Full wwPDB EM Validation Report (i)

Jun 1, 2024 – 10:43 AM EDT

PDB ID	:	7UOO
EMDB ID	:	EMD-26651
Title	:	Nucleoplasmic pre-60S intermediate of the Nog2 containing pre-rotation state
Authors	:	Sekulski, K.; Cruz, V.E.; Weirich, C.S.; Erzberger, J.P.
Deposited on	:	2022-04-13
Resolution	:	2.34 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 (i) 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 (1)) were used in the production of this report:

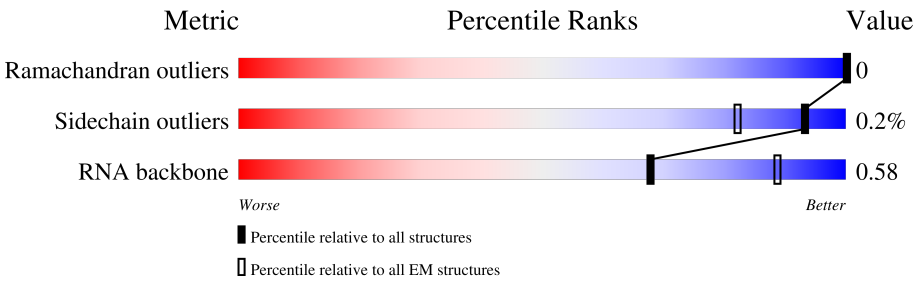
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.34 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	7%, 84%, 16%
2	1	3396	14%, 72%, 16%, •, 12%
3	2	158	6%, 83%, 17%
4	3	121	74%, 79%, 21%, •
5	5	120	61%, 61%, 39%
6	6	87	43%, 46%, 21%, 33%
7	8	165	87%, 96%, •
8	9	175	19%, 67%, 33%

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Mol	Chain	Length	Quality of chain
9	B	387	99%
10	C	362	5%, 99%
11	D	297	52%, 91%, 9%
12	E	176	10%, 88%, 12%
13	F	244	90%, 10%
14	G	256	11%, 88%, 12%
15	H	191	8%, 100%
16	I	166	45%, 79%, 21%
17	J	174	96%, 98%
18	K	376	67%, 71%, 29%
19	L	199	19%, 90%, 10%
20	M	138	8%, 99%
21	N	204	6%, 93%, 7%
22	O	199	99%
23	P	184	95%, 5%
24	Q	186	8%, 79%, 21%
25	R	189	6%, 83%, 17%
26	S	172	15%, 99%
27	T	160	28%, 71%, 29%
28	U	121	11%, 88%, 12%
29	V	137	7%, 99%
30	W	312	32%, 75%, 25%
31	X	142	98%
32	Y	127	98%
33	Z	136	7%, 99%

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Mol	Chain	Length	Quality of chain
34	a	149	13% 62% 38%
35	b	647	22% 99%
36	c	105	15% 92% 8%
37	d	113	10% 95% 5%
38	e	130	98%
39	f	107	99%
40	g	121	9% 93% 7%
41	h	120	99%
42	i	100	23% 99%
43	j	88	95% 5%
44	k	78	24% 99%
45	l	51	98%
46	m	486	20% 95%
47	n	605	23% 61% 39%
48	o	220	34% 60% 40%
49	p	92	9% 98%
50	q	455	23% 34% 66%
51	r	261	5% 88% 12%
52	s	520	7% 14% 86%
53	t	322	59% 89% 11%
54	u	199	5% 75% 25%
55	v	344	49% 85% 15%
56	w	203	45% 96%
57	x	515	38% 97%
58	y	245	12% 100%

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Mol	Chain	Length	Quality of chain
59	z	106	15% 82% 18%
60	4	593	32% 90% • 9%

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 157947 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	2991	64043	28619	11563	20870	2991	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
			Total	C	N	O	S		
7	8	158	1196	750	216	228	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	W	234	1887	1194	323	364	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called Pescadillo homolog.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 57 is a protein called RSA4 isoform 1.

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

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

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

- Molecule 59 is a protein called UPF0642 protein YBL028C.

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

- Molecule 60 is a protein called Probable metalloprotease ARX1.

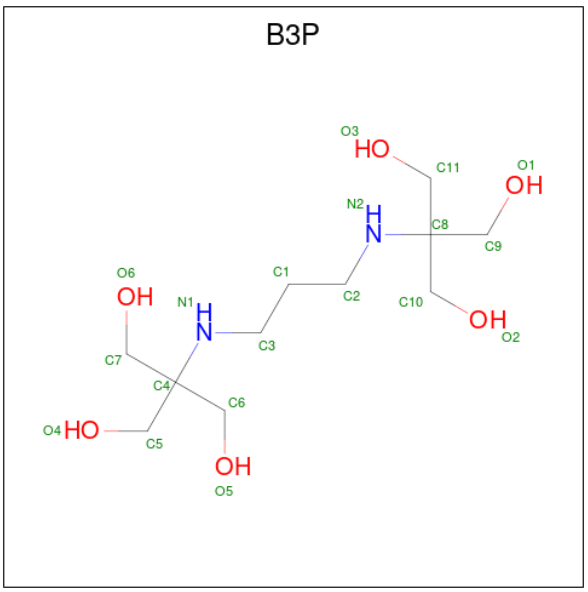
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	4	538	4166	2633	718	800	15	0	0

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

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

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

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

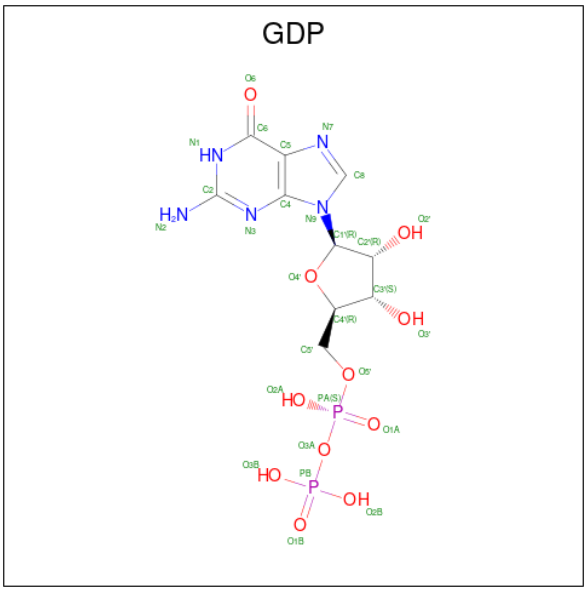


Mol	Chain	Residues	Atoms				AltConf
62	1	1	Total	C	N	O	0
			19	11	2	6	
62	1	1	Total	C	N	O	0
			19	11	2	6	
62	1	1	Total	C	N	O	0
			19	11	2	6	

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

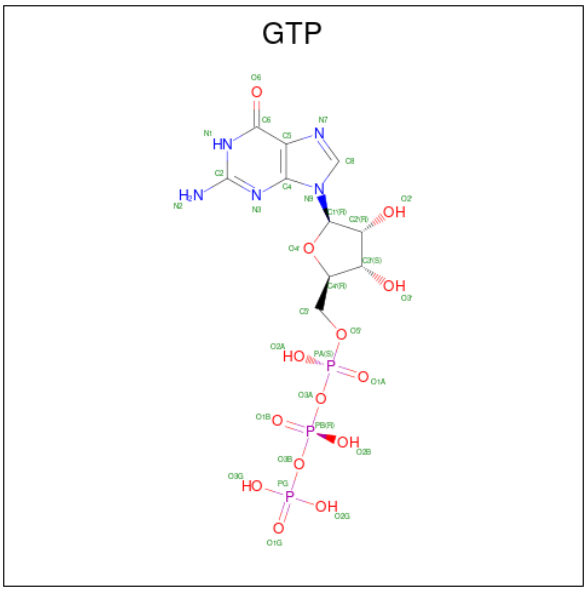
Mol	Chain	Residues	Atoms		AltConf
63	I	1	Total	Zn	0
			1	1	
63	g	1	Total	Zn	0
			1	1	
63	j	1	Total	Zn	0
			1	1	
63	p	1	Total	Zn	0
			1	1	
63	u	1	Total	Zn	0
			1	1	

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 65 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
65	m	1	32	10	5	14	3	0

- Molecule 66 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 67 is water.

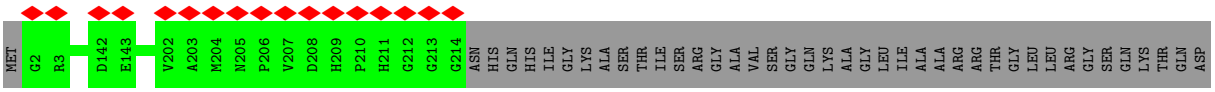
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
67	1	346	346	346	0
67	2	6	6	6	0
67	C	3	3	3	0
67	F	1	1	1	0
67	N	3	3	3	0
67	O	1	1	1	0
67	R	2	2	2	0
67	V	1	1	1	0
67	X	1	1	1	0
67	b	3	3	3	0
67	d	1	1	1	0
67	j	2	2	2	0
67	m	3	3	3	0

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.

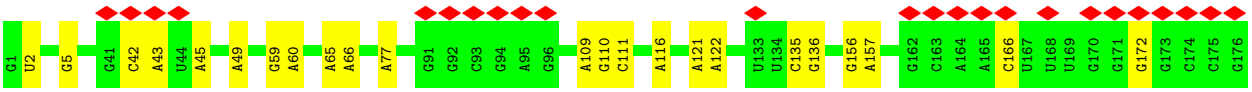
- Molecule 1: 60S ribosomal protein L2-A

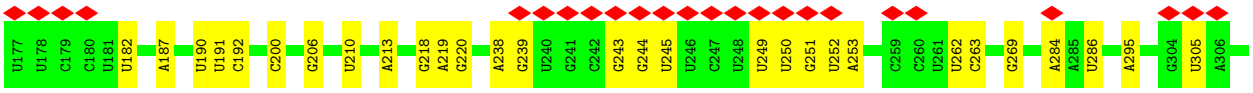
Chain A:

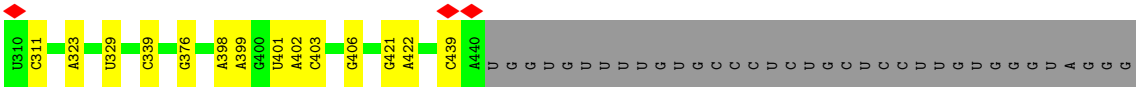


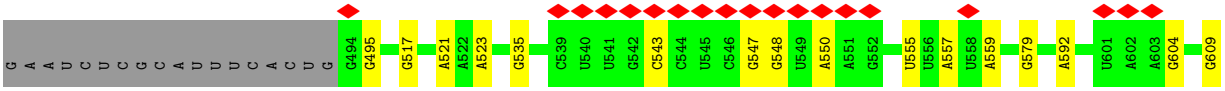
- Molecule 2: 25S rRNA

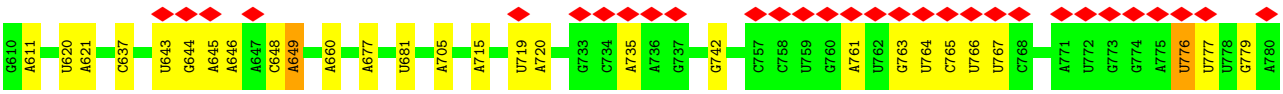
Chain 1:

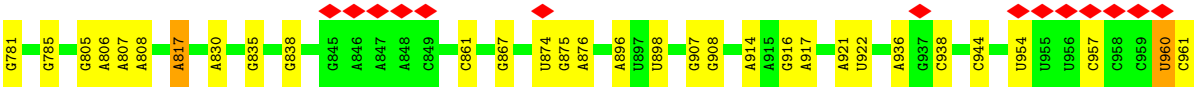


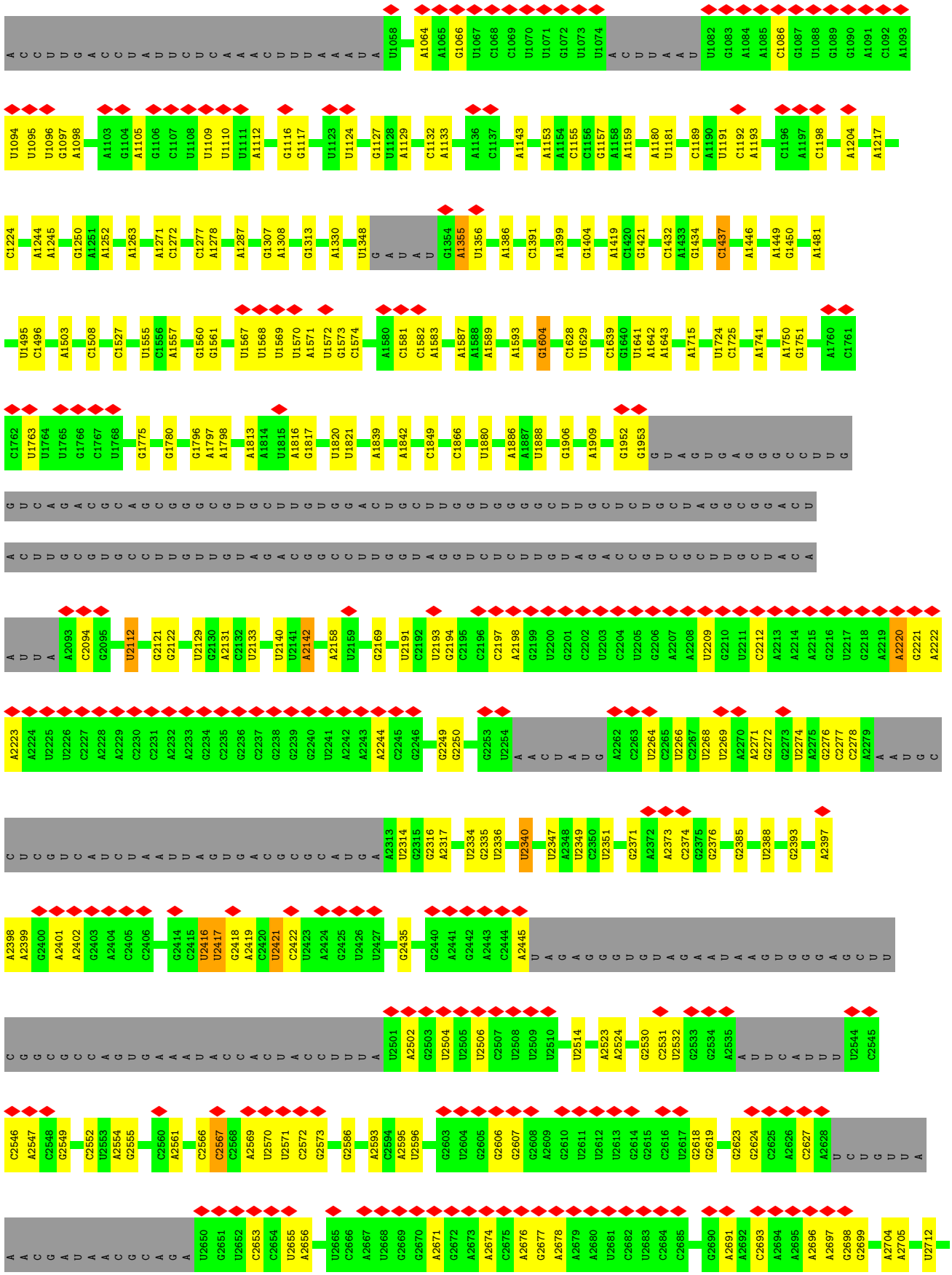








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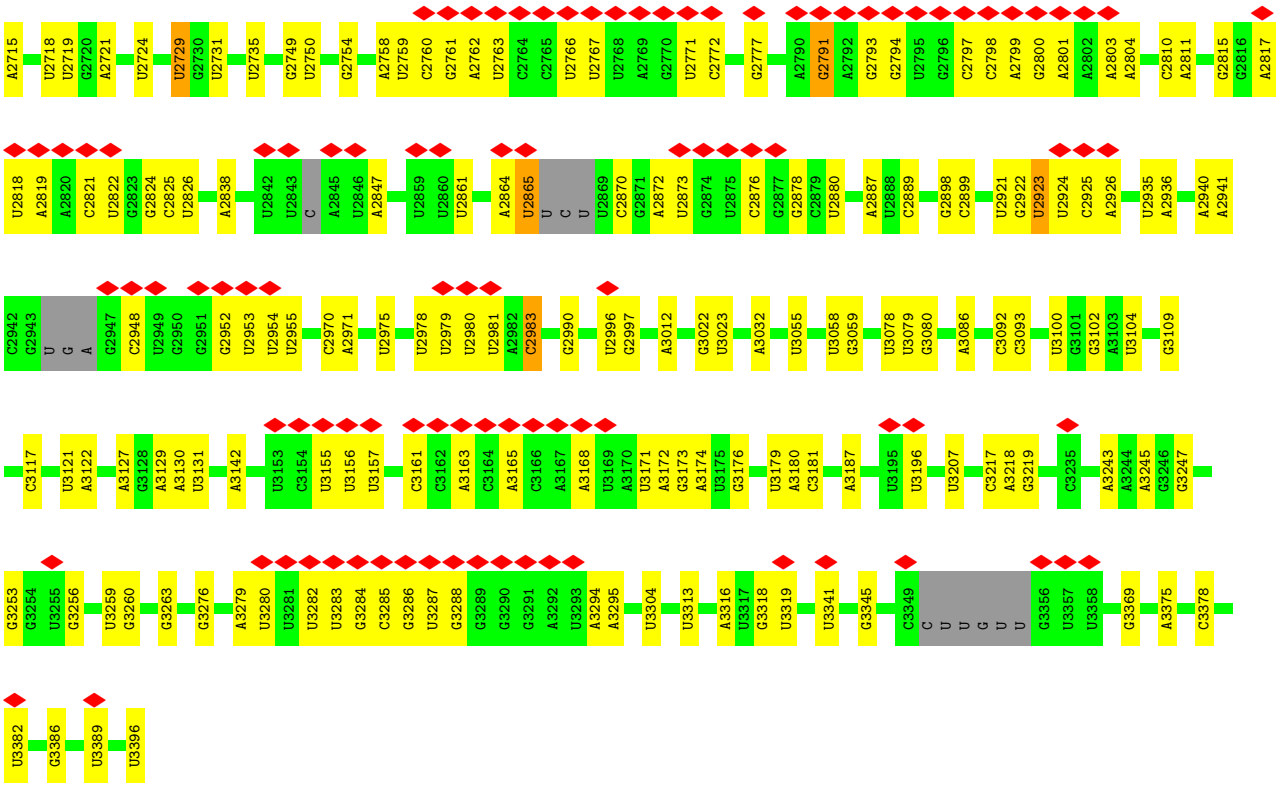
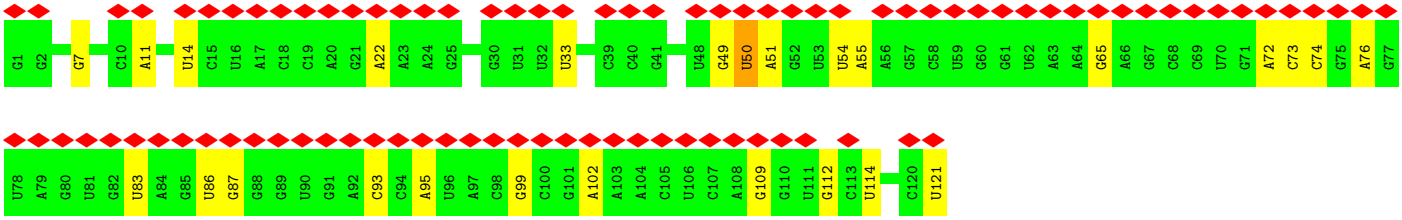


- Molecule 3: 5.8S rRNA

Chain 2:

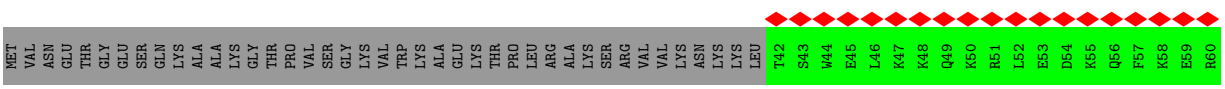
- Molecule 4: 5S rRNA

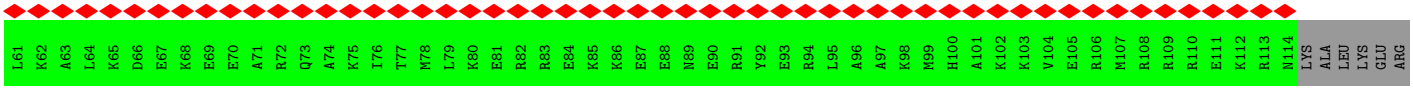
Chain 3:



- Molecule 5: rRNA-processing protein

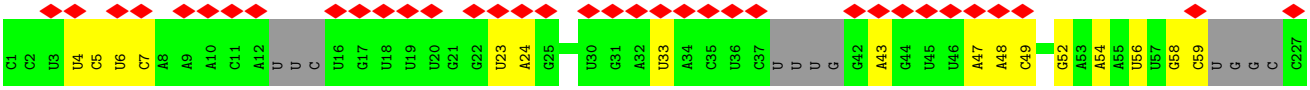
Chain 5:





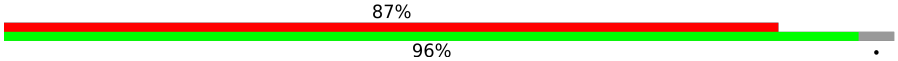
• Molecule 6: ITS2 rRNA

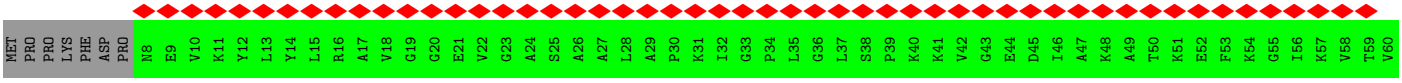
Chain 6:

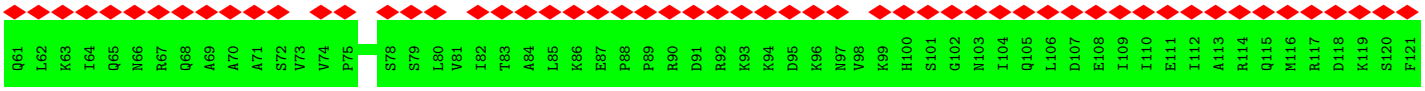


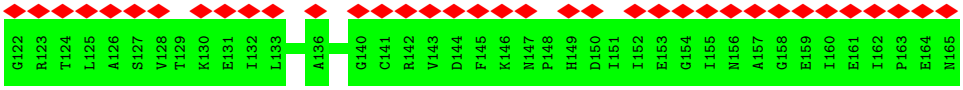
• Molecule 7: 60S ribosomal protein L12-A

Chain 8:



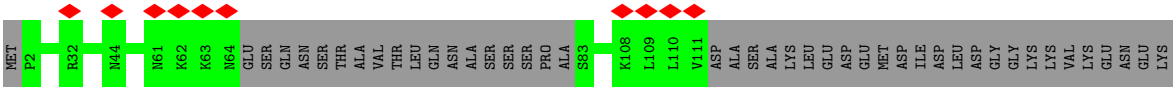


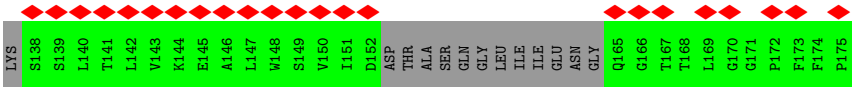




• Molecule 8: Ribosome biogenesis protein ALB1

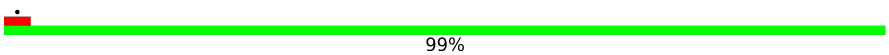
Chain 9:

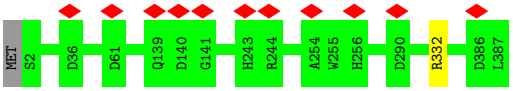




• Molecule 9: 60S ribosomal protein L3

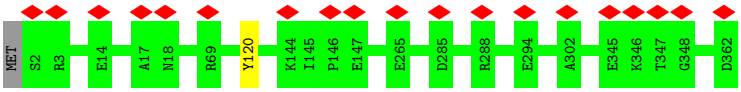
Chain B:





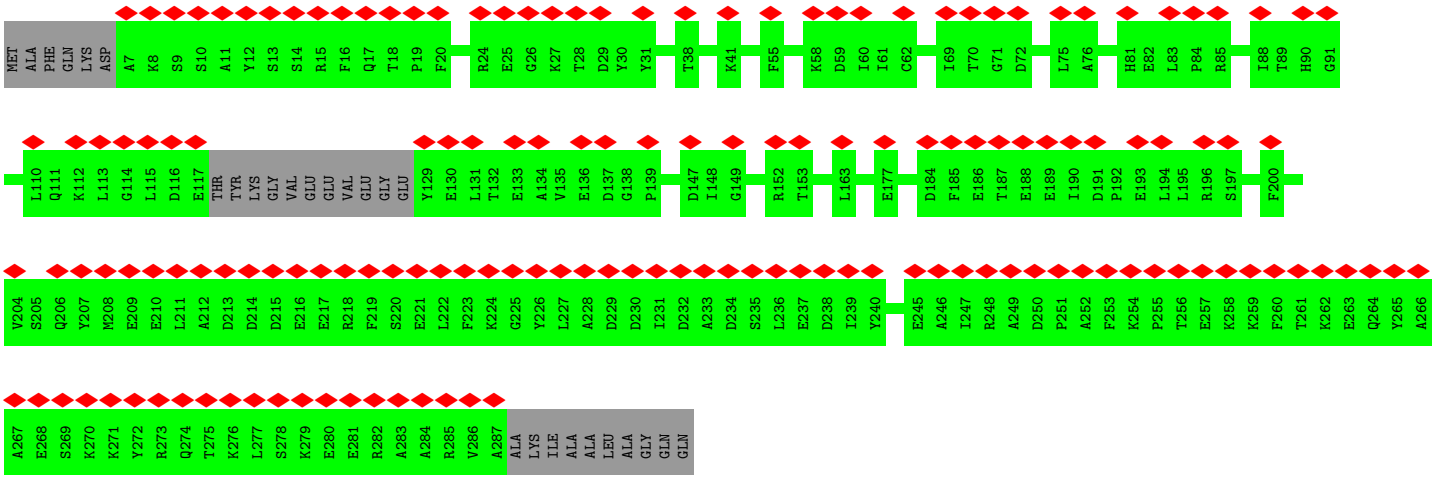
• Molecule 10: 60S ribosomal protein L4-A

Chain C: 5% 99%



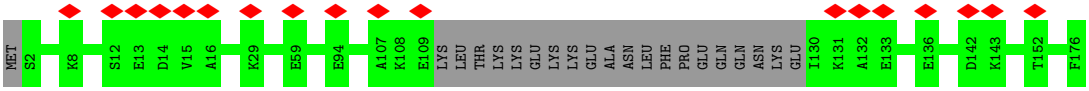
• Molecule 11: 60S ribosomal protein L5

Chain D: 52% 91% 9%



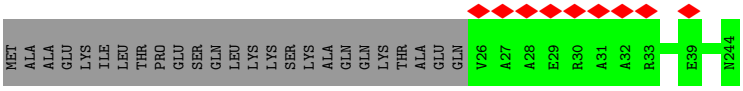
• Molecule 12: 60S ribosomal protein L6-A

Chain E: 10% 88% 12%



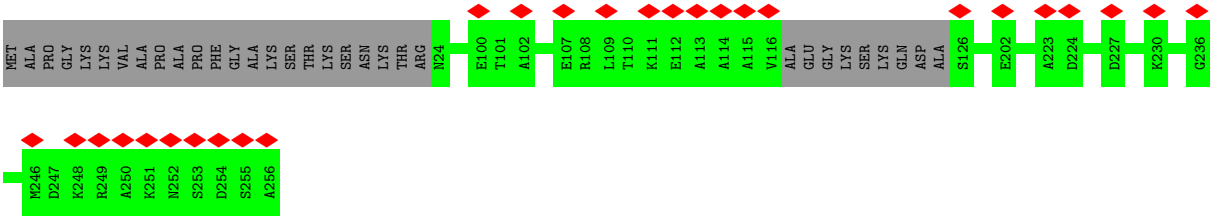
• Molecule 13: 60S ribosomal protein L7-A

Chain F: 90% 10%



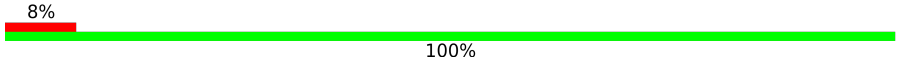
• Molecule 14: 60S ribosomal protein L8-A

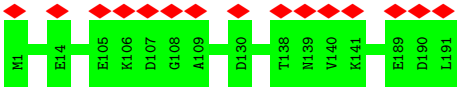
Chain G: 11% 88% 12%



• Molecule 15: 60S ribosomal protein L9-A

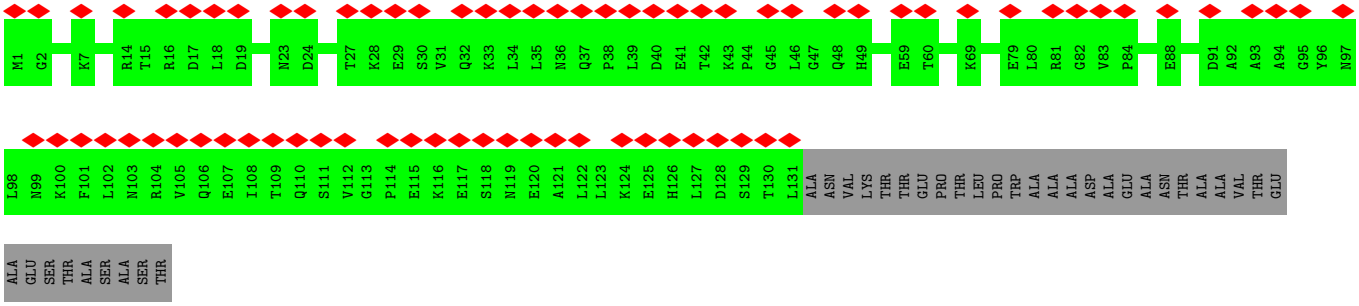
Chain H:





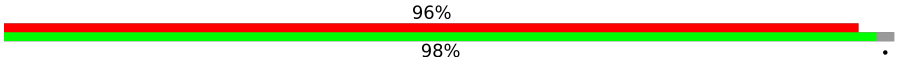
• Molecule 16: Bud site selection protein 20

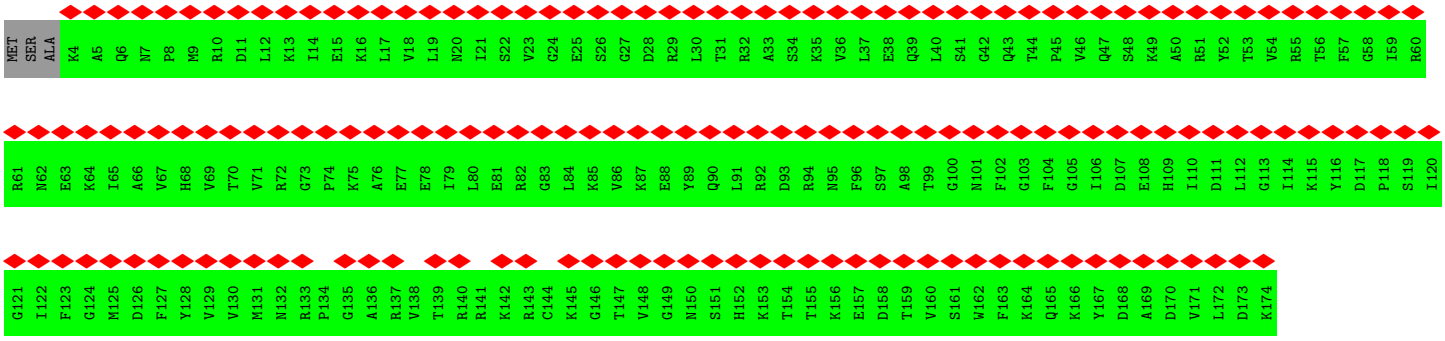
Chain I:



• Molecule 17: 60S ribosomal protein L11-A

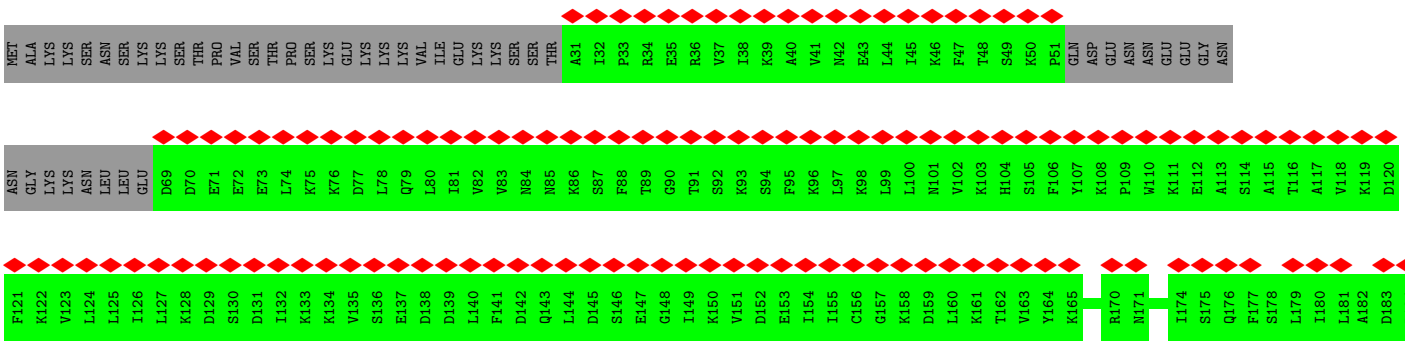
Chain J:

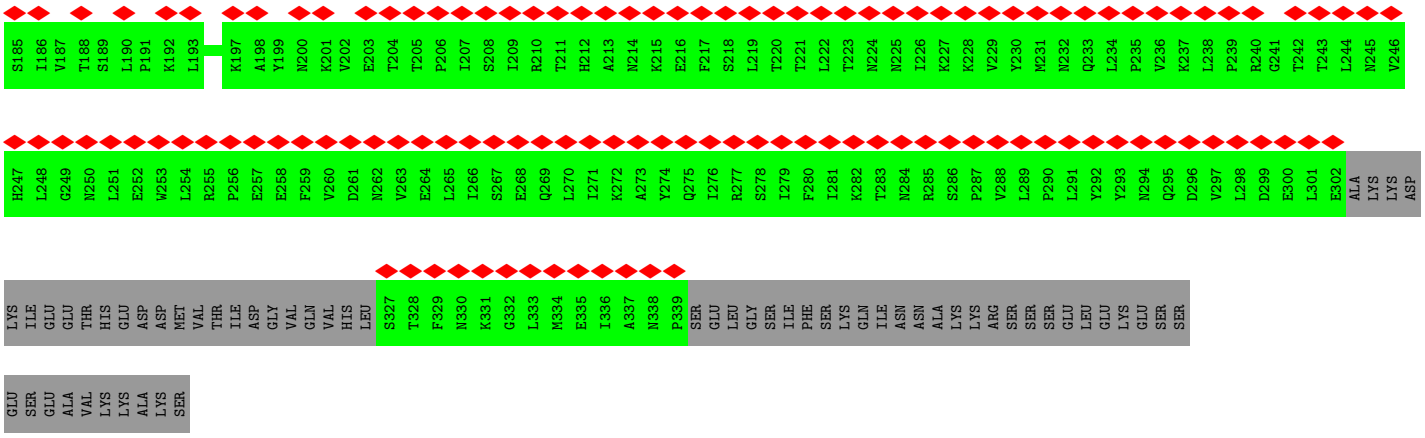




• Molecule 18: Proteasome-interacting protein CIC1

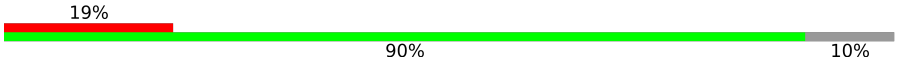
Chain K:

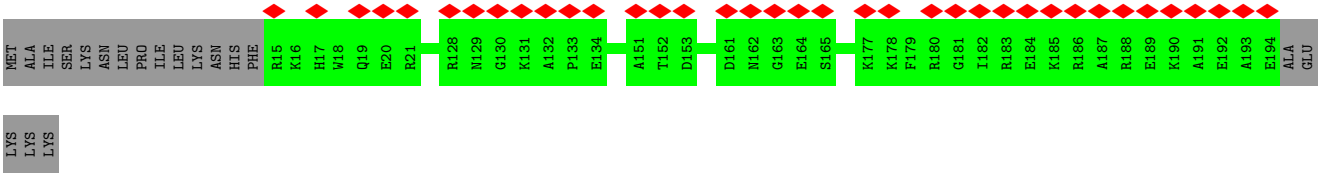




- Molecule 19: 60S ribosomal protein L13-A

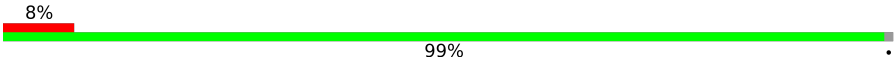
Chain L:

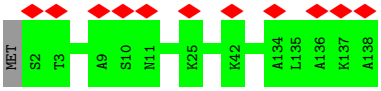




- Molecule 20: 60S ribosomal protein L14-A

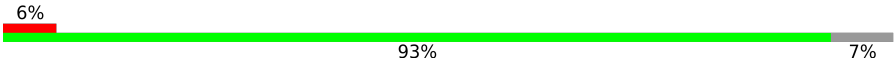
Chain M:

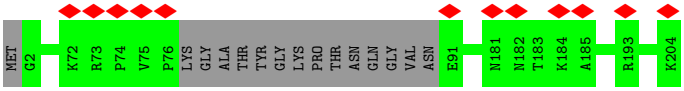




- Molecule 21: 60S ribosomal protein L15-A

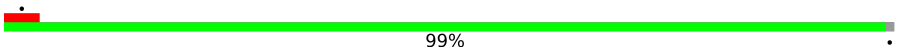
Chain N:

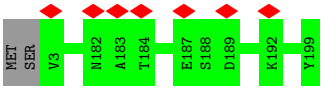




- Molecule 22: 60S ribosomal protein L16-A

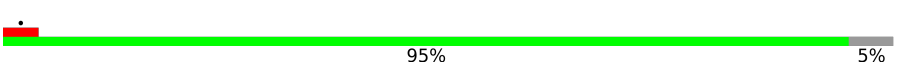
Chain O:

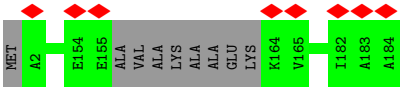




- Molecule 23: 60S ribosomal protein L17-A

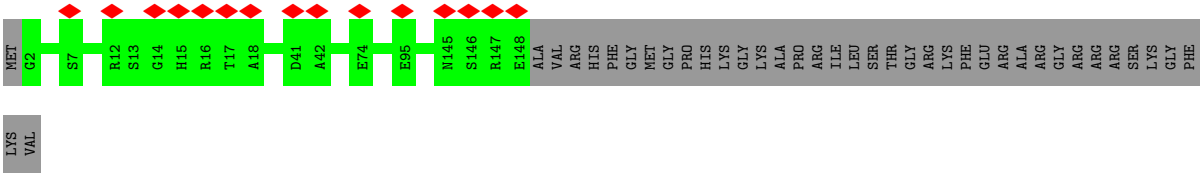
Chain P:





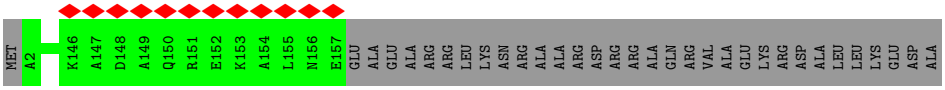
• Molecule 24: 60S ribosomal protein L18-A

Chain Q:



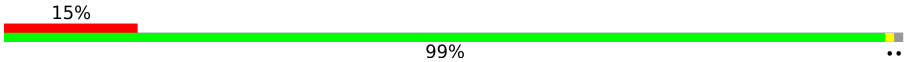
• Molecule 25: 60S ribosomal protein L19-A

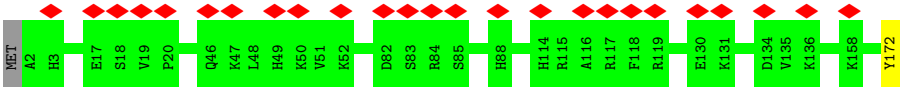
Chain R:



• Molecule 26: 60S ribosomal protein L20-A

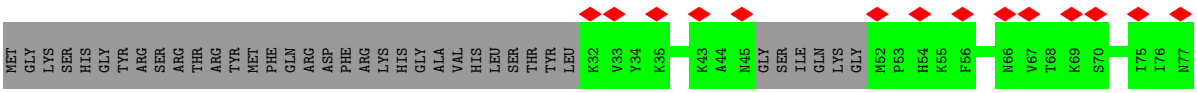
Chain S:

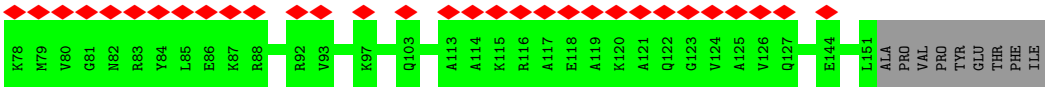




• Molecule 27: 60S ribosomal protein L21-A

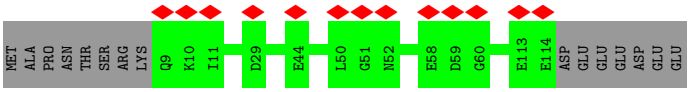
Chain T:





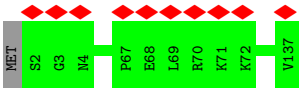
• Molecule 28: 60S ribosomal protein L22-A

Chain U:



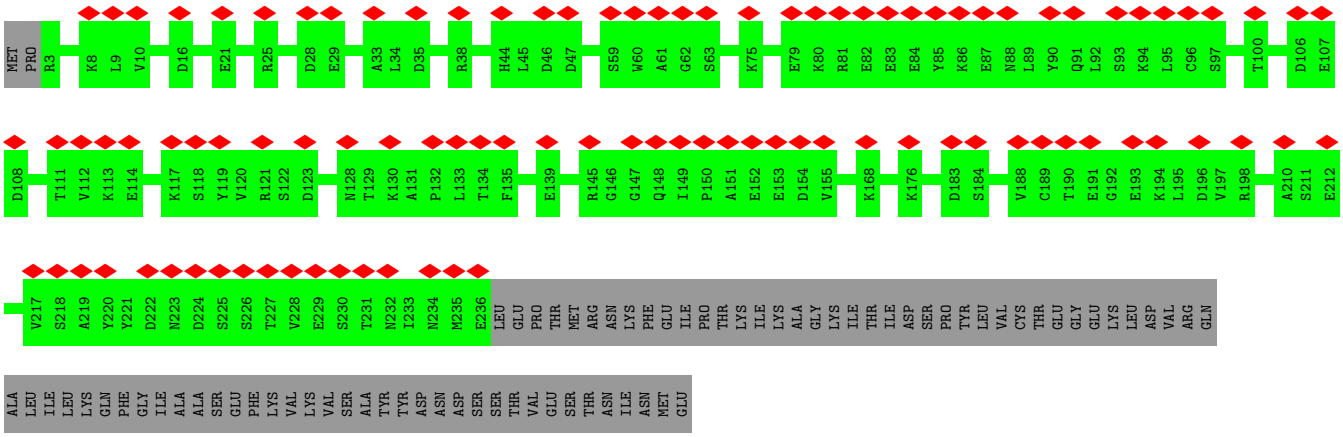
• Molecule 29: 60S ribosomal protein L23-A

Chain V: 7% 99%



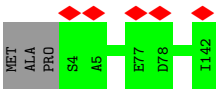
• Molecule 30: Ribosome assembly factor MRT4

Chain W: 32% 75% 25%



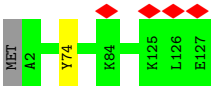
• Molecule 31: 60S ribosomal protein L25

Chain X: 98%



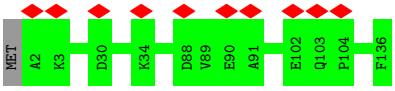
• Molecule 32: 60S ribosomal protein L26-A

Chain Y: 98%



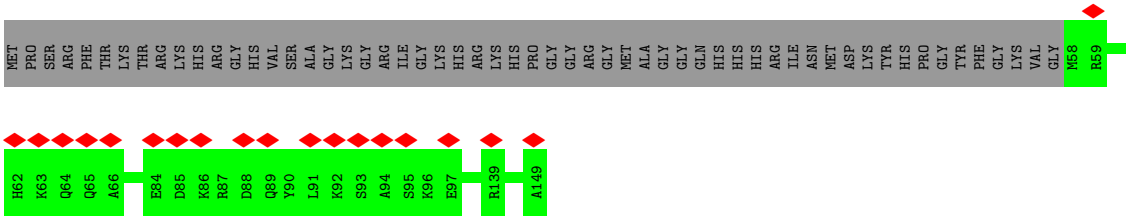
• Molecule 33: 60S ribosomal protein L27-A

Chain Z: 7% 99%



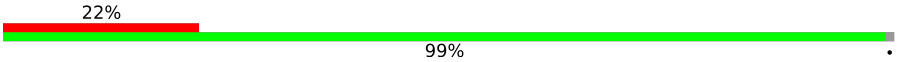
• Molecule 34: 60S ribosomal protein L28

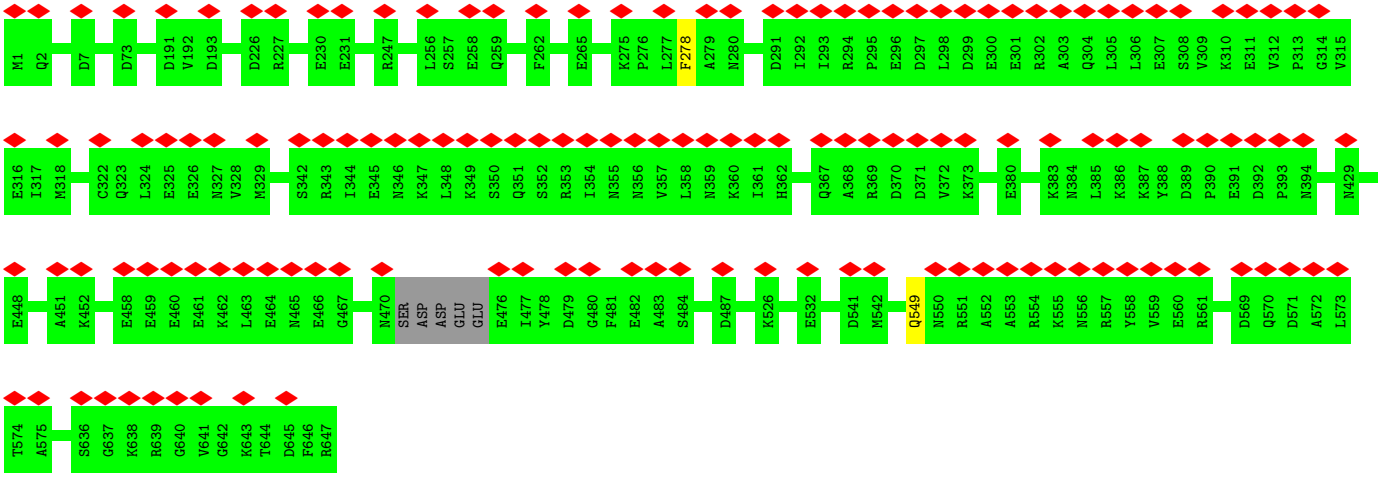
Chain a: 13% 62% 38%



• Molecule 35: Nucleolar GTP-binding protein 1

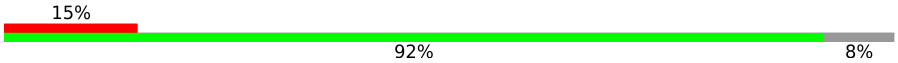
Chain b:

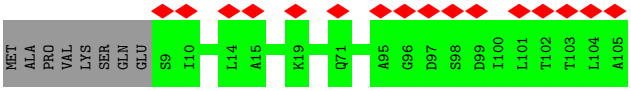




• Molecule 36: 60S ribosomal protein L30

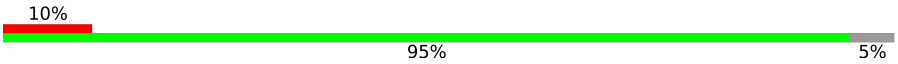
Chain c:

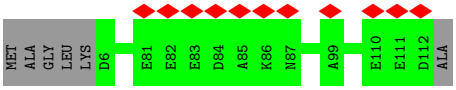




• Molecule 37: 60S ribosomal protein L31-A

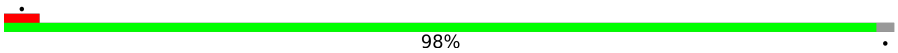
Chain d:

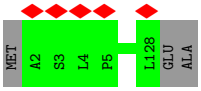




• Molecule 38: 60S ribosomal protein L32

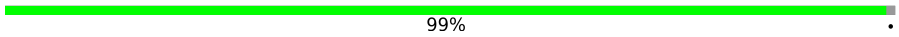
Chain e:





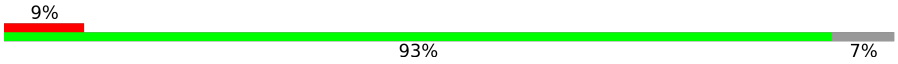
• Molecule 39: 60S ribosomal protein L33-A

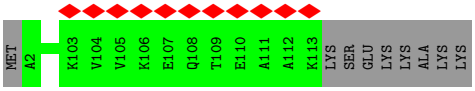
Chain f:



• Molecule 40: 60S ribosomal protein L34-A

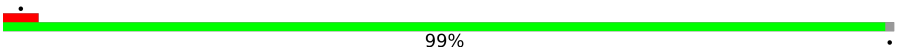
Chain g:

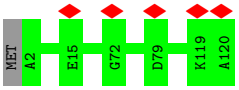




• Molecule 41: 60S ribosomal protein L35-A

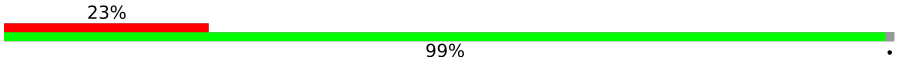
Chain h:

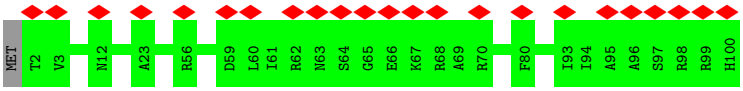




• Molecule 42: 60S ribosomal protein L36-A

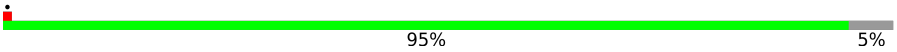
Chain i:

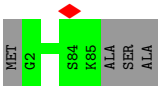




• Molecule 43: 60S ribosomal protein L37-A

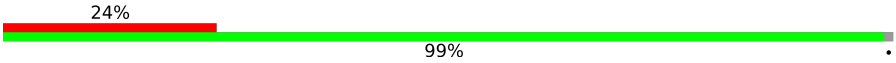
Chain j:

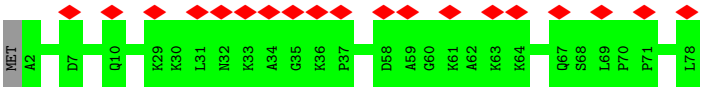




• Molecule 44: 60S ribosomal protein L38

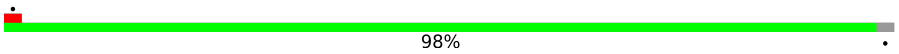
Chain k:





• Molecule 45: 60S ribosomal protein L39

Chain l:



• Molecule 46: Nucleolar GTP-binding protein 2

Chain m: 20% 95%

MET G2 T3 G4 K5 K6 E7 K8 S9 R10 R11 I12 R13 E14 GLY ASP THR LYS ASP G20 N21 L22 R23 V24 K25 F29 D32 S33 K34 S44 G45 K46 R49 N50 K51 K52 G53 N54 L55 I56 D68 G97 E98 T99 Q100 K101 E119 E120 K121 D122 A123 D124 E125

A129 D133 T134 K144 R151 L152 A153 A154 S155 N156 L157 E158 D159 E172 E173 K174 Q175 V176 L177 D178 A179 T180 L181 G182 L183 M184 G185 N186 Q187 E188 D189 K190 E191 N192 S196 A197 A198 K199 D312 N325 W353 S374 S375 K376 D377 S378 E379 T394

K422 K440 G441 G442 E443 E470 K471 E472 GLY GLU GLU LYS PRO LYS LYS LYS GLU VAL GLU LYS THR ALA

• Molecule 47: Pescadillo homolog

Chain n: 23% 61% 39%

M1 K5 R104 D110 S111 K119 E120 S124 D127 A128 I129 R130 D131 I132 D133 D134 F142 N149 Q150 D158 K161 V170 R174 K184 N191 I192 K193 G194 E195 E196 V197 R198 F205 P206 E207 N208 I209 P210 S211 D212 V213 D214 H230

Y234 T238 D239 S240 G241 L242 I243 K247 L248 D249 L250 K251 K252 D253 K254 I255 I256 S257 G258 L259 S260 S261 Y262 I263 L264 E265 S266 R267 GLN GLU ASP SER LEU LEU LEU LYS LEU ASP PRO THR GLU ILE GLU GLU ASP VAL LYS VAL GLU SER LEU ASP ALA SER THR LEU LYS SER ALA

LEU ASN ALA ASP GLU ALA ASN THR ASP GLU THR GLU LYS GLU GLU GLU GLU GLN GLU LYS LYS GLN GLU LYS GLU GLN GLU LYS GLU GLN ASN GLU GLU THR GLU LEU ASP THR PHE GLU ASP ASN ASN LYS ASN LYS GLY ASP ILE LEU ILE GLN PRO SER K351 Y352 D353 S354 P355 V356 A357

S358 L359 F360 S361 A362 F363 V367 S368 R369 E370 V371 P372 I373 D374 I375 L376 E377 L381 S382 C383 N386 V387 I388 S389 E390 A391 A392 M393 D394 Q395 I396 GLU ASN LYS LYS ASP ILE ASP MET S405 K406 V407 T408 H409 Q410 I411 V412 D413 R414 P415 V416 L417 K418 N419 K420 V421 A422

G423 R424 T425 Y426 I427 Q428 P429 Q430 W431 D434 C435 I436 M437 K438 G439 E440 L441 V442 P443 A444 N445 K446 Y447 L448 P449 G450 E451 A452 L453 H456 L457 S458 P459 W460 GLY ASP ALA ILE GLY TYR ASP PRO THR ALA PRO VAL GLU GLU GLY GLU GLU GLU GLU SER GLU SER GLU SER

GLU SER GLU ASP GLN VAL GLU GLU GLU ASP GLN GLU VAL VAL ALA GLY GLU GLU ASP ASP ASP ASP GLU GLU LEU GLN ALA LYS GLU LEU GLU LEU GLU ALA GLN GLY ILE LYS TYR SER GLU THR SER GLU ALA ASP LYS ASP VAL ASN LYS SER LYS ASN LYS LEU LYS LYS ARG LYS

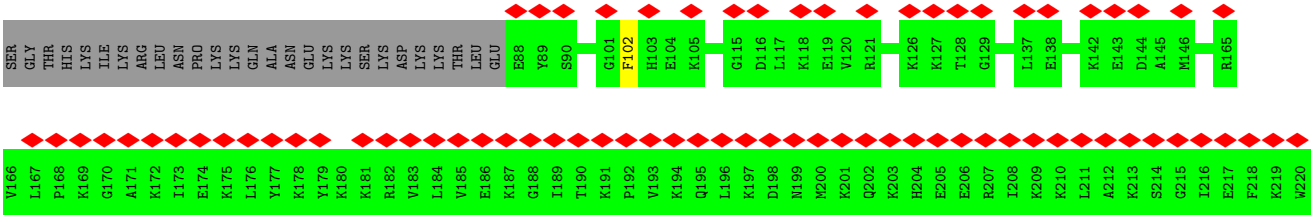
VAL ASP GLU GLU GLU GLU LYS LYS LEU LYS MET ILE MET MET SER ASN LYS GLN LYS LYS LEU TYR LYS LYS MET LYS TYR SER ASN ALA LYS LYS GLU GLU GLN ALA GLU ASN LEU LYS LYS LYS LYS LYS GLN ILE ALA LYS GLN LYS ALA LYS LEU ASN LYS LEU ASP SER LYS

LYS

• Molecule 48: Ribosome biogenesis protein 15

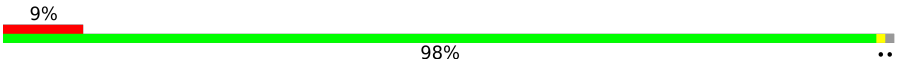
Chain o: 34% 60% 40%

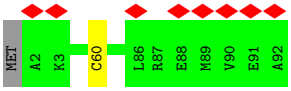
MET VAL LYS SER THR SER LYS THR SER THR LYS GLU THR VAL THR LYS GLN PRO THR GLU GLU GLU LYS PRO ILE GLN GLU GLU LYS GLU GLU LEU ALA LEU GLU THR SER SER SER SER SER ASP GLU GLU GLU ASP GLU LYS ASP GLU ASP GLU ILE GLU GLY LEU ALA ALA SER ASP ASP GLU GLU



- Molecule 49: 60S ribosomal protein L43-A

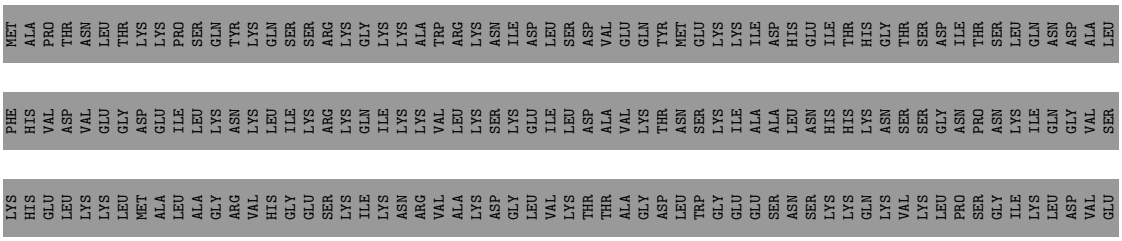
Chain p:

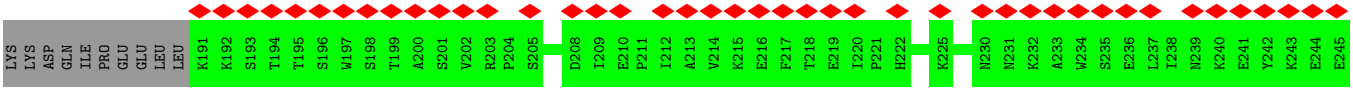


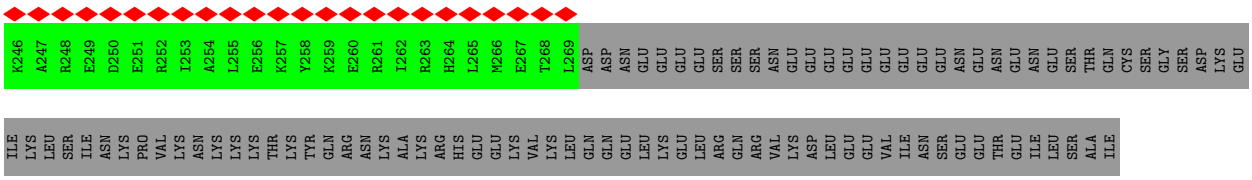


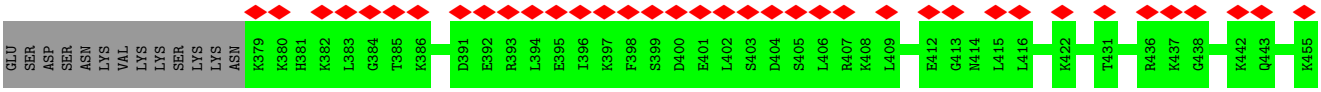
- Molecule 50: Ribosome biogenesis protein NOP53

Chain q:



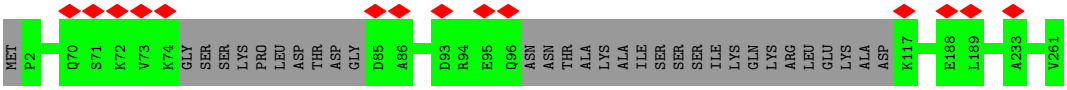






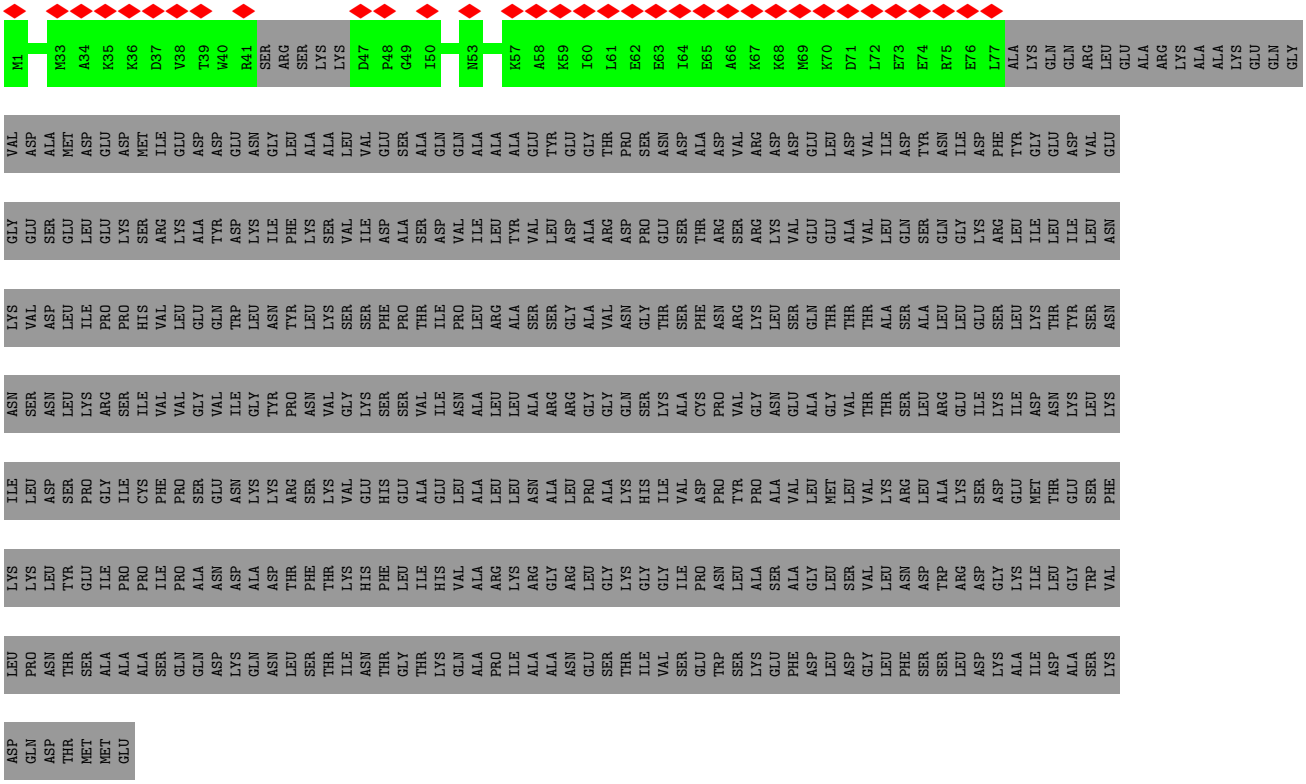
- Molecule 51: Ribosome biogenesis protein NSA2

Chain r:



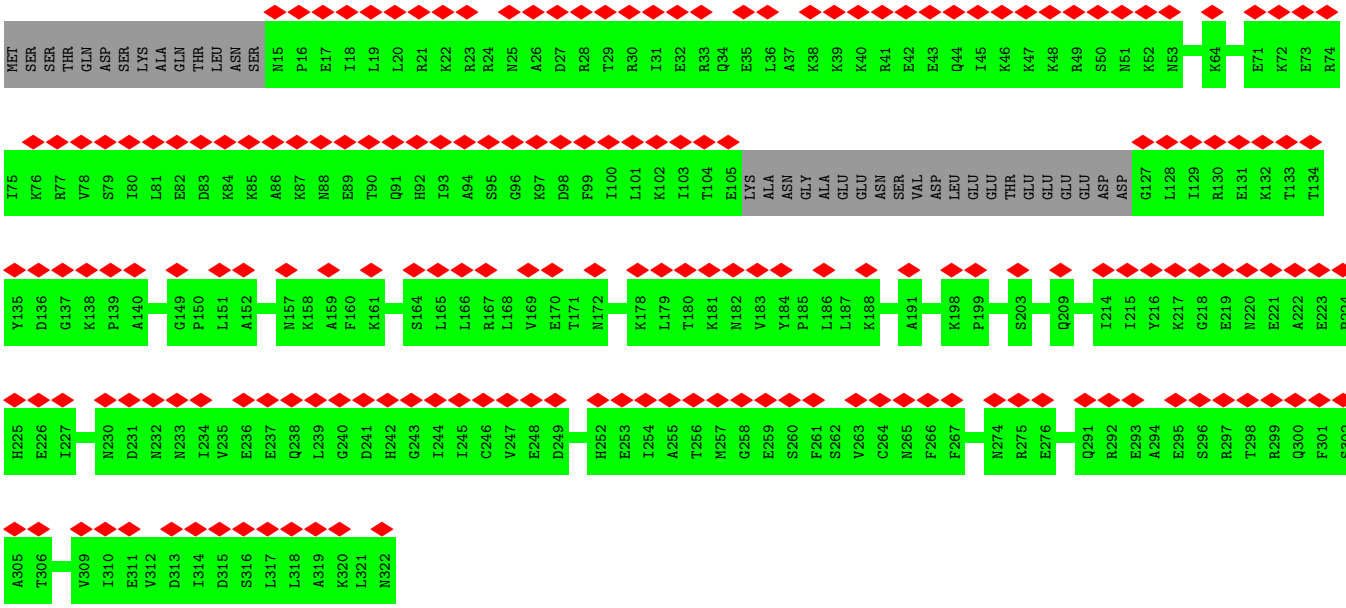
- Molecule 52: Nuclear GTP-binding protein NUG1

Chain s:



- Molecule 53: Ribosome biogenesis protein RLP7

Chain t:



- Molecule 54: Ribosome biogenesis protein RLP24

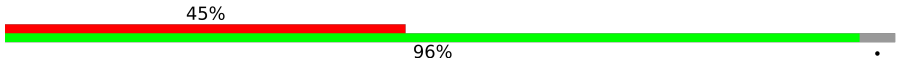
Chain u:

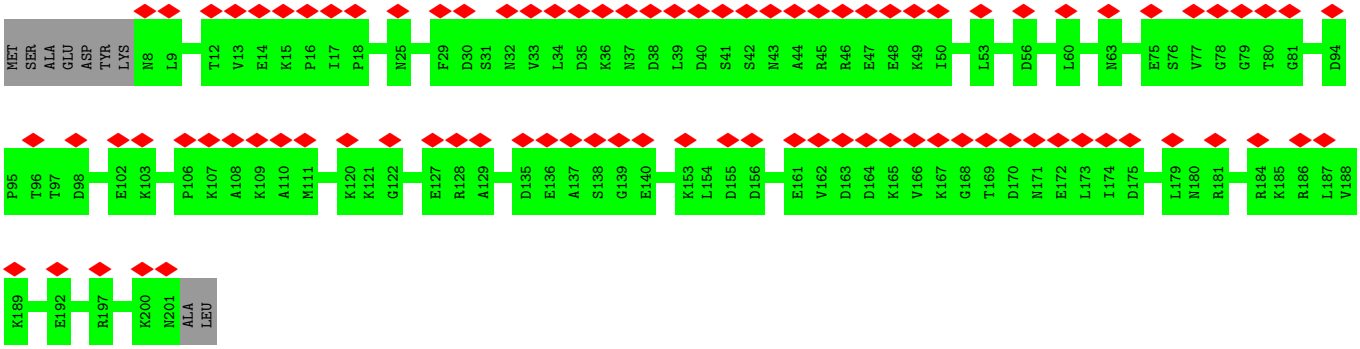
• Molecule 55: Ribosome production factor 2 homolog

Chain v:

• Molecule 56: Ribosome biogenesis regulatory protein

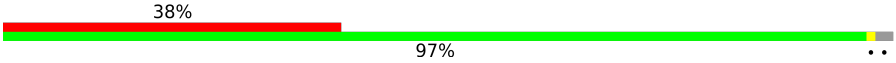
Chain w:

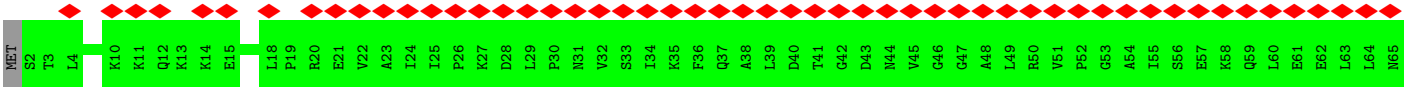


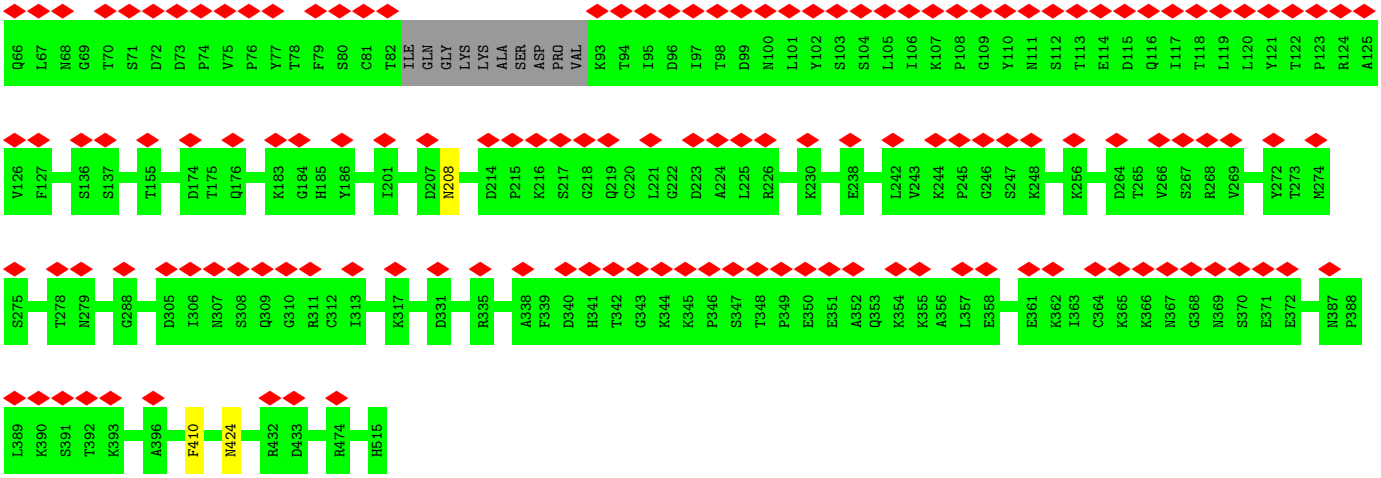


• Molecule 57: RSA4 isoform 1

Chain x:

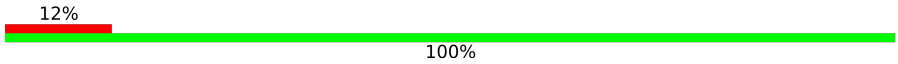


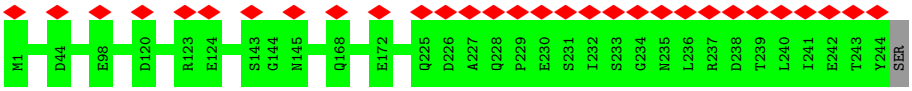




- Molecule 58: Eukaryotic translation initiation factor 6

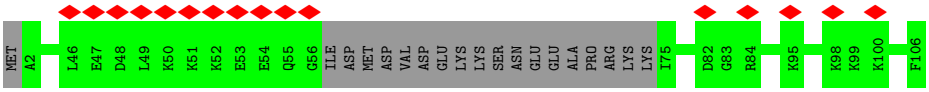
Chain y:





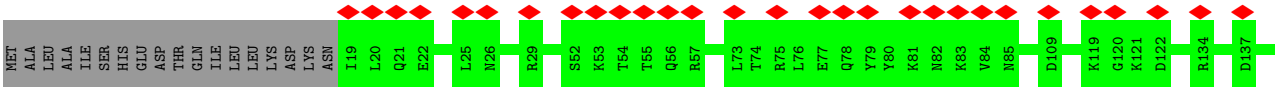
- Molecule 59: UPF0642 protein YBL028C

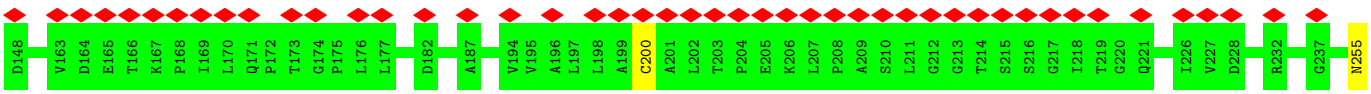
Chain z:

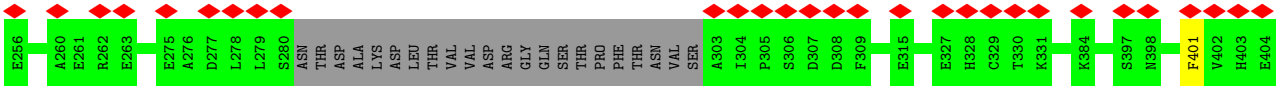


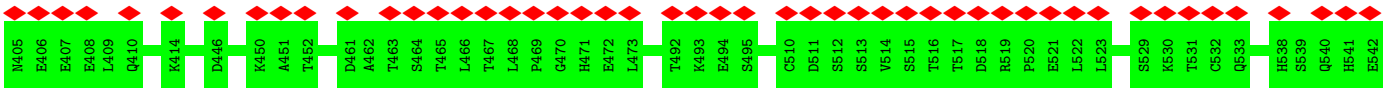
- Molecule 60: Probable metalloprotease ARX1

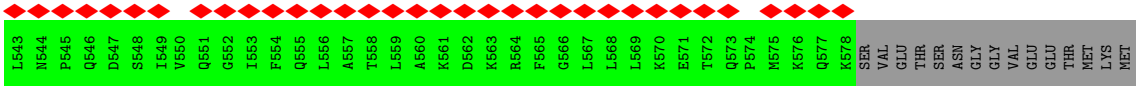
Chain 4:










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
MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1358921	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	0.265	Depositor
Minimum map value	-0.116	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	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: GTP, OMC, ZN, 1MA, MG, OMU, OMG, K, 5MC, GDP, PSU, B3P, A2M

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	0.57	0/2241
2	1	0.30	0/70356	0.83	19/109681 (0.0%)
3	2	0.31	0/3724	0.80	0/5798
4	3	0.19	0/2861	0.78	0/4457
5	5	0.24	0/649	0.51	0/848
6	6	0.23	0/1367	0.86	0/2118
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	0.51	0/3792
11	D	0.24	0/2227	0.49	0/3004
12	E	0.25	0/1251	0.49	0/1682
13	F	0.26	0/1798	0.49	0/2420
14	G	0.25	0/1784	0.46	0/2408
15	H	0.26	0/1539	0.51	0/2073
16	I	0.24	0/1075	0.48	0/1443
17	J	0.25	0/1389	0.52	0/1860
18	K	0.24	0/2190	0.47	0/2955
19	L	0.25	0/1460	0.56	0/1960
20	M	0.24	0/1074	0.50	0/1446
21	N	0.25	0/1654	0.59	0/2213
22	O	0.27	0/1585	0.50	0/2128
23	P	0.25	0/1410	0.56	0/1893
24	Q	0.25	0/1153	0.53	0/1555
25	R	0.25	0/1275	0.53	0/1702
26	S	0.26	0/1473	0.51	0/1980
27	T	0.25	0/916	0.50	0/1226
28	U	0.27	0/861	0.50	0/1167
29	V	0.27	0/1018	0.54	0/1369
30	W	0.25	0/1919	0.48	0/2586
31	X	0.25	0/1103	0.50	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	0.48	0/1497
34	a	0.24	0/747	0.46	0/1008
35	b	0.25	0/5270	0.50	0/7080
36	c	0.26	0/751	0.46	0/1008
37	d	0.24	0/887	0.53	0/1191
38	e	0.24	0/1041	0.51	0/1394
39	f	0.27	0/868	0.57	0/1168
40	g	0.25	0/891	0.56	0/1191
41	h	0.26	0/978	0.51	0/1301
42	i	0.24	0/778	0.54	0/1034
43	j	0.26	0/680	0.59	0/901
44	k	0.25	0/618	0.52	0/826
45	l	0.24	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	0.25	0/1129	0.48	0/1502
49	p	0.25	0/701	0.56	0/934
50	q	0.25	0/1321	0.48	0/1766
51	r	0.25	0/1892	0.51	0/2528
52	s	0.25	0/608	0.49	0/798
53	t	0.25	0/2333	0.50	0/3128
54	u	0.26	0/1287	0.54	0/1711
55	v	0.25	0/2410	0.48	0/3220
56	w	0.24	0/1565	0.46	0/2108
57	x	0.24	0/4022	0.50	0/5460
58	y	0.24	0/1872	0.52	0/2548
59	z	0.24	0/721	0.46	0/948
60	4	0.24	0/4242	0.47	0/5758
All	All	0.27	0/165978	0.69	19/239876 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	406	G	O4'-C1'-N9	9.18	115.54	108.20
2	1	1495	U	C2-N1-C1'	6.90	125.98	117.70
2	1	1495	U	C6-N1-C1'	-6.65	111.89	121.20
2	1	1604	G	C4-N9-C1'	6.52	134.97	126.50
2	1	1496	C	C2-N1-C1'	6.35	125.79	118.80
2	1	922	U	C2-N1-C1'	6.13	125.06	117.70
2	1	835	G	O4'-C1'-N9	6.12	113.10	108.20
2	1	2112	U	C2-N1-C1'	6.00	124.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	922	U	C6-N1-C1'	-5.96	112.85	121.20
2	1	2112	U	C6-N1-C1'	-5.85	113.01	121.20
2	1	1496	C	C6-N1-C1'	-5.76	113.89	120.80
2	1	1604	G	C8-N9-C1'	-5.34	120.05	127.00
2	1	3058	U	C2-N1-C1'	5.32	124.09	117.70
2	1	3058	U	C6-N1-C1'	-5.28	113.81	121.20
2	1	2212	C	C2-N1-C1'	5.25	124.58	118.80
2	1	2567	C	C2-N1-C1'	5.11	124.43	118.80
2	1	2983	C	C2-N1-C1'	5.10	124.41	118.80
2	1	1355	A	P-O3'-C3'	5.08	125.79	119.70
2	1	961	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/254 (83%)	201 (95%)	10 (5%)	0	100	100
5	5	71/120 (59%)	70 (99%)	1 (1%)	0	100	100
7	8	156/165 (94%)	152 (97%)	4 (3%)	0	100	100
8	9	110/175 (63%)	109 (99%)	1 (1%)	0	100	100
9	B	384/387 (99%)	379 (99%)	5 (1%)	0	100	100
10	C	359/362 (99%)	349 (97%)	10 (3%)	0	100	100
11	D	266/297 (90%)	254 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	E	151/176 (86%)	148 (98%)	3 (2%)	0	100	100
13	F	217/244 (89%)	214 (99%)	3 (1%)	0	100	100
14	G	220/256 (86%)	216 (98%)	4 (2%)	0	100	100
15	H	189/191 (99%)	183 (97%)	6 (3%)	0	100	100
16	I	129/166 (78%)	127 (98%)	2 (2%)	0	100	100
17	J	169/174 (97%)	166 (98%)	3 (2%)	0	100	100
18	K	262/376 (70%)	257 (98%)	5 (2%)	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	185/204 (91%)	179 (97%)	6 (3%)	0	100	100
22	O	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
23	P	171/184 (93%)	165 (96%)	6 (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%)	106 (96%)	4 (4%)	0	100	100
28	U	104/121 (86%)	101 (97%)	3 (3%)	0	100	100
29	V	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
30	W	232/312 (74%)	226 (97%)	6 (3%)	0	100	100
31	X	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
32	Y	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
33	Z	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
34	a	90/149 (60%)	86 (96%)	4 (4%)	0	100	100
35	b	638/647 (99%)	618 (97%)	20 (3%)	0	100	100
36	c	95/105 (90%)	95 (100%)	0	0	100	100
37	d	105/113 (93%)	105 (100%)	0	0	100	100
38	e	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
39	f	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
40	g	110/121 (91%)	109 (99%)	1 (1%)	0	100	100
41	h	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
42	i	97/100 (97%)	93 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	j	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
44	k	75/78 (96%)	75 (100%)	0	0	100	100
45	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
46	m	462/486 (95%)	454 (98%)	8 (2%)	0	100	100
47	n	363/605 (60%)	353 (97%)	10 (3%)	0	100	100
48	o	131/220 (60%)	128 (98%)	3 (2%)	0	100	100
49	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
50	q	152/455 (33%)	143 (94%)	9 (6%)	0	100	100
51	r	224/261 (86%)	219 (98%)	5 (2%)	0	100	100
52	s	68/520 (13%)	66 (97%)	2 (3%)	0	100	100
53	t	283/322 (88%)	275 (97%)	8 (3%)	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	192/203 (95%)	187 (97%)	5 (3%)	0	100	100
57	x	500/515 (97%)	487 (97%)	13 (3%)	0	100	100
58	y	242/245 (99%)	231 (96%)	11 (4%)	0	100	100
59	z	83/106 (78%)	83 (100%)	0	0	100	100
60	4	534/593 (90%)	529 (99%)	5 (1%)	0	100	100
All	All	10648/12924 (82%)	10393 (98%)	255 (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	67/106 (63%)	67 (100%)	0	100	100
7	8	129/136 (95%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	9	106/153 (69%)	106 (100%)	0	100	100
9	B	322/323 (100%)	321 (100%)	1 (0%)	92	96
10	C	288/289 (100%)	287 (100%)	1 (0%)	92	96
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%)	171 (100%)	0	100	100
16	I	117/141 (83%)	117 (100%)	0	100	100
17	J	148/150 (99%)	148 (100%)	0	100	100
18	K	247/346 (71%)	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	165/176 (94%)	165 (100%)	0	100	100
22	O	160/162 (99%)	160 (100%)	0	100	100
23	P	141/146 (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	92
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	211/281 (75%)	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%)	566 (100%)	2 (0%)	91	95
36	c	81/88 (92%)	81 (100%)	0	100	100
37	d	94/97 (97%)	94 (100%)	0	100	100
38	e	109/111 (98%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	f	90/91 (99%)	90 (100%)	0	100	100
40	g	95/103 (92%)	95 (100%)	0	100	100
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	81/82 (99%)	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	45/46 (98%)	45 (100%)	0	100	100
46	m	411/428 (96%)	409 (100%)	2 (0%)	88	93
47	n	332/548 (61%)	331 (100%)	1 (0%)	92	96
48	o	118/199 (59%)	117 (99%)	1 (1%)	81	89
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%)	203 (100%)	0	100	100
52	s	65/445 (15%)	65 (100%)	0	100	100
53	t	256/287 (89%)	256 (100%)	0	100	100
54	u	133/180 (74%)	133 (100%)	0	100	100
55	v	264/309 (85%)	264 (100%)	0	100	100
56	w	172/179 (96%)	172 (100%)	0	100	100
57	x	442/451 (98%)	439 (99%)	3 (1%)	84	90
58	y	210/211 (100%)	210 (100%)	0	100	100
59	z	77/95 (81%)	77 (100%)	0	100	100
60	4	471/520 (91%)	468 (99%)	3 (1%)	86	92
All	All	9306/11137 (84%)	9289 (100%)	17 (0%)	93	96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	B	332	ARG
10	C	120	TYR
26	S	172	TYR
32	Y	74	TYR
35	b	278	PHE
35	b	549	GLN
46	m	325	ASN

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Mol	Chain	Res	Type
46	m	353	TRP
47	n	427	ILE
48	o	102	PHE
49	p	60	CYS
57	x	208	ASN
57	x	410	PHE
57	x	424	ASN
60	4	200	CYS
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
46	m	227	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	2976/3396 (87%)	509 (17%)	4 (0%)
3	2	157/158 (99%)	26 (16%)	0
4	3	120/121 (99%)	26 (21%)	0
6	6	54/87 (62%)	18 (33%)	0
All	All	3307/3762 (87%)	579 (17%)	4 (0%)

All (579) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	2	U
2	1	5	G
2	1	42	C
2	1	43	A
2	1	45	A
2	1	49	A
2	1	59	G
2	1	60	A
2	1	65	A
2	1	66	A
2	1	77	A
2	1	109	A

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Mol	Chain	Res	Type
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	172	G
2	1	182	U
2	1	187	A
2	1	190	U
2	1	191	U
2	1	192	C
2	1	200	C
2	1	206	G
2	1	210	U
2	1	213	A
2	1	218	G
2	1	219	A
2	1	220	G
2	1	238	A
2	1	239	G
2	1	243	G
2	1	244	G
2	1	245	U
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	284	A
2	1	286	U
2	1	295	A
2	1	305	U
2	1	311	C
2	1	323	A

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Mol	Chain	Res	Type
2	1	329	U
2	1	339	C
2	1	376	G
2	1	398	A
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	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	548	G
2	1	550	A
2	1	555	U
2	1	557	A
2	1	559	A
2	1	579	G
2	1	592	A
2	1	604	G
2	1	609	G
2	1	611	A
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	705	A
2	1	715	A

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Mol	Chain	Res	Type
2	1	719	U
2	1	720	A
2	1	735	A
2	1	742	G
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	776	PSU
2	1	777	U
2	1	779	G
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	936	A
2	1	938	C
2	1	944	C
2	1	954	U
2	1	957	C
2	1	960	PSU
2	1	971	G
2	1	973	A
2	1	974	G
2	1	975	C
2	1	976	U
2	1	979	U
2	1	980	A

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Mol	Chain	Res	Type
2	1	993	G
2	1	1064	A
2	1	1066	G
2	1	1086	C
2	1	1094	U
2	1	1095	U
2	1	1096	U
2	1	1097	G
2	1	1098	A
2	1	1105	A
2	1	1109	U
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	1157	G
2	1	1159	A
2	1	1180	A
2	1	1181	U
2	1	1189	C
2	1	1191	U
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	1244	A
2	1	1245	A
2	1	1250	G
2	1	1252	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	1313	G
2	1	1330	A
2	1	1348	U
2	1	1356	U
2	1	1386	A
2	1	1391	C
2	1	1399	A
2	1	1404	G
2	1	1419	A
2	1	1421	G
2	1	1432	C
2	1	1434	G
2	1	1437	OMC
2	1	1446	A
2	1	1481	A
2	1	1503	A
2	1	1508	C
2	1	1527	C
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	1583	A
2	1	1587	A
2	1	1589	A
2	1	1593	A
2	1	1604	G
2	1	1628	C
2	1	1629	U
2	1	1639	C

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Mol	Chain	Res	Type
2	1	1641	U
2	1	1642	A
2	1	1643	A
2	1	1715	A
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	1775	G
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	1820	U
2	1	1821	U
2	1	1839	A
2	1	1842	A
2	1	1849	C
2	1	1866	C
2	1	1880	U
2	1	1886	A
2	1	1906	G
2	1	1909	A
2	1	1952	G
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	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	2209	U
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	2271	A
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	2376	G
2	1	2385	G
2	1	2388	U
2	1	2393	G
2	1	2397	A
2	1	2398	A
2	1	2399	A
2	1	2401	A
2	1	2402	A
2	1	2416	PSU
2	1	2417	OMU
2	1	2418	G
2	1	2419	A
2	1	2421	OMU
2	1	2422	C
2	1	2435	G
2	1	2445	A

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Mol	Chain	Res	Type
2	1	2502	A
2	1	2504	U
2	1	2506	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	2546	C
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	2596	U
2	1	2606	G
2	1	2607	G
2	1	2618	G
2	1	2619	G
2	1	2623	G
2	1	2624	G
2	1	2627	C
2	1	2653	C
2	1	2655	U
2	1	2656	A
2	1	2671	A
2	1	2674	A
2	1	2676	A
2	1	2677	G
2	1	2678	A

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Mol	Chain	Res	Type
2	1	2691	A
2	1	2693	C
2	1	2696	A
2	1	2697	A
2	1	2698	G
2	1	2699	G
2	1	2704	A
2	1	2705	A
2	1	2712	U
2	1	2715	A
2	1	2718	U
2	1	2719	U
2	1	2721	A
2	1	2729	OMU
2	1	2731	U
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	2791	OMG
2	1	2794	G
2	1	2797	C
2	1	2798	C
2	1	2799	A
2	1	2800	G
2	1	2801	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

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Mol	Chain	Res	Type
2	1	2819	A
2	1	2821	C
2	1	2822	U
2	1	2824	G
2	1	2825	C
2	1	2838	A
2	1	2847	A
2	1	2861	U
2	1	2864	A
2	1	2865	PSU
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	2923	PSU
2	1	2924	U
2	1	2925	C
2	1	2926	A
2	1	2935	U
2	1	2936	A
2	1	2940	A
2	1	2941	A
2	1	2948	OMC
2	1	2952	G
2	1	2953	U
2	1	2954	U
2	1	2955	U
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

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Mol	Chain	Res	Type
2	1	3022	G
2	1	3023	U
2	1	3032	A
2	1	3055	U
2	1	3059	G
2	1	3078	U
2	1	3079	U
2	1	3080	G
2	1	3086	A
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	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	3180	A
2	1	3181	C
2	1	3187	A
2	1	3196	U
2	1	3207	U
2	1	3217	C
2	1	3218	A

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Mol	Chain	Res	Type
2	1	3219	G
2	1	3243	A
2	1	3245	A
2	1	3247	G
2	1	3253	G
2	1	3256	G
2	1	3259	U
2	1	3260	G
2	1	3263	G
2	1	3276	G
2	1	3279	A
2	1	3280	U
2	1	3282	U
2	1	3283	U
2	1	3284	G
2	1	3285	C
2	1	3286	G
2	1	3287	U
2	1	3288	G
2	1	3294	A
2	1	3295	A
2	1	3304	U
2	1	3313	U
2	1	3316	A
2	1	3318	G
2	1	3319	U
2	1	3341	U
2	1	3345	G
2	1	3369	G
2	1	3375	A
2	1	3378	C
2	1	3382	U
2	1	3386	G
2	1	3389	U
2	1	3396	U
3	2	23	U
3	2	34	U
3	2	35	C
3	2	38	U
3	2	52	A
3	2	59	A
3	2	62	C

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Mol	Chain	Res	Type
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	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	22	A
4	3	33	U
4	3	49	G
4	3	50	PSU
4	3	51	A
4	3	54	U
4	3	55	A
4	3	65	G
4	3	72	A
4	3	73	C
4	3	74	C
4	3	76	A
4	3	83	U
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

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Mol	Chain	Res	Type
4	3	112	G
4	3	114	U
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	24	A
6	6	33	U
6	6	43	A
6	6	47	A
6	6	48	A
6	6	49	C
6	6	52	G
6	6	54	A
6	6	56	U
6	6	58	G
6	6	59	C
6	6	228	U
6	6	231	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	1355	A
2	1	1568	U
2	1	3121	U
2	1	3283	U

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

58 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	2975	2	18,21,22	1.11	1 (5%)	22,30,33	1.50	4 (18%)
4	PSU	3	50	4	18,21,22	1.19	2 (11%)	22,30,33	1.50	4 (18%)
2	OMG	1	2815	2	18,26,27	1.11	2 (11%)	19,38,41	0.88	1 (5%)
3	PSU	2	73	3	18,21,22	1.10	1 (5%)	22,30,33	1.47	4 (18%)
2	1MA	1	2142	2,61	16,25,26	0.98	2 (12%)	18,37,40	1.09	2 (11%)
2	OMG	1	908	2	18,26,27	1.11	2 (11%)	19,38,41	0.89	1 (5%)
2	OMU	1	1888	2	19,22,23	3.00	7 (36%)	26,31,34	1.95	8 (30%)
2	A2M	1	1449	2,61	18,25,26	1.45	1 (5%)	18,36,39	0.97	1 (5%)
2	OMG	1	2922	2	18,26,27	1.13	2 (11%)	19,38,41	0.83	1 (5%)
2	PSU	1	2923	2	18,21,22	1.25	2 (11%)	22,30,33	1.38	4 (18%)
2	PSU	1	986	2	18,21,22	1.11	1 (5%)	22,30,33	1.36	4 (18%)
2	PSU	1	990	2	18,21,22	1.15	1 (5%)	22,30,33	1.45	4 (18%)
2	OMC	1	650	2	19,22,23	0.52	0	26,31,34	0.67	0
2	OMC	1	2959	2	19,22,23	0.58	0	26,31,34	0.76	0
2	A2M	1	817	2,61	18,25,26	1.39	1 (5%)	18,36,39	1.09	2 (11%)
2	PSU	1	2349	2,61	18,21,22	1.12	1 (5%)	22,30,33	1.35	4 (18%)
2	A2M	1	807	2	18,25,26	1.47	1 (5%)	18,36,39	1.01	0
2	OMU	1	898	2	19,22,23	2.88	8 (42%)	26,31,34	1.68	5 (19%)
2	PSU	1	776	2	18,21,22	1.19	1 (5%)	22,30,33	1.47	5 (22%)
2	OMG	1	805	2	18,26,27	1.14	2 (11%)	19,38,41	0.85	1 (5%)
2	OMU	1	2347	2	19,22,23	2.90	7 (36%)	26,31,34	1.67	4 (15%)
2	PSU	1	1124	2	18,21,22	1.19	1 (5%)	22,30,33	1.46	5 (22%)
2	OMC	1	663	2	19,22,23	0.55	0	26,31,34	0.65	0
2	OMU	1	2729	2	19,22,23	2.92	8 (42%)	26,31,34	1.74	5 (19%)
2	OMU	1	2724	2	19,22,23	2.90	8 (42%)	26,31,34	1.67	4 (15%)
2	OMG	1	2793	2	18,26,27	1.10	2 (11%)	19,38,41	0.95	1 (5%)
2	PSU	1	2266	2	18,21,22	1.16	1 (5%)	22,30,33	1.42	4 (18%)
2	A2M	1	1133	2	18,25,26	1.49	1 (5%)	18,36,39	0.97	0
2	OMC	1	2948	2	19,22,23	0.53	0	26,31,34	0.76	0
2	PSU	1	2129	2	18,21,22	1.18	2 (11%)	22,30,33	1.41	4 (18%)
2	OMC	1	2197	2	19,22,23	0.48	0	26,31,34	0.62	0
2	OMU	1	2417	2	19,22,23	2.92	8 (42%)	26,31,34	1.64	4 (15%)
2	A2M	1	649	2	18,25,26	1.50	1 (5%)	18,36,39	0.97	1 (5%)
2	PSU	1	2865	2	18,21,22	1.20	3 (16%)	22,30,33	1.44	4 (18%)
2	OMG	1	1450	2	18,26,27	1.14	2 (11%)	19,38,41	0.79	1 (5%)
2	PSU	1	966	2	18,21,22	1.21	3 (16%)	22,30,33	1.43	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PSU	1	2735	2	18,21,22	1.10	1 (5%)	22,30,33	1.49	4 (18%)
2	A2M	1	2220	2	18,25,26	1.53	1 (5%)	18,36,39	1.09	1 (5%)
2	PSU	1	2826	2,61	18,21,22	1.07	1 (5%)	22,30,33	1.53	4 (18%)
2	OMU	1	2921	2	19,22,23	2.94	8 (42%)	26,31,34	1.68	5 (19%)
2	PSU	1	2264	2	18,21,22	1.21	3 (16%)	22,30,33	1.48	4 (18%)
2	OMC	1	2337	2	19,22,23	0.54	0	26,31,34	0.64	0
2	PSU	1	960	2	18,21,22	1.18	2 (11%)	22,30,33	1.41	4 (18%)
2	PSU	1	2133	2	18,21,22	1.07	1 (5%)	22,30,33	1.49	4 (18%)
2	OMC	1	1437	2	19,22,23	0.61	0	26,31,34	0.97	1 (3%)
2	PSU	1	2416	2	18,21,22	1.18	2 (11%)	22,30,33	1.50	4 (18%)
2	PSU	1	2191	2	18,21,22	1.09	1 (5%)	22,30,33	1.45	4 (18%)
2	5MC	1	2870	2	18,22,23	0.92	2 (11%)	26,32,35	1.13	2 (7%)
2	5MC	1	2278	2	18,22,23	0.94	2 (11%)	26,32,35	1.10	3 (11%)
2	A2M	1	876	2	18,25,26	1.44	1 (5%)	18,36,39	0.93	0
2	PSU	1	2314	2	18,21,22	1.17	1 (5%)	22,30,33	1.44	4 (18%)
2	PSU	1	2351	2	18,21,22	1.06	1 (5%)	22,30,33	1.46	4 (18%)
2	OMU	1	2421	2	19,22,23	2.96	8 (42%)	26,31,34	1.71	5 (19%)
2	PSU	1	1110	2	18,21,22	1.15	1 (5%)	22,30,33	1.47	5 (22%)
2	PSU	1	2880	2	18,21,22	1.19	2 (11%)	22,30,33	1.44	5 (22%)
2	OMG	1	2791	2	18,26,27	1.08	2 (11%)	19,38,41	0.90	1 (5%)
2	OMG	1	867	2	18,26,27	1.14	2 (11%)	19,38,41	0.86	1 (5%)
2	PSU	1	2340	2	18,21,22	1.03	1 (5%)	22,30,33	1.44	4 (18%)

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	2975	2	-	0/7/25/26	0/2/2/2
4	PSU	3	50	4	-	2/7/25/26	0/2/2/2
2	OMG	1	2815	2	-	0/5/27/28	0/3/3/3
3	PSU	2	73	3	-	0/7/25/26	0/2/2/2
2	1MA	1	2142	2,61	-	2/3/25/26	0/3/3/3
2	OMG	1	908	2	-	0/5/27/28	0/3/3/3
2	OMU	1	1888	2	-	2/9/27/28	0/2/2/2
2	A2M	1	1449	2,61	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	1	2922	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2923	2	-	2/7/25/26	0/2/2/2
2	PSU	1	986	2	-	2/7/25/26	0/2/2/2
2	PSU	1	990	2	-	0/7/25/26	0/2/2/2
2	OMC	1	650	2	-	0/9/27/28	0/2/2/2
2	OMC	1	2959	2	-	0/9/27/28	0/2/2/2
2	A2M	1	817	2,61	-	2/5/27/28	0/3/3/3
2	PSU	1	2349	2,61	-	0/7/25/26	0/2/2/2
2	A2M	1	807	2	-	0/5/27/28	0/3/3/3
2	OMU	1	898	2	-	0/9/27/28	0/2/2/2
2	PSU	1	776	2	-	2/7/25/26	0/2/2/2
2	OMG	1	805	2	-	1/5/27/28	0/3/3/3
2	OMU	1	2347	2	-	0/9/27/28	0/2/2/2
2	PSU	1	1124	2	-	0/7/25/26	0/2/2/2
2	OMC	1	663	2	-	0/9/27/28	0/2/2/2
2	OMU	1	2729	2	-	2/9/27/28	0/2/2/2
2	OMU	1	2724	2	-	1/9/27/28	0/2/2/2
2	OMG	1	2793	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2266	2	-	0/7/25/26	0/2/2/2
2	A2M	1	1133	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	2129	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2197	2	-	2/9/27/28	0/2/2/2
2	OMU	1	2417	2	-	2/9/27/28	0/2/2/2
2	A2M	1	649	2	-	3/5/27/28	0/3/3/3
2	PSU	1	2865	2	-	2/7/25/26	0/2/2/2
2	OMG	1	1450	2	-	2/5/27/28	0/3/3/3
2	PSU	1	966	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2735	2	-	0/7/25/26	0/2/2/2
2	A2M	1	2220	2	-	2/5/27/28	0/3/3/3
2	PSU	1	2826	2,61	-	2/7/25/26	0/2/2/2
2	OMU	1	2921	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2264	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2337	2	-	0/9/27/28	0/2/2/2
2	PSU	1	960	2	-	2/7/25/26	0/2/2/2
2	PSU	1	2133	2	-	0/7/25/26	0/2/2/2
2	OMC	1	1437	2	-	4/9/27/28	0/2/2/2
2	PSU	1	2416	2	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	1	2191	2	-	0/7/25/26	0/2/2/2
2	5MC	1	2870	2	-	0/7/25/26	0/2/2/2
2	5MC	1	2278	2	-	0/7/25/26	0/2/2/2
2	A2M	1	876	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2314	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2351	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2421	2	-	2/9/27/28	0/2/2/2
2	PSU	1	1110	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2880	2	-	0/7/25/26	0/2/2/2
2	OMG	1	2791	2	-	3/5/27/28	0/3/3/3
2	OMG	1	867	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2340	2	-	3/7/25/26	0/2/2/2

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	1888	OMU	C2-N1	7.59	1.50	1.38
2	1	2421	OMU	C2-N1	7.15	1.49	1.38
2	1	2921	OMU	C2-N1	7.13	1.49	1.38
2	1	2347	OMU	C2-N1	7.05	1.49	1.38
2	1	2417	OMU	C2-N1	7.01	1.49	1.38
2	1	2729	OMU	C2-N1	6.99	1.49	1.38
2	1	898	OMU	C2-N1	6.95	1.49	1.38
2	1	2724	OMU	C2-N1	6.90	1.49	1.38
2	1	2417	OMU	C2-N3	6.67	1.49	1.38
2	1	2421	OMU	C2-N3	6.65	1.49	1.38
2	1	2724	OMU	C2-N3	6.60	1.49	1.38
2	1	2921	OMU	C2-N3	6.60	1.49	1.38
2	1	2729	OMU	C2-N3	6.57	1.49	1.38
2	1	1888	OMU	C2-N3	6.52	1.49	1.38
2	1	2347	OMU	C2-N3	6.43	1.49	1.38
2	1	898	OMU	C2-N3	6.31	1.49	1.38
2	1	2921	OMU	C6-C5	5.87	1.48	1.35
2	1	2421	OMU	C6-C5	5.86	1.48	1.35
2	1	2729	OMU	C6-C5	5.84	1.48	1.35
2	1	1888	OMU	C6-C5	5.82	1.48	1.35
2	1	898	OMU	C6-C5	5.81	1.48	1.35
2	1	2724	OMU	C6-C5	5.79	1.48	1.35
2	1	2417	OMU	C6-C5	5.79	1.48	1.35
2	1	2347	OMU	C6-C5	5.69	1.48	1.35
2	1	807	A2M	O5'-C5'	-4.74	1.33	1.44
2	1	2220	A2M	O5'-C5'	-4.73	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	876	A2M	O5'-C5'	-4.67	1.33	1.44
2	1	649	A2M	O5'-C5'	-4.60	1.33	1.44
2	1	1133	A2M	O5'-C5'	-4.57	1.33	1.44
2	1	817	A2M	O5'-C5'	-4.55	1.33	1.44
2	1	1449	A2M	O5'-C5'	-4.53	1.33	1.44
2	1	2421	OMU	C4-N3	3.56	1.44	1.38
2	1	2921	OMU	C4-N3	3.50	1.44	1.38
2	1	2729	OMU	C4-N3	3.46	1.44	1.38
2	1	2417	OMU	C4-N3	3.45	1.44	1.38
2	1	2724	OMU	C4-N3	3.35	1.44	1.38
2	1	898	OMU	C4-N3	3.27	1.44	1.38
2	1	2347	OMU	C4-N3	3.26	1.44	1.38
2	1	1888	OMU	C4-N3	3.18	1.44	1.38
2	1	2865	PSU	C2-N1	3.17	1.41	1.36
4	3	50	PSU	C2-N1	3.14	1.41	1.36
2	1	2264	PSU	C2-N1	3.11	1.40	1.36
2	1	2129	PSU	C2-N1	3.11	1.40	1.36
2	1	2923	PSU	C2-N1	3.07	1.40	1.36
2	1	1110	PSU	C2-N1	3.06	1.40	1.36
2	1	1124	PSU	C2-N1	3.00	1.40	1.36
2	1	2975	PSU	C2-N1	3.00	1.40	1.36
2	1	1888	OMU	O2-C2	-2.99	1.17	1.23
2	1	2880	PSU	C2-N1	2.99	1.40	1.36
2	1	776	PSU	C2-N1	2.98	1.40	1.36
2	1	966	PSU	C2-N1	2.93	1.40	1.36
2	1	2314	PSU	C2-N1	2.92	1.40	1.36
2	1	990	PSU	C2-N1	2.91	1.40	1.36
2	1	2347	OMU	O4-C4	-2.90	1.18	1.24
2	1	2191	PSU	C2-N1	2.89	1.40	1.36
2	1	2351	PSU	C2-N1	2.88	1.40	1.36
2	1	2922	OMG	C8-N7	-2.88	1.30	1.35
2	1	2266	PSU	C2-N1	2.88	1.40	1.36
2	1	2416	PSU	C2-N1	2.87	1.40	1.36
2	1	1450	OMG	C8-N7	-2.85	1.30	1.35
2	1	2735	PSU	C2-N1	2.85	1.40	1.36
2	1	960	PSU	C2-N1	2.85	1.40	1.36
2	1	1888	OMU	O4-C4	-2.85	1.19	1.24
3	2	73	PSU	C2-N1	2.82	1.40	1.36
2	1	898	OMU	O4-C4	-2.81	1.19	1.24
2	1	867	OMG	C8-N7	-2.81	1.30	1.35
2	1	805	OMG	C8-N7	-2.81	1.30	1.35
2	1	898	OMU	O2-C2	-2.78	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2133	PSU	C2-N1	2.78	1.40	1.36
2	1	2347	OMU	O2-C2	-2.78	1.18	1.23
2	1	2826	PSU	C2-N1	2.77	1.40	1.36
2	1	2349	PSU	C2-N1	2.77	1.40	1.36
2	1	908	OMG	C8-N7	-2.76	1.30	1.35
2	1	2278	5MC	C6-C5	2.74	1.39	1.34
2	1	2724	OMU	O4-C4	-2.73	1.19	1.24
2	1	2815	OMG	C8-N7	-2.73	1.30	1.35
2	1	2142	1MA	C8-N7	-2.72	1.30	1.35
2	1	2421	OMU	O4-C4	-2.66	1.19	1.24
2	1	2340	PSU	C2-N1	2.65	1.40	1.36
2	1	2791	OMG	C8-N7	-2.65	1.30	1.35
2	1	986	PSU	C2-N1	2.64	1.40	1.36
2	1	2729	OMU	O4-C4	-2.64	1.19	1.24
2	1	2921	OMU	O4-C4	-2.63	1.19	1.24
2	1	2729	OMU	O2-C2	-2.63	1.18	1.23
2	1	2793	OMG	C8-N7	-2.62	1.30	1.35
2	1	2724	OMU	O2-C2	-2.61	1.18	1.23
2	1	2417	OMU	O4-C4	-2.60	1.19	1.24
2	1	2417	OMU	O2-C2	-2.57	1.18	1.23
2	1	2921	OMU	O2-C2	-2.55	1.18	1.23
2	1	2421	OMU	O2-C2	-2.54	1.18	1.23
2	1	2870	5MC	C6-C5	2.53	1.38	1.34
2	1	1450	OMG	C5-C6	-2.43	1.42	1.47
2	1	867	OMG	C5-C6	-2.40	1.42	1.47
2	1	2922	OMG	C5-C6	-2.33	1.42	1.47
2	1	805	OMG	C5-C6	-2.32	1.42	1.47
2	1	2870	5MC	C6-N1	-2.23	1.34	1.38
2	1	2815	OMG	C5-C6	-2.22	1.42	1.47
2	1	2142	1MA	C5-C4	-2.21	1.37	1.43
2	1	2793	OMG	C5-C6	-2.21	1.42	1.47
2	1	2278	5MC	C6-N1	-2.20	1.34	1.38
2	1	1888	OMU	C6-N1	2.20	1.43	1.38
2	1	908	OMG	C5-C6	-2.19	1.43	1.47
2	1	2791	OMG	C5-C6	-2.18	1.43	1.47
2	1	966	PSU	C6-N1	2.16	1.39	1.36
2	1	960	PSU	C4-N3	2.12	1.42	1.38
2	1	2729	OMU	C5-C4	2.12	1.48	1.43
2	1	2416	PSU	C6-N1	2.12	1.39	1.36
2	1	2421	OMU	C5-C4	2.11	1.48	1.43
4	3	50	PSU	C6-N1	2.11	1.39	1.36
2	1	2921	OMU	C6-N1	2.10	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2880	PSU	C4-N3	2.09	1.42	1.38
2	1	2347	OMU	C6-N1	2.09	1.43	1.38
2	1	2729	OMU	C6-N1	2.09	1.43	1.38
2	1	2264	PSU	C4-N3	2.08	1.42	1.38
2	1	2865	PSU	C6-N1	2.07	1.39	1.36
2	1	2921	OMU	C5-C4	2.07	1.48	1.43
2	1	2923	PSU	C6-N1	2.07	1.39	1.36
2	1	2421	OMU	C6-N1	2.07	1.43	1.38
2	1	898	OMU	C6-N1	2.06	1.43	1.38
2	1	2264	PSU	C6-N1	2.05	1.39	1.36
2	1	898	OMU	C5-C4	2.05	1.48	1.43
2	1	2417	OMU	C5-C4	2.04	1.48	1.43
2	1	2724	OMU	C6-N1	2.04	1.42	1.38
2	1	2724	OMU	C5-C4	2.04	1.48	1.43
2	1	2865	PSU	C4-N3	2.03	1.42	1.38
2	1	966	PSU	C4-N3	2.03	1.42	1.38
2	1	2129	PSU	C6-N1	2.02	1.39	1.36
2	1	2417	OMU	C6-N1	2.00	1.42	1.38

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2729	OMU	C4-N3-C2	-5.45	119.39	126.58
2	1	2421	OMU	C4-N3-C2	-5.26	119.65	126.58
2	1	898	OMU	C4-N3-C2	-5.23	119.69	126.58
2	1	2921	OMU	C4-N3-C2	-5.22	119.70	126.58
2	1	2347	OMU	C4-N3-C2	-5.16	119.77	126.58
2	1	2724	OMU	C4-N3-C2	-5.09	119.86	126.58
2	1	2417	OMU	C4-N3-C2	-4.91	120.11	126.58
2	1	1888	OMU	C4-N3-C2	-4.73	120.35	126.58
2	1	1888	OMU	C1'-N1-C2	4.41	125.55	117.57
2	1	2865	PSU	C6-C5-C4	4.38	121.26	118.20
4	3	50	PSU	C6-C5-C4	4.28	121.19	118.20
2	1	2826	PSU	C6-C5-C4	4.23	121.16	118.20
2	1	2264	PSU	C6-C5-C4	4.19	121.13	118.20
2	1	2416	PSU	C6-C5-C4	4.19	121.13	118.20
2	1	2735	PSU	C6-C5-C4	4.12	121.08	118.20
2	1	776	PSU	C6-C5-C4	4.00	121.00	118.20
2	1	2975	PSU	C6-C5-C4	3.98	120.98	118.20
2	1	2729	OMU	N3-C2-N1	3.97	120.17	114.89
2	1	2314	PSU	C6-C5-C4	3.95	120.96	118.20
2	1	1888	OMU	N3-C2-N1	3.95	120.13	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2351	PSU	C6-C5-C4	3.94	120.95	118.20
2	1	1110	PSU	C6-C5-C4	3.93	120.94	118.20
2	1	990	PSU	C6-C5-C4	3.92	120.94	118.20
2	1	898	OMU	N3-C2-N1	3.89	120.06	114.89
3	2	73	PSU	C6-C5-C4	3.89	120.92	118.20
2	1	2129	PSU	C6-C5-C4	3.84	120.88	118.20
2	1	2880	PSU	C6-C5-C4	3.84	120.88	118.20
2	1	966	PSU	C6-C5-C4	3.83	120.88	118.20
2	1	2923	PSU	C6-C5-C4	3.83	120.87	118.20
2	1	2421	OMU	N3-C2-N1	3.81	119.94	114.89
2	1	2921	OMU	N3-C2-N1	3.69	119.78	114.89
2	1	2724	OMU	N3-C2-N1	3.68	119.77	114.89
2	1	2340	PSU	C6-C5-C4	3.65	120.75	118.20
2	1	2347	OMU	N3-C2-N1	3.64	119.72	114.89
2	1	1124	PSU	C6-C5-C4	3.63	120.74	118.20
2	1	2191	PSU	C6-C5-C4	3.62	120.73	118.20
2	1	2266	PSU	C6-C5-C4	3.54	120.67	118.20
2	1	2133	PSU	C6-C5-C4	3.48	120.63	118.20
2	1	2417	OMU	N3-C2-N1	3.47	119.49	114.89
2	1	2347	OMU	C5-C4-N3	3.44	119.99	114.84
2	1	2870	5MC	C5-C6-N1	-3.38	119.86	123.34
2	1	2729	OMU	C5-C4-N3	3.37	119.89	114.84
2	1	2421	OMU	C5-C4-N3	3.34	119.83	114.84
2	1	960	PSU	C6-C5-C4	3.33	120.53	118.20
2	1	2921	OMU	C5-C4-N3	3.32	119.80	114.84
2	1	2724	OMU	C5-C4-N3	3.32	119.80	114.84
2	1	2417	OMU	C5-C4-N3	3.25	119.70	114.84
2	1	898	OMU	C5-C4-N3	3.25	119.70	114.84
2	1	2278	5MC	C5-C6-N1	-3.18	120.07	123.34
2	1	2349	PSU	O4-C4-N3	-3.15	114.07	120.12
2	1	1888	OMU	C5-C4-N3	3.15	119.56	114.84
2	1	986	PSU	C6-C5-C4	3.01	120.30	118.20
2	1	2865	PSU	C4-N3-C2	-2.99	122.03	126.34
2	1	2826	PSU	C4-N3-C2	-2.98	122.04	126.34
2	1	2133	PSU	C4-N3-C2	-2.95	122.09	126.34
2	1	2264	PSU	C4-N3-C2	-2.95	122.09	126.34
3	2	73	PSU	C4-N3-C2	-2.95	122.09	126.34
2	1	990	PSU	C4-N3-C2	-2.94	122.09	126.34
2	1	2133	PSU	O4-C4-N3	-2.94	114.47	120.12
2	1	2735	PSU	C4-N3-C2	-2.94	122.11	126.34
2	1	986	PSU	O4-C4-N3	-2.92	114.51	120.12
2	1	2347	OMU	O4-C4-C5	-2.92	120.02	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2417	OMU	O4-C4-C5	-2.91	120.04	125.16
2	1	2975	PSU	C4-N3-C2	-2.90	122.16	126.34
2	1	2880	PSU	C4-N3-C2	-2.89	122.17	126.34
4	3	50	PSU	C4-N3-C2	-2.88	122.19	126.34
2	1	2351	PSU	C4-N3-C2	-2.88	122.19	126.34
2	1	2416	PSU	C4-N3-C2	-2.87	122.21	126.34
2	1	776	PSU	C4-N3-C2	-2.86	122.22	126.34
2	1	2421	OMU	O4-C4-C5	-2.86	120.13	125.16
2	1	2314	PSU	C4-N3-C2	-2.86	122.22	126.34
2	1	1124	PSU	C4-N3-C2	-2.85	122.24	126.34
2	1	2191	PSU	O4-C4-N3	-2.85	114.66	120.12
2	1	960	PSU	C4-N3-C2	-2.83	122.26	126.34
2	1	2266	PSU	C4-N3-C2	-2.82	122.27	126.34
2	1	2724	OMU	O4-C4-C5	-2.82	120.20	125.16
2	1	1110	PSU	C4-N3-C2	-2.81	122.28	126.34
2	1	2921	OMU	O4-C4-C5	-2.80	120.23	125.16
2	1	966	PSU	C4-N3-C2	-2.80	122.31	126.34
2	1	2191	PSU	C4-N3-C2	-2.80	122.31	126.34
2	1	2129	PSU	C4-N3-C2	-2.79	122.32	126.34
2	1	960	PSU	O4-C4-N3	-2.78	114.78	120.12
2	1	2729	OMU	O4-C4-C5	-2.78	120.28	125.16
2	1	2340	PSU	C4-N3-C2	-2.76	122.36	126.34
2	1	2923	PSU	C4-N3-C2	-2.75	122.38	126.34
2	1	2340	PSU	O4-C4-N3	-2.73	114.88	120.12
2	1	1437	OMC	C1'-N1-C2	2.71	124.46	118.42
2	1	1124	PSU	O4-C4-N3	-2.69	114.96	120.12
2	1	986	PSU	C4-N3-C2	-2.68	122.48	126.34
2	1	2923	PSU	O4-C4-N3	-2.67	115.00	120.12
2	1	2266	PSU	O4-C4-N3	-2.65	115.03	120.12
2	1	2975	PSU	O4-C4-N3	-2.65	115.05	120.12
2	1	2349	PSU	C6-C5-C4	2.63	120.04	118.20
2	1	2278	5MC	C5-C4-N3	-2.62	118.84	121.67
2	1	1888	OMU	O4-C4-C5	-2.62	120.55	125.16
2	1	2351	PSU	O4-C4-N3	-2.61	115.11	120.12
2	1	1110	PSU	O4-C4-N3	-2.60	115.14	120.12
3	2	73	PSU	O4-C4-N3	-2.58	115.18	120.12
2	1	966	PSU	O4-C4-N3	-2.57	115.18	120.12
2	1	898	OMU	O4-C4-C5	-2.55	120.67	125.16
2	1	990	PSU	O4-C4-N3	-2.50	115.33	120.12
2	1	2793	OMG	O6-C6-C5	2.49	129.24	124.37
2	1	2826	PSU	O4-C4-N3	-2.49	115.35	120.12
4	3	50	PSU	O4-C4-N3	-2.48	115.36	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2735	PSU	O4-C4-N3	-2.48	115.36	120.12
2	1	2880	PSU	O4-C4-N3	-2.48	115.37	120.12
2	1	776	PSU	O4-C4-N3	-2.45	115.41	120.12
2	1	2129	PSU	O4-C4-N3	-2.45	115.42	120.12
2	1	2314	PSU	O4-C4-N3	-2.44	115.43	120.12
2	1	2349	PSU	C4-N3-C2	-2.44	122.82	126.34
2	1	2791	OMG	O6-C6-C5	2.44	129.13	124.37
2	1	2815	OMG	O6-C6-C5	2.43	129.12	124.37
2	1	2142	1MA	N1-C6-N6	2.40	125.88	119.77
2	1	2922	OMG	O6-C6-C5	2.40	129.06	124.37
2	1	2416	PSU	O4-C4-N3	-2.40	115.52	120.12
2	1	908	OMG	O6-C6-C5	2.38	129.03	124.37
2	1	817	A2M	C3'-C2'-C1'	-2.38	98.42	102.89
2	1	1888	OMU	O2-C2-N3	-2.38	117.07	121.50
2	1	2264	PSU	O4-C4-N3	-2.37	115.58	120.12
2	1	2133	PSU	N1-C2-N3	2.37	117.81	115.13
2	1	2729	OMU	O2-C2-N1	-2.34	119.68	122.79
2	1	2865	PSU	O4-C4-N3	-2.32	115.66	120.12
2	1	2870	5MC	C5-C4-N3	-2.31	119.18	121.67
2	1	2826	PSU	N1-C2-N3	2.27	117.70	115.13
2	1	1888	OMU	C6-N1-C2	-2.25	118.11	120.99
2	1	867	OMG	O6-C6-C5	2.25	128.76	124.37
2	1	2142	1MA	C5-C6-N1	-2.22	110.58	113.90
2	1	805	OMG	O6-C6-C5	2.21	128.68	124.37
2	1	776	PSU	O4'-C1'-C2'	2.20	108.24	105.14
2	1	1124	PSU	O4'-C1'-C2'	2.19	108.23	105.14
3	2	73	PSU	N1-C2-N3	2.18	117.61	115.13
2	1	2416	PSU	O4'-C1'-C2'	2.17	108.20	105.14
2	1	2735	PSU	N1-C2-N3	2.15	117.57	115.13
2	1	2975	PSU	N1-C2-N3	2.15	117.57	115.13
4	3	50	PSU	N1-C2-N3	2.15	117.56	115.13
2	1	990	PSU	N1-C2-N3	2.14	117.56	115.13
2	1	898	OMU	O2-C2-N1	-2.13	119.95	122.79
2	1	1110	PSU	N1-C2-N3	2.13	117.55	115.13
2	1	960	PSU	N1-C2-N3	2.13	117.55	115.13
2	1	1450	OMG	O6-C6-C5	2.12	128.52	124.37
2	1	1110	PSU	O4'-C1'-C2'	2.11	108.12	105.14
2	1	2191	PSU	N1-C2-N3	2.11	117.52	115.13
2	1	2421	OMU	O2-C2-N1	-2.11	119.98	122.79
2	1	2314	PSU	N1-C2-N3	2.10	117.51	115.13
2	1	2880	PSU	N1-C2-N3	2.10	117.51	115.13
2	1	1124	PSU	N1-C2-N3	2.10	117.50	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	2264	PSU	N1-C2-N3	2.09	117.50	115.13
2	1	2351	PSU	N1-C2-N3	2.09	117.50	115.13
2	1	776	PSU	N1-C2-N3	2.09	117.49	115.13
2	1	2923	PSU	N1-C2-N3	2.08	117.49	115.13
2	1	1449	A2M	C2-N1-C6	-2.08	115.20	118.75
2	1	1888	OMU	C1'-N1-C6	-2.08	116.32	120.84
2	1	817	A2M	C2-N1-C6	-2.07	115.21	118.75
2	1	2340	PSU	N1-C2-N3	2.07	117.48	115.13
2	1	2865	PSU	N1-C2-N3	2.07	117.47	115.13
2	1	966	PSU	N1-C2-N3	2.06	117.46	115.13
2	1	986	PSU	N1-C2-N3	2.05	117.45	115.13
2	1	2220	A2M	C2-N1-C6	-2.04	115.27	118.75
2	1	649	A2M	C2-N1-C6	-2.04	115.27	118.75
2	1	2278	5MC	O2-C2-N3	-2.03	119.03	122.33
2	1	2880	PSU	O4'-C1'-C2'	2.03	108.00	105.14
2	1	2266	PSU	N1-C2-N3	2.02	117.42	115.13
2	1	2129	PSU	N1-C2-N3	2.02	117.42	115.13
2	1	2921	OMU	O2-C2-N1	-2.02	120.10	122.79
2	1	2349	PSU	N1-C2-N3	2.01	117.41	115.13

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	649	A2M	C3'-C4'-C5'-O5'
2	1	776	PSU	C3'-C4'-C5'-O5'
2	1	776	PSU	O4'-C4'-C5'-O5'
2	1	960	PSU	C3'-C4'-C5'-O5'
2	1	960	PSU	O4'-C4'-C5'-O5'
2	1	1437	OMC	C1'-C2'-O2'-CM2
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	C3'-C4'-C5'-O5'
2	1	2340	PSU	O4'-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	2724	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
2	1	2791	OMG	O4'-C4'-C5'-O5'
2	1	2865	PSU	O4'-C4'-C5'-O5'
2	1	2923	PSU	O4'-C1'-C5-C4
2	1	2923	PSU	O4'-C1'-C5-C6
2	1	2948	OMC	C3'-C4'-C5'-O5'
2	1	2948	OMC	O4'-C4'-C5'-O5'
4	3	50	PSU	C3'-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	2340	PSU	C3'-C4'-C5'-O5'
2	1	2421	OMU	O4'-C4'-C5'-O5'
2	1	2729	OMU	O4'-C4'-C5'-O5'
2	1	2791	OMG	C3'-C4'-C5'-O5'
2	1	2865	PSU	C3'-C4'-C5'-O5'
2	1	1450	OMG	C3'-C4'-C5'-O5'
2	1	2142	1MA	C3'-C4'-C5'-O5'
2	1	2220	A2M	O4'-C4'-C5'-O5'
2	1	2729	OMU	C3'-C4'-C5'-O5'
2	1	2416	PSU	O4'-C4'-C5'-O5'
2	1	1437	OMC	C3'-C4'-C5'-O5'
2	1	2416	PSU	C3'-C4'-C5'-O5'
2	1	2826	PSU	O4'-C4'-C5'-O5'
2	1	817	A2M	C4'-C5'-O5'-P
2	1	2340	PSU	C4'-C5'-O5'-P
2	1	805	OMG	C3'-C2'-O2'-CM2
2	1	649	A2M	C4'-C5'-O5'-P
2	1	986	PSU	O4'-C4'-C5'-O5'
2	1	2791	OMG	C4'-C5'-O5'-P
2	1	1437	OMC	C2'-C1'-N1-C2
2	1	817	A2M	O4'-C4'-C5'-O5'
2	1	2826	PSU	C3'-C4'-C5'-O5'
2	1	986	PSU	C3'-C4'-C5'-O5'
2	1	2416	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	b	801	61	24,30,30	0.94	1 (4%)	30,47,47	1.25	4 (13%)
65	GTP	m	501	66,61	26,34,34	1.24	1 (3%)	32,54,54	1.52	7 (21%)
62	B3P	1	3479	-	18,18,18	1.55	3 (16%)	21,23,23	1.92	6 (28%)
62	B3P	1	3480	-	18,18,18	1.52	2 (11%)	21,23,23	2.00	6 (28%)
62	B3P	1	3478	61	18,18,18	1.60	3 (16%)	21,23,23	1.83	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	b	801	61	-	3/12/32/32	0/3/3/3
65	GTP	m	501	66,61	-	5/18/38/38	0/3/3/3
62	B3P	1	3479	-	-	10/28/28/28	-
62	B3P	1	3480	-	-	7/28/28/28	-
62	B3P	1	3478	61	-	12/28/28/28	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	1	3480	B3P	C6-C4	5.29	1.59	1.53
62	1	3478	B3P	C6-C4	4.99	1.59	1.53
62	1	3479	B3P	C6-C4	4.80	1.59	1.53
65	m	501	GTP	C5-C6	-4.26	1.38	1.47
62	1	3479	B3P	C7-C4	2.68	1.56	1.53
62	1	3478	B3P	C7-C4	2.52	1.56	1.53
64	b	801	GDP	C6-N1	-2.42	1.34	1.37
62	1	3480	B3P	C7-C4	2.29	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	1	3478	B3P	C9-C8	2.16	1.56	1.53
62	1	3479	B3P	C11-C8	2.15	1.56	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	1	3480	B3P	O5-C6-C4	5.10	121.96	111.63
62	1	3478	B3P	O5-C6-C4	5.02	121.80	111.63
62	1	3479	B3P	O5-C6-C4	5.02	121.80	111.63
62	1	3480	B3P	C2-N2-C8	-4.06	110.31	116.08
62	1	3479	B3P	C3-N1-C4	-3.92	110.51	116.08
62	1	3478	B3P	C3-N1-C4	-3.63	110.92	116.08
62	1	3480	B3P	C3-N1-C4	-3.56	111.02	116.08
65	m	501	GTP	C5-C6-N1	3.31	119.79	113.95
64	b	801	GDP	PA-O3A-PB	-3.26	121.62	132.83
65	m	501	GTP	C8-N7-C5	3.21	109.11	102.99
62	1	3479	B3P	C2-N2-C8	-3.14	111.63	116.08
65	m	501	GTP	C2-N1-C6	-3.08	119.43	125.10
64	b	801	GDP	C3'-C2'-C1'	2.81	105.20	100.98
65	m	501	GTP	PA-O3A-PB	-2.80	123.20	132.83
62	1	3480	B3P	O6-C7-C4	-2.76	106.04	111.63
62	1	3478	B3P	C2-N2-C8	-2.74	112.19	116.08
62	1	3479	B3P	O6-C7-C4	-2.67	106.23	111.63
62	1	3480	B3P	O3-C11-C8	-2.58	106.40	111.63
62	1	3479	B3P	O4-C5-C4	-2.56	106.44	111.63
62	1	3478	B3P	O6-C7-C4	-2.52	106.52	111.63
62	1	3478	B3P	O4-C5-C4	-2.48	106.62	111.63
62	1	3479	B3P	O3-C11-C8	-2.40	106.78	111.63
65	m	501	GTP	O6-C6-C5	-2.38	119.72	124.37
65	m	501	GTP	PB-O3B-PG	-2.32	124.88	132.83
64	b	801	GDP	C8-N7-C5	2.32	107.40	102.99
64	b	801	GDP	C5-C6-N1	2.31	118.02	113.95
62	1	3478	B3P	O3-C11-C8	-2.23	107.12	111.63
62	1	3480	B3P	O4-C5-C4	-2.08	107.42	111.63
65	m	501	GTP	C3'-C2'-C1'	2.03	104.04	100.98

There are no chirality outliers.

All (37) 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

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Mol	Chain	Res	Type	Atoms
62	1	3478	B3P	C7-C4-C6-O5
62	1	3478	B3P	N2-C8-C9-O1
62	1	3478	B3P	C10-C8-C9-O1
62	1	3478	B3P	C11-C8-C9-O1
62	1	3478	B3P	O3-C11-C8-N2
62	1	3478	B3P	O3-C11-C8-C9
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	C10-C8-N2-C2
62	1	3479	B3P	C11-C8-N2-C2
62	1	3479	B3P	O3-C11-C8-N2
62	1	3479	B3P	O3-C11-C8-C9
62	1	3479	B3P	O3-C11-C8-C10
62	1	3480	B3P	N1-C4-C5-O4
62	1	3480	B3P	C6-C4-C5-O4
62	1	3480	B3P	C7-C4-C5-O4
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
65	m	501	GTP	C5'-O5'-PA-O3A
62	1	3479	B3P	C1-C2-N2-C8
62	1	3480	B3P	C3-C1-C2-N2
65	m	501	GTP	O4'-C4'-C5'-O5'
65	m	501	GTP	C3'-C4'-C5'-O5'
62	1	3478	B3P	C5-C4-C7-O6
64	b	801	GDP	C5'-O5'-PA-O3A
64	b	801	GDP	C5'-O5'-PA-O2A
65	m	501	GTP	C5'-O5'-PA-O2A
62	1	3479	B3P	C10-C8-C9-O1
62	1	3478	B3P	C6-C4-C7-O6
65	m	501	GTP	C5'-O5'-PA-O1A
62	1	3478	B3P	C11-C8-N2-C2

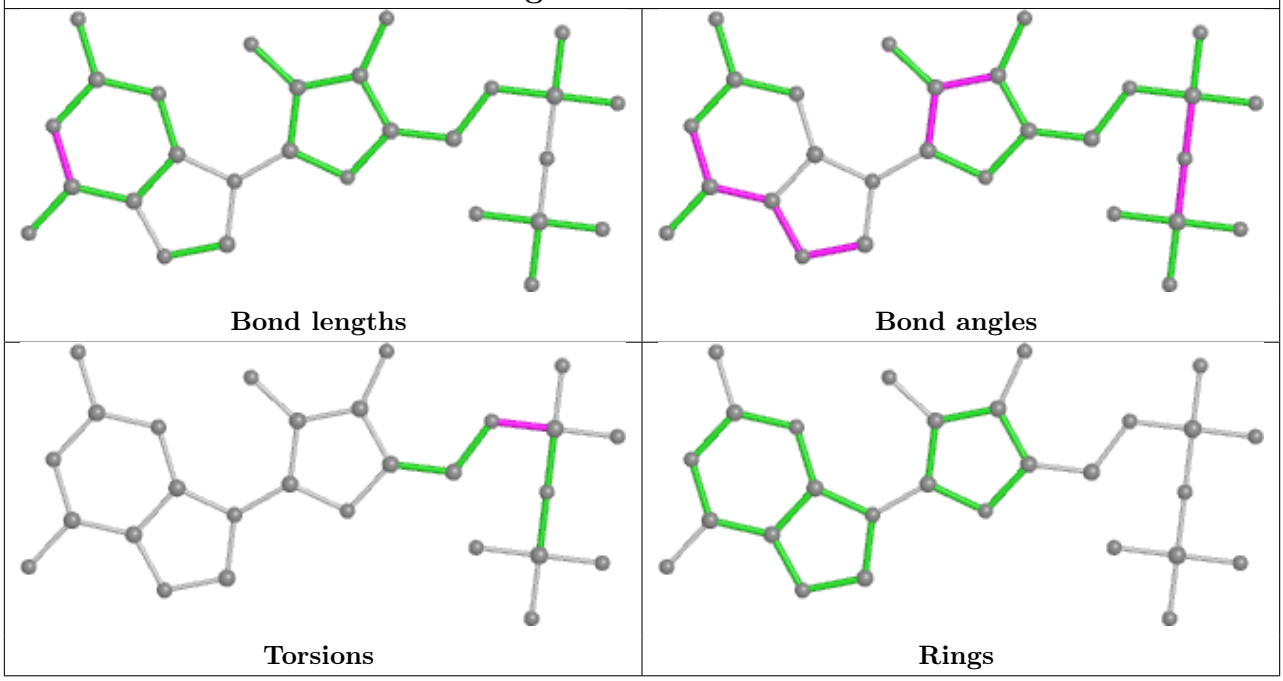
There are no ring outliers.

No monomer is involved in short contacts.

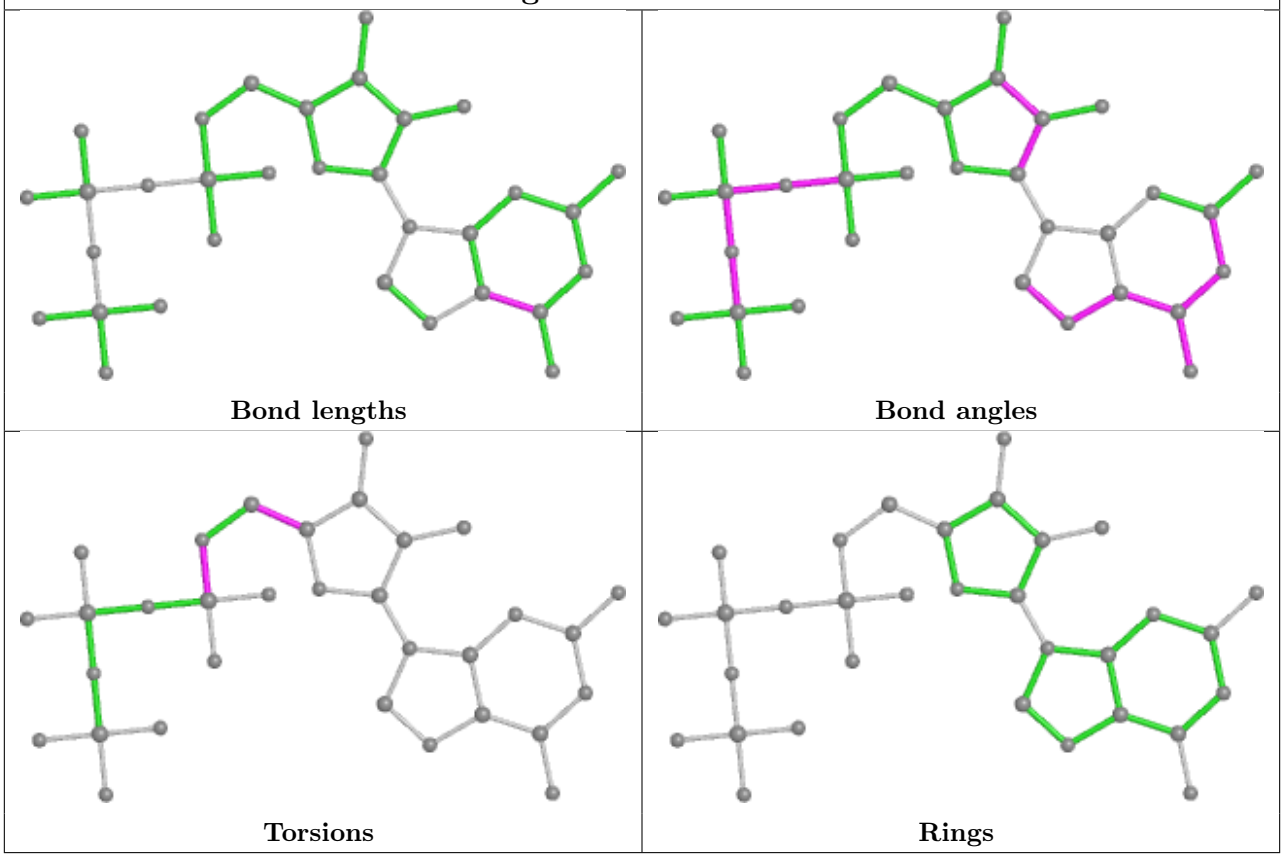
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

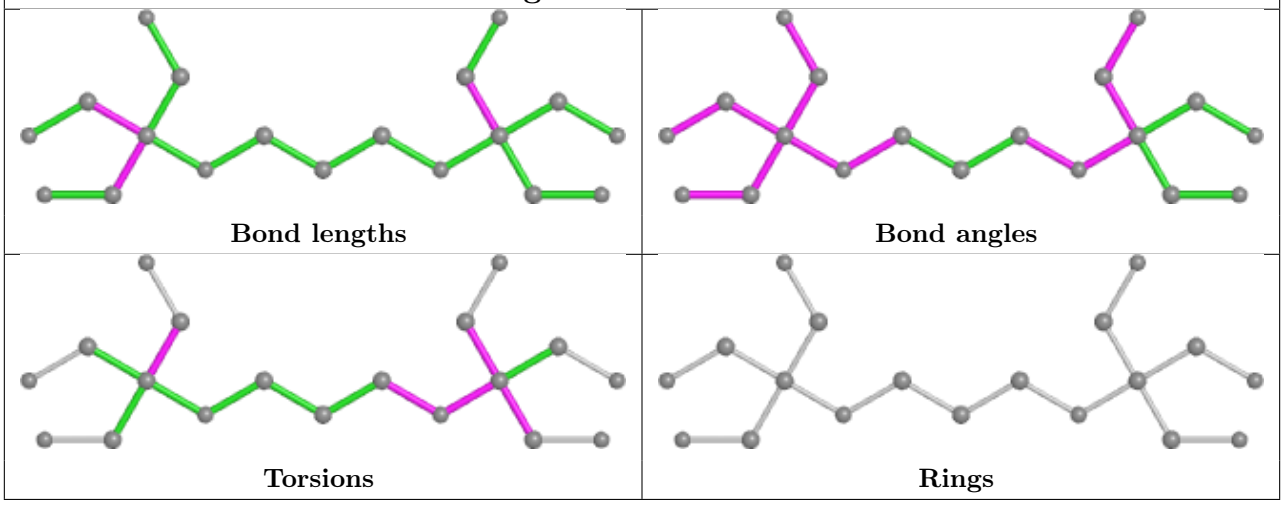
Ligand GDP b 801

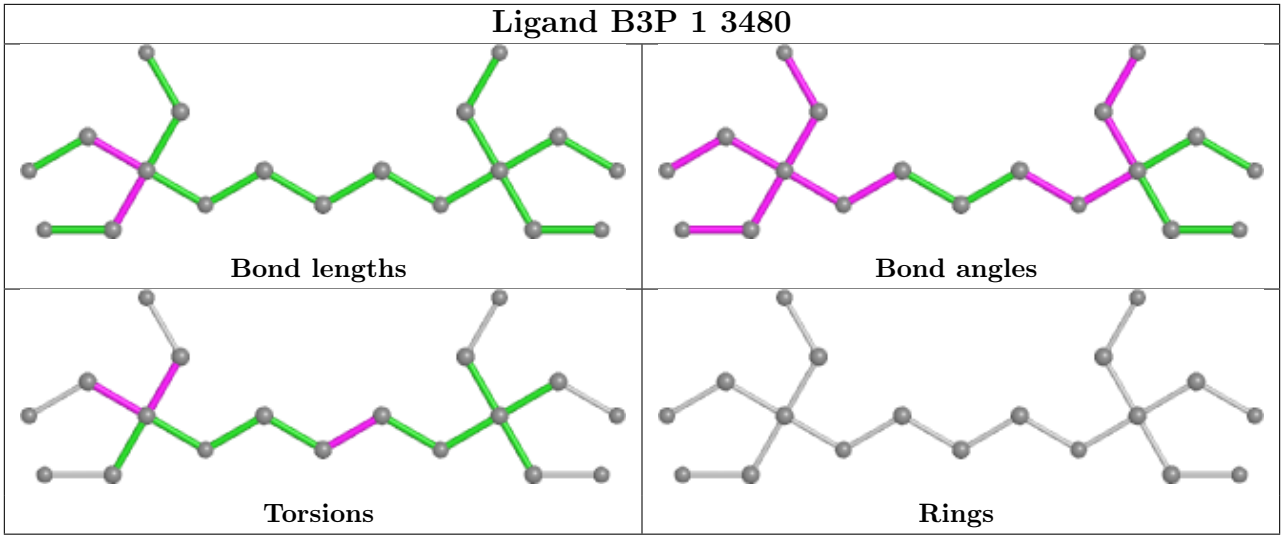


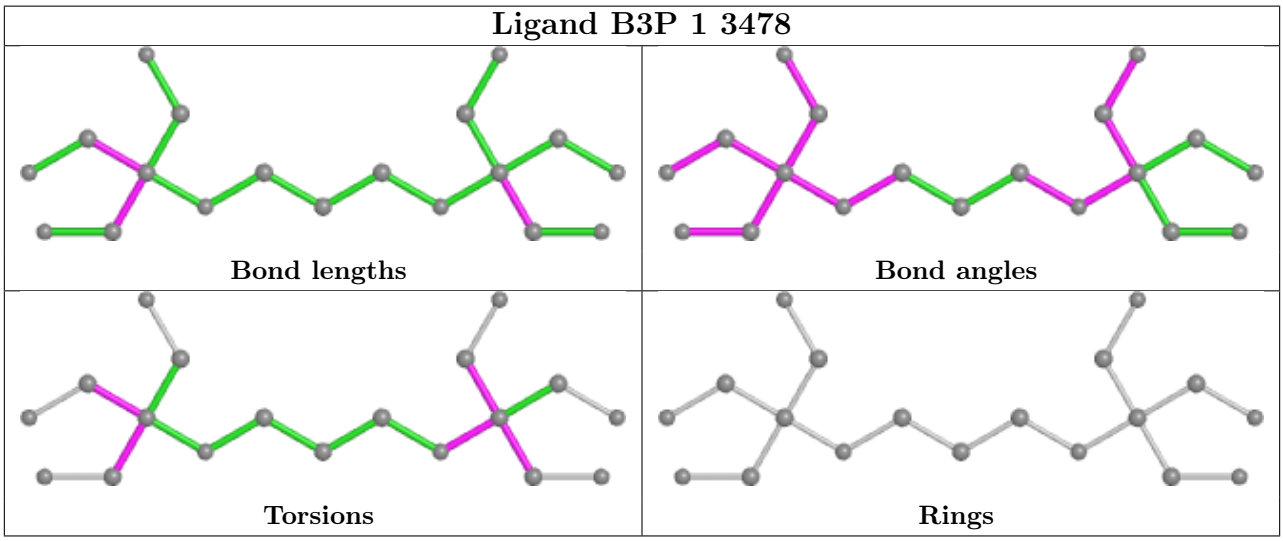
Ligand GTP m 501



Ligand B3P 1 3479







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.

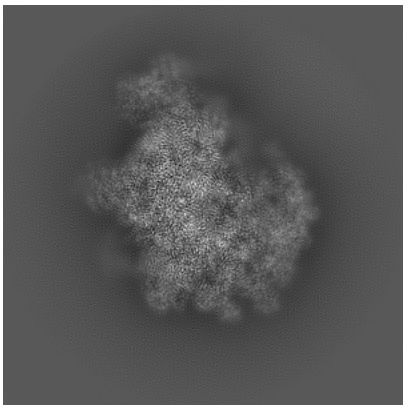
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26651. These allow visual inspection of the internal detail of the map and identification of artifacts.

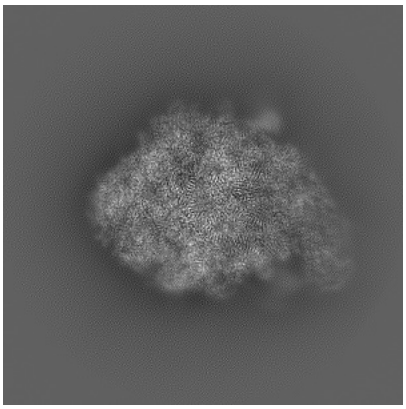
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

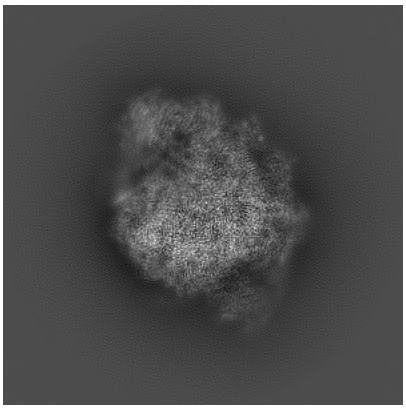
6.1.1 Primary map



X

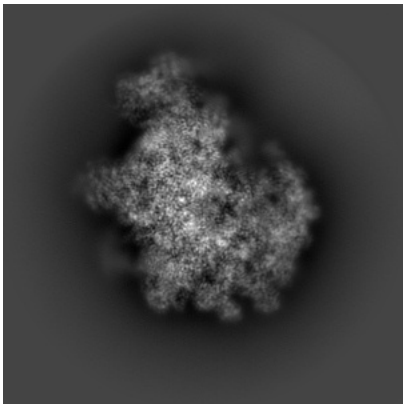


Y

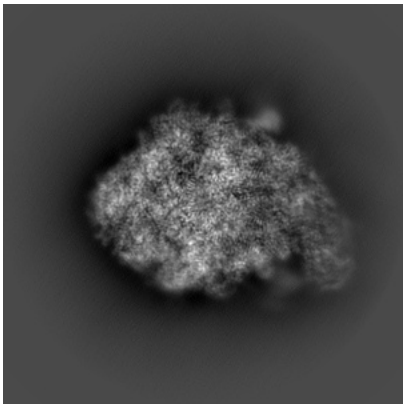


Z

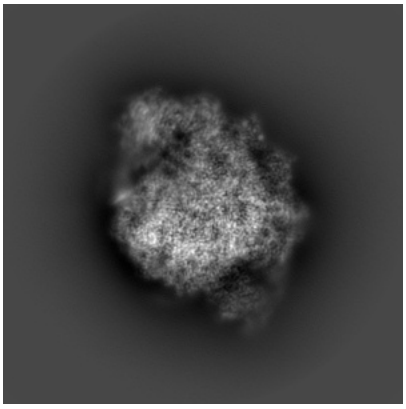
6.1.2 Raw map



X



Y

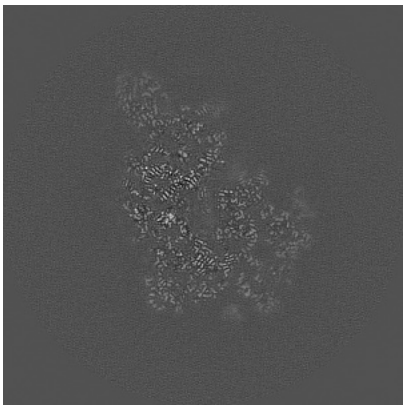


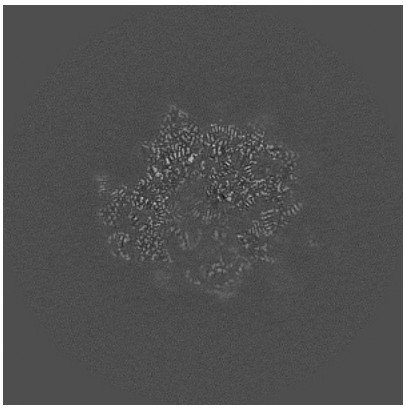
Z

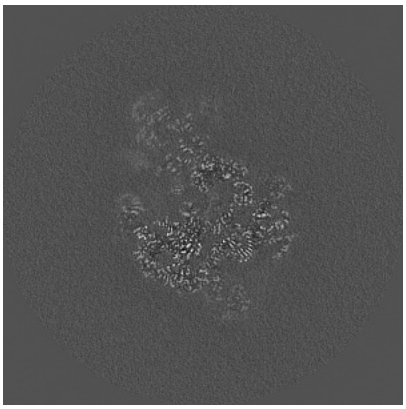
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

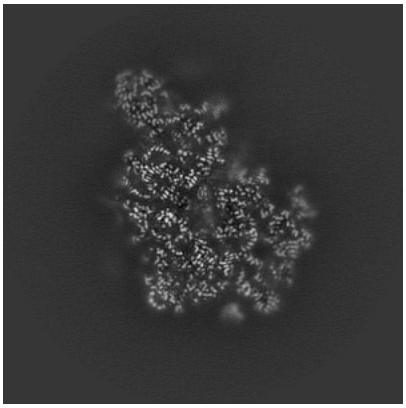
6.2.1 Primary map

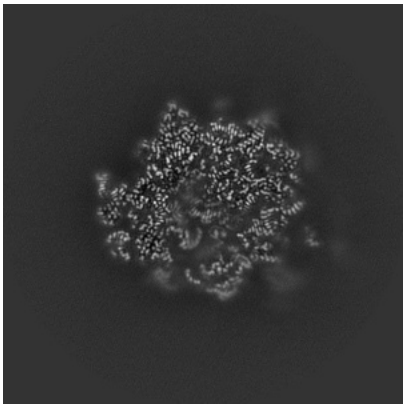

X Index: 200

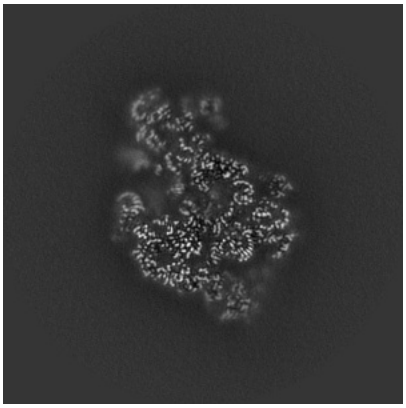

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

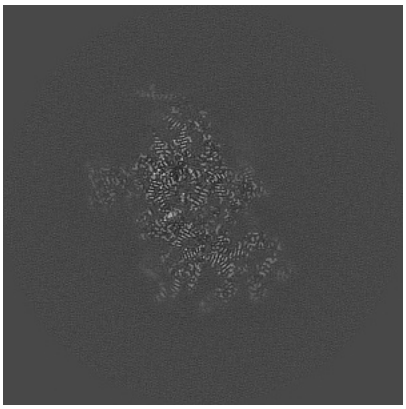

Y Index: 200


Z Index: 200

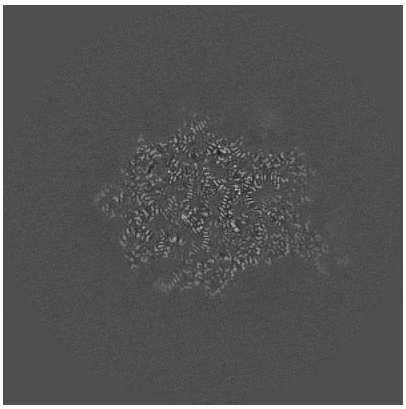
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

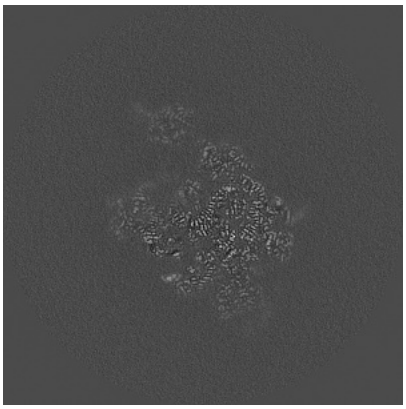
6.3.1 Primary map



X Index: 227

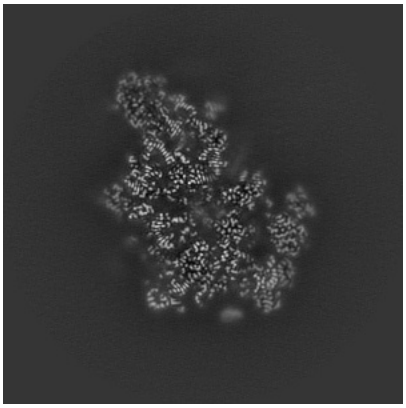


Y Index: 179

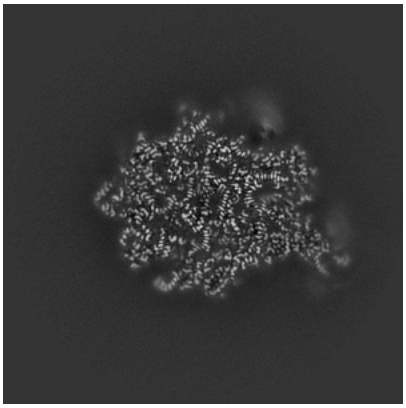


Z Index: 220

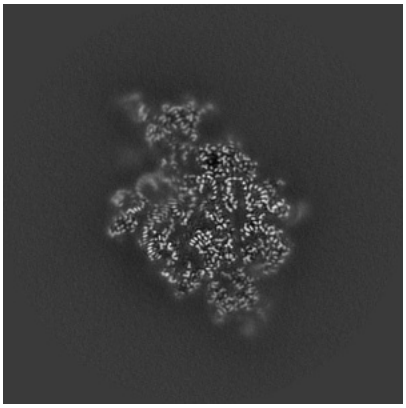
6.3.2 Raw map



X Index: 205



Y Index: 179

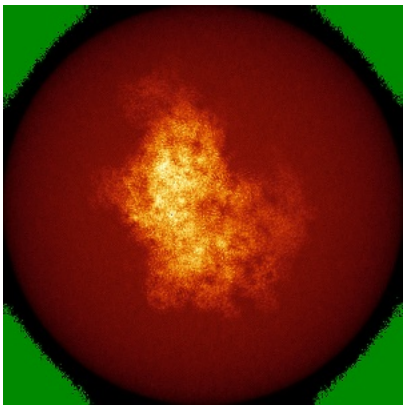


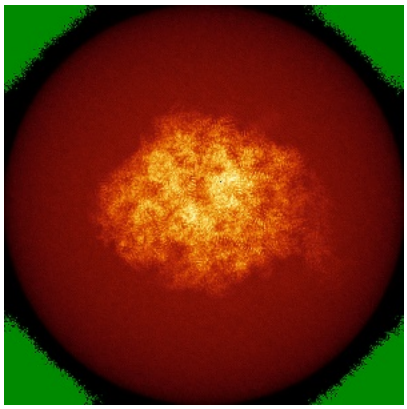
Z Index: 213

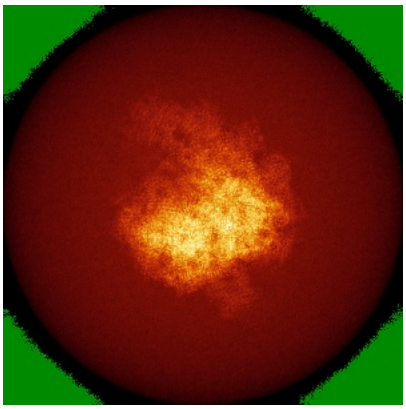
The images above show the largest variance slices of the map in three orthogonal directions.

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

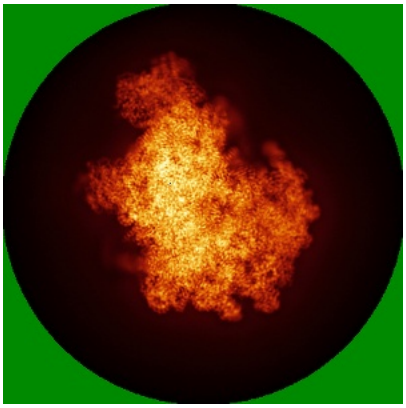
6.4.1 Primary map


X

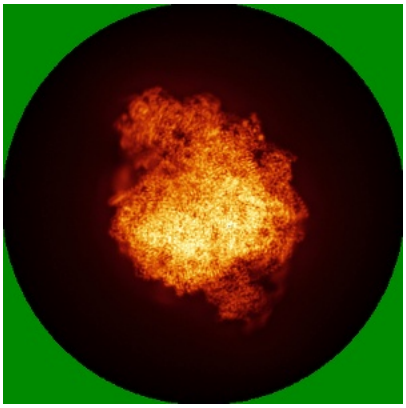

Y


Z

6.4.2 Raw map


X

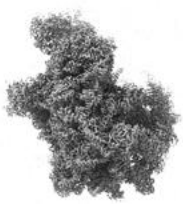
Y


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.

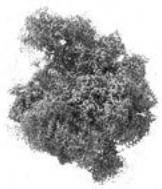
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y



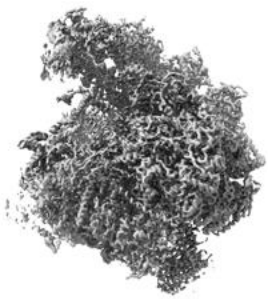
Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

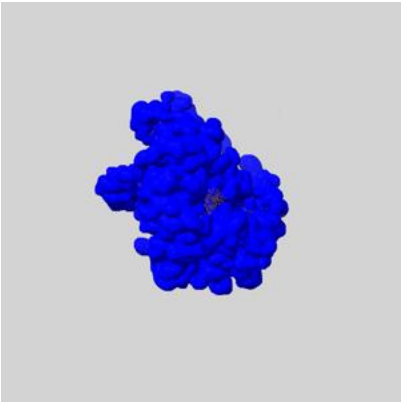
6.6 Mask visualisation (i)

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

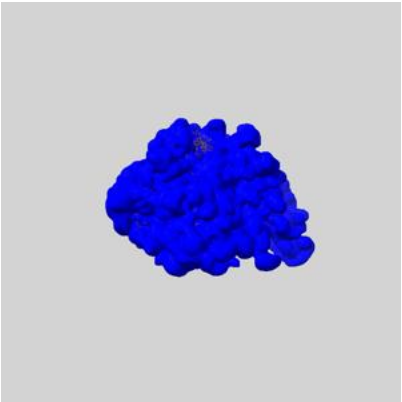
A mask typically either:

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

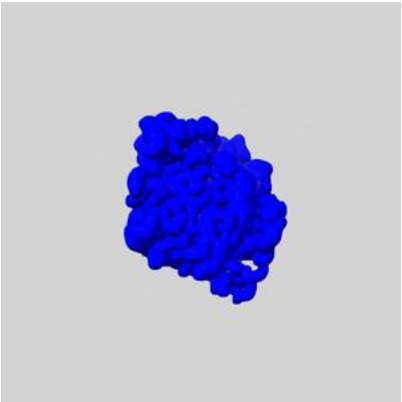
6.6.1 emd_26651_msk_1.map (i)



X



Y

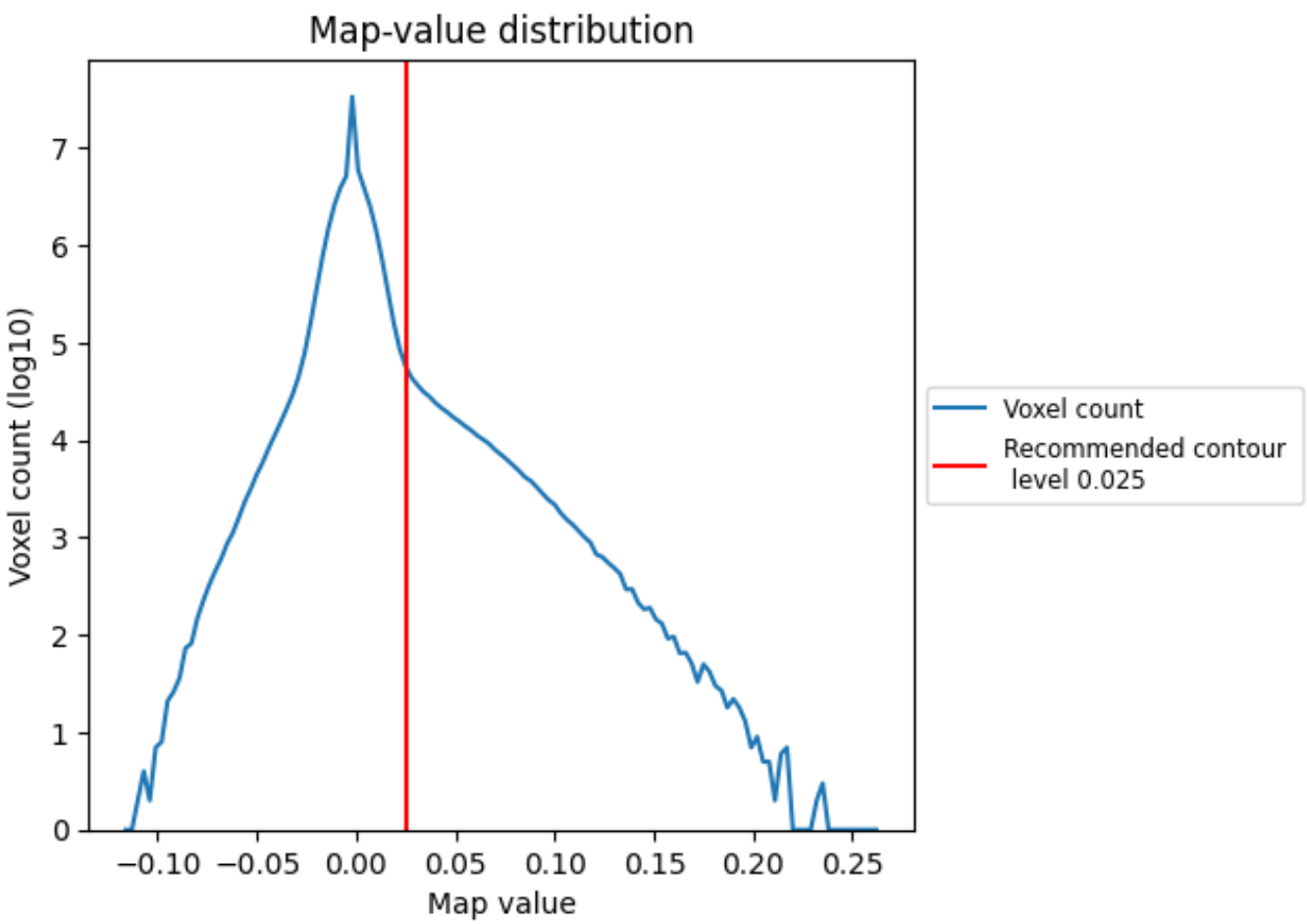


Z

7 Map analysis (i)

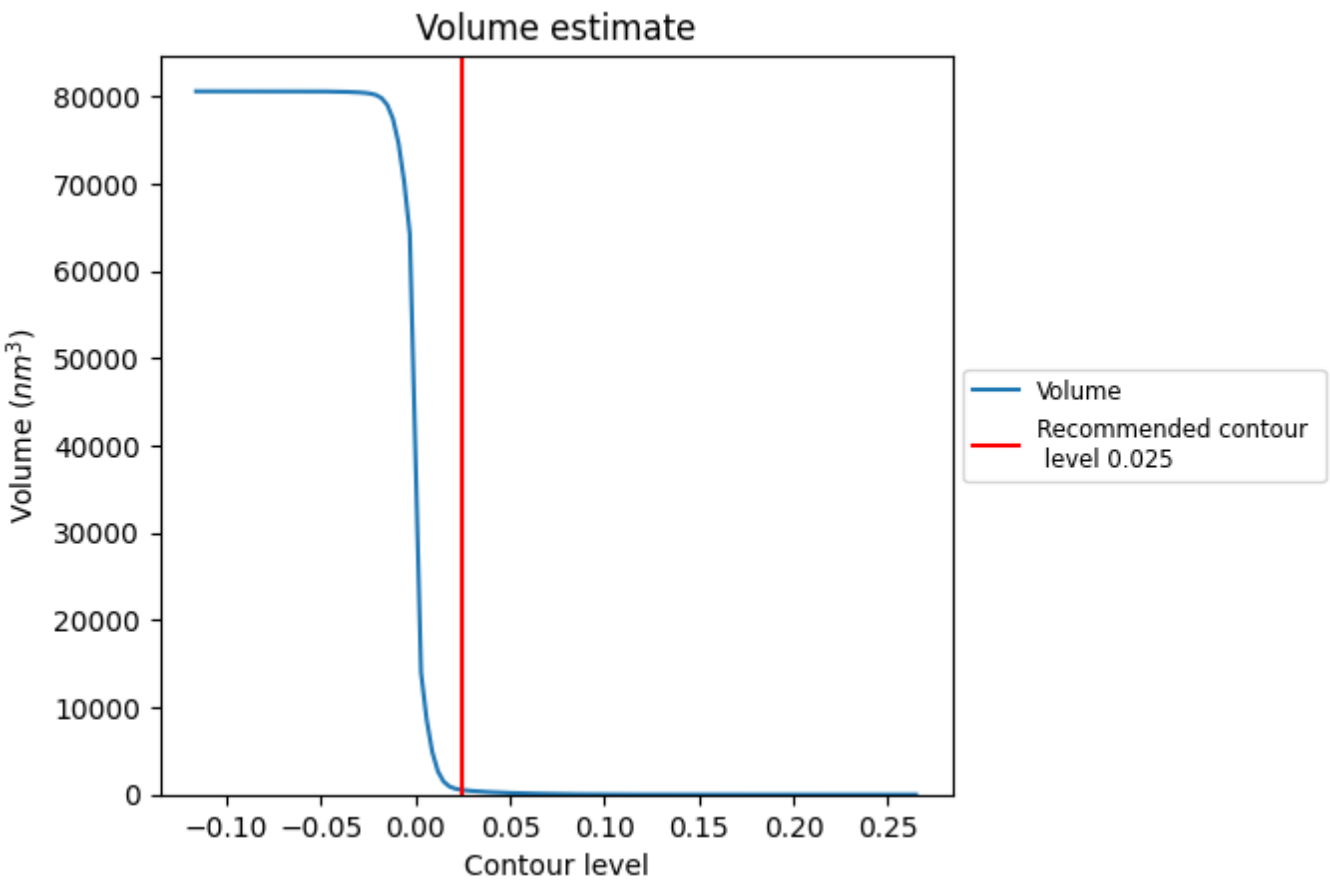
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

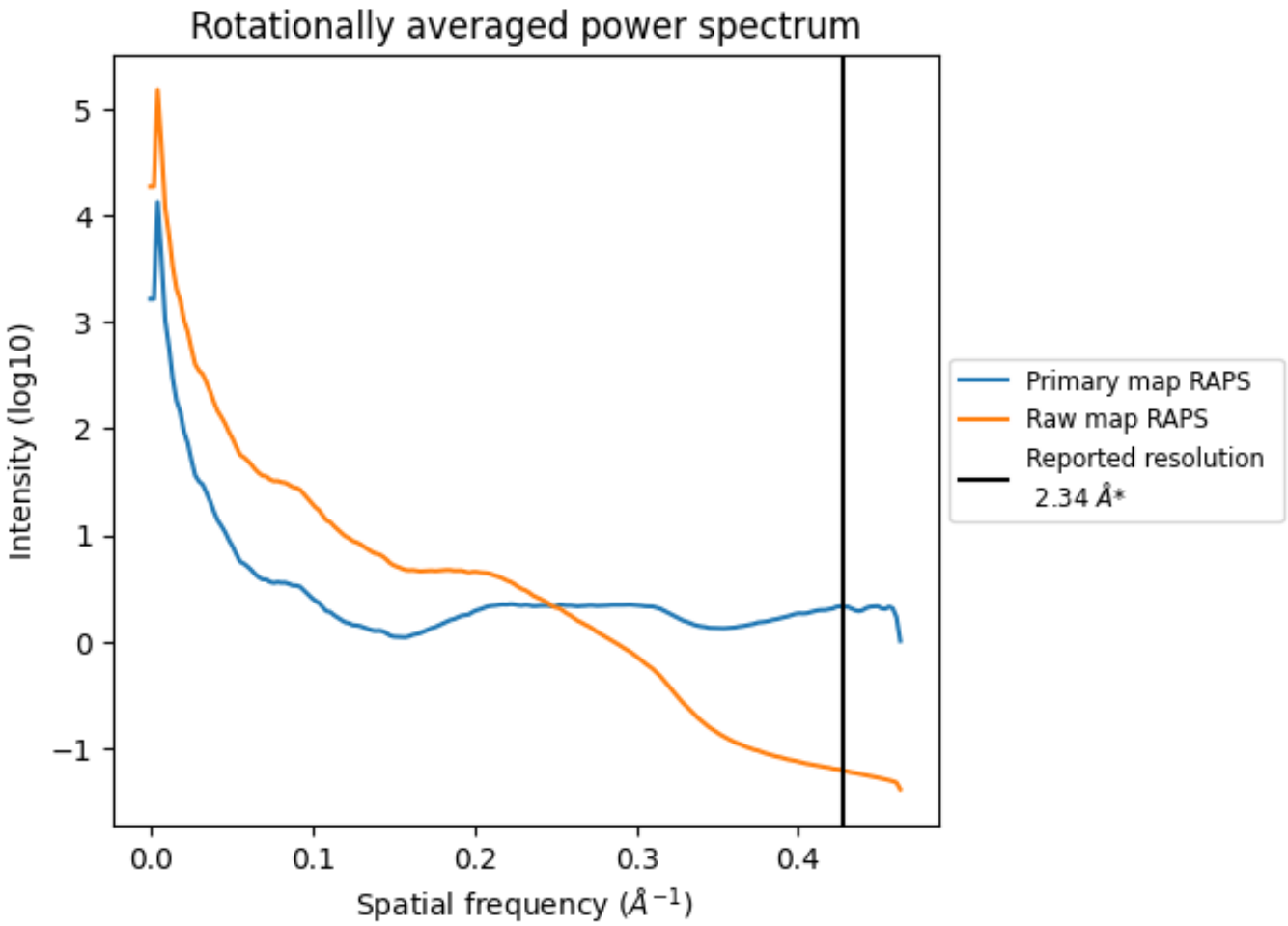
7.2 Volume estimate (i)



The volume at the recommended contour level is 526 nm^3; this corresponds to an approximate mass of 475 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)

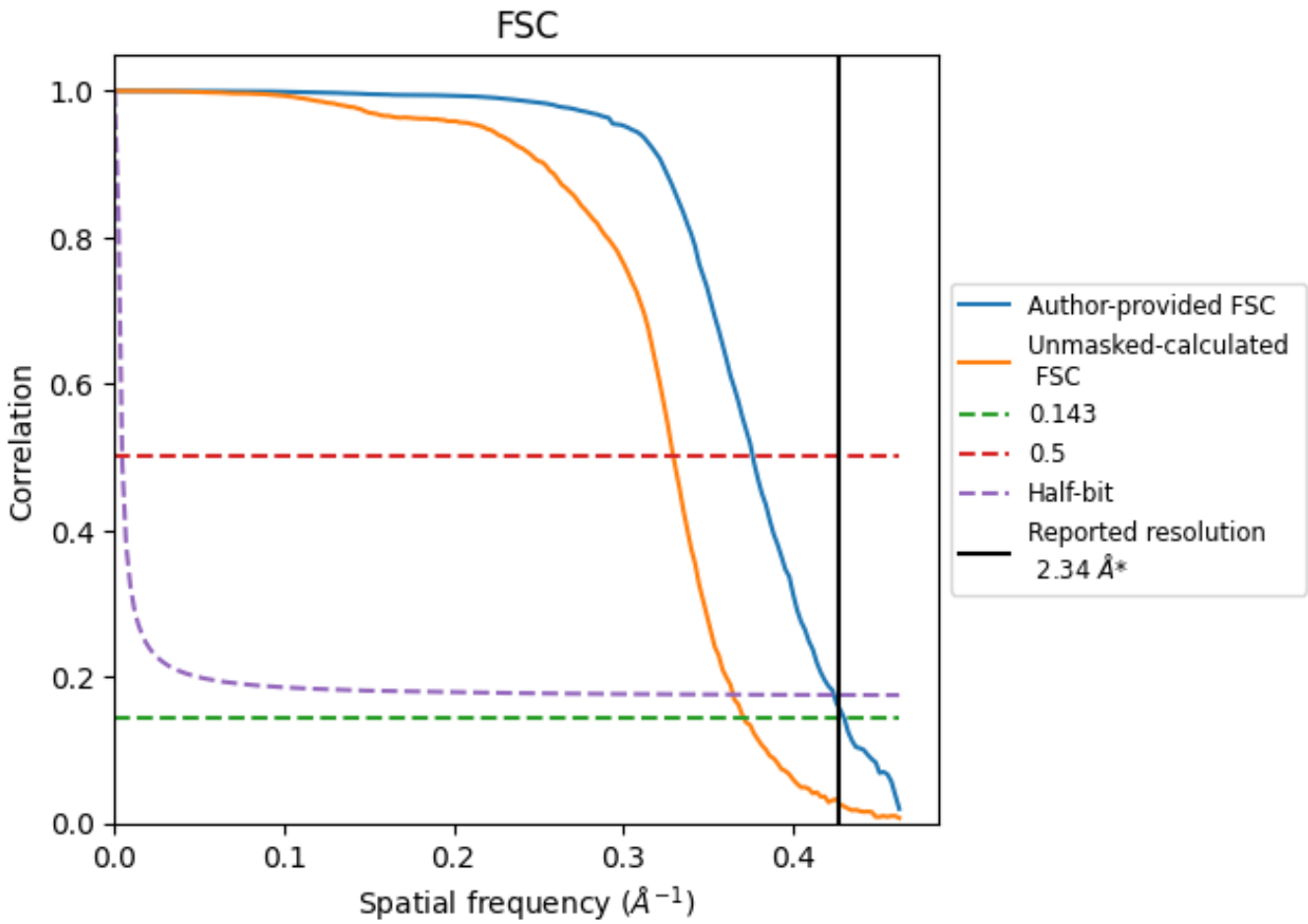


*Reported resolution corresponds to spatial frequency of 0.427 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.427 Å^{-1}

8.2 Resolution estimates (i)

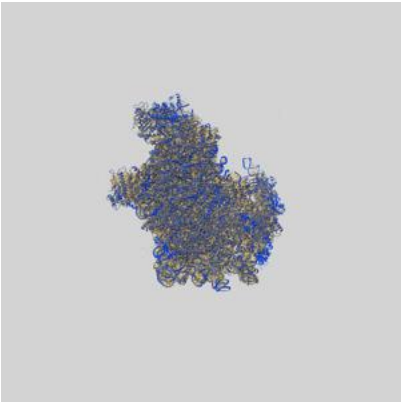
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.34	-	-
Author-provided FSC curve	2.32	2.66	2.36
Unmasked-calculated*	2.69	3.03	2.74

*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 2.69 differs from the reported value 2.34 by more than 10 %

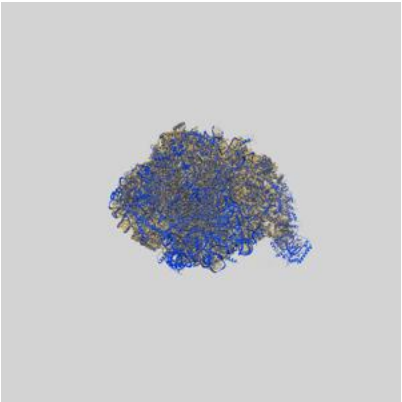
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26651 and PDB model 7UOO. Per-residue inclusion information can be found in section 3 on page 18.

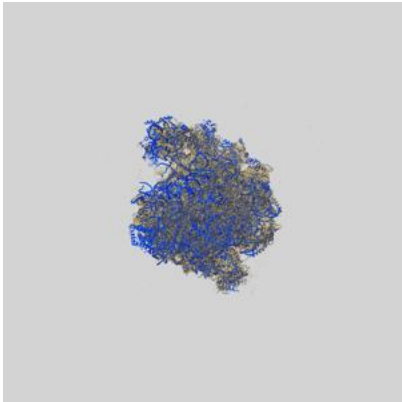
9.1 Map-model overlay (i)



X



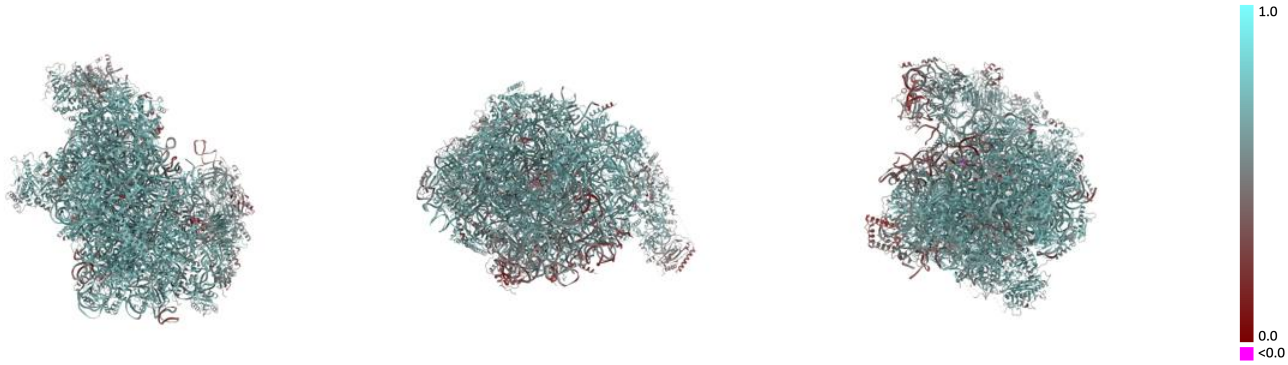
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

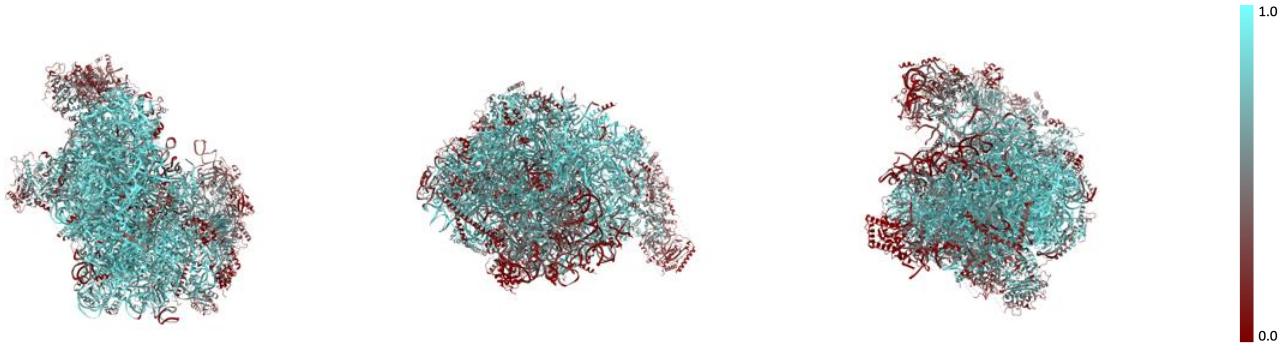
9.2 Q-score mapped to coordinate model (i)



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.

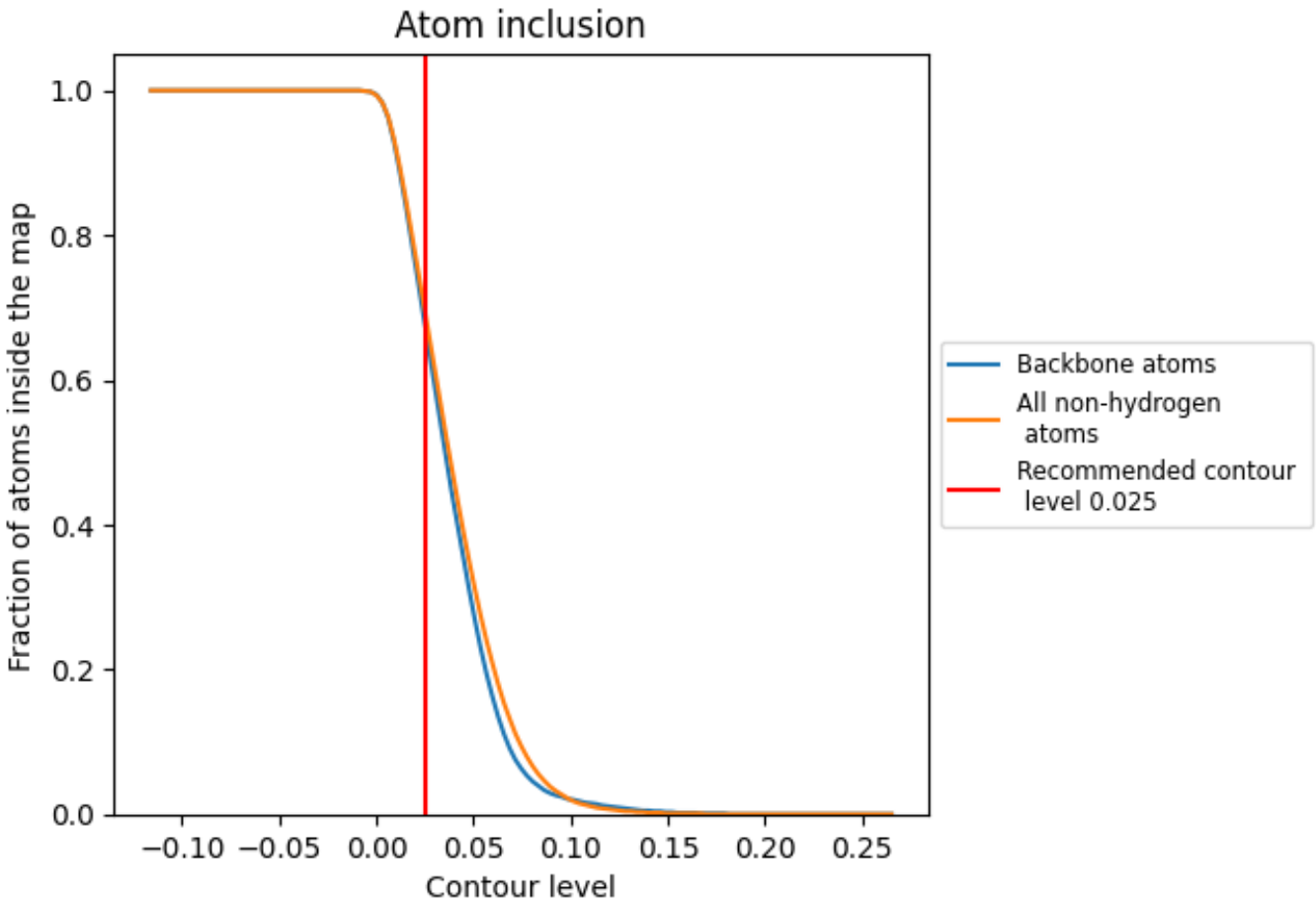
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.6330
1	0.7900	0.6380
2	0.9300	0.6910
3	0.2640	0.4310
4	0.5360	0.6280
5	0.0390	0.4230
6	0.3410	0.5170
8	0.1130	0.5020
9	0.6050	0.6370
A	0.8460	0.7120
B	0.8950	0.7100
C	0.8460	0.6980
D	0.3470	0.5510
E	0.7300	0.6580
F	0.8460	0.6890
G	0.7610	0.6670
H	0.7480	0.6600
I	0.4000	0.6440
J	0.0540	0.3820
K	0.1060	0.4760
L	0.6970	0.6430
M	0.7910	0.6690
N	0.8800	0.7130
O	0.8860	0.7040
P	0.8640	0.7040
Q	0.7540	0.6560
R	0.8520	0.6870
S	0.7240	0.6510
T	0.4450	0.5680
U	0.7190	0.6480
V	0.8440	0.6900
W	0.4550	0.5870
X	0.8470	0.7010
Y	0.8440	0.6960
Z	0.7800	0.6700

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Chain	Atom inclusion	Q-score
a	0.6820	0.6550
b	0.6550	0.6360
c	0.7290	0.6570
d	0.8020	0.6850
e	0.8580	0.7060
f	0.9310	0.7130
g	0.8430	0.6910
h	0.8410	0.6920
i	0.5910	0.6200
j	0.9530	0.7360
k	0.6110	0.6310
l	0.9520	0.7390
m	0.7050	0.6560
n	0.5190	0.6220
o	0.3740	0.5250
p	0.8180	0.6980
q	0.3490	0.5870
r	0.8180	0.6830
s	0.4260	0.5750
t	0.3330	0.5580
u	0.7770	0.6670
v	0.3830	0.5870
w	0.4280	0.5770
x	0.4900	0.5840
y	0.7560	0.6610
z	0.6850	0.6360