	120.98	118.20
2	1	867	OMG	O6-C6-N1	-3.96	115.97	120.65
2	1	1124	PSU	C6-C5-C4	3.91	120.93	118.20
2	1	2340	PSU	C6-C5-C4	3.90	120.92	118.20
2	1	2880	PSU	C6-C5-C4	3.89	120.92	118.20
2	1	2133	PSU	C6-C5-C4	3.88	120.91	118.20
2	1	2791	OMG	O6-C6-N1	-3.88	116.07	120.65
2	1	2815	OMG	O6-C6-N1	-3.85	116.11	120.65
2	1	805	OMG	O6-C6-N1	-3.84	116.12	120.65
2	1	908	OMG	O6-C6-N1	-3.83	116.13	120.65
3	2	73	PSU	C6-C5-C4	3.78	120.84	118.20
2	1	966	PSU	C6-C5-C4	3.76	120.83	118.20
2	1	2266	PSU	C6-C5-C4	3.75	120.82	118.20
2	1	2129	PSU	C6-C5-C4	3.71	120.79	118.20
2	1	776	PSU	C6-C5-C4	3.67	120.77	118.20
2	1	2793	OMG	O6-C6-N1	-3.63	116.36	120.65
2	1	2870	5MC	C5-C6-N1	-3.62	119.61	123.34
2	1	2191	PSU	C6-C5-C4	3.49	120.64	118.20
2	1	1450	OMG	O6-C6-N1	-3.41	116.62	120.65
2	1	2791	OMG	O6-C6-C5	3.32	130.86	124.37
2	1	867	OMG	O6-C6-C5	3.32	130.86	124.37
2	1	908	OMG	O6-C6-C5	3.30	130.83	124.37
2	1	2815	OMG	O6-C6-C5	3.29	130.81	124.37
2	1	805	OMG	O6-C6-C5	3.29	130.80	124.37
2	1	2278	5MC	C5-C6-N1	-3.28	119.97	123.34
2	1	2793	OMG	O6-C6-C5	3.28	130.77	124.37
2	1	960	PSU	C6-C5-C4	3.24	120.47	118.20
2	1	1437	OMC	C1'-N1-C2	3.18	125.53	118.42
2	1	986	PSU	C6-C5-C4	3.17	120.41	118.20
2	1	1450	OMG	O6-C6-C5	3.09	130.40	124.37
2	1	2349	PSU	O4-C4-N3	-3.08	114.22	120.12
2	1	2975	PSU	C4-N3-C2	-3.00	122.02	126.34
2	1	2129	PSU	C4-N3-C2	-2.97	122.07	126.34
3	2	73	PSU	C4-N3-C2	-2.95	122.08	126.34
2	1	2191	PSU	C4-N3-C2	-2.94	122.10	126.34
4	3	50	PSU	C4-N3-C2	-2.94	122.10	126.34
2	1	2416	PSU	C4-N3-C2	-2.93	122.12	126.34
2	1	2133	PSU	C4-N3-C2	-2.92	122.13	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2735	PSU	C4-N3-C2	-2.92	122.14	126.34
2	1	2865	PSU	C4-N3-C2	-2.91	122.14	126.34
2	1	2880	PSU	C4-N3-C2	-2.91	122.15	126.34
2	1	1124	PSU	C4-N3-C2	-2.90	122.16	126.34
2	1	2826	PSU	C4-N3-C2	-2.89	122.17	126.34
2	1	990	PSU	C4-N3-C2	-2.89	122.18	126.34
2	1	776	PSU	C4-N3-C2	-2.88	122.19	126.34
2	1	986	PSU	O4-C4-N3	-2.88	114.60	120.12
2	1	2314	PSU	C4-N3-C2	-2.87	122.20	126.34
2	1	966	PSU	C4-N3-C2	-2.87	122.20	126.34
2	1	2349	PSU	C6-C5-C4	2.87	120.21	118.20
2	1	2133	PSU	O4-C4-N3	-2.86	114.64	120.12
2	1	2351	PSU	C4-N3-C2	-2.85	122.23	126.34
2	1	2264	PSU	C4-N3-C2	-2.84	122.25	126.34
2	1	960	PSU	O4-C4-N3	-2.83	114.69	120.12
2	1	2266	PSU	C4-N3-C2	-2.83	122.26	126.34
2	1	1110	PSU	C4-N3-C2	-2.81	122.28	126.34
2	1	2340	PSU	C4-N3-C2	-2.79	122.32	126.34
2	1	986	PSU	C4-N3-C2	-2.75	122.37	126.34
2	1	960	PSU	C4-N3-C2	-2.74	122.39	126.34
2	1	2191	PSU	O4-C4-N3	-2.73	114.89	120.12
2	1	2349	PSU	C4-N3-C2	-2.69	122.47	126.34
2	1	1888	OMU	O2-C2-N1	2.66	126.32	122.79
2	1	2278	5MC	C5-C4-N3	-2.65	118.81	121.67
2	1	776	PSU	O4-C4-N3	-2.64	115.06	120.12
2	1	2340	PSU	O4-C4-N3	-2.62	115.10	120.12
2	1	2129	PSU	O4-C4-N3	-2.62	115.10	120.12
2	1	1124	PSU	O4-C4-N3	-2.61	115.12	120.12
2	1	1888	OMU	C1'-N1-C2	2.61	122.29	117.57
2	1	966	PSU	O4-C4-N3	-2.57	115.19	120.12
2	1	2351	PSU	O4-C4-N3	-2.57	115.20	120.12
2	1	2735	PSU	O4-C4-N3	-2.56	115.22	120.12
2	1	2266	PSU	O4-C4-N3	-2.55	115.22	120.12
2	1	1110	PSU	O4-C4-N3	-2.54	115.25	120.12
2	1	2880	PSU	O4-C4-N3	-2.53	115.26	120.12
3	2	73	PSU	O4-C4-N3	-2.50	115.33	120.12
2	1	817	A2M	C3'-C2'-C1'	-2.50	98.20	102.89
2	1	2975	PSU	O4-C4-N3	-2.49	115.35	120.12
2	1	2314	PSU	O4-C4-N3	-2.49	115.35	120.12
2	1	2142	1MA	N1-C6-N6	2.48	126.07	119.77
2	1	2729	OMU	CM2-O2'-C2'	-2.48	108.03	114.52
2	1	2417	OMU	CM2-O2'-C2'	-2.44	108.11	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	990	PSU	O4-C4-N3	-2.44	115.44	120.12
2	1	2264	PSU	O4-C4-N3	-2.44	115.44	120.12
2	1	2133	PSU	N1-C2-N3	2.42	117.87	115.13
4	3	50	PSU	O4-C4-N3	-2.41	115.50	120.12
2	1	2826	PSU	O4-C4-N3	-2.41	115.50	120.12
2	1	2865	PSU	O4-C4-N3	-2.36	115.59	120.12
2	1	2416	PSU	O4-C4-N3	-2.32	115.66	120.12
2	1	1888	OMU	CM2-O2'-C2'	-2.31	108.45	114.52
2	1	2421	OMU	CM2-O2'-C2'	-2.31	108.46	114.52
2	1	2729	OMU	C4-N3-C2	-2.31	123.53	126.58
2	1	2421	OMU	C4-N3-C2	-2.30	123.55	126.58
2	1	2948	OMC	C1'-N1-C2	2.30	123.55	118.42
2	1	1888	OMU	O2-C2-N3	-2.26	117.30	121.50
2	1	898	OMU	C4-N3-C2	-2.25	123.61	126.58
2	1	2417	OMU	C4-N3-C2	-2.23	123.64	126.58
2	1	2351	PSU	N1-C2-N3	2.23	117.65	115.13
2	1	2975	PSU	N1-C2-N3	2.22	117.64	115.13
2	1	776	PSU	N1-C2-N3	2.21	117.64	115.13
2	1	2191	PSU	N1-C2-N3	2.21	117.63	115.13
2	1	2735	PSU	N1-C2-N3	2.20	117.62	115.13
2	1	2142	1MA	C5-C6-N1	-2.20	110.61	113.90
2	1	2724	OMU	C4-N3-C2	-2.19	123.69	126.58
3	2	73	PSU	N1-C2-N3	2.19	117.61	115.13
2	1	2870	5MC	C5-C4-N3	-2.16	119.34	121.67
2	1	1437	OMC	C1'-N1-C6	-2.14	116.17	120.84
2	1	990	PSU	N1-C2-N3	2.13	117.55	115.13
2	1	2220	A2M	C2-N1-C6	-2.12	115.12	118.75
2	1	776	PSU	O4'-C1'-C2'	2.11	108.13	105.14
2	1	2826	PSU	N1-C2-N3	2.11	117.52	115.13
2	1	1124	PSU	N1-C2-N3	2.11	117.52	115.13
2	1	2266	PSU	N1-C2-N3	2.11	117.52	115.13
2	1	2340	PSU	N1-C2-N3	2.11	117.52	115.13
2	1	2880	PSU	N1-C2-N3	2.11	117.52	115.13
2	1	1110	PSU	N1-C2-N3	2.11	117.52	115.13
2	1	960	PSU	O4'-C1'-C2'	2.10	108.10	105.14
2	1	986	PSU	N1-C2-N3	2.10	117.51	115.13
4	3	50	PSU	N1-C2-N3	2.09	117.50	115.13
2	1	2865	PSU	N1-C2-N3	2.09	117.50	115.13
2	1	2314	PSU	N1-C2-N3	2.09	117.49	115.13
2	1	2349	PSU	N1-C2-N3	2.08	117.49	115.13
2	1	2278	5MC	O2-C2-N3	-2.07	118.96	122.33
2	1	649	A2M	C2-N1-C6	-2.07	115.20	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	807	A2M	C2-N1-C6	-2.07	115.22	118.75
2	1	898	OMU	CM2-O2'-C2'	-2.06	109.12	114.52
2	1	2220	A2M	O4'-C4'-C3'	2.06	109.19	105.11
2	1	2266	PSU	O4'-C1'-C2'	2.05	108.04	105.14
2	1	2416	PSU	O4'-C1'-C2'	2.05	108.04	105.14
2	1	2416	PSU	N1-C2-N3	2.05	117.45	115.13
2	1	1449	A2M	C2-N1-C6	-2.04	115.26	118.75
2	1	2349	PSU	O4'-C1'-C2'	2.03	108.01	105.14
2	1	2129	PSU	N1-C2-N3	2.03	117.43	115.13
2	1	2191	PSU	O4'-C1'-C2'	2.03	108.01	105.14
2	1	2264	PSU	N1-C2-N3	2.02	117.42	115.13
2	1	2347	OMU	C4-N3-C2	-2.02	123.92	126.58
2	1	960	PSU	N1-C2-N3	2.02	117.42	115.13
2	1	966	PSU	N1-C2-N3	2.01	117.41	115.13

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	649	A2M	C3'-C4'-C5'-O5'
2	1	960	PSU	C3'-C4'-C5'-O5'
2	1	960	PSU	O4'-C4'-C5'-O5'
2	1	1450	OMG	O4'-C4'-C5'-O5'
2	1	1888	OMU	O4'-C1'-N1-C2
2	1	1888	OMU	O4'-C1'-N1-C6
2	1	2142	1MA	O4'-C4'-C5'-O5'
2	1	2197	OMC	C3'-C4'-C5'-O5'
2	1	2197	OMC	O4'-C4'-C5'-O5'
2	1	2220	A2M	O4'-C4'-C5'-O5'
2	1	2220	A2M	C3'-C4'-C5'-O5'
2	1	2417	OMU	C3'-C4'-C5'-O5'
2	1	2417	OMU	O4'-C4'-C5'-O5'
2	1	2421	OMU	C3'-C4'-C5'-O5'
2	1	2421	OMU	O4'-C4'-C5'-O5'
2	1	2948	OMC	C3'-C4'-C5'-O5'
2	1	2948	OMC	O4'-C4'-C5'-O5'
4	3	50	PSU	O4'-C4'-C5'-O5'
2	1	649	A2M	O4'-C4'-C5'-O5'
2	1	1437	OMC	O4'-C4'-C5'-O5'
2	1	1450	OMG	C3'-C4'-C5'-O5'
2	1	2340	PSU	O4'-C4'-C5'-O5'
2	1	2416	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	3	50	PSU	C3'-C4'-C5'-O5'
2	1	2142	1MA	C3'-C4'-C5'-O5'
2	1	2340	PSU	C3'-C4'-C5'-O5'
2	1	2416	PSU	O4'-C4'-C5'-O5'
2	1	2865	PSU	O4'-C4'-C5'-O5'
2	1	2826	PSU	O4'-C4'-C5'-O5'
2	1	776	PSU	C3'-C4'-C5'-O5'
2	1	2865	PSU	C3'-C4'-C5'-O5'
2	1	2347	OMU	C3'-C4'-C5'-O5'
2	1	2729	OMU	O4'-C4'-C5'-O5'
2	1	1437	OMC	C3'-C4'-C5'-O5'
2	1	2729	OMU	C3'-C4'-C5'-O5'
2	1	776	PSU	O4'-C4'-C5'-O5'
2	1	2340	PSU	C4'-C5'-O5'-P
2	1	2220	A2M	C3'-C2'-O2'-CM'
2	1	649	A2M	C4'-C5'-O5'-P
2	1	908	OMG	C3'-C2'-O2'-CM2
2	1	2416	PSU	C4'-C5'-O5'-P
2	1	2826	PSU	C3'-C4'-C5'-O5'
2	1	817	A2M	C4'-C5'-O5'-P
2	1	1450	OMG	C1'-C2'-O2'-CM2
2	1	1437	OMC	C2'-C1'-N1-C2
2	1	2347	OMU	O4'-C4'-C5'-O5'
2	1	817	A2M	O4'-C4'-C5'-O5'
2	1	776	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 92 ligands modelled in this entry, 87 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
64	GDP	m	501	61,65	24,30,30	0.94	1 (4%)	30,47,47	1.26	4 (13%)
62	B3P	1	3479	-	18,18,18	1.48	2 (11%)	21,23,23	1.99	6 (28%)
62	B3P	1	3478	61	18,18,18	1.50	2 (11%)	21,23,23	1.95	6 (28%)
64	GDP	b	801	61	24,30,30	0.95	1 (4%)	30,47,47	1.26	4 (13%)
62	B3P	1	3480	-	18,18,18	1.52	2 (11%)	21,23,23	1.99	6 (28%)

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
64	GDP	m	501	61,65	-	3/12/32/32	0/3/3/3
62	B3P	1	3479	-	-	10/28/28/28	-
62	B3P	1	3478	61	-	7/28/28/28	-
64	GDP	b	801	61	-	5/12/32/32	0/3/3/3
62	B3P	1	3480	-	-	6/28/28/28	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	1	3480	B3P	C6-C4	5.08	1.59	1.53
62	1	3478	B3P	C6-C4	5.03	1.59	1.53
62	1	3479	B3P	C6-C4	4.68	1.59	1.53
62	1	3479	B3P	C7-C4	2.79	1.56	1.53
62	1	3480	B3P	C7-C4	2.58	1.56	1.53
64	m	501	GDP	C6-N1	-2.55	1.34	1.37
64	b	801	GDP	C6-N1	-2.40	1.34	1.37
62	1	3478	B3P	C7-C4	2.35	1.56	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	1	3480	B3P	O5-C6-C4	5.04	121.83	111.63
62	1	3478	B3P	O5-C6-C4	4.99	121.75	111.63
62	1	3479	B3P	O5-C6-C4	4.93	121.62	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	1	3479	B3P	C2-N2-C8	-4.32	109.95	116.08
62	1	3480	B3P	C2-N2-C8	-3.93	110.50	116.08
62	1	3480	B3P	C3-N1-C4	-3.92	110.52	116.08
62	1	3478	B3P	C3-N1-C4	-3.77	110.72	116.08
62	1	3478	B3P	C2-N2-C8	-3.74	110.77	116.08
62	1	3479	B3P	C3-N1-C4	-3.31	111.38	116.08
64	b	801	GDP	PA-O3A-PB	-3.16	121.97	132.83
64	m	501	GDP	PA-O3A-PB	-2.99	122.57	132.83
64	b	801	GDP	C3'-C2'-C1'	2.83	105.24	100.98
62	1	3478	B3P	O6-C7-C4	-2.78	106.00	111.63
64	m	501	GDP	C3'-C2'-C1'	2.76	105.13	100.98
62	1	3479	B3P	O6-C7-C4	-2.76	106.06	111.63
62	1	3480	B3P	O6-C7-C4	-2.65	106.27	111.63
62	1	3480	B3P	O3-C11-C8	-2.62	106.33	111.63
62	1	3479	B3P	O4-C5-C4	-2.60	106.36	111.63
62	1	3479	B3P	O3-C11-C8	-2.47	106.63	111.63
62	1	3478	B3P	O3-C11-C8	-2.46	106.65	111.63
62	1	3478	B3P	O4-C5-C4	-2.45	106.68	111.63
64	b	801	GDP	C8-N7-C5	2.36	107.48	102.99
64	m	501	GDP	C8-N7-C5	2.33	107.44	102.99
64	m	501	GDP	C5-C6-N1	2.33	118.07	113.95
64	b	801	GDP	C5-C6-N1	2.27	117.95	113.95
62	1	3480	B3P	O4-C5-C4	-2.24	107.09	111.63

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	1	3478	B3P	N1-C4-C6-O5
62	1	3478	B3P	C5-C4-C6-O5
62	1	3478	B3P	C7-C4-C6-O5
62	1	3478	B3P	O3-C11-C8-N2
62	1	3478	B3P	O3-C11-C8-C10
62	1	3479	B3P	N1-C4-C5-O4
62	1	3479	B3P	C6-C4-C5-O4
62	1	3479	B3P	C7-C4-C5-O4
62	1	3479	B3P	N1-C4-C6-O5
62	1	3479	B3P	C5-C4-C6-O5
62	1	3479	B3P	C7-C4-C6-O5
62	1	3480	B3P	N1-C4-C5-O4
62	1	3480	B3P	C6-C4-C5-O4
62	1	3480	B3P	C7-C4-C5-O4

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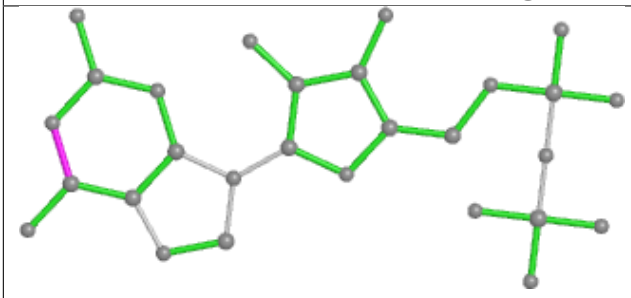
Mol	Chain	Res	Type	Atoms
62	1	3480	B3P	N1-C4-C6-O5
62	1	3480	B3P	C5-C4-C6-O5
62	1	3480	B3P	C7-C4-C6-O5
64	b	801	GDP	C5'-O5'-PA-O1A
64	b	801	GDP	C5'-O5'-PA-O2A
64	m	501	GDP	PA-O3A-PB-O3B
64	b	801	GDP	O4'-C4'-C5'-O5'
64	b	801	GDP	C3'-C4'-C5'-O5'
62	1	3479	B3P	O3-C11-C8-N2
62	1	3479	B3P	C7-C4-N1-C3
62	1	3478	B3P	C2-C1-C3-N1
62	1	3478	B3P	O3-C11-C8-C9
64	m	501	GDP	PA-O3A-PB-O2B
62	1	3479	B3P	O3-C11-C8-C10
62	1	3479	B3P	C5-C4-N1-C3
64	m	501	GDP	PA-O3A-PB-O1B
64	b	801	GDP	C5'-O5'-PA-O3A

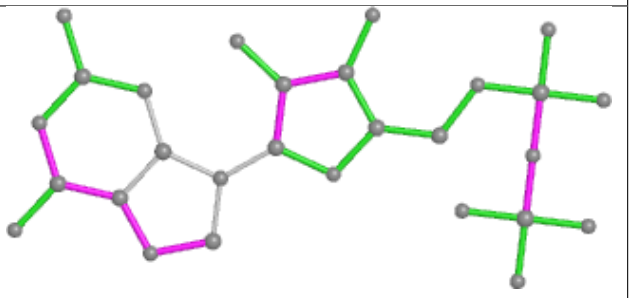
There are no ring outliers.

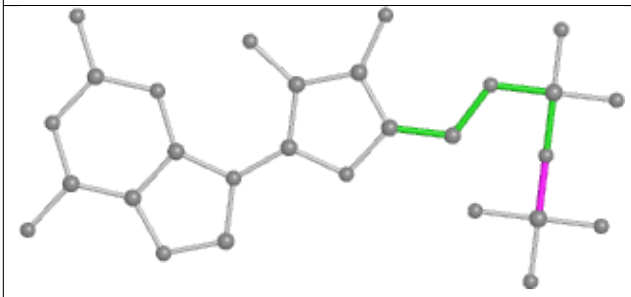
No monomer is involved in short contacts.

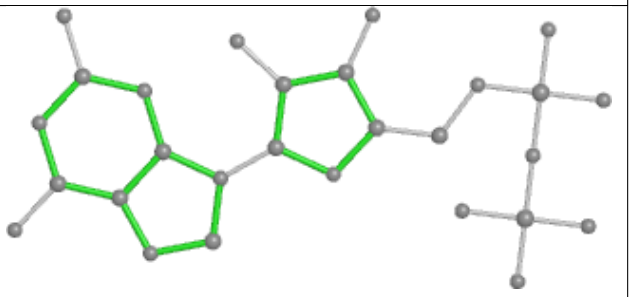
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand GDP m 501

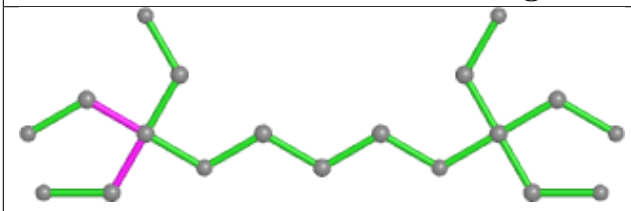

Bond lengths


Bond angles


Torsions


Rings

Ligand B3P 1 3479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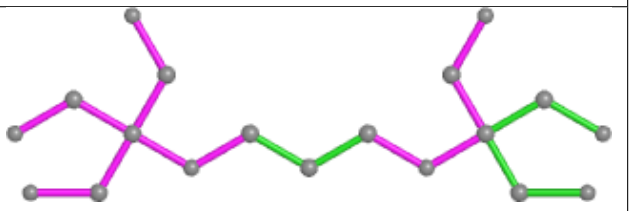
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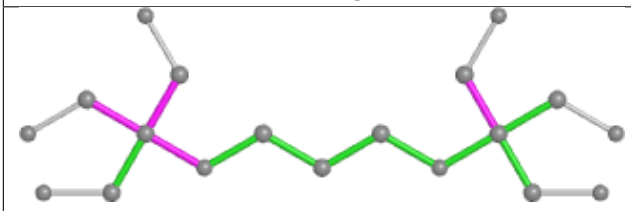
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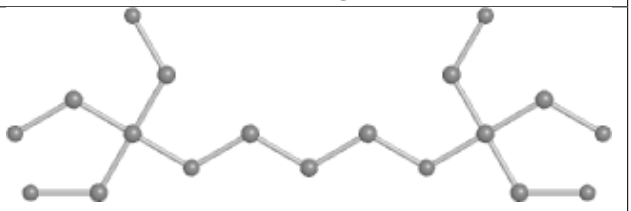
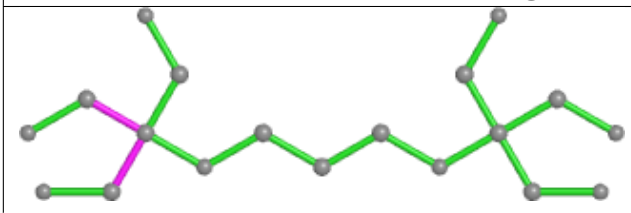
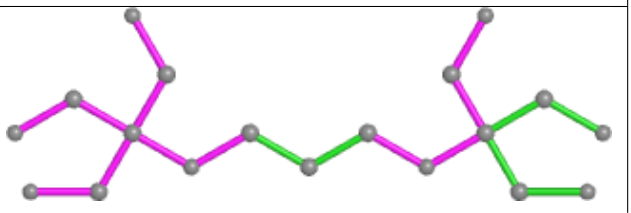
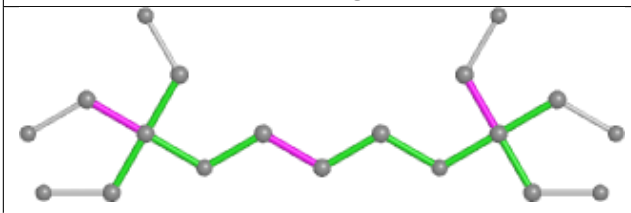
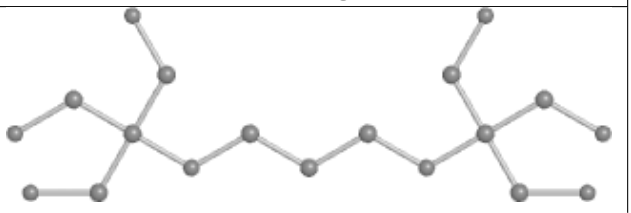

Rings

Ligand B3P 1 3478

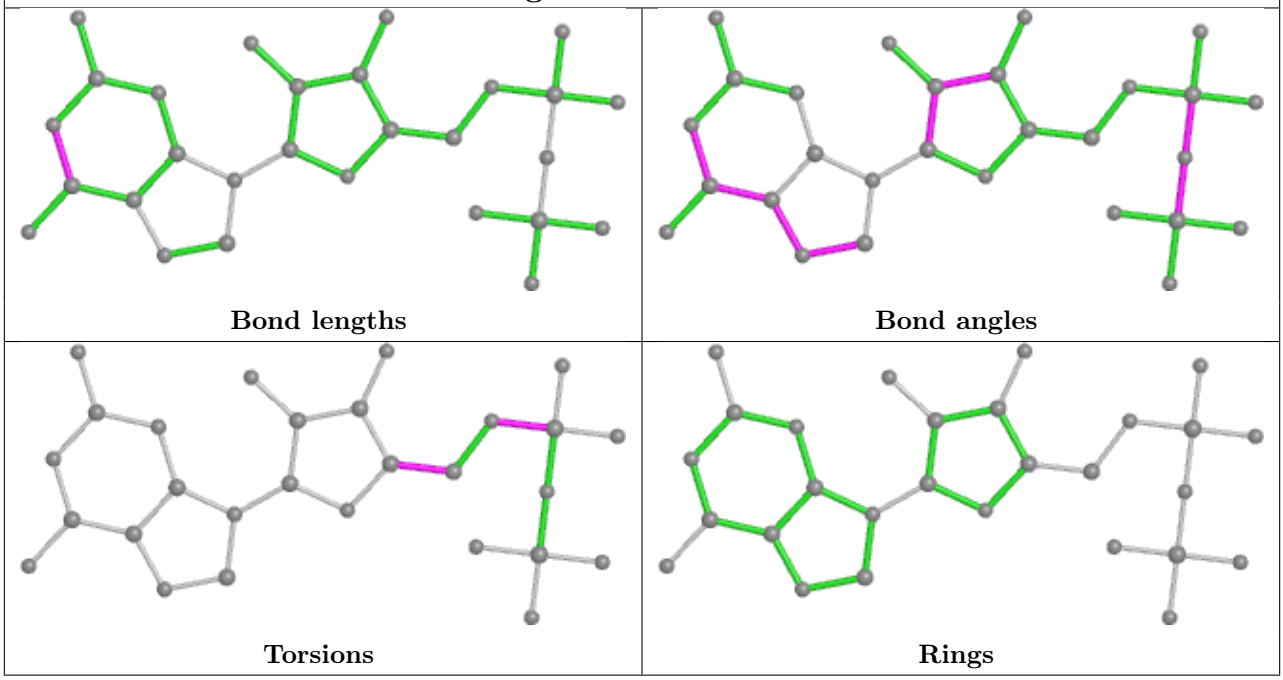

Bond lengths


Bond angles

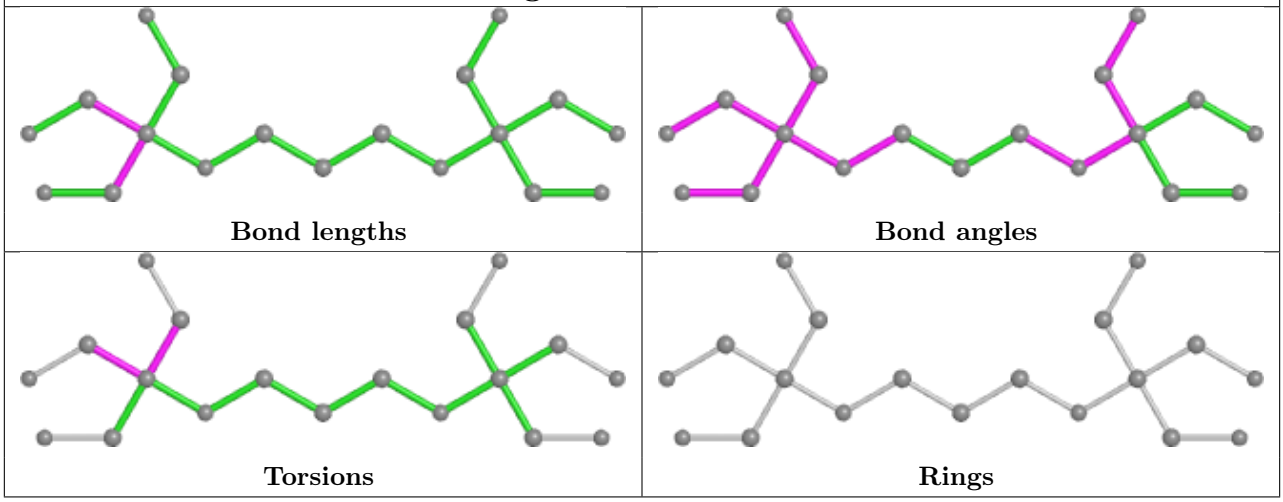

Torsions


Rings

Ligand GDP b 801



Ligand B3P 1 3480



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

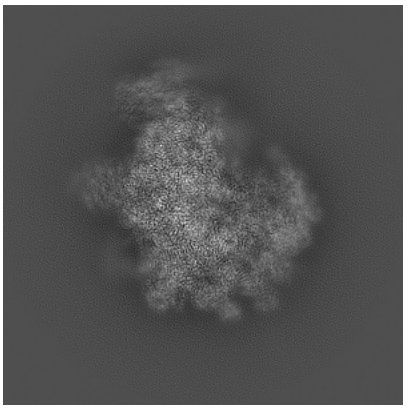
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26703. 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

6.1.1 Primary map



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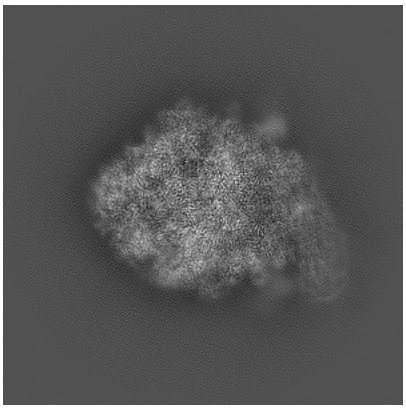

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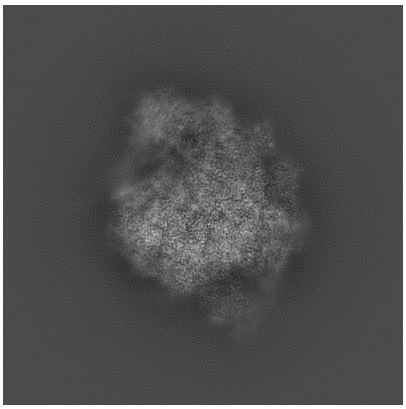
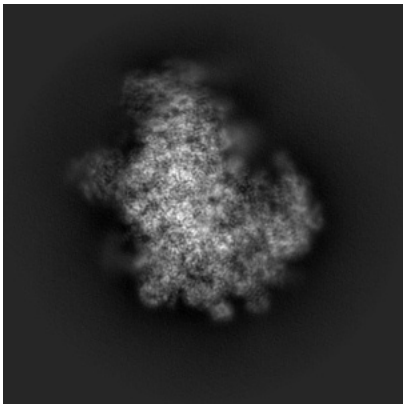
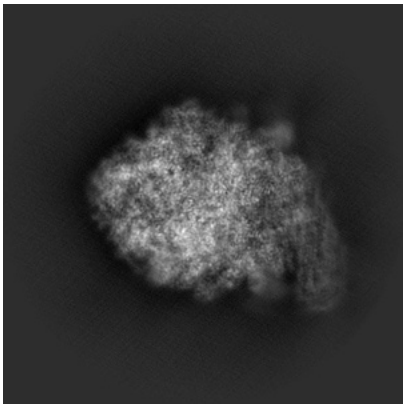


Z

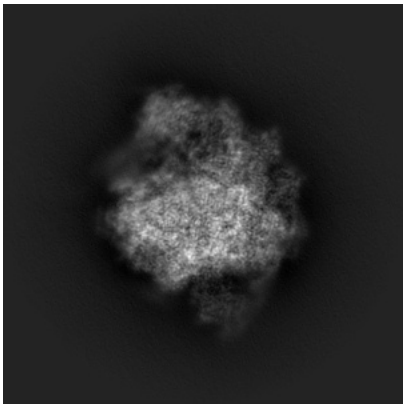
6.1.2 Raw map



X



Y

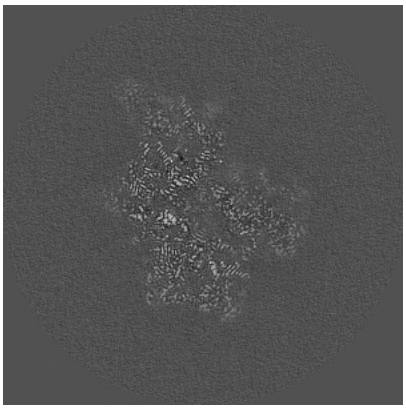


Z

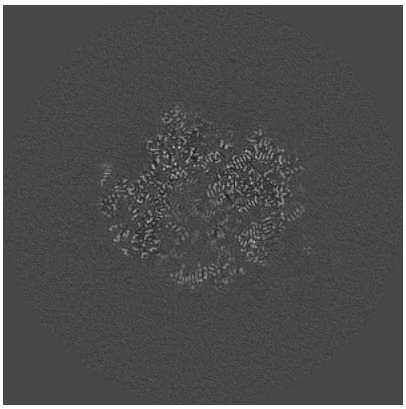
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

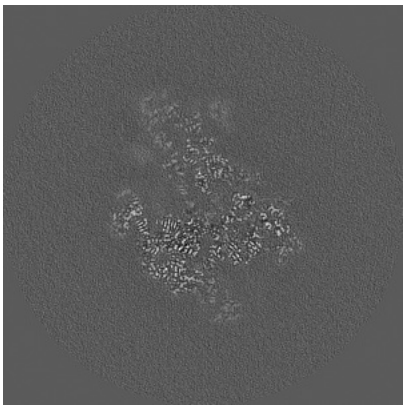
6.2.1 Primary map



X Index: 200

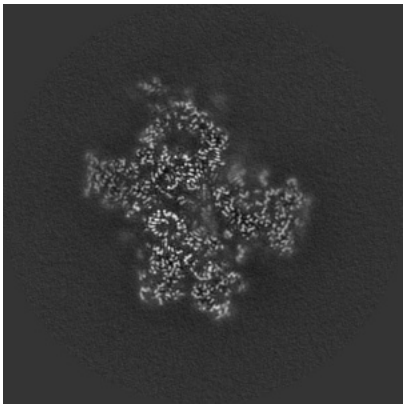


Y Index: 200

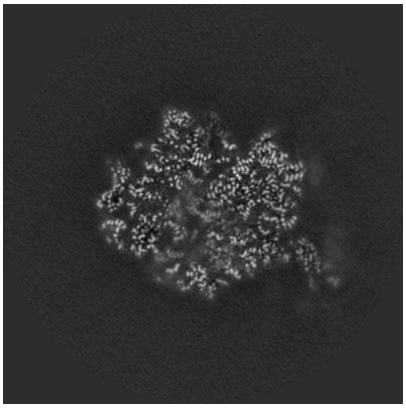


Z Index: 200

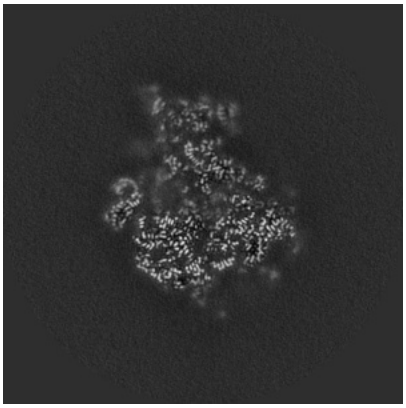
6.2.2 Raw map



X Index: 200



Y Index: 200

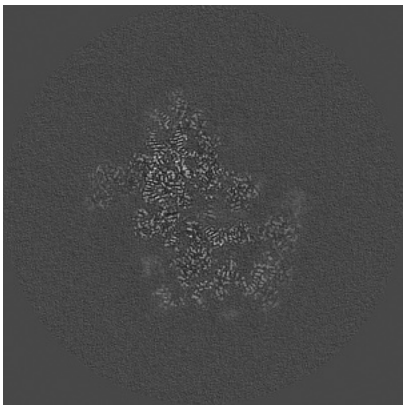


Z Index: 200

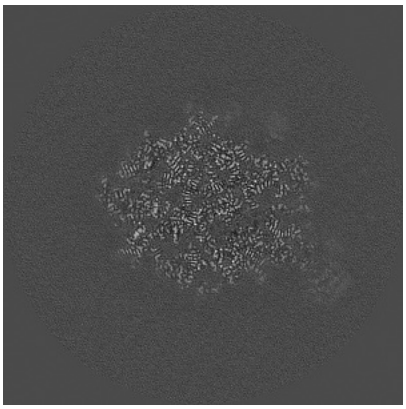
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

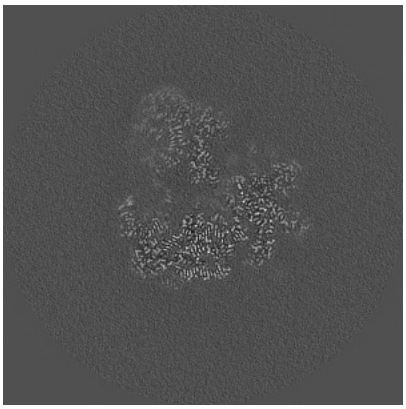
6.3.1 Primary map



X Index: 222

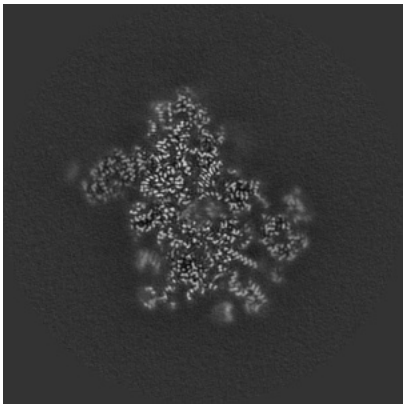


Y Index: 172

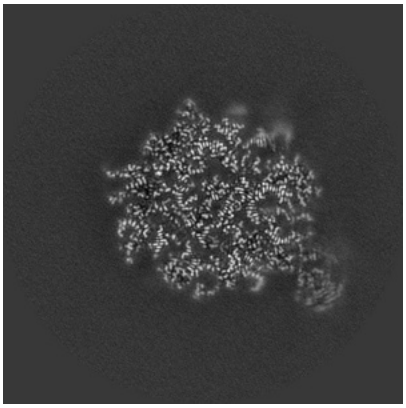


Z Index: 186

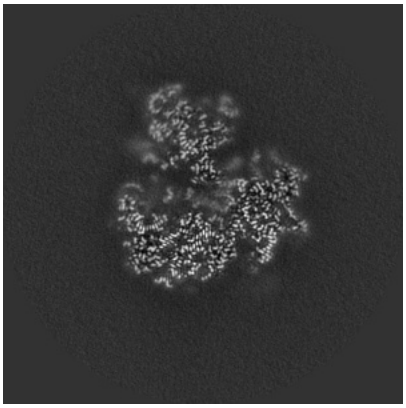
6.3.2 Raw map



X Index: 217



Y Index: 179

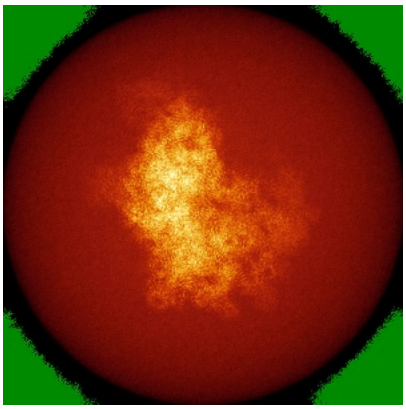


Z Index: 187

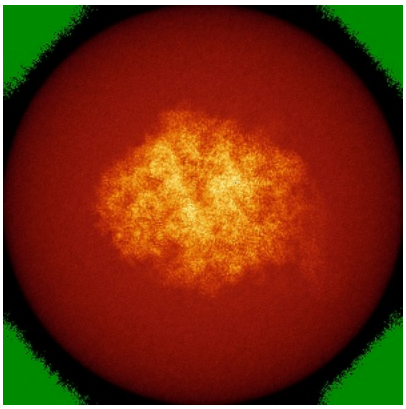
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

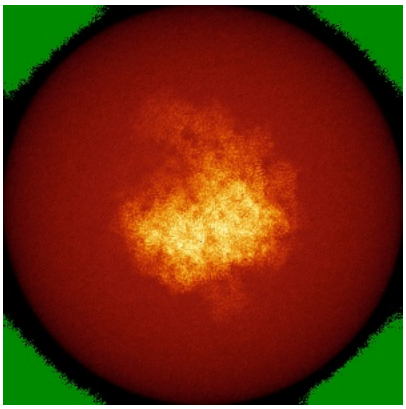
6.4.1 Primary map



X

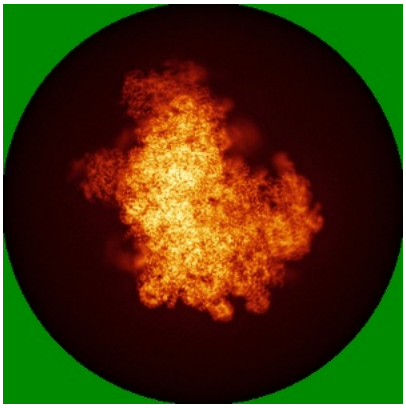


Y

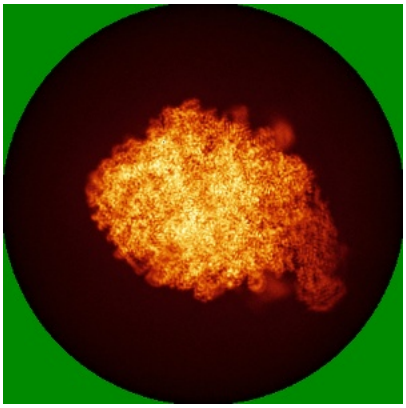


Z

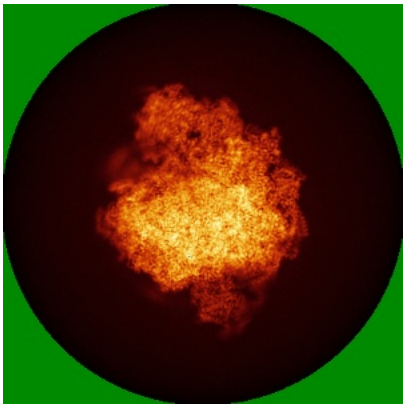
6.4.2 Raw map



X



Y

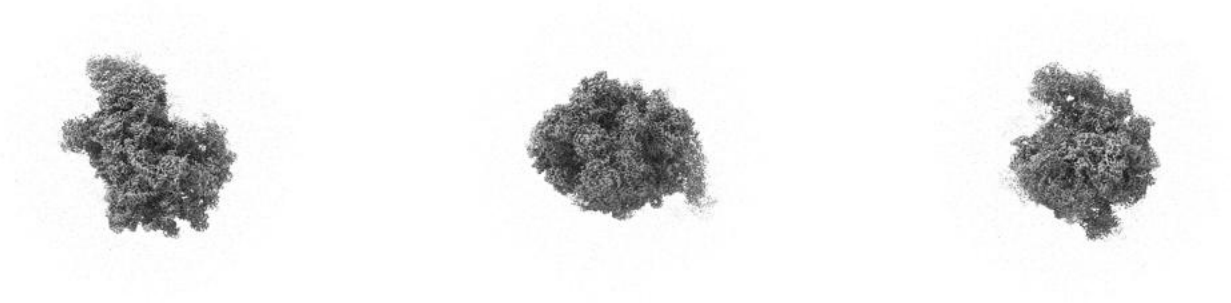


Z

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)

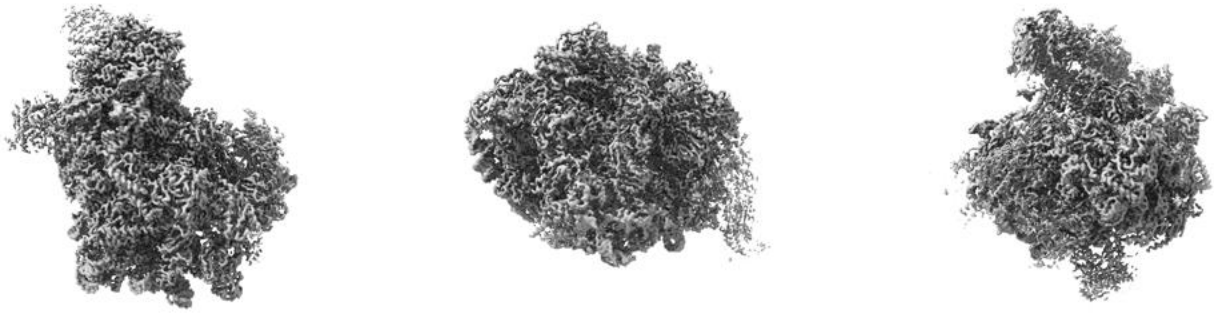
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. 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



X Y Z

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.

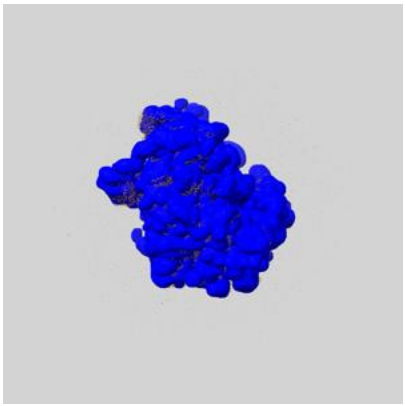
6.6 Mask visualisation (i)

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

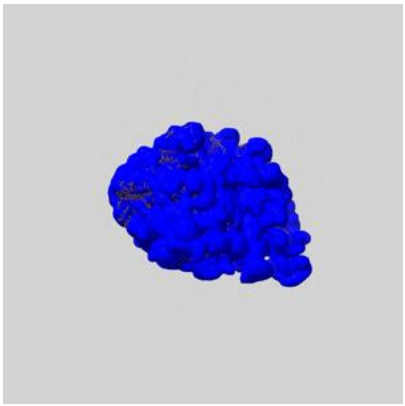
A mask typically either:

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

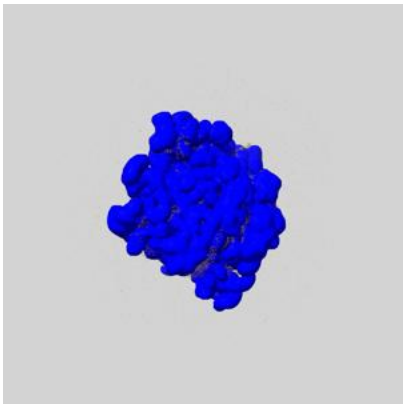
6.6.1 emd_26703_msk_1.map (i)



X



Y

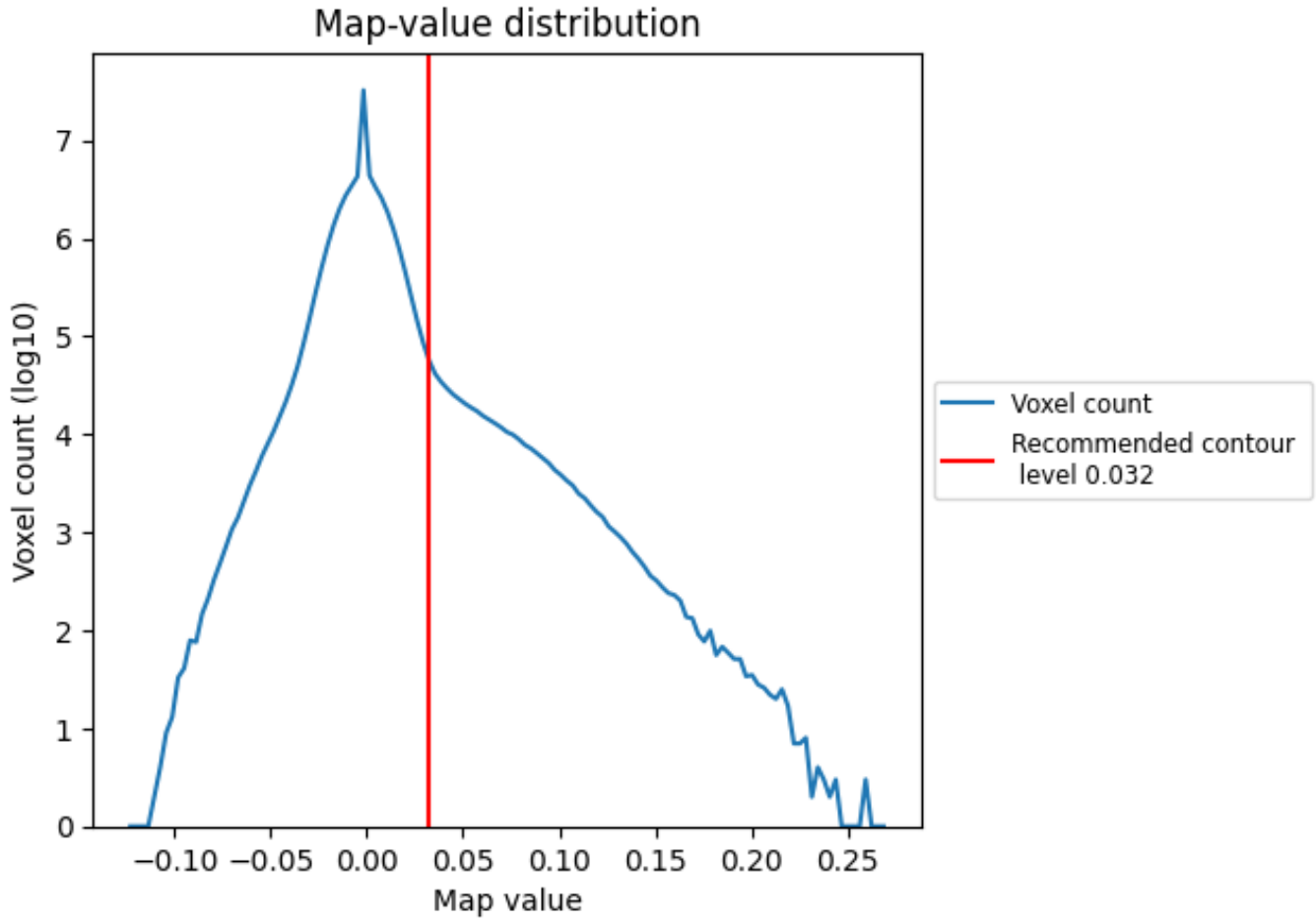


Z

7 Map analysis

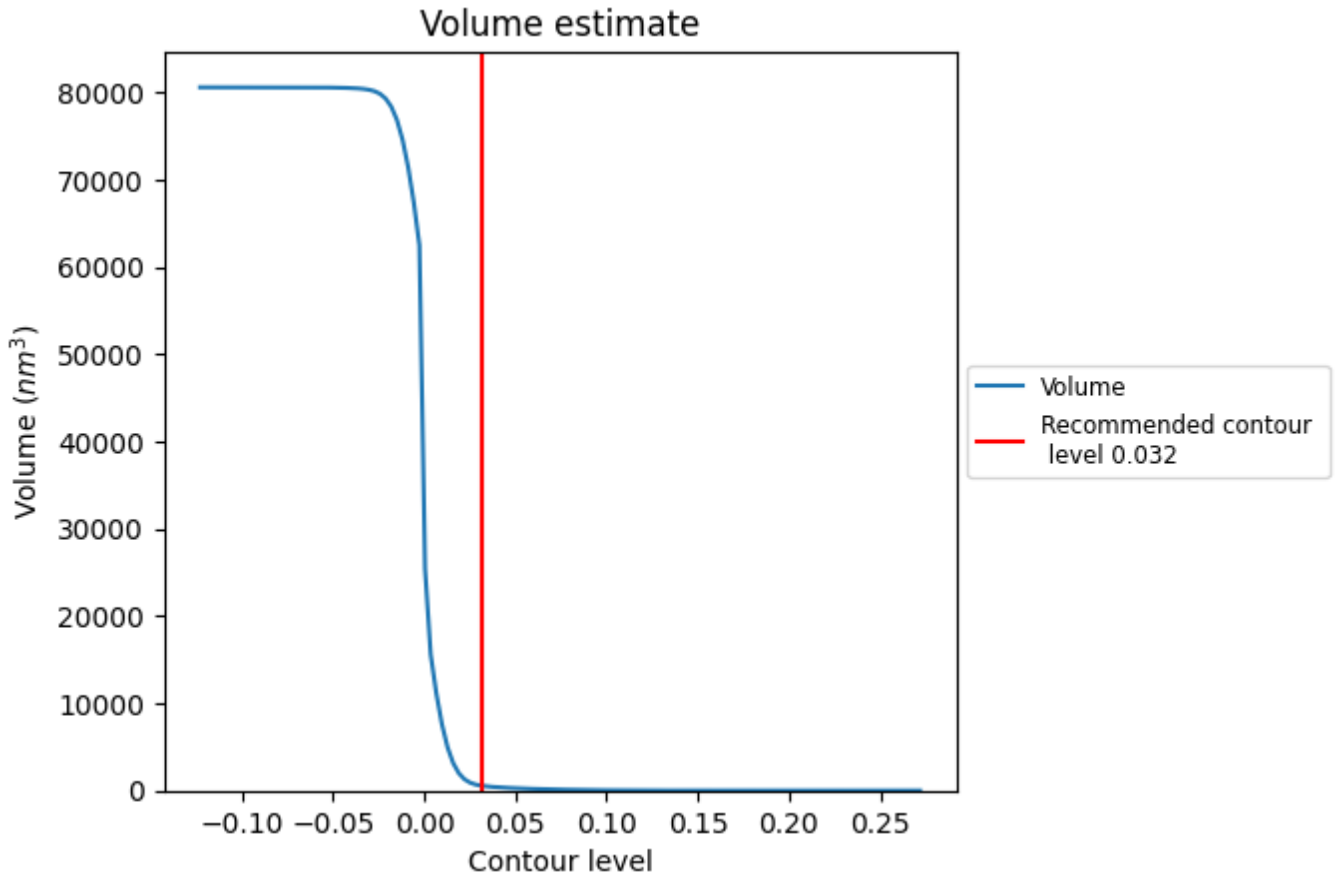
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

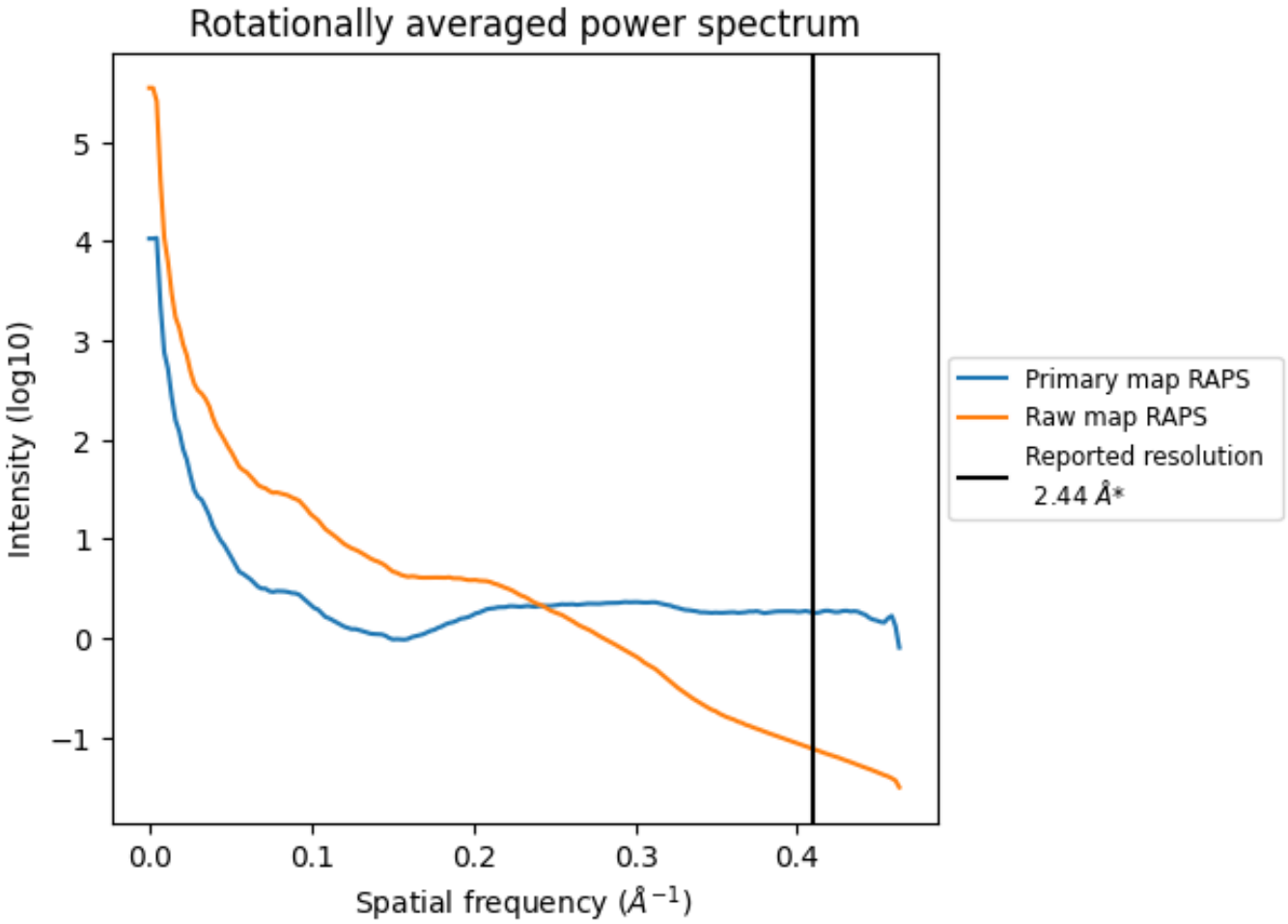
7.2 Volume estimate



The volume at the recommended contour level is 540 nm^3; this corresponds to an approximate mass of 488 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)

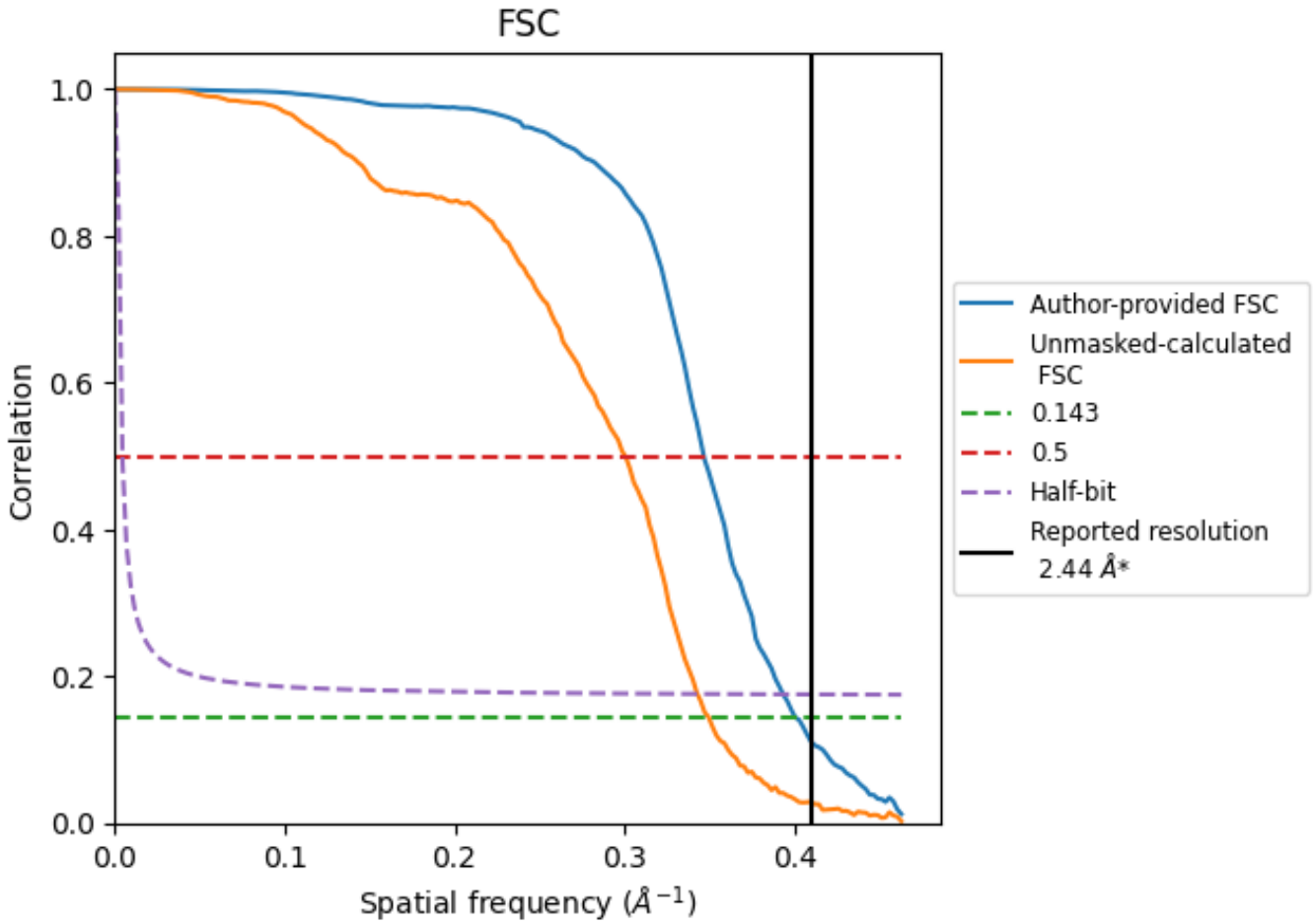


*Reported resolution corresponds to spatial frequency of 0.410 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.410 Å^{-1}

8.2 Resolution estimates (i)

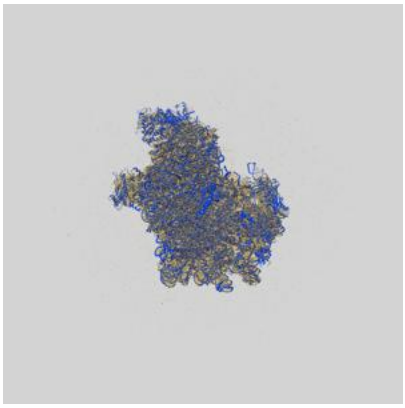
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.49	2.88	2.54
Unmasked-calculated*	2.86	3.33	2.92

*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 2.86 differs from the reported value 2.44 by more than 10 %

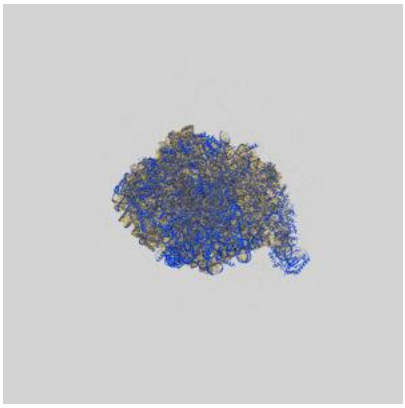
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26703 and PDB model 7UQZ. Per-residue inclusion information can be found in section 3 on page 18.

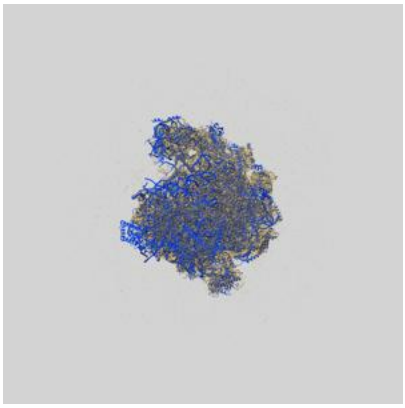
9.1 Map-model overlay



X



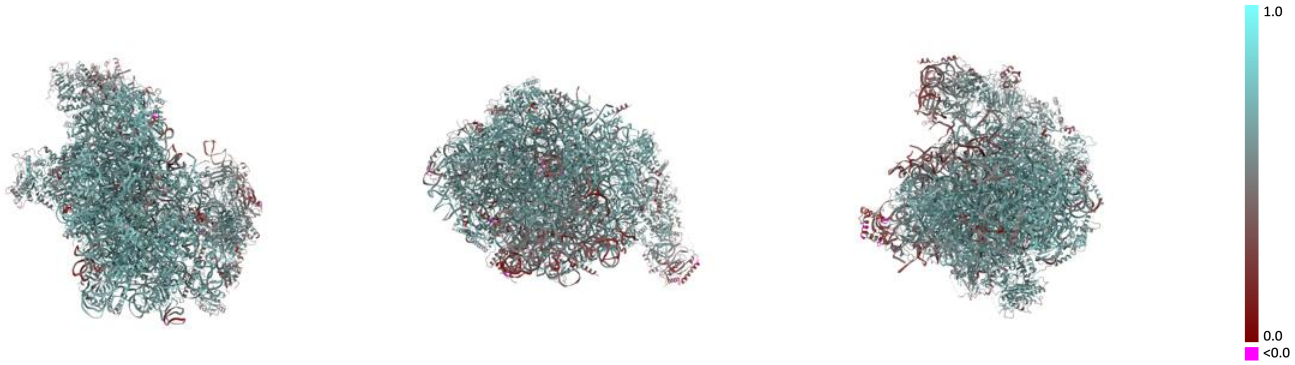
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

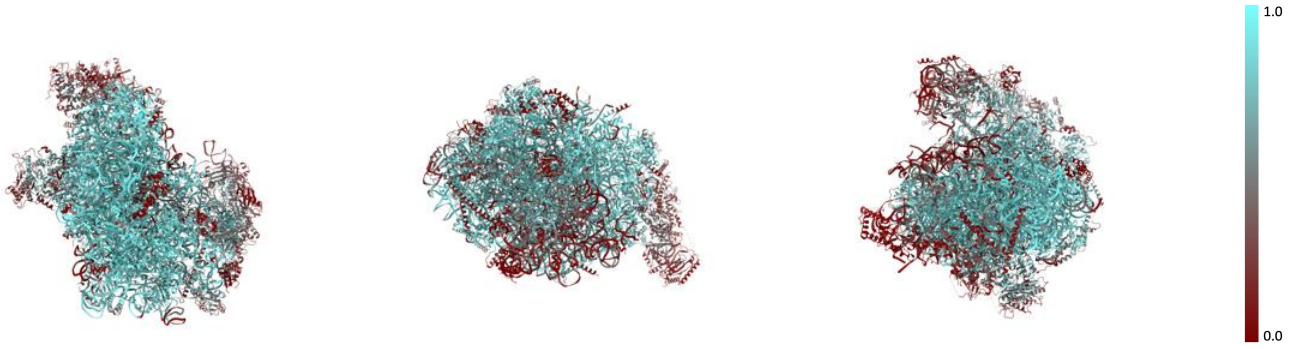
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

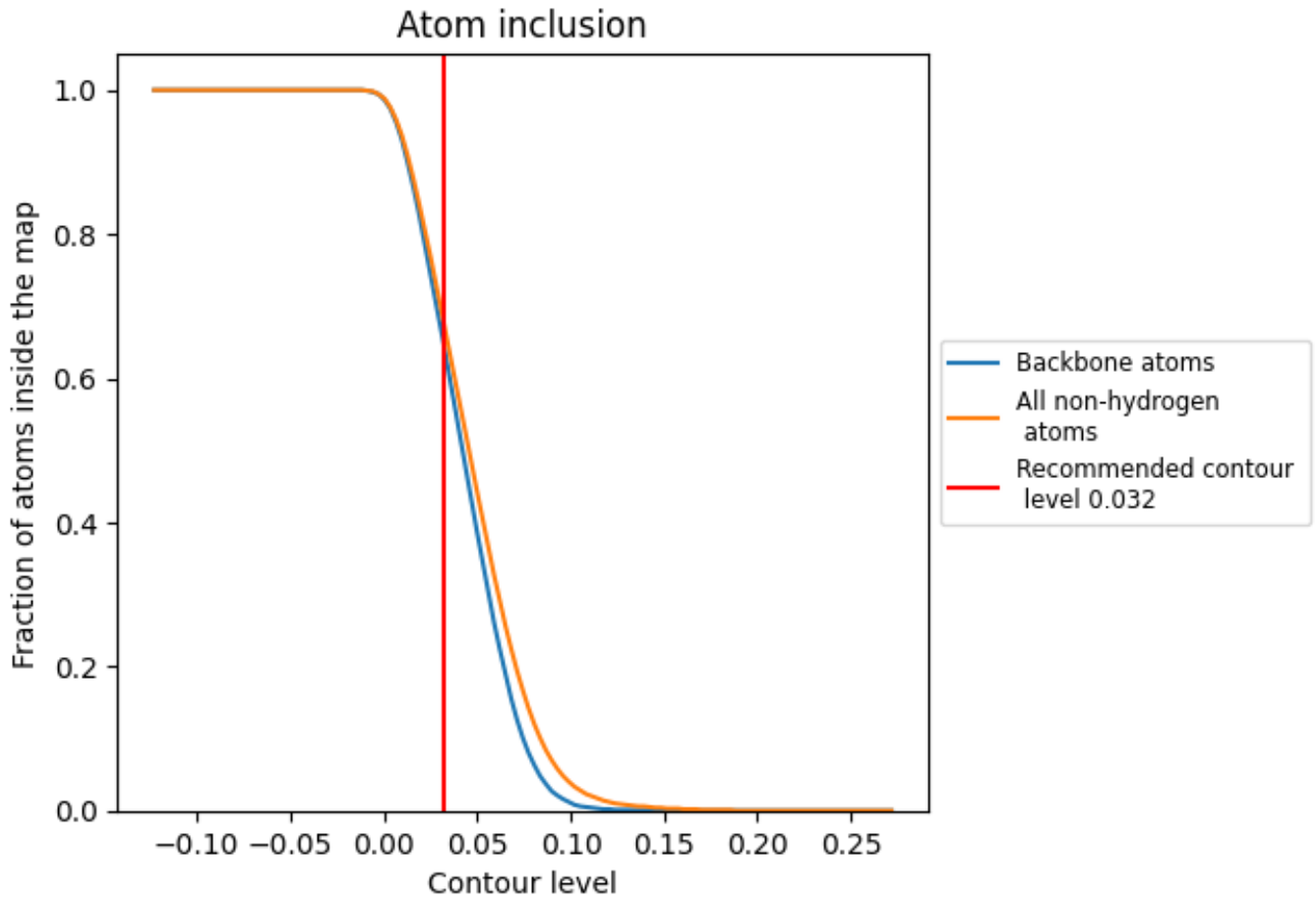
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 68% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6790	0.6080
1	0.7760	0.6170
2	0.9180	0.6710
3	0.2750	0.4030
4	0.4660	0.5930
5	0.0520	0.3360
6	0.2490	0.4640
8	0.1660	0.4710
9	0.5360	0.6130
A	0.8550	0.6970
B	0.9040	0.7000
C	0.8540	0.6800
D	0.3680	0.5160
E	0.7230	0.6440
F	0.8490	0.6750
G	0.7500	0.6430
H	0.7880	0.6510
I	0.0440	0.5310
J	0.0770	0.3090
K	0.0770	0.3900
L	0.7160	0.6260
M	0.8080	0.6580
N	0.8720	0.6950
O	0.8850	0.6920
P	0.8520	0.6820
Q	0.7320	0.6360
R	0.8430	0.6680
S	0.7270	0.6340
T	0.4390	0.5390
U	0.7120	0.6200
V	0.8350	0.6770
W	0.4690	0.5600
X	0.8420	0.6890
Y	0.8410	0.6790
Z	0.7620	0.6440

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.6680	0.6190
b	0.6780	0.6160
c	0.7050	0.6280
d	0.8040	0.6670
e	0.8590	0.6870
f	0.9110	0.7000
g	0.8250	0.6700
h	0.8420	0.6770
i	0.5580	0.5970
j	0.9410	0.7150
k	0.6130	0.6140
l	0.9180	0.7140
m	0.6810	0.6290
n	0.4310	0.5790
o	0.2700	0.4650
p	0.8240	0.6720
q	0.2630	0.5370
r	0.8030	0.6670
s	0.4110	0.5190
t	0.2300	0.5060
u	0.7650	0.6370
v	0.4100	0.5520
w	0.4300	0.5420
x	0.5060	0.5540
y	0.7850	0.6510
z	0.6380	0.6200