



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:11 AM UTC

PDB ID : 7UOO / pdb_00007uoo
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

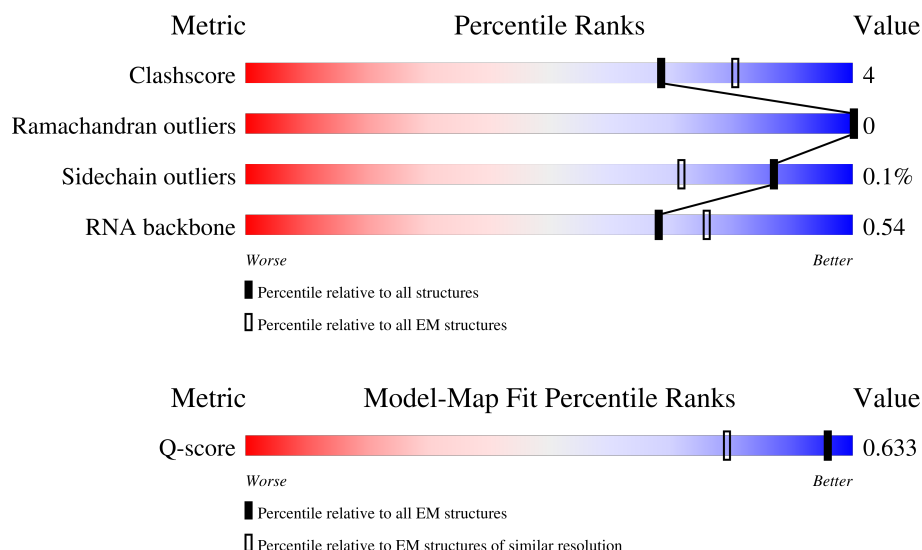
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4520 (1.84 - 2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	
2	1	3396	
3	2	158	

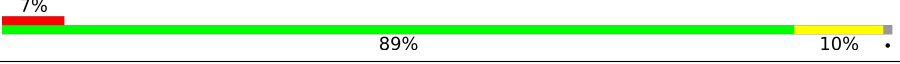
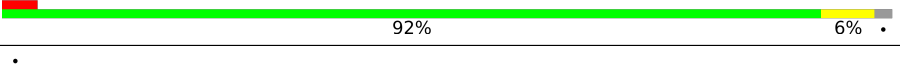
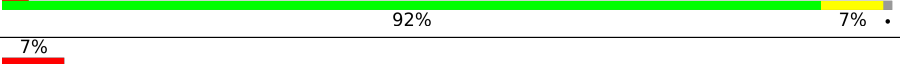
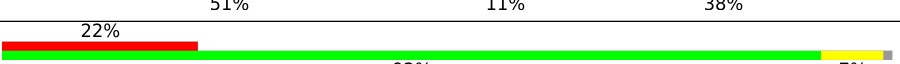
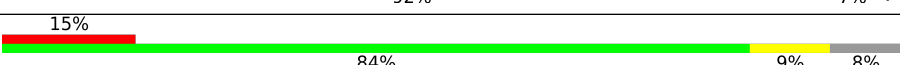
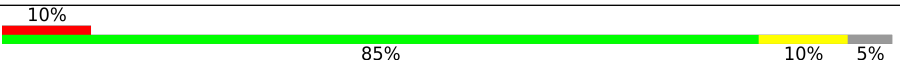
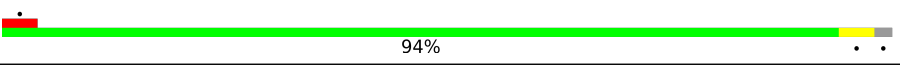
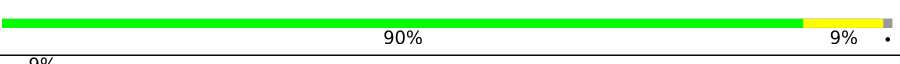
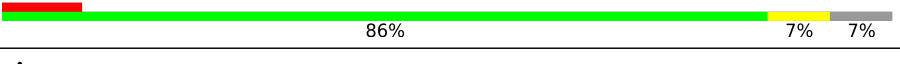
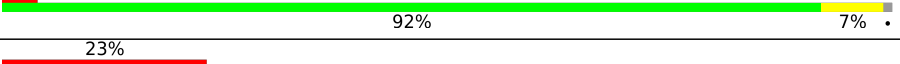
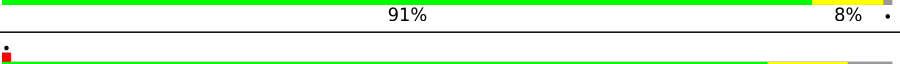
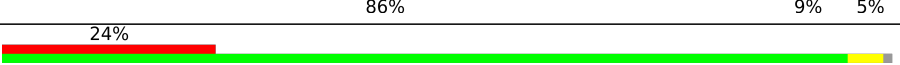
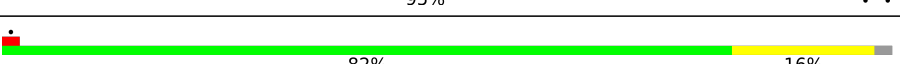
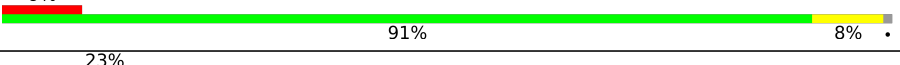
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Mol	Chain	Length	Quality of chain
4	3	121	
5	5	120	
6	6	87	
7	8	165	
8	9	175	
9	B	387	
10	C	362	
11	D	297	
12	E	176	
13	F	244	
14	G	256	
15	H	191	
16	I	166	
17	J	174	
18	K	376	
19	L	199	
20	M	138	
21	N	204	
22	O	199	
23	P	184	
24	Q	186	
25	R	189	
26	S	172	
27	T	160	
28	U	121	

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Mol	Chain	Length	Quality of chain
29	V	137	
30	W	312	
31	X	142	
32	Y	127	
33	Z	136	
34	a	149	
35	b	647	
36	c	105	
37	d	113	
38	e	130	
39	f	107	
40	g	121	
41	h	120	
42	i	100	
43	j	88	
44	k	78	
45	l	51	
46	m	486	
47	n	605	
48	o	220	
49	p	92	
50	q	455	
51	r	261	
52	s	520	
53	t	322	

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Mol	Chain	Length	Quality of chain
54	u	199	
55	v	344	
56	w	203	
57	x	515	
58	y	245	
59	z	106	
60	4	593	

2 Entry composition

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
1	A	213	Total	C	N	O	S	0	0
			1634	1023	326	284	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	2991	Total	C	N	O	P	0	0
			64043	28619	11563	20870	2991		

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

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

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

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

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

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

- Molecule 6 is a RNA chain called ITS2 rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called Pescadillo homolog.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 57 is a protein called RSA4 isoform 1.

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

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

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

- Molecule 59 is a protein called UPF0642 protein YBL028C.

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

- Molecule 60 is a protein called Probable metalloprotease ARX1.

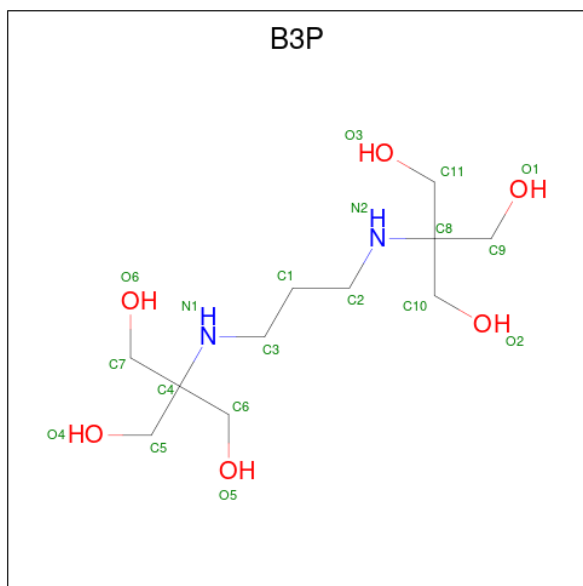
Mol	Chain	Residues	Atoms					AltConf	Trace
60	4	538	Total	C	N	O	S	0	0
			4166	2633	718	800	15		

- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 62 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula:

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

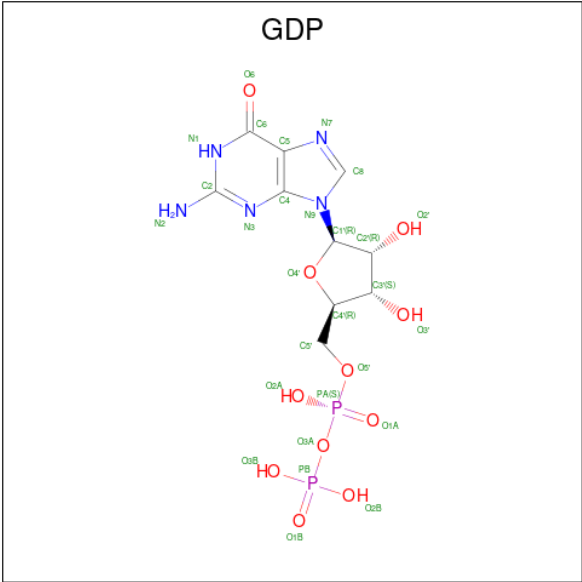


Mol	Chain	Residues	Atoms				AltConf
62	1	1	Total	C	N	O	0
			19	11	2	6	
62	1	1	Total	C	N	O	0
			19	11	2	6	
62	1	1	Total	C	N	O	0
			19	11	2	6	

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

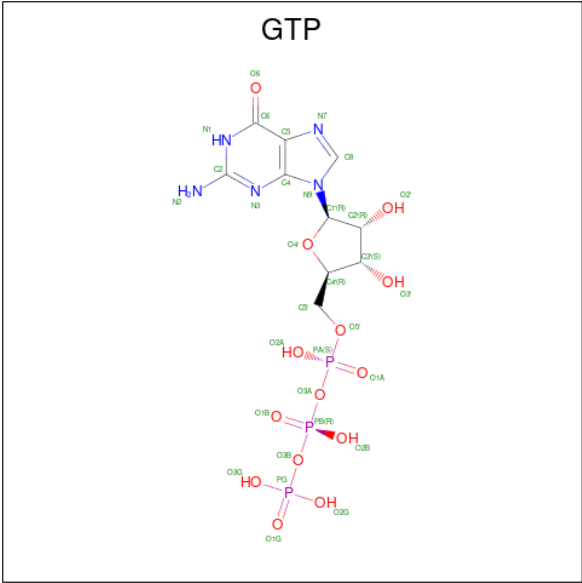
Mol	Chain	Residues	Atoms		AltConf
63	I	1	Total	Zn	0
			1	1	
63	g	1	Total	Zn	0
			1	1	
63	j	1	Total	Zn	0
			1	1	
63	p	1	Total	Zn	0
			1	1	
63	u	1	Total	Zn	0
			1	1	

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



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

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



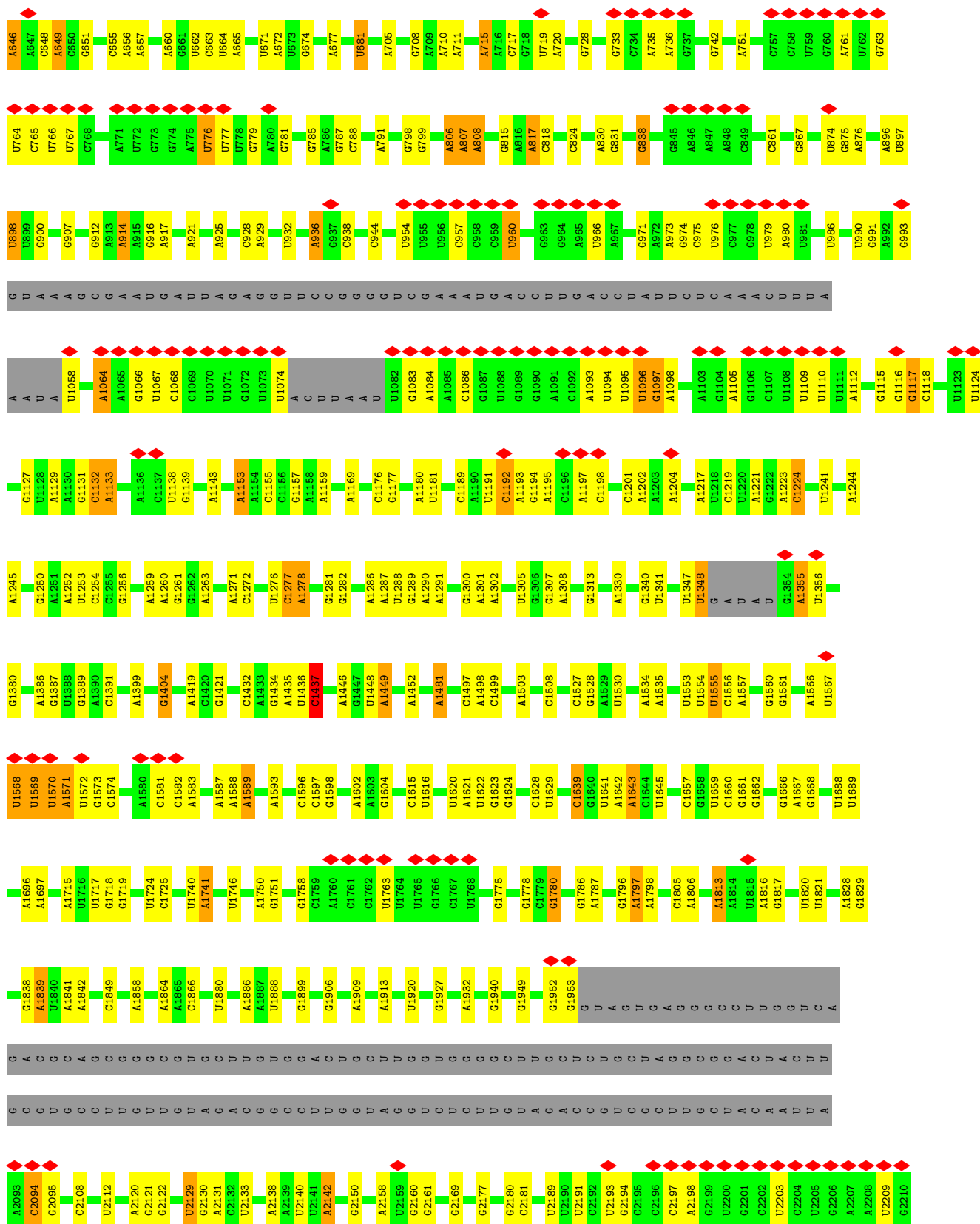
Mol	Chain	Residues	Atoms					AltConf
65	m	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

- Molecule 67 is water.

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



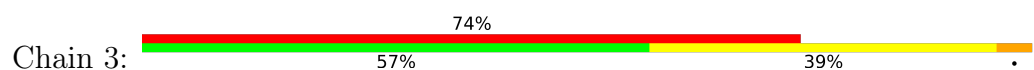




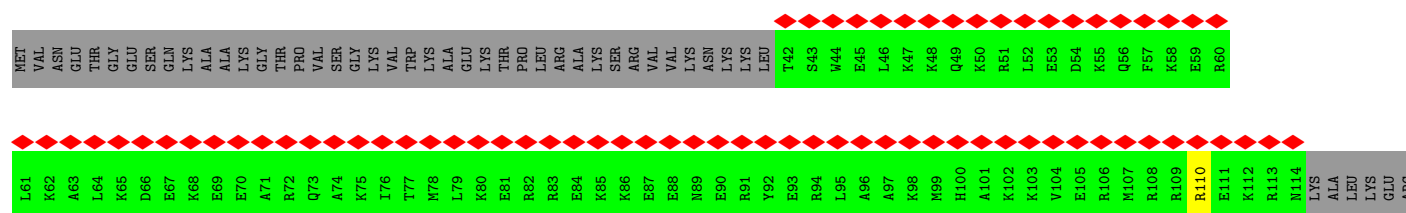
• Molecule 3: 5.8S rRNA



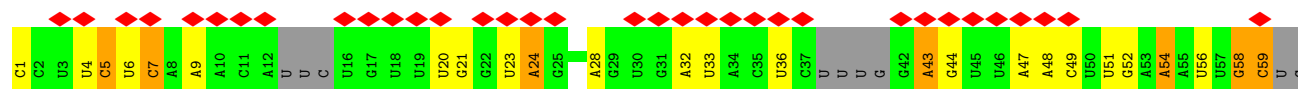
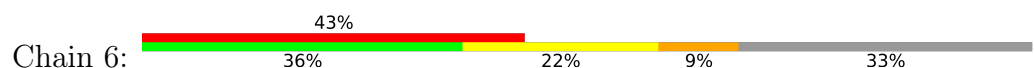
• Molecule 4: 5S rRNA



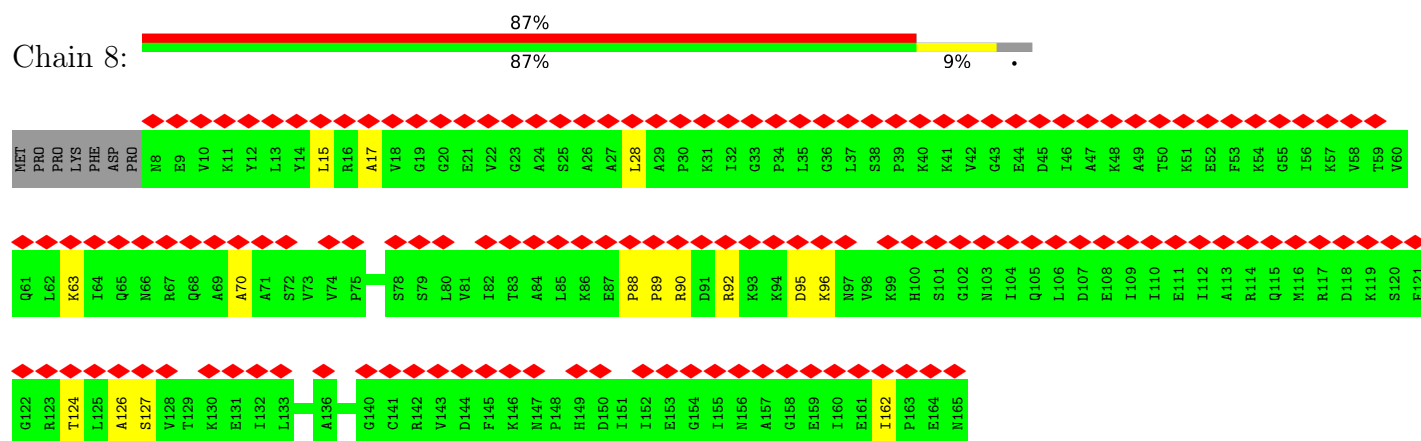
• Molecule 5: rRNA-processing protein



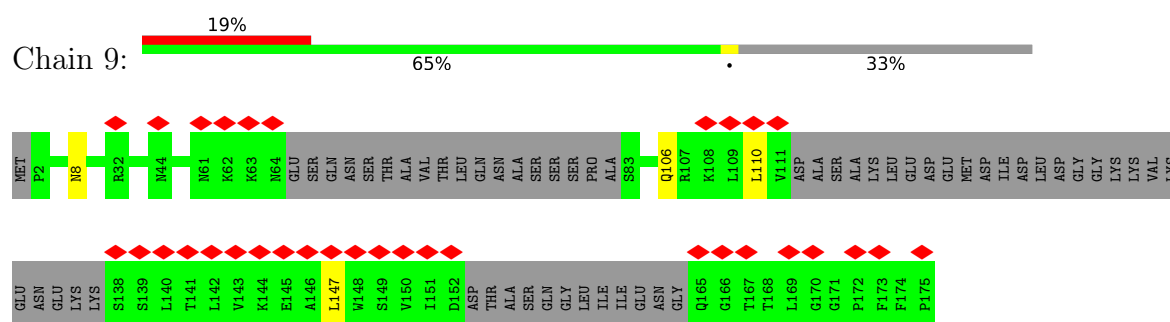
• Molecule 6: ITS2 rRNA



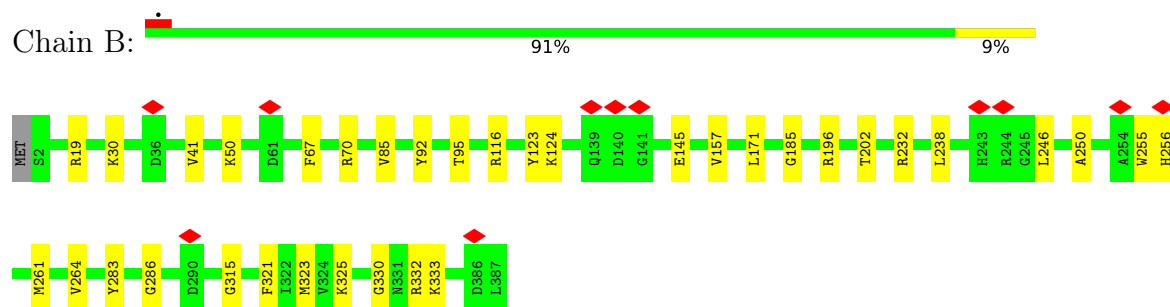
• Molecule 7: 60S ribosomal protein L12-A



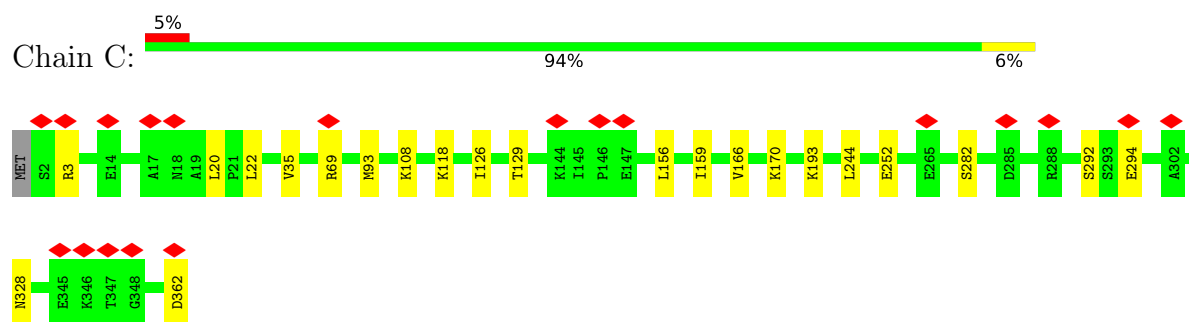
• Molecule 8: Ribosome biogenesis protein ALB1



• Molecule 9: 60S ribosomal protein L3

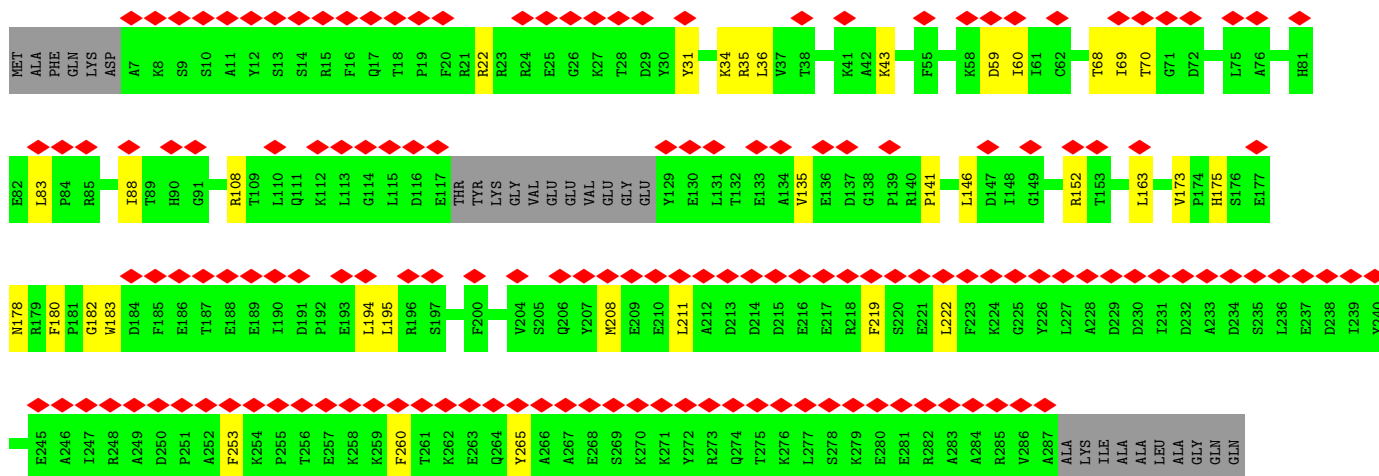


• Molecule 10: 60S ribosomal protein L4-A

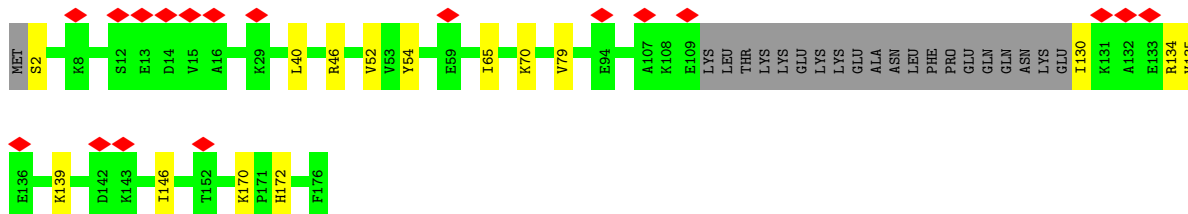
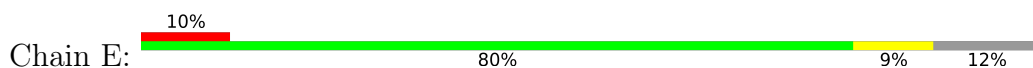


• Molecule 11: 60S ribosomal protein L5

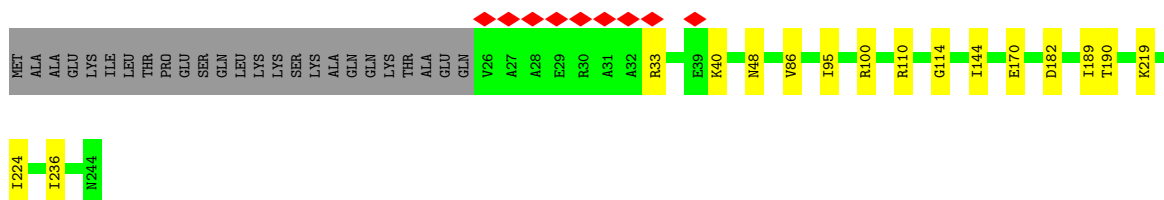
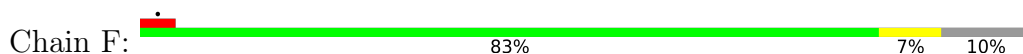




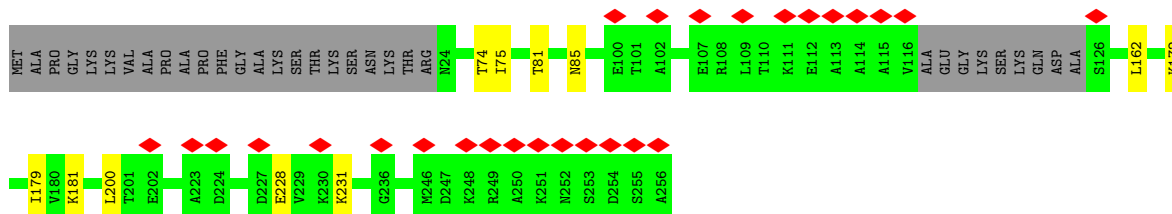
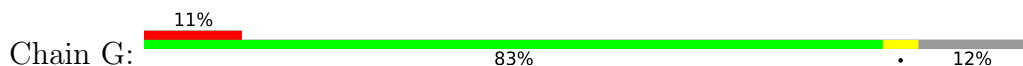
- Molecule 12: 60S ribosomal protein L6-A



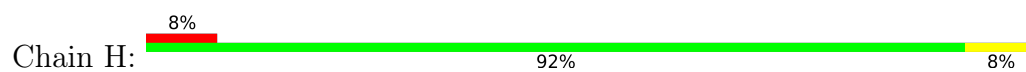
- Molecule 13: 60S ribosomal protein L7-A



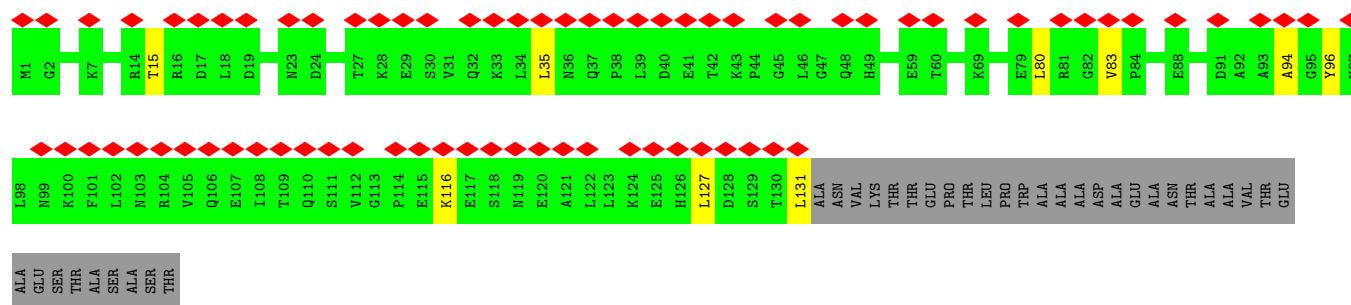
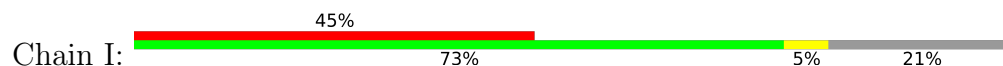
- Molecule 14: 60S ribosomal protein L8-A



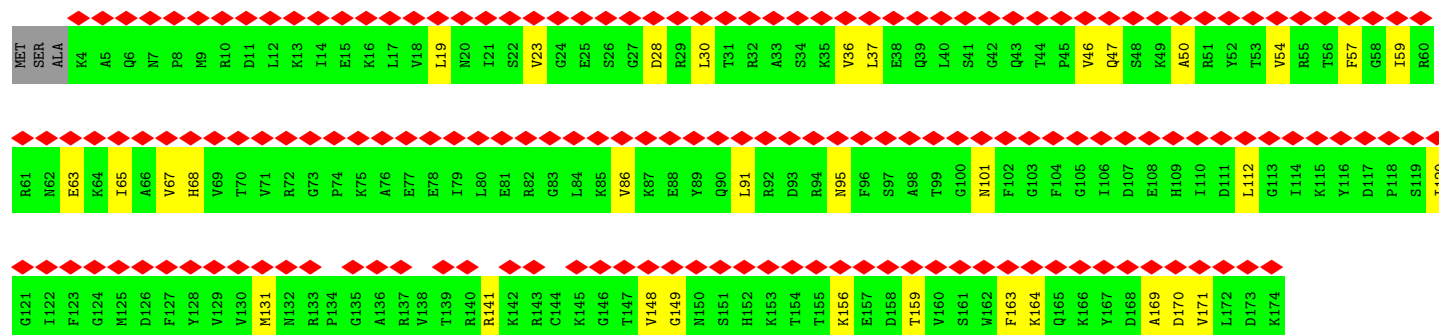
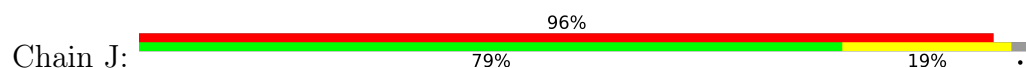
- Molecule 15: 60S ribosomal protein L9-A



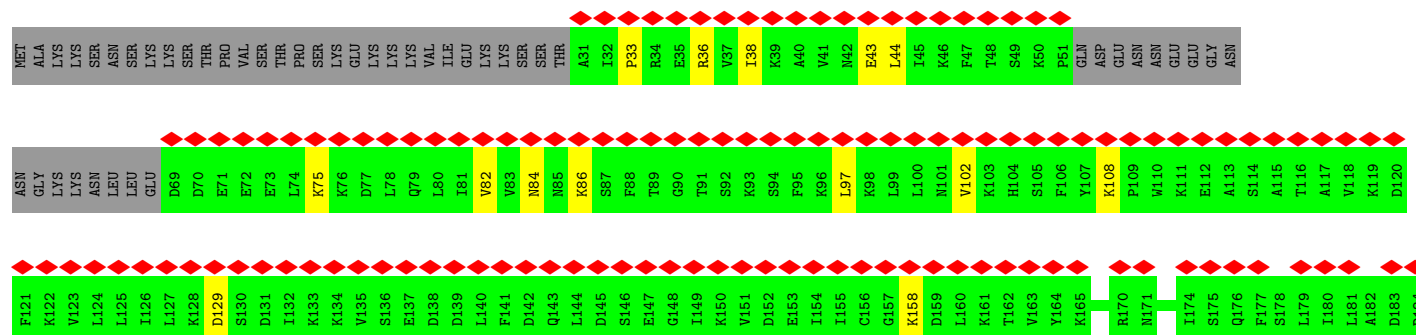
• Molecule 16: Bud site selection protein 20

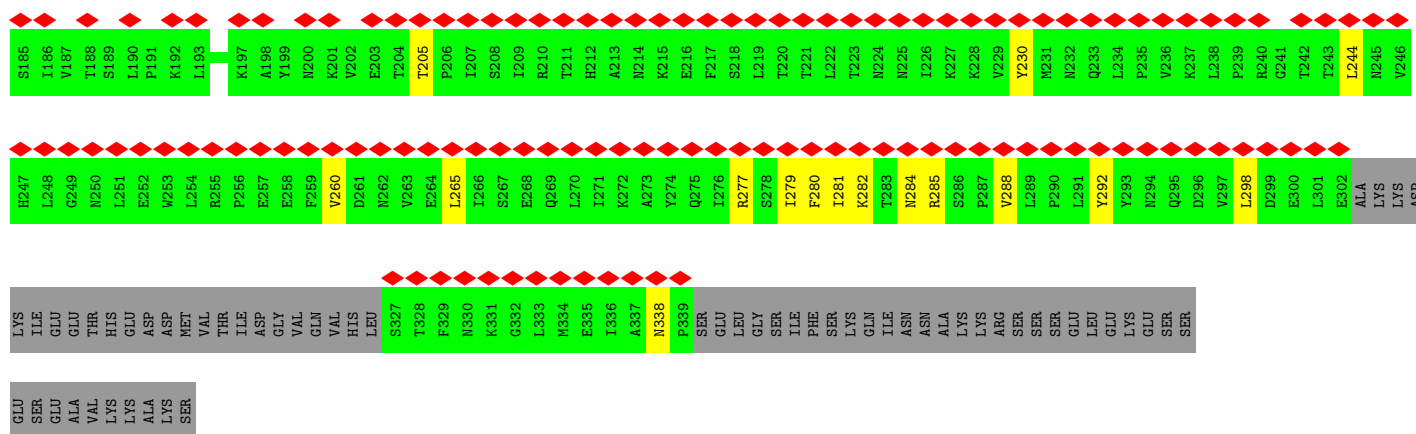


• Molecule 17: 60S ribosomal protein L11-A

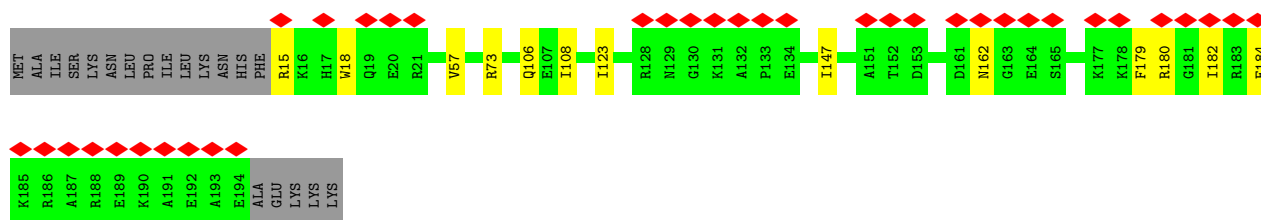
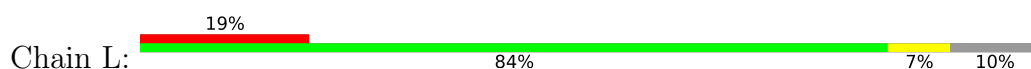


• Molecule 18: Proteasome-interacting protein CIC1

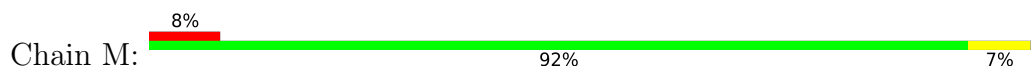




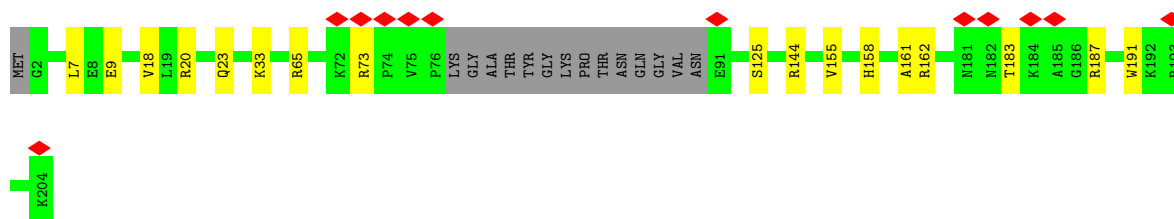
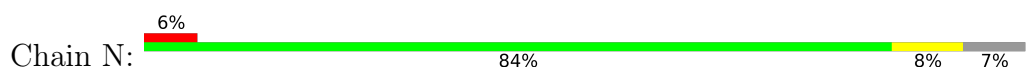
• Molecule 19: 60S ribosomal protein L13-A



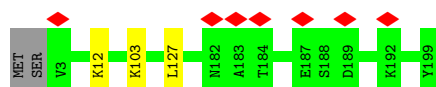
• Molecule 20: 60S ribosomal protein L14-A



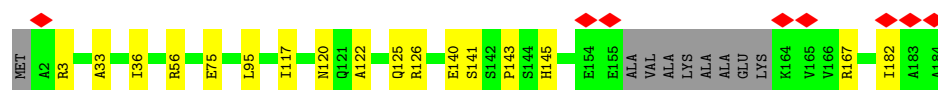
• Molecule 21: 60S ribosomal protein L15-A



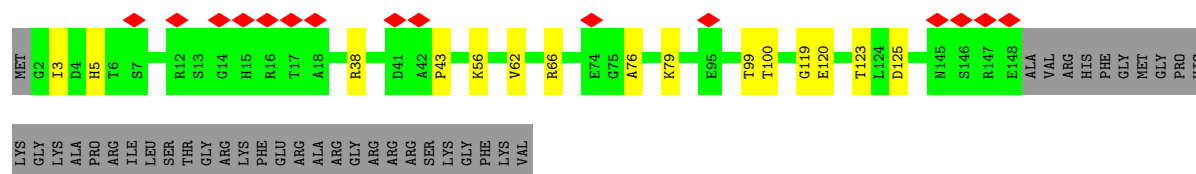
• Molecule 22: 60S ribosomal protein L16-A



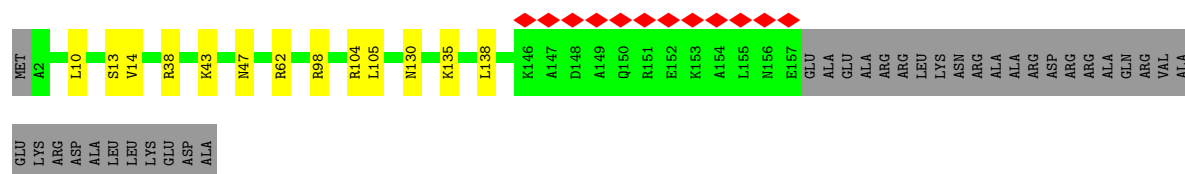
• Molecule 23: 60S ribosomal protein L17-A

Chain P: 

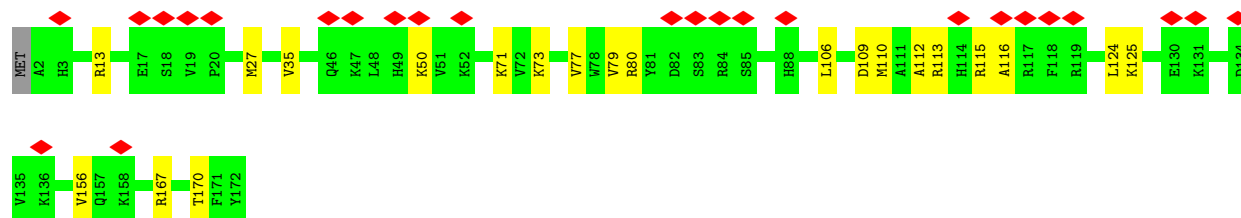
• Molecule 24: 60S ribosomal protein L18-A

Chain Q: 

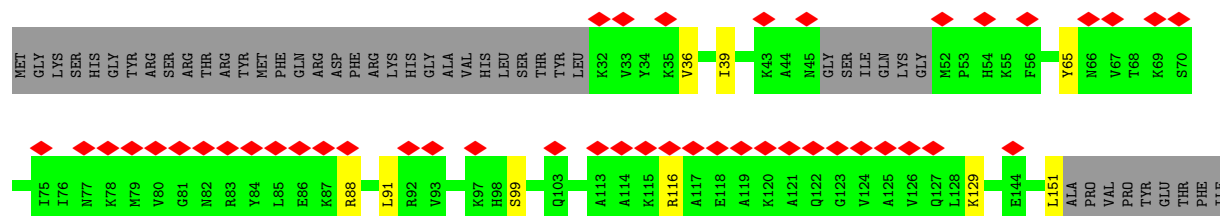
• Molecule 25: 60S ribosomal protein L19-A

Chain R: 

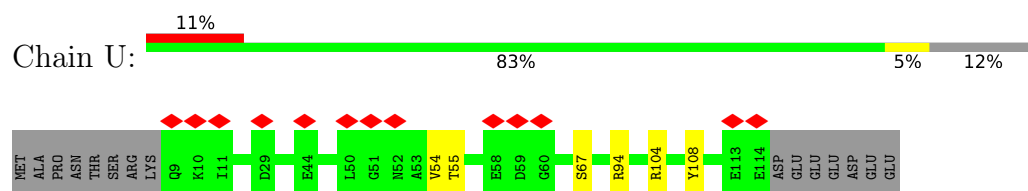
• Molecule 26: 60S ribosomal protein L20-A

Chain S: 

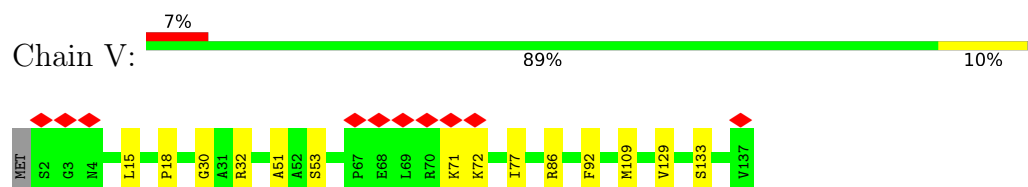
• Molecule 27: 60S ribosomal protein L21-A

Chain T: 

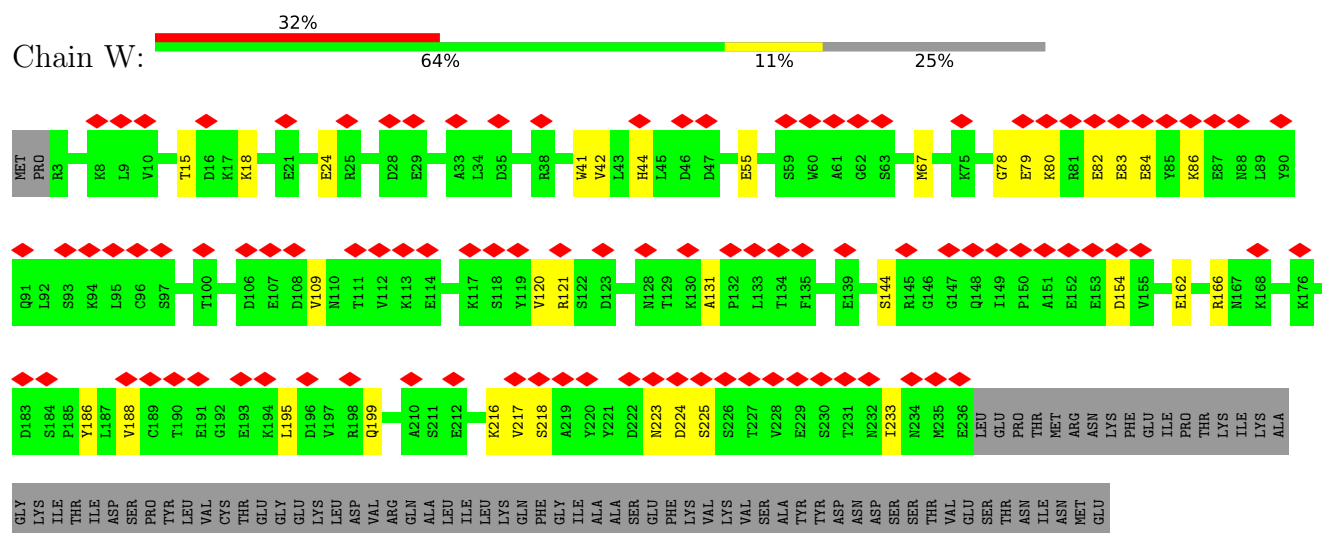
- Molecule 28: 60S ribosomal protein L22-A



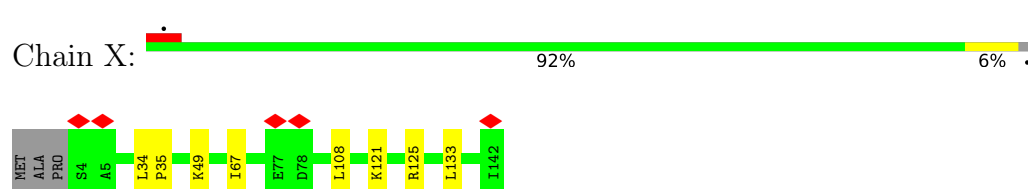
- Molecule 29: 60S ribosomal protein L23-A



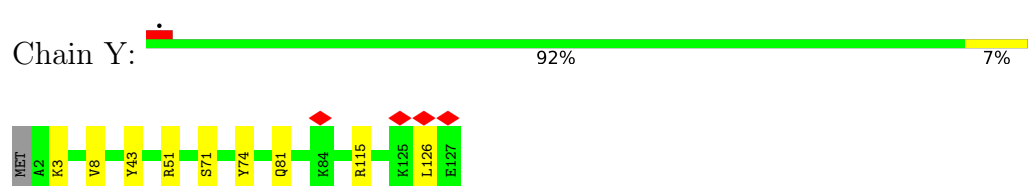
- Molecule 30: Ribosome assembly factor MRT4



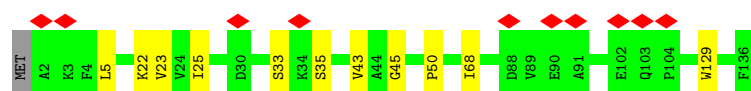
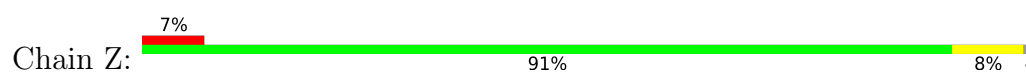
- Molecule 31: 60S ribosomal protein L25



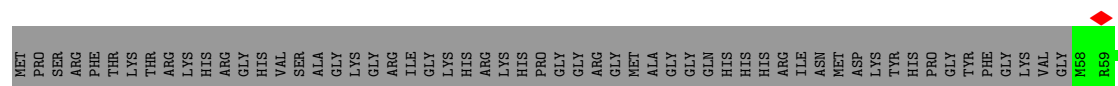
- Molecule 32: 60S ribosomal protein L26-A



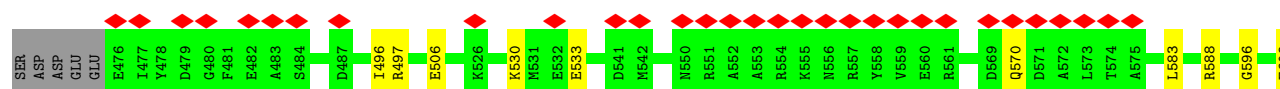
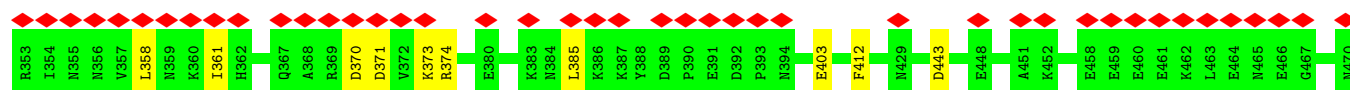
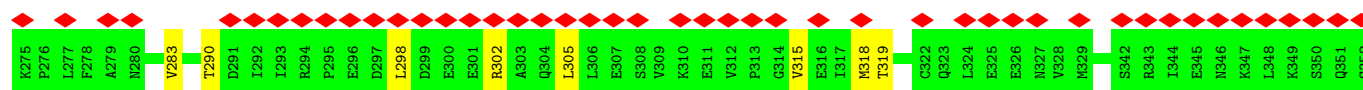
- Molecule 33: 60S ribosomal protein L27-A



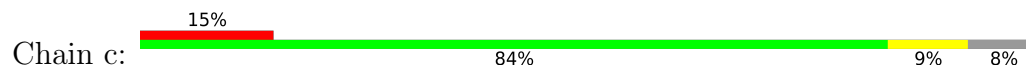
• Molecule 34: 60S ribosomal protein L28



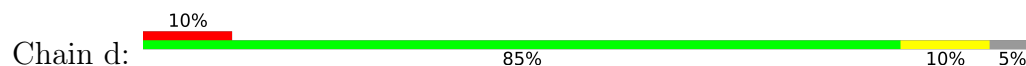
• Molecule 35: Nucleolar GTP-binding protein 1

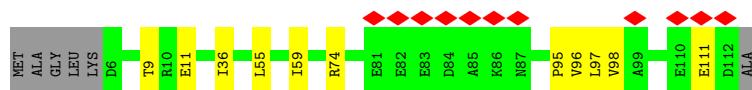


• Molecule 36: 60S ribosomal protein L30



• Molecule 37: 60S ribosomal protein L31-A





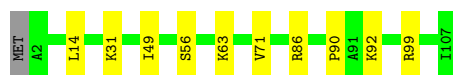
- Molecule 38: 60S ribosomal protein L32

Chain e: 94%



- Molecule 39: 60S ribosomal protein L33-A

Chain f: 90%



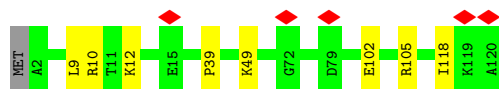
- Molecule 40: 60S ribosomal protein L34-A

Chain g: 9% 86% 7% 7%



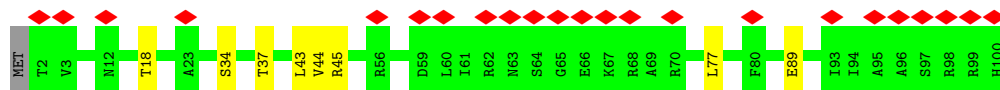
- Molecule 41: 60S ribosomal protein L35-A

Chain h: 92% 7%



- Molecule 42: 60S ribosomal protein L36-A

Chain i: 23% 91% 8%

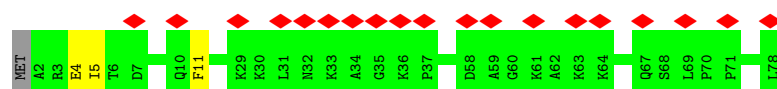
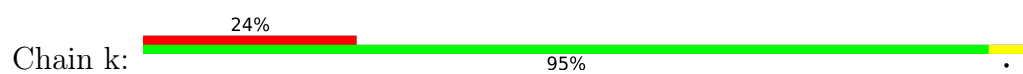


- Molecule 43: 60S ribosomal protein L37-A

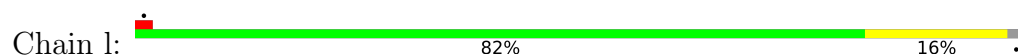
Chain j: 86% 9% 5%



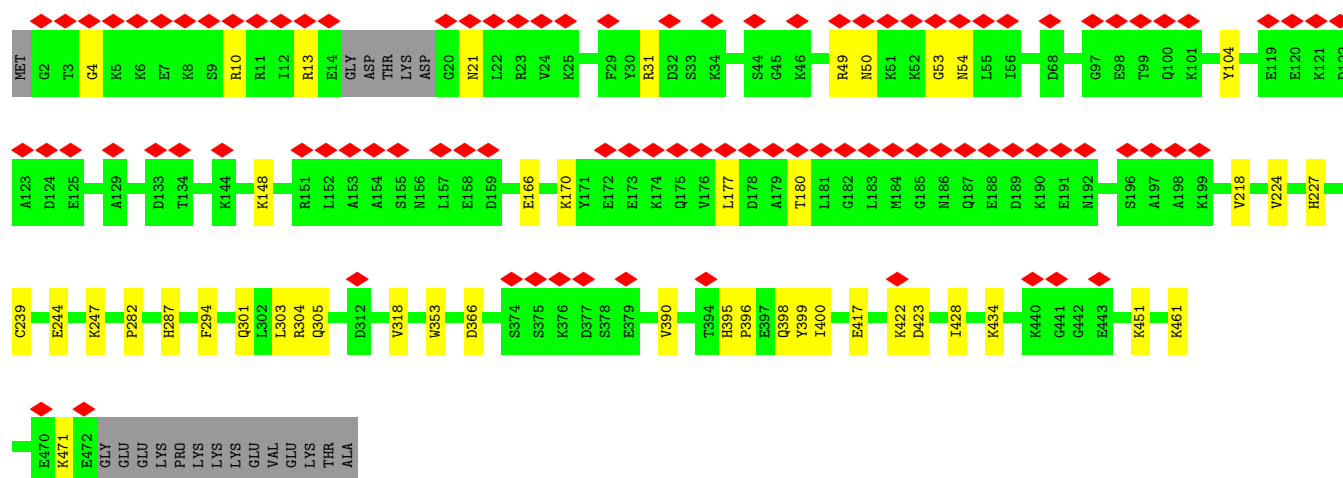
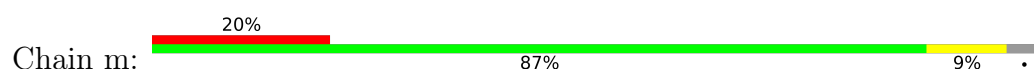
- Molecule 44: 60S ribosomal protein L38



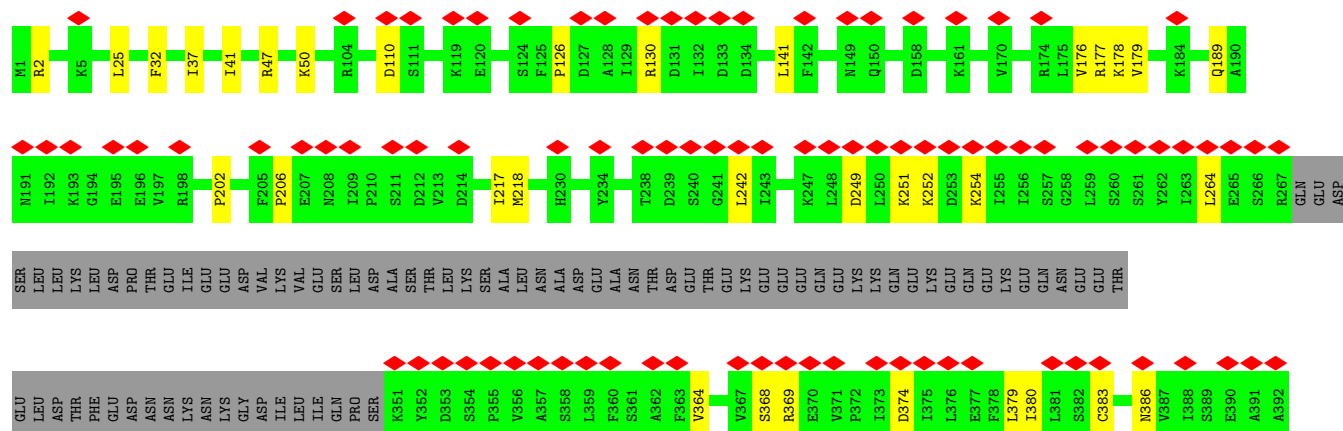
- Molecule 45: 60S ribosomal protein L39

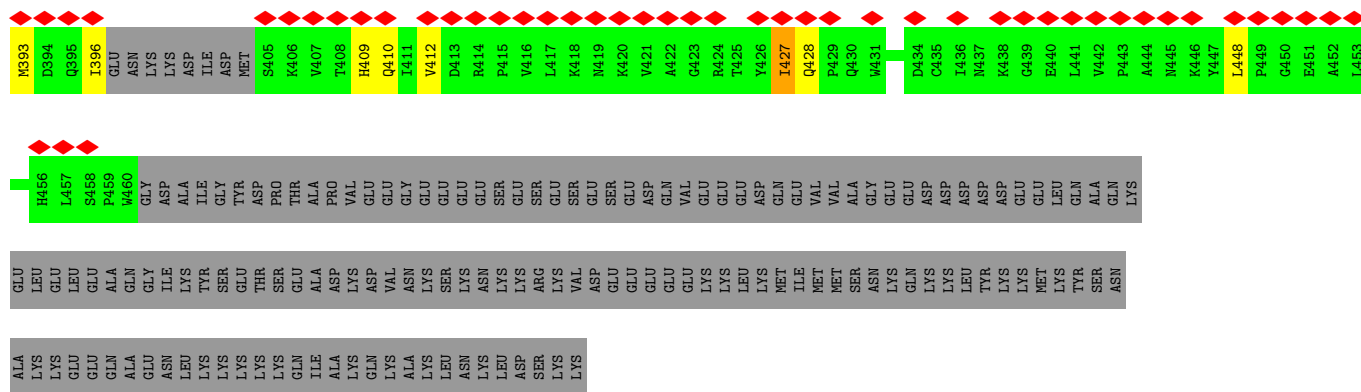


- Molecule 46: Nucleolar GTP-binding protein 2

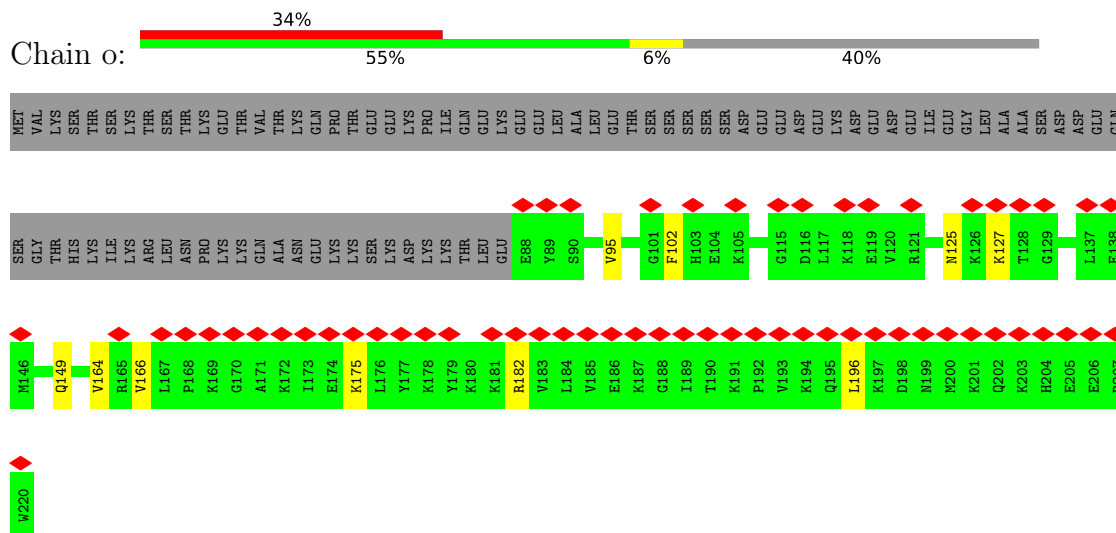


- Molecule 47: Pescadillo homolog

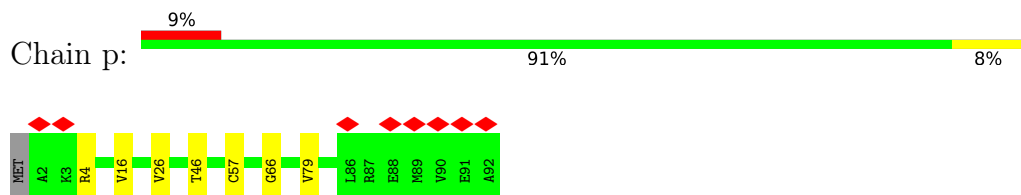




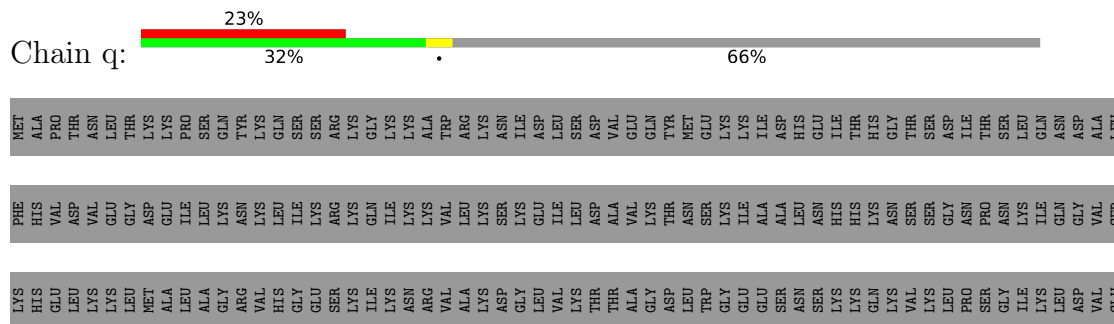
• Molecule 48: Ribosome biogenesis protein 15



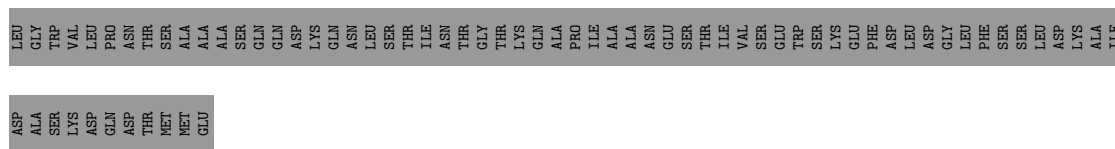
• Molecule 49: 60S ribosomal protein L43-A



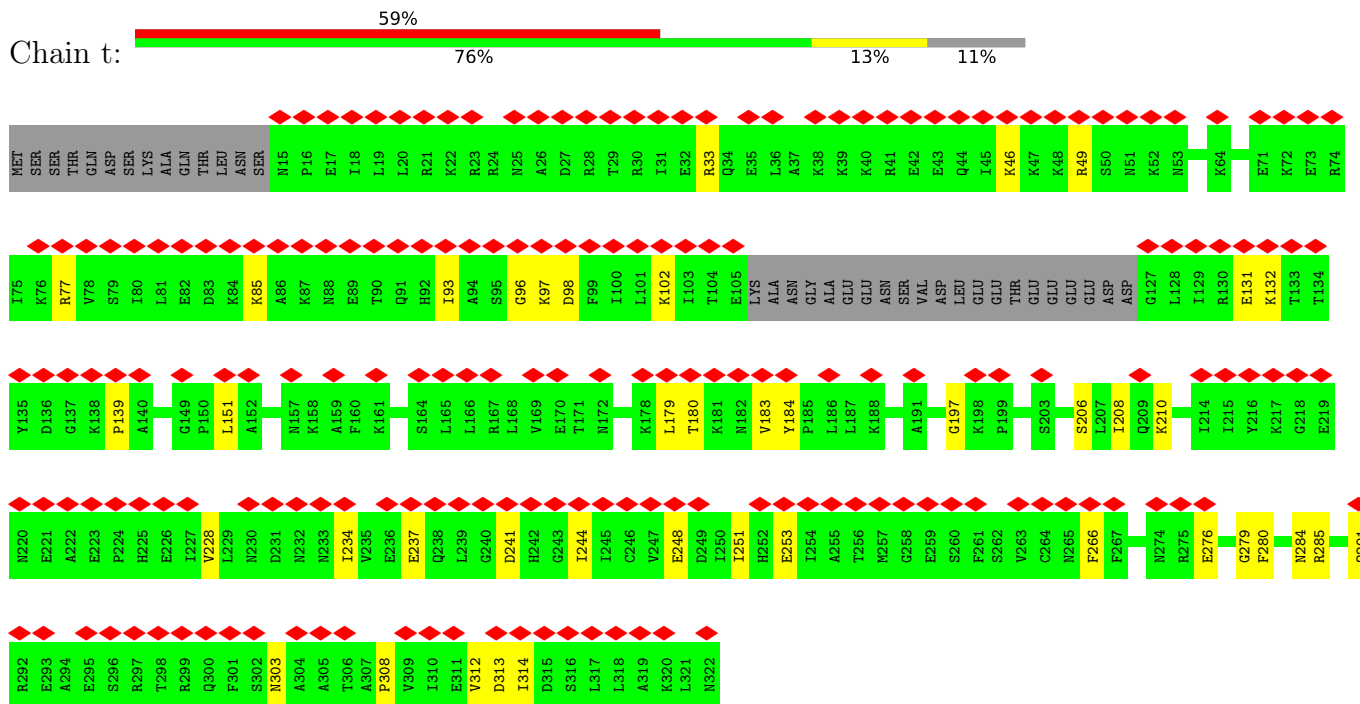
• Molecule 50: Ribosome biogenesis protein NOP53



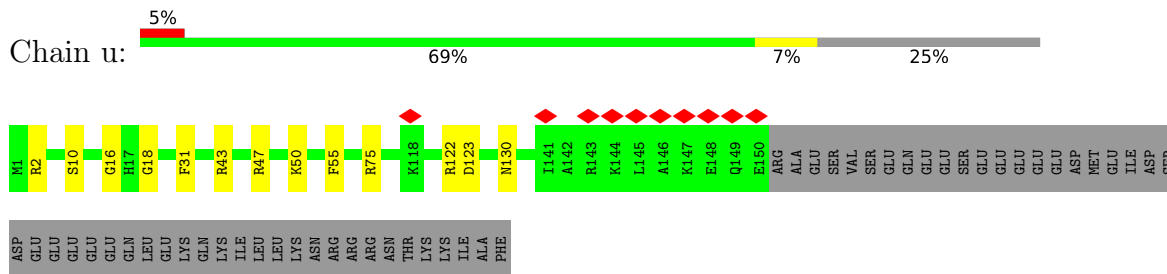




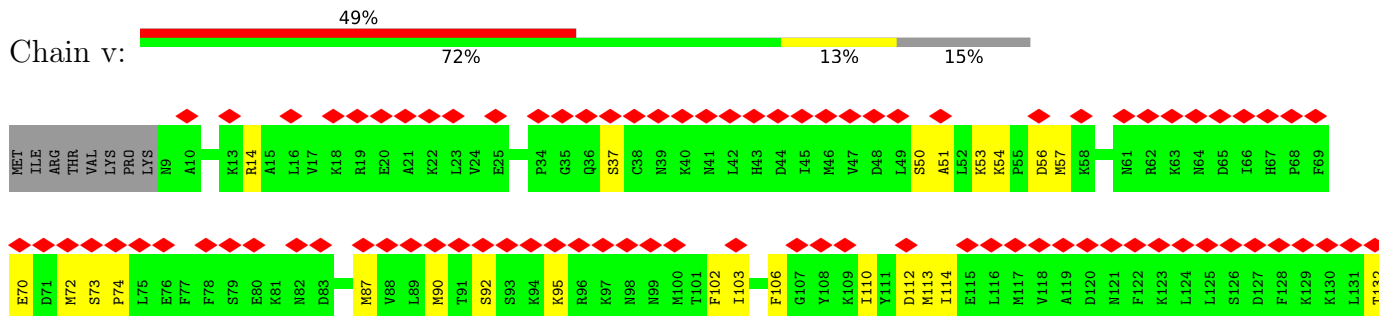
- Molecule 53: Ribosome biogenesis protein RLP7

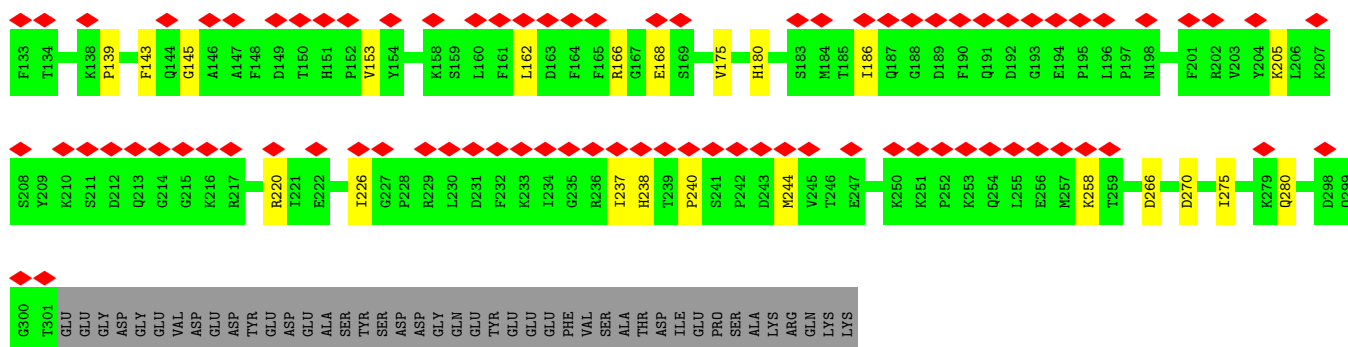


- Molecule 54: Ribosome biogenesis protein RLP24

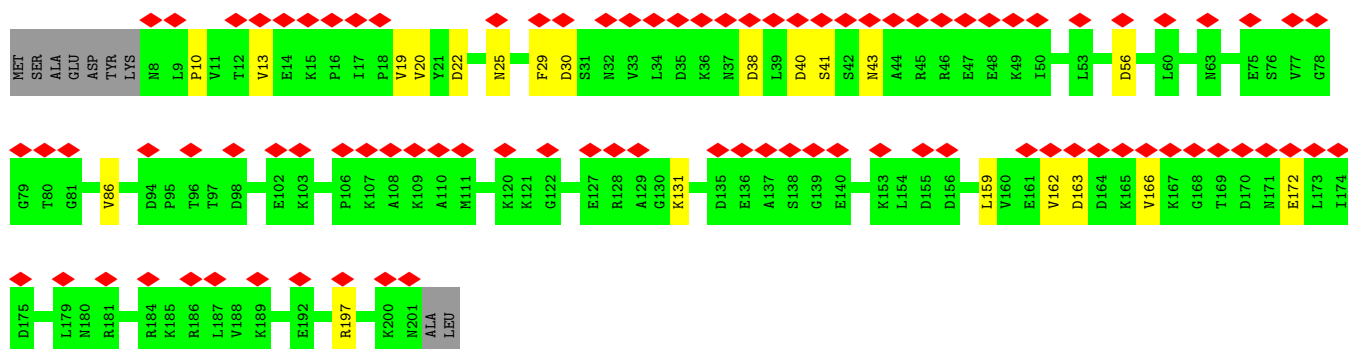
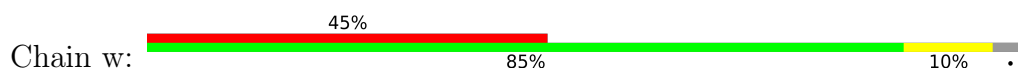


- Molecule 55: Ribosome production factor 2 homolog

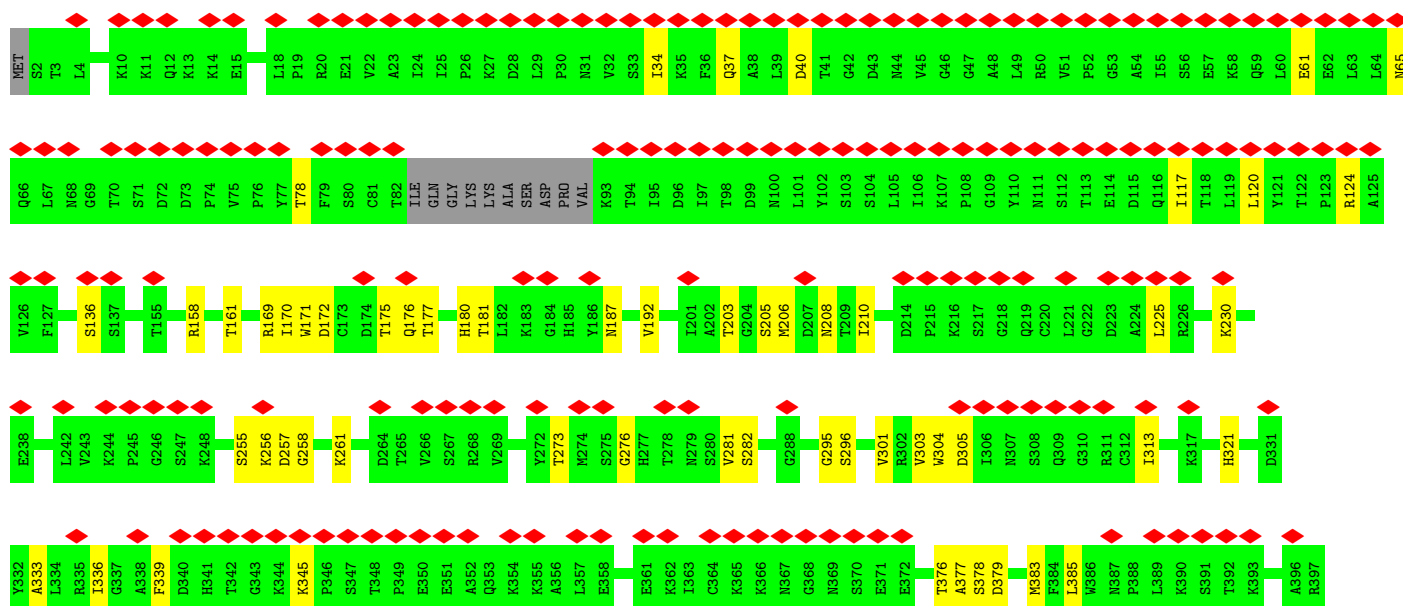
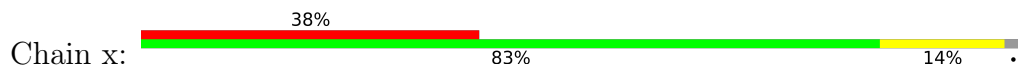




• Molecule 56: Ribosome biogenesis regulatory protein

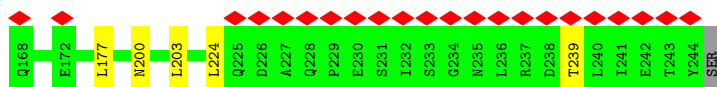
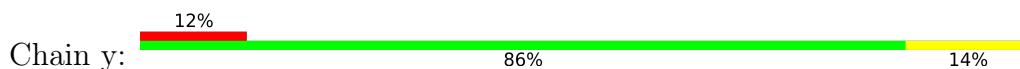


• Molecule 57: RSA4 isoform 1

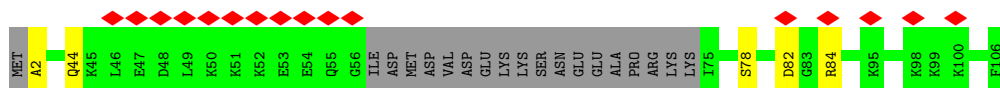
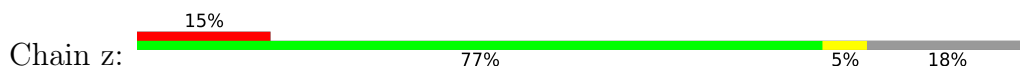




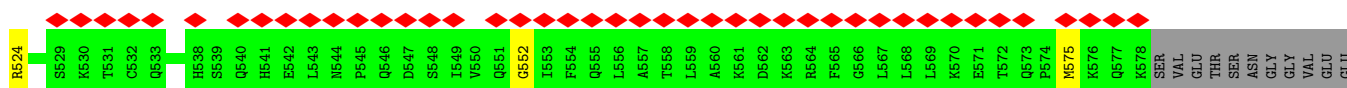
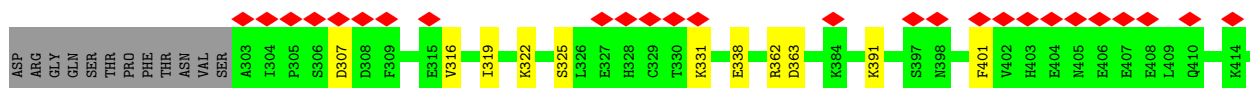
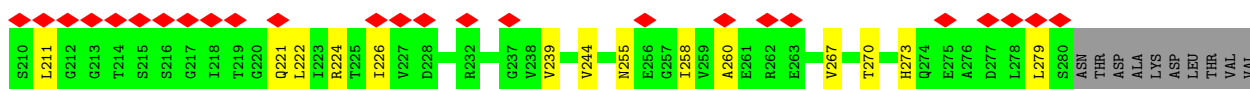
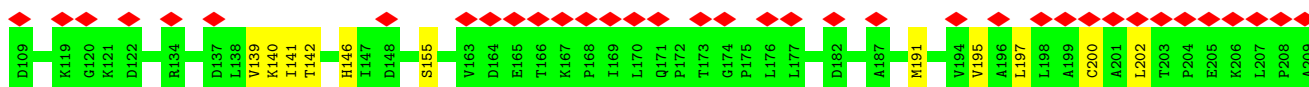
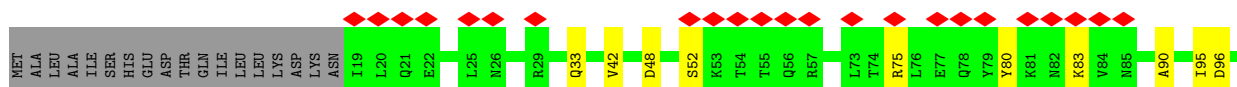
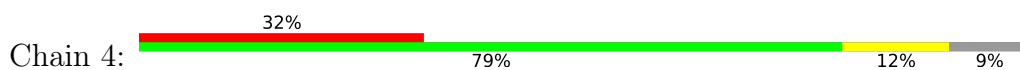
- Molecule 58: Eukaryotic translation initiation factor 6



- Molecule 59: UPF0642 protein YBL028C



- Molecule 60: Probable metalloprotease ARX1



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, GTP, 5MC, GDP, K, ZN, A2M, MG, OMU, OMG, OMC, B3P, PSU

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	0.13	0/1666	0.34	0/2241
2	1	0.16	0/70356	0.30	0/109681
3	2	0.16	0/3724	0.29	0/5798
4	3	0.09	0/2861	0.22	0/4457
5	5	0.11	0/649	0.22	0/848
6	6	0.12	0/1367	0.28	0/2118
7	8	0.11	0/1210	0.28	0/1627
8	9	0.11	0/948	0.25	0/1264
9	B	0.14	0/3152	0.34	0/4239
10	C	0.13	0/2801	0.33	0/3792
11	D	0.10	0/2227	0.27	0/3004
12	E	0.12	0/1251	0.31	0/1682
13	F	0.14	0/1798	0.31	0/2420
14	G	0.13	0/1784	0.30	0/2408
15	H	0.13	0/1539	0.32	0/2073
16	I	0.12	0/1075	0.31	0/1443
17	J	0.10	0/1389	0.29	0/1860
18	K	0.11	0/2190	0.29	0/2955
19	L	0.13	0/1460	0.31	0/1960
20	M	0.13	0/1074	0.29	0/1446
21	N	0.15	0/1654	0.34	0/2213
22	O	0.16	0/1585	0.30	0/2128
23	P	0.15	0/1410	0.36	0/1893
24	Q	0.12	0/1153	0.28	0/1555
25	R	0.14	0/1275	0.29	0/1702
26	S	0.11	0/1473	0.28	0/1980
27	T	0.11	0/916	0.25	0/1226
28	U	0.13	0/861	0.38	0/1167
29	V	0.13	0/1018	0.33	0/1369
30	W	0.11	0/1919	0.28	0/2586
31	X	0.12	0/1103	0.32	0/1484
32	Y	0.12	0/1004	0.32	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.11	0/1118	0.28	0/1497
34	a	0.11	0/747	0.25	0/1008
35	b	0.14	0/5270	0.32	0/7080
36	c	0.12	0/751	0.30	0/1008
37	d	0.13	0/887	0.32	0/1191
38	e	0.12	0/1041	0.30	0/1394
39	f	0.14	0/868	0.33	0/1168
40	g	0.15	0/891	0.32	0/1191
41	h	0.15	0/978	0.28	0/1301
42	i	0.11	0/778	0.29	0/1034
43	j	0.15	0/680	0.37	0/901
44	k	0.12	0/618	0.30	0/826
45	l	0.16	0/443	0.33	0/588
46	m	0.13	0/3828	0.30	0/5154
47	n	0.13	0/3085	0.30	0/4166
48	o	0.11	0/1129	0.30	0/1502
49	p	0.14	0/701	0.36	0/934
50	q	0.14	0/1321	0.33	0/1766
51	r	0.12	0/1892	0.29	0/2528
52	s	0.12	0/608	0.23	0/798
53	t	0.13	0/2333	0.28	0/3128
54	u	0.14	0/1287	0.28	0/1711
55	v	0.11	0/2410	0.29	0/3220
56	w	0.11	0/1565	0.27	0/2108
57	x	0.11	0/4022	0.34	0/5460
58	y	0.13	0/1872	0.35	0/2548
59	z	0.13	0/721	0.24	0/948
60	4	0.12	0/4242	0.27	0/5758
All	All	0.14	0/165978	0.30	0/239876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1634	0	1685	20	0
2	1	64043	0	32237	379	0
3	2	3353	0	1695	24	0
4	3	2579	0	1304	28	0
5	5	645	0	688	1	0
6	6	1227	0	622	16	0
7	8	1196	0	1257	13	0
8	9	937	0	1008	4	0
9	B	3081	0	3165	23	0
10	C	2749	0	2863	15	0
11	D	2180	0	2134	25	0
12	E	1230	0	1320	17	0
13	F	1761	0	1843	12	0
14	G	1753	0	1845	15	0
15	H	1518	0	1587	10	0
16	I	1059	0	1089	7	0
17	J	1368	0	1401	25	0
18	K	2155	0	2230	21	0
19	L	1438	0	1493	10	0
20	M	1059	0	1154	7	0
21	N	1620	0	1679	18	0
22	O	1555	0	1659	3	0
23	P	1388	0	1423	17	0
24	Q	1136	0	1214	14	0
25	R	1258	0	1342	8	0
26	S	1437	0	1475	17	0
27	T	905	0	957	8	0
28	U	844	0	855	5	0
29	V	1003	0	1048	8	0
30	W	1887	0	1917	22	0
31	X	1088	0	1175	5	0
32	Y	993	0	1081	7	0
33	Z	1092	0	1155	6	0
34	a	731	0	773	10	0
35	b	5185	0	5251	33	0
36	c	743	0	797	6	0
37	d	873	0	914	6	0
38	e	1020	0	1090	4	0
39	f	850	0	880	6	0
40	g	881	0	945	5	0
41	h	969	0	1078	6	0
42	i	771	0	849	6	0
43	j	665	0	668	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	k	612	0	682	2	0
45	l	436	0	475	6	0
46	m	3754	0	3822	35	0
47	n	3014	0	3094	28	0
48	o	1107	0	1159	9	0
49	p	694	0	734	6	0
50	q	1298	0	1343	14	0
51	r	1860	0	1965	14	0
52	s	602	0	661	2	0
53	t	2306	0	2454	30	0
54	u	1265	0	1314	11	0
55	v	2366	0	2452	45	0
56	w	1541	0	1597	21	0
57	x	3927	0	3893	46	0
58	y	1849	0	1836	22	0
59	z	714	0	760	5	0
60	4	4166	0	4248	41	0
61	1	77	0	0	0	0
61	R	1	0	0	0	0
61	V	1	0	0	0	0
61	b	1	0	0	0	0
61	m	1	0	0	0	0
62	1	57	0	78	6	0
63	I	1	0	0	0	0
63	g	1	0	0	0	0
63	j	1	0	0	0	0
63	p	1	0	0	0	0
63	u	1	0	0	0	0
64	b	28	0	12	0	0
65	m	32	0	12	0	0
66	m	1	0	0	0	0
67	1	346	0	0	0	0
67	2	6	0	0	0	0
67	C	3	0	0	0	0
67	F	1	0	0	0	0
67	N	3	0	0	0	0
67	O	1	0	0	0	0
67	R	2	0	0	0	0
67	V	1	0	0	0	0
67	X	1	0	0	0	0
67	b	3	0	0	0	0
67	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	j	2	0	0	0	0
67	m	3	0	0	0	0
All	All	157947	0	125436	1032	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1032) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y:43:TYR:CE1	32:Y:126:LEU:HD13	1.68	1.29
55:v:132:THR:HG22	55:v:226:ILE:CG2	1.75	1.17
32:Y:43:TYR:HE1	32:Y:126:LEU:CD1	1.59	1.15
55:v:132:THR:CG2	55:v:226:ILE:HG21	1.78	1.14
14:G:74:THR:CG2	21:N:18:VAL:HG21	1.77	1.14
56:w:19:VAL:HG13	56:w:29:PHE:O	1.49	1.12
12:E:52:VAL:HG21	12:E:65:ILE:HG21	1.23	1.11
7:8:15:LEU:CD2	7:8:28:LEU:HD11	1.84	1.08
14:G:74:THR:HG21	21:N:18:VAL:HG21	1.37	1.06
4:3:39:C:C6	17:J:46:VAL:HG21	1.91	1.04
12:E:52:VAL:CG2	12:E:65:ILE:HG21	1.88	1.03
11:D:182:GLY:HA2	11:D:194:LEU:HD23	1.39	0.99
12:E:65:ILE:CD1	12:E:79:VAL:HG21	1.91	0.99
4:3:39:C:C5	17:J:46:VAL:HG21	1.97	0.98
55:v:132:THR:HG22	55:v:226:ILE:HG21	0.99	0.98
12:E:65:ILE:HD12	12:E:79:VAL:HG21	1.40	0.97
24:Q:3:ILE:HD11	24:Q:5:HIS:CE1	1.99	0.97
12:E:65:ILE:HD12	12:E:79:VAL:CG2	1.97	0.95
2:1:2426:U:H3	2:1:2603:G:H1	1.01	0.95
4:3:39:C:C6	17:J:46:VAL:CG2	2.53	0.91
32:Y:43:TYR:HE1	32:Y:126:LEU:HD13	0.76	0.90
14:G:74:THR:CG2	21:N:18:VAL:CG2	2.50	0.90
11:D:182:GLY:CA	11:D:194:LEU:HD23	2.05	0.87
1:A:104:LEU:CD1	1:A:158:ILE:HD11	2.03	0.86
17:J:156:LYS:O	17:J:159:THR:HG22	1.76	0.85
14:G:74:THR:HG22	21:N:18:VAL:CG2	2.05	0.85
57:x:78:THR:HG23	57:x:124:ARG:HG3	1.60	0.83
2:1:2442:G:H1	2:1:2505:U:H3	1.28	0.82
11:D:163:LEU:CD1	11:D:173:VAL:HG11	2.10	0.82
2:1:173:G:H1	2:1:245:U:H3	1.27	0.80
7:8:15:LEU:HD23	7:8:28:LEU:HD11	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:132:THR:CG2	55:v:226:ILE:CG2	2.50	0.78
12:E:52:VAL:CG2	12:E:65:ILE:CG2	2.61	0.78
8:9:106:GLN:O	8:9:110:LEU:HD13	1.82	0.78
30:W:186:TYR:CE2	30:W:188:VAL:HG22	2.19	0.77
53:t:312:VAL:HG12	53:t:313:ASP:N	1.99	0.77
55:v:132:THR:HA	55:v:226:ILE:HD13	1.66	0.76
2:1:170:G:H1	2:1:248:U:H3	1.32	0.76
2:1:2203:U:H3	2:1:2239:G:H1	1.31	0.76
46:m:104:TYR:O	55:v:275:ILE:HG12	1.86	0.74
2:1:1132:C:H2'	2:1:1133:A2M:H8	1.69	0.74
56:w:19:VAL:HG13	56:w:29:PHE:C	2.14	0.73
35:b:609:GLU:HG3	45:l:36:ARG:HB3	1.69	0.71
30:W:186:TYR:HE2	30:W:188:VAL:HG22	1.54	0.71
1:A:104:LEU:HD11	1:A:158:ILE:HD11	1.72	0.71
2:1:2219:A:H2'	2:1:2220:A2M:H8	1.73	0.71
24:Q:3:ILE:CD1	24:Q:5:HIS:CE1	2.72	0.70
53:t:312:VAL:HG12	53:t:313:ASP:H	1.56	0.70
12:E:65:ILE:CD1	12:E:79:VAL:CG2	2.62	0.70
24:Q:3:ILE:HD11	24:Q:5:HIS:HE1	1.53	0.69
60:4:155:SER:HB3	60:4:504:CYS:HB3	1.74	0.69
57:x:34:ILE:HG22	57:x:117:ILE:HB	1.74	0.69
57:x:418:VAL:HG23	57:x:452:TRP:CZ2	2.27	0.69
7:8:15:LEU:HD22	7:8:28:LEU:HD11	1.73	0.69
2:1:3268:A:OP1	12:E:46:ARG:NH2	2.27	0.68
20:M:48:GLY:HA3	20:M:53:VAL:HB	1.76	0.67
15:H:83:THR:HG23	15:H:84:LYS:HG3	1.76	0.67
60:4:195:VAL:HG11	60:4:524:ARG:HH21	1.58	0.67
11:D:163:LEU:HD11	11:D:173:VAL:CG1	2.25	0.66
2:1:2830:G:H2'	2:1:2831:G:C8	2.31	0.66
2:1:1858:A:H1'	40:g:4:ARG:HD3	1.77	0.65
50:q:214:VAL:HG12	50:q:215:LYS:H	1.60	0.65
57:x:418:VAL:HG11	57:x:459:LEU:HD21	1.77	0.65
23:P:125:GLN:HB3	23:P:141:SER:HB2	1.78	0.65
2:1:2248:C:H2'	46:m:304:ARG:HH21	1.62	0.65
50:q:214:VAL:HG12	50:q:215:LYS:N	2.12	0.65
12:E:65:ILE:HD11	12:E:79:VAL:HG21	1.75	0.65
57:x:418:VAL:HG23	57:x:452:TRP:HZ2	1.60	0.65
2:1:1387:G:HO2'	12:E:2:SER:N	1.96	0.64
53:t:312:VAL:CG1	53:t:313:ASP:H	2.10	0.64
32:Y:43:TYR:CE1	32:Y:126:LEU:CD1	2.51	0.64
30:W:44:HIS:HB2	30:W:216:LYS:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2569:A:O2'	53:t:33:ARG:NH1	2.31	0.64
2:1:1661:G:H2'	2:1:1662:G:C8	2.33	0.64
2:1:600:G:N2	2:1:603:A:OP2	2.31	0.64
2:1:2359:C:H4'	2:1:2399:A:H4'	1.79	0.63
58:y:1:MET:HB2	58:y:224:LEU:HB3	1.79	0.63
13:F:110:ARG:HB3	24:Q:3:ILE:HG22	1.80	0.63
18:K:298:LEU:HD21	48:o:196:LEU:HD11	1.80	0.63
3:2:63:G:O2'	41:h:49:LYS:NZ	2.31	0.63
55:v:51:ALA:HA	55:v:54:LYS:HD2	1.80	0.63
57:x:78:THR:HG23	57:x:124:ARG:CG	2.28	0.62
21:N:33:LYS:O	21:N:65:ARG:NH2	2.32	0.62
11:D:83:LEU:HB3	11:D:88:ILE:HB	1.81	0.62
23:P:33:ALA:O	23:P:36:ILE:HG22	2.00	0.62
23:P:33:ALA:HA	23:P:36:ILE:HG22	1.82	0.62
60:4:244:VAL:HG22	60:4:319:ILE:HG23	1.81	0.62
2:1:2761:G:H1	2:1:2799:A:H61	1.46	0.62
35:b:187:ILE:HG13	35:b:188:THR:HG23	1.82	0.61
2:1:1241:U:O2'	46:m:148:LYS:NZ	2.32	0.61
3:2:128:U:O4	47:n:47:ARG:NH2	2.33	0.61
53:t:312:VAL:CG1	53:t:313:ASP:N	2.63	0.61
55:v:145:GLY:HA3	55:v:186:ILE:HD12	1.80	0.61
55:v:162:LEU:O	55:v:166:ARG:HB2	2.00	0.61
58:y:114:VAL:HG11	58:y:177:LEU:HD23	1.83	0.61
14:G:74:THR:HG22	21:N:18:VAL:HG22	1.80	0.61
2:1:3217:C:C4	23:P:182:ILE:HG23	2.35	0.61
30:W:78:GLY:HA3	30:W:84:GLU:HA	1.82	0.60
2:1:1571:A:OP2	53:t:284:ASN:ND2	2.35	0.60
10:C:35:VAL:HG21	10:C:244:LEU:HD21	1.83	0.60
55:v:153:VAL:HG22	55:v:237:ILE:HD13	1.84	0.60
2:1:838:G:O6	49:p:4:ARG:NH2	2.35	0.60
2:1:1570:U:H1'	53:t:279:GLY:HA2	1.83	0.60
55:v:220:ARG:NH1	56:w:10:PRO:O	2.34	0.60
2:1:1115:G:N2	2:1:1115:G:OP2	2.35	0.60
60:4:197:LEU:HD22	60:4:226:ILE:HD12	1.84	0.60
60:4:202:LEU:HB3	60:4:520:PRO:HB2	1.84	0.60
14:G:75:ILE:HD11	21:N:18:VAL:HG13	1.83	0.60
35:b:443:ASP:O	54:u:75:ARG:NH1	2.35	0.60
26:S:80:ARG:NE	26:S:124:LEU:HD11	2.16	0.60
2:1:1657:C:O2'	2:1:1797:A:OP2	2.19	0.59
2:1:2211:U:H3	2:1:2234:G:H1	1.50	0.59
2:1:439:C:O2'	2:1:494:G:N2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:73:SER:OG	55:v:74:PRO:HD3	2.02	0.59
2:1:2898:G:N2	51:r:7:ILE:H	2.01	0.59
2:1:1553:U:H4'	2:1:1554:U:H5'	1.84	0.59
4:3:87:G:H2'	4:3:88:G:H8	1.66	0.59
25:R:105:LEU:HD23	25:R:138:LEU:HD23	1.85	0.59
32:Y:3:LYS:HD2	32:Y:8:VAL:HG23	1.84	0.59
43:j:21:ARG:NH2	43:j:41:ALA:O	2.29	0.59
51:r:22:GLU:OE2	51:r:25:ARG:NH2	2.35	0.59
60:4:211:LEU:HD13	60:4:552:GLY:HA3	1.85	0.59
2:1:3233:C:H2'	2:1:3234:A:C8	2.38	0.59
1:A:104:LEU:CD1	1:A:158:ILE:CD1	2.79	0.59
2:1:799:G:O2'	19:L:18:TRP:NE1	2.36	0.59
2:1:1566:A:H2	50:q:432:ARG:HB2	1.67	0.59
41:h:9:LEU:HA	41:h:12:LYS:HZ3	1.68	0.58
60:4:75:ARG:NH2	60:4:575:MET:SD	2.76	0.58
39:f:56:SER:O	39:f:63:LYS:NZ	2.35	0.58
2:1:498:A:OP1	39:f:86:ARG:NH1	2.35	0.58
25:R:98:ARG:NH2	25:R:130:ASN:OD1	2.32	0.58
1:A:21:ARG:HD3	2:1:824:C:H5''	1.86	0.58
2:1:86:G:N2	2:1:99:A:OP2	2.34	0.58
2:1:2894:C:OP1	15:H:168:ARG:NH1	2.37	0.58
16:I:83:VAL:O	54:u:47:ARG:NH2	2.37	0.58
29:V:30:GLY:O	29:V:32:ARG:NH1	2.36	0.58
60:4:423:MET:HE1	60:4:432:CYS:HB2	1.85	0.58
2:1:1261:G:H4'	2:1:1278:A:H2	1.68	0.58
2:1:1481:A:N3	2:1:1858:A:O2'	2.36	0.58
18:K:84:ASN:ND2	18:K:86:LYS:O	2.36	0.58
2:1:2764:C:N3	2:1:2794:G:C2	2.72	0.58
18:K:75:LYS:HE2	18:K:285:ARG:HG3	1.86	0.58
60:4:362:ARG:NH1	60:4:363:ASP:O	2.37	0.58
2:1:305:U:OP1	2:1:2777:G:N2	2.37	0.58
11:D:163:LEU:CD1	11:D:173:VAL:CG1	2.79	0.58
46:m:4:GLY:O	46:m:13:ARG:NH1	2.35	0.58
2:1:655:C:H2'	2:1:656:A:H8	1.68	0.57
2:1:3045:G:OP1	9:B:19:ARG:NH2	2.36	0.57
30:W:188:VAL:O	30:W:199:GLN:NE2	2.34	0.57
55:v:50:SER:HB2	55:v:57:MET:HG3	1.86	0.57
2:1:2160:G:H2'	2:1:2161:G:H8	1.68	0.57
57:x:78:THR:CG2	57:x:124:ARG:HG3	2.33	0.57
1:A:80:GLU:HG3	49:p:66:GLY:HA2	1.86	0.57
2:1:2396:G:H2'	2:1:2398:A:H5'	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:36:C:OP2	5:5:110:ARG:NH2	2.37	0.57
35:b:497:ARG:NH2	54:u:123:ASP:OD1	2.33	0.57
35:b:264:ILE:HD12	35:b:302:ARG:HD3	1.86	0.57
53:t:77:ARG:NH2	53:t:303:ASN:OD1	2.38	0.57
6:6:32:A:H4'	18:K:285:ARG:HH12	1.69	0.57
18:K:75:LYS:HA	18:K:284:ASN:HB3	1.86	0.57
57:x:406:ASN:ND2	57:x:448:TYR:O	2.37	0.57
2:1:711:A:OP1	34:a:65:GLN:NE2	2.38	0.57
34:a:100:PRO:HG2	34:a:123:VAL:HG12	1.85	0.57
1:A:7:ASN:OD1	1:A:10:LYS:NZ	2.38	0.57
2:1:595:G:OP1	13:F:33:ARG:NH2	2.37	0.57
55:v:205:LYS:HB2	55:v:226:ILE:HD12	1.87	0.57
2:1:100:A:H2'	2:1:101:G:N3	2.20	0.56
55:v:226:ILE:O	55:v:226:ILE:HG22	2.05	0.56
56:w:19:VAL:HG12	56:w:20:VAL:N	2.20	0.56
2:1:1305:U:O4	9:B:256:HIS:ND1	2.32	0.56
2:1:2220:A2M:HM'2	2:1:2221:G:H5'	1.87	0.56
2:1:2966:G:O6	46:m:31:ARG:NH2	2.38	0.56
46:m:400:ILE:HG13	46:m:428:ILE:HD11	1.87	0.56
47:n:179:VAL:HG21	47:n:379:LEU:HD11	1.87	0.56
59:z:82:ASP:OD2	59:z:84:ARG:NH1	2.39	0.56
60:4:319:ILE:O	60:4:504:CYS:HA	2.04	0.56
3:2:12:A:OP1	23:P:3:ARG:NH1	2.39	0.56
2:1:1717:U:H2'	2:1:1718:G:C8	2.41	0.56
50:q:214:VAL:CG1	50:q:215:LYS:H	2.18	0.56
9:B:85:VAL:HG22	9:B:202:THR:HG22	1.88	0.56
55:v:106:PHE:HB3	55:v:244:MET:HE2	1.87	0.56
60:4:338:GLU:OE1	60:4:441:ARG:NH1	2.36	0.56
2:1:3343:G:O2'	2:1:3362:A:N6	2.39	0.56
57:x:210:ILE:HB	57:x:225:LEU:HB2	1.87	0.56
2:1:2681:U:H2'	2:1:2682:C:H6	1.70	0.56
6:6:51:U:O2'	6:6:54:A:N7	2.37	0.55
13:F:95:ILE:O	13:F:100:ARG:NH2	2.39	0.55
2:1:2403:G:H2'	2:1:2404:A:H8	1.71	0.55
10:C:69:ARG:HD2	35:b:636:SER:HA	1.88	0.55
24:Q:100:THR:HG22	24:Q:120:GLU:HG2	1.87	0.55
57:x:470:VAL:HB	57:x:480:VAL:HG12	1.88	0.55
47:n:178:LYS:HB2	47:n:189:GLN:HB3	1.87	0.55
35:b:570:GLN:NE2	60:4:260:ALA:O	2.35	0.55
46:m:104:TYR:HA	55:v:275:ILE:HD11	1.87	0.55
2:1:3165:A:H62	2:1:3285:C:H42	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:228:U:H3'	53:t:46:LYS:HE2	1.87	0.55
17:J:47:GLN:HG3	17:J:67:VAL:HG12	1.87	0.55
18:K:82:VAL:HB	18:K:244:LEU:HB3	1.89	0.55
10:C:20:LEU:HD11	10:C:252:GLU:HG3	1.87	0.55
17:J:101:ASN:HD22	17:J:131:MET:H	1.54	0.55
55:v:153:VAL:HG22	55:v:237:ILE:CD1	2.36	0.55
57:x:61:GLU:OE2	57:x:65:ASN:ND2	2.36	0.55
6:6:58:G:OP1	6:6:58:G:N2	2.39	0.55
53:t:206:SER:O	53:t:210:LYS:HB2	2.06	0.55
31:X:34:LEU:HD12	31:X:35:PRO:HD2	1.89	0.55
51:r:2:PRO:HB2	51:r:6:TYR:CG	2.41	0.55
2:1:1940:G:H21	2:1:3362:A:H8	1.53	0.55
12:E:65:ILE:HD12	12:E:79:VAL:HG22	1.87	0.55
40:g:42:PRO:HB2	40:g:51:LEU:HD12	1.88	0.55
13:F:48:ASN:ND2	13:F:182:ASP:OD2	2.40	0.54
2:1:99:A:H2'	2:1:100:A:C8	2.42	0.54
2:1:3217:C:N3	23:P:182:ILE:HG23	2.22	0.54
10:C:3:ARG:NE	10:C:22:LEU:O	2.39	0.54
47:n:218:MET:HE1	50:q:416:LEU:HD22	1.89	0.54
51:r:140:GLY:O	51:r:143:ARG:NH1	2.40	0.54
27:T:88:ARG:NH1	56:w:172:GLU:OE2	2.40	0.54
56:w:19:VAL:CG1	56:w:29:PHE:O	2.39	0.54
58:y:123:ARG:NH1	58:y:126:GLU:OE1	2.40	0.54
2:1:283:G:H2'	2:1:284:A:C8	2.43	0.54
23:P:56:ARG:NH2	23:P:75:GLU:OE2	2.33	0.54
23:P:120:ASN:OD1	23:P:145:HIS:HB2	2.07	0.54
41:h:102:GLU:OE2	41:h:105:ARG:NH2	2.36	0.54
47:n:141:LEU:HD21	50:q:416:LEU:HD23	1.90	0.54
53:t:197:GLY:HA3	53:t:314:ILE:HB	1.88	0.54
57:x:230:LYS:HB3	57:x:256:LYS:HB3	1.88	0.54
58:y:129:ILE:HG23	58:y:133:LEU:HD12	1.88	0.54
34:a:132:LYS:NZ	34:a:136:GLU:OE2	2.39	0.54
2:1:1097:G:O5'	27:T:129:LYS:NZ	2.41	0.54
17:J:163:PHE:HE1	17:J:169:ALA:HB3	1.72	0.54
30:W:82:GLU:HG2	30:W:83:GLU:HG3	1.90	0.54
2:1:2418:G:N7	46:m:13:ARG:NH2	2.56	0.54
6:6:5:C:N4	6:6:24:A:OP2	2.38	0.54
9:B:19:ARG:NH1	9:B:232:ARG:O	2.40	0.54
30:W:86:LYS:NZ	30:W:223:ASN:OD1	2.40	0.54
1:A:112:ILE:HD13	49:p:79:VAL:HG22	1.90	0.54
2:1:394:G:N1	2:1:397:A:OP2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:36:U:O3'	18:K:277:ARG:NH1	2.40	0.54
17:J:91:LEU:HD12	17:J:95:ASN:HD22	1.72	0.54
55:v:54:LYS:HB3	55:v:57:MET:HE3	1.90	0.54
2:1:2966:G:H2'	2:1:2967:A:C8	2.43	0.54
17:J:156:LYS:O	17:J:159:THR:CG2	2.54	0.54
2:1:1667:A:H2'	2:1:1668:G:C8	2.42	0.53
10:C:328:ASN:OD1	13:F:48:ASN:ND2	2.38	0.53
34:a:82:ILE:O	34:a:87:ARG:NH2	2.40	0.53
36:c:30:THR:HG23	36:c:91:SER:HB2	1.90	0.53
58:y:28:VAL:HG12	58:y:50:HIS:HB3	1.89	0.53
2:1:1253:U:H5'	2:1:1254:C:H5'	1.90	0.53
2:1:2514:U:OP2	2:1:2586:G:N2	2.37	0.53
18:K:97:LEU:HD11	18:K:205:THR:HB	1.90	0.53
32:Y:71:SER:N	32:Y:81:GLN:O	2.39	0.53
57:x:258:GLY:HA2	57:x:281:VAL:HG23	1.90	0.53
57:x:301:VAL:HG21	57:x:376:THR:HG21	1.89	0.53
4:3:100:C:OP2	55:v:95:LYS:NZ	2.36	0.53
25:R:105:LEU:HD22	25:R:135:LYS:HG3	1.88	0.53
53:t:102:LYS:HB2	53:t:131:GLU:HG3	1.90	0.53
2:1:1256:G:H4'	7:8:127:SER:HB2	1.90	0.53
2:1:1621:A:H2'	2:1:1622:U:C6	2.44	0.53
3:2:66:A:OP1	41:h:10:ARG:NH2	2.41	0.53
4:3:78:U:H2'	4:3:79:A:H8	1.74	0.53
30:W:42:VAL:HG23	30:W:218:SER:HB3	1.90	0.53
30:W:224:ASP:OD1	30:W:225:SER:N	2.42	0.53
34:a:76:ASP:HB3	34:a:116:GLY:HA3	1.91	0.53
56:w:163:ASP:HB3	56:w:166:VAL:HG23	1.91	0.53
2:1:2094:C:H2'	2:1:2095:G:H8	1.74	0.53
2:1:2679:A:H2'	17:J:57:PHE:HE2	1.74	0.53
7:8:15:LEU:C	7:8:15:LEU:HD12	2.34	0.53
14:G:228:GLU:HA	14:G:231:LYS:HE2	1.91	0.53
16:I:80:LEU:O	16:I:116:LYS:NZ	2.36	0.53
16:I:94:ALA:HB2	54:u:10:SER:HB3	1.91	0.53
18:K:129:ASP:HB3	18:K:158:LYS:HE2	1.90	0.53
57:x:136:SER:N	57:x:512:LEU:O	2.41	0.53
57:x:158:ARG:NH2	57:x:172:ASP:OD1	2.41	0.53
2:1:619:A:OP1	23:P:167:ARG:NH1	2.37	0.53
2:1:1192:C:C4	52:s:6:ARG:HB2	2.44	0.53
10:C:156:LEU:HD12	10:C:159:ILE:HD12	1.91	0.53
57:x:61:GLU:O	57:x:65:ASN:ND2	2.42	0.53
57:x:418:VAL:CG2	57:x:452:TRP:CZ2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:y:126:GLU:HG2	58:y:137:VAL:HG11	1.89	0.53
2:1:1778:G:O2'	2:1:1780:G:OP2	2.26	0.53
47:n:364:VAL:HG22	47:n:386:ASN:HB2	1.91	0.53
1:A:180:LEU:HD11	49:p:26:VAL:HG21	1.91	0.53
38:e:79:VAL:HG13	38:e:111:ARG:HG2	1.91	0.53
57:x:40:ASP:N	57:x:40:ASP:OD1	2.42	0.53
60:4:507:ILE:HD12	60:4:522:LEU:HD11	1.90	0.53
2:1:1197:A:H1'	52:s:16:LYS:HG3	1.91	0.53
2:1:1786:G:H2'	2:1:1787:A:C8	2.44	0.53
4:3:89:G:N2	4:3:92:A:OP1	2.42	0.53
2:1:3067:C:H3'	25:R:62:ARG:HH22	1.74	0.52
15:H:90:MET:HE2	15:H:179:ILE:HG22	1.92	0.52
2:1:674:G:O6	24:Q:56:LYS:NZ	2.43	0.52
2:1:3157:U:H4'	2:1:3158:G:H5'	1.91	0.52
17:J:164:LYS:HE2	17:J:170:ASP:HA	1.92	0.52
18:K:282:LYS:HB3	18:K:288:VAL:HG12	1.90	0.52
60:4:191:MET:HE1	60:4:319:ILE:HB	1.92	0.52
18:K:102:VAL:HA	18:K:265:LEU:HD23	1.91	0.52
2:1:361:A:O3'	43:j:45:ARG:NH2	2.41	0.52
2:1:3295:A:H2'	2:1:3296:A:C8	2.45	0.52
48:o:95:VAL:HG12	48:o:164:VAL:HG22	1.90	0.52
57:x:282:SER:N	57:x:295:GLY:O	2.42	0.52
58:y:107:VAL:HG23	58:y:108:ILE:HG13	1.92	0.52
10:C:362:ASP:OD2	26:S:125:LYS:NZ	2.42	0.52
45:l:5:LYS:HE2	45:l:13:MET:HE1	1.91	0.52
57:x:339:PHE:HE1	57:x:345:LYS:HG2	1.74	0.52
4:3:103:A:H2'	4:3:104:A:H8	1.74	0.52
26:S:79:VAL:HG11	26:S:106:LEU:HD21	1.91	0.52
47:n:409:HIS:HD2	47:n:427:ILE:HD11	1.75	0.52
26:S:77:VAL:HG11	26:S:106:LEU:HD22	1.92	0.52
2:1:1348:U:OP1	24:Q:38:ARG:NH2	2.43	0.52
46:m:282:PRO:HG2	55:v:275:ILE:CD1	2.38	0.52
37:d:55:LEU:HB2	37:d:95:PRO:HD3	1.92	0.52
42:i:45:ARG:NH2	42:i:89:GLU:OE2	2.40	0.52
46:m:177:LEU:O	46:m:180:THR:OG1	2.27	0.52
58:y:114:VAL:HG12	58:y:115:ALA:N	2.25	0.52
2:1:646:A:H1'	2:1:2375:G:C6	2.44	0.52
2:1:1696:A:H2'	2:1:1697:A:C8	2.45	0.52
2:1:3275:U:O2'	39:f:99:ARG:NH1	2.42	0.51
6:6:32:A:O2'	18:K:285:ARG:NH1	2.43	0.51
36:c:17:VAL:HG11	36:c:92:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:n:206:PRO:HG2	53:t:228:VAL:HB	1.93	0.51
47:n:368:SER:HB2	47:n:412:VAL:HG12	1.92	0.51
2:1:2793:OMG:C2	2:1:2794:G:H1'	2.45	0.51
2:1:3343:G:H21	2:1:3362:A:H2	1.58	0.51
4:3:100:C:O2'	55:v:70:GLU:OE2	2.27	0.51
7:8:92:ARG:O	7:8:96:LYS:NZ	2.42	0.51
35:b:5:TRP:CD1	35:b:69:PRO:HG3	2.45	0.51
39:f:14:LEU:HD11	39:f:31:LYS:HB2	1.92	0.51
2:1:2364:G:H22	2:1:2396:G:H1'	1.76	0.51
6:6:59:C:H5''	48:o:175:LYS:HD2	1.92	0.51
57:x:192:VAL:HG12	57:x:203:THR:HG22	1.91	0.51
2:1:1219:C:O2'	2:1:1286:A:N1	2.43	0.51
2:1:3322:A:H2'	2:1:3323:A:C8	2.45	0.51
2:1:12:A:H2'	2:1:13:A:C8	2.46	0.51
2:1:3121:U:H1'	2:1:3122:A:H5''	1.91	0.51
35:b:371:ASP:OD1	35:b:373:LYS:NZ	2.38	0.51
2:1:733:G:N2	2:1:736:A:OP2	2.36	0.51
3:2:154:C:H5''	14:G:181:LYS:HD2	1.93	0.51
46:m:166:GLU:OE2	46:m:170:LYS:NZ	2.43	0.51
56:w:22:ASP:OD2	56:w:25:ASN:ND2	2.43	0.51
18:K:108:LYS:HE3	18:K:230:TYR:HE2	1.76	0.51
30:W:79:GLU:HG3	30:W:80:LYS:HG3	1.92	0.51
4:3:39:C:C6	17:J:46:VAL:HG23	2.42	0.51
6:6:7:C:H5	6:6:21:G:H1	1.57	0.51
28:U:54:VAL:HG22	28:U:67:SER:CB	2.41	0.51
2:1:1639:C:OP2	40:g:74:ARG:NH1	2.43	0.50
2:1:1899:G:O2'	2:1:2334:U:O4	2.25	0.50
2:1:2689:A:O2'	2:1:2690:G:N2	2.44	0.50
2:1:2898:G:H22	51:r:7:ILE:H	1.57	0.50
2:1:2901:G:O2'	2:1:3024:A:N1	2.42	0.50
33:Z:5:LEU:HD11	36:c:35:ARG:HD2	1.92	0.50
36:c:74:ASN:OD1	36:c:74:ASN:N	2.44	0.50
55:v:113:MET:HB2	55:v:238:HIS:HB3	1.93	0.50
57:x:276:GLY:H	57:x:304:TRP:HH2	1.58	0.50
11:D:108:ARG:HE	11:D:253:PHE:HB2	1.76	0.50
46:m:390:VAL:HG12	46:m:451:LYS:HG2	1.93	0.50
60:4:42:VAL:HG21	60:4:141:ILE:HG21	1.94	0.50
2:1:655:C:H2'	2:1:656:A:C8	2.45	0.50
2:1:2250:G:H1	2:1:2266:PSU:HN3	1.59	0.50
2:1:2367:A:H2'	2:1:2368:A:C8	2.46	0.50
2:1:2659:G:OP1	55:v:14:ARG:NH2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:n:393:MET:O	47:n:396:ILE:HG13	2.11	0.50
2:1:173:G:O6	2:1:245:U:O4	2.30	0.50
2:1:643:U:H3'	2:1:644:G:C8	2.46	0.50
35:b:80:ASP:OD2	35:b:245:HIS:NE2	2.37	0.50
58:y:118:HIS:HB3	58:y:121:ILE:HG23	1.94	0.50
2:1:1347:U:H2'	2:1:1355:A:H61	1.76	0.50
26:S:80:ARG:HG2	26:S:124:LEU:HD11	1.94	0.50
49:p:46:THR:OG1	49:p:57:CYS:SG	2.64	0.50
55:v:87:MET:HB2	55:v:103:ILE:HB	1.92	0.50
4:3:44:C:H4'	11:D:152:ARG:HG3	1.93	0.50
39:f:49:ILE:HD11	39:f:71:VAL:HG22	1.94	0.49
50:q:214:VAL:CG1	50:q:215:LYS:N	2.75	0.49
55:v:102:PHE:HB2	55:v:114:ILE:HG22	1.93	0.49
2:1:900:G:H1'	2:1:1589:A:N6	2.27	0.49
9:B:92:TYR:HB2	9:B:157:VAL:HB	1.94	0.49
23:P:33:ALA:HB1	23:P:117:ILE:HG12	1.94	0.49
25:R:10:LEU:O	25:R:14:VAL:HG23	2.12	0.49
2:1:3347:A:H2'	2:1:3348:G:C8	2.48	0.49
9:B:67:PHE:HA	9:B:70:ARG:HD2	1.93	0.49
17:J:148:VAL:HG12	17:J:149:GLY:N	2.27	0.49
36:c:24:THR:HG22	36:c:91:SER:HB3	1.94	0.49
1:A:181:LYS:HB2	1:A:184:ARG:HG3	1.93	0.49
22:O:12:LYS:O	26:S:167:ARG:NH2	2.39	0.49
53:t:85:LYS:HD3	53:t:96:GLY:HA2	1.94	0.49
57:x:205:SER:OG	57:x:206:MET:N	2.45	0.49
2:1:2949:U:H2'	2:1:2950:G:C8	2.48	0.49
2:1:3153:U:OP2	2:1:3293:U:O2'	2.29	0.49
55:v:226:ILE:CG2	55:v:226:ILE:O	2.60	0.49
56:w:19:VAL:HG22	56:w:30:ASP:CB	2.42	0.49
2:1:501:A:H2'	2:1:502:U:C6	2.47	0.49
57:x:426:ILE:HB	57:x:440:PHE:HB2	1.95	0.49
2:1:708:G:O6	34:a:63:LYS:NZ	2.45	0.49
2:1:1596:C:H2'	2:1:1597:C:C6	2.48	0.49
8:9:147:LEU:HD12	60:4:279:LEU:HD13	1.95	0.49
26:S:27:MET:HE2	27:T:151:LEU:HD11	1.95	0.49
30:W:144:SER:OG	30:W:154:ASP:OD1	2.31	0.49
30:W:162:GLU:OE1	30:W:166:ARG:NH1	2.46	0.49
46:m:282:PRO:CG	55:v:275:ILE:HD11	2.42	0.49
55:v:139:PRO:HB3	55:v:180:HIS:NE2	2.27	0.49
2:1:110:G:OP2	19:L:73:ARG:NH2	2.38	0.49
46:m:301:GLN:OE1	46:m:305:GLN:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:n:410:GLN:HG2	47:n:412:VAL:HG13	1.95	0.49
2:1:2180:G:H2'	2:1:2181:C:C6	2.48	0.49
57:x:487:ASP:HB3	57:x:506:LYS:HB2	1.95	0.49
58:y:142:ILE:HG13	58:y:148:VAL:HG12	1.95	0.49
60:4:316:VAL:HG22	60:4:508:VAL:HG22	1.95	0.49
2:1:567:G:H2'	2:1:568:G:C8	2.48	0.48
2:1:2522:G:O2'	2:1:2524:A:OP2	2.26	0.48
2:1:2724:OMU:OP2	55:v:258:LYS:NZ	2.44	0.48
2:1:2940:A:H2'	9:B:255:TRP:HB3	1.94	0.48
16:I:15:THR:O	54:u:43:ARG:NH2	2.45	0.48
26:S:13:ARG:NH2	26:S:50:LYS:O	2.46	0.48
39:f:90:PRO:HB2	39:f:92:LYS:HG2	1.95	0.48
60:4:224:ARG:NH2	60:4:267:VAL:HG23	2.27	0.48
2:1:2761:G:H1	2:1:2799:A:N6	2.11	0.48
10:C:126:ILE:O	10:C:129:THR:OG1	2.27	0.48
17:J:54:VAL:HG12	17:J:57:PHE:H	1.77	0.48
19:L:123:ILE:HG22	41:h:118:ILE:HG12	1.94	0.48
35:b:107:GLN:NE2	35:b:111:ASP:OD1	2.45	0.48
2:1:662:U:H2'	2:1:663:OMC:C6	2.48	0.48
29:V:71:LYS:O	29:V:72:LYS:HG3	2.13	0.48
53:t:280:PHE:O	53:t:285:ARG:NH1	2.45	0.48
2:1:33:G:H5''	21:N:73:ARG:HH21	1.78	0.48
62:1:3478:B3P:O5	62:1:3478:B3P:O4	2.31	0.48
11:D:146:LEU:HD22	11:D:163:LEU:HD22	1.94	0.48
2:1:1437:OMC:HM22	10:C:93:MET:HG3	1.95	0.48
2:1:2768:U:H2'	2:1:2769:A:H8	1.77	0.48
6:6:228:U:O2'	53:t:49:ARG:NH1	2.46	0.48
10:C:292:SER:OG	10:C:294:GLU:OE1	2.31	0.48
11:D:69:ILE:HG13	11:D:70:THR:HG23	1.96	0.48
2:1:339:C:OP1	2:1:1380:G:O2'	2.29	0.48
2:1:541:U:H2'	2:1:542:G:H8	1.78	0.48
2:1:664:U:H2'	2:1:665:A:H8	1.78	0.48
53:t:208:ILE:HD12	53:t:251:ILE:HG12	1.95	0.48
2:1:29:C:H4'	2:1:62:A:H4'	1.96	0.48
2:1:1805:C:H2'	2:1:1806:A:H8	1.79	0.48
4:3:87:G:H2'	4:3:88:G:C8	2.46	0.48
6:6:28:A:OP1	48:o:125:ASN:ND2	2.45	0.48
36:c:9:SER:OG	36:c:10:ILE:N	2.47	0.48
46:m:224:VAL:O	46:m:318:VAL:HA	2.14	0.48
2:1:1841:A:H1'	45:l:45:ARG:HH22	1.78	0.48
34:a:71:PRO:HG2	34:a:109:TYR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:x:161:THR:HB	57:x:171:TRP:HE1	1.79	0.48
2:1:791:A:OP1	10:C:108:LYS:NZ	2.42	0.48
2:1:2242:A:O2'	2:1:2244:A:OP1	2.31	0.48
2:1:2797:C:OP1	56:w:197:ARG:NH1	2.41	0.48
2:1:3050:U:O2'	54:u:16:GLY:O	2.24	0.48
2:1:3295:A:H2'	2:1:3296:A:H8	1.79	0.48
9:B:41:VAL:HA	9:B:185:GLY:HA3	1.94	0.48
60:4:96:ASP:HB2	60:4:140:LYS:HE2	1.96	0.48
2:1:1288:U:H2'	2:1:1289:G:H8	1.79	0.48
2:1:2685:C:H2'	2:1:2686:A:C8	2.49	0.48
2:1:2744:U:H2'	2:1:2745:G:C8	2.49	0.48
2:1:2821:C:OP1	2:1:2822:U:O2'	2.31	0.48
2:1:2862:U:H1'	35:b:92:LYS:HE3	1.96	0.48
2:1:2899:C:O2'	2:1:2901:G:OP2	2.32	0.48
2:1:3113:A:OP1	15:H:73:SER:OG	2.29	0.48
3:2:9:A:H2'	3:2:10:A:C8	2.49	0.48
3:2:135:G:H5''	31:X:49:LYS:HD3	1.96	0.48
33:Z:25:ILE:HA	33:Z:43:VAL:HG12	1.95	0.48
47:n:41:ILE:HD13	50:q:207:LEU:HD21	1.95	0.48
55:v:53:LYS:HE3	55:v:56:ASP:HB2	1.96	0.48
2:1:428:A:H2'	2:1:429:U:C6	2.49	0.47
2:1:1281:G:H2'	2:1:1282:G:H8	1.79	0.47
2:1:1534:A:H2'	2:1:1535:A:C8	2.49	0.47
17:J:86:VAL:HG21	17:J:112:LEU:HD23	1.96	0.47
29:V:77:ILE:HD12	29:V:109:MET:HE1	1.95	0.47
34:a:94:ALA:HB2	34:a:121:VAL:HG22	1.96	0.47
47:n:428:GLN:NE2	47:n:448:LEU:O	2.42	0.47
2:1:3348:G:H1	2:1:3357:U:H3	1.61	0.47
58:y:15:VAL:HA	58:y:61:ARG:HG2	1.95	0.47
2:1:283:G:H2'	2:1:284:A:H8	1.78	0.47
56:w:38:ASP:HA	56:w:43:ASN:HD22	1.78	0.47
2:1:1221:A:H61	30:W:24:GLU:HG2	1.79	0.47
13:F:224:ILE:HD11	26:S:35:VAL:HG12	1.97	0.47
24:Q:62:VAL:HG13	24:Q:66:ARG:HD2	1.96	0.47
55:v:132:THR:HG22	55:v:226:ILE:HD13	1.96	0.47
2:1:2994:A:O2'	3:2:1:A:N1	2.43	0.47
9:B:171:LEU:HD21	9:B:333:LYS:HB2	1.97	0.47
35:b:506:GLU:HA	37:d:97:LEU:HD13	1.96	0.47
47:n:126:PRO:HB2	47:n:130:ARG:HH21	1.79	0.47
53:t:180:THR:H	53:t:183:VAL:HB	1.78	0.47
2:1:1666:G:H2'	2:1:1667:A:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2568:C:O2'	2:1:2569:A:O4'	2.32	0.47
7:8:63:LYS:HG3	7:8:70:ALA:HB3	1.95	0.47
8:9:8:ASN:O	22:O:103:LYS:NZ	2.48	0.47
9:B:202:THR:O	59:z:44:GLN:NE2	2.37	0.47
27:T:36:VAL:HG13	27:T:65:TYR:HA	1.97	0.47
37:d:11:GLU:OE2	37:d:74:ARG:NH2	2.46	0.47
46:m:417:GLU:HB2	46:m:434:LYS:HE3	1.96	0.47
47:n:249:ASP:HB3	47:n:252:LYS:HB2	1.96	0.47
56:w:19:VAL:CG1	56:w:20:VAL:N	2.77	0.47
60:4:466:LEU:HB3	60:4:469:PRO:HD2	1.95	0.47
2:1:563:U:H2'	2:1:564:G:H8	1.79	0.47
2:1:1194:G:H2'	2:1:1195:A:C8	2.49	0.47
2:1:2357:A:H2'	2:1:2358:A:C8	2.50	0.47
3:2:63:G:H22	3:2:97:A:H2	1.62	0.47
11:D:141:PRO:HD2	56:w:86:VAL:HG21	1.97	0.47
46:m:282:PRO:HG2	55:v:275:ILE:HD11	1.97	0.47
47:n:380:ILE:O	47:n:383:CYS:C	2.57	0.47
53:t:139:PRO:HA	53:t:179:LEU:O	2.15	0.47
2:1:1277:C:HO2'	2:1:1278:A:H8	1.60	0.47
2:1:2108:C:H1'	2:1:3344:A:H8	1.79	0.47
2:1:2357:A:H2'	2:1:2358:A:H8	1.80	0.47
3:2:49:G:O2'	41:h:39:PRO:O	2.31	0.47
4:3:78:U:H2'	4:3:79:A:C8	2.50	0.47
13:F:86:VAL:O	13:F:114:GLY:HA2	2.14	0.47
26:S:80:ARG:CG	26:S:124:LEU:HD11	2.45	0.47
2:1:646:A:H1'	2:1:2375:G:N1	2.30	0.47
2:1:710:A:H2'	2:1:711:A:C8	2.49	0.47
2:1:1645:U:O2'	47:n:50:LYS:NZ	2.46	0.47
2:1:2426:U:O4	2:1:2603:G:O6	2.32	0.47
15:H:5:GLN:HE22	15:H:7:GLU:HB3	1.80	0.47
35:b:403:GLU:HG3	35:b:412:PHE:HB3	1.97	0.47
46:m:353:TRP:HA	46:m:366:ASP:O	2.15	0.47
2:1:643:U:H3'	2:1:644:G:H8	1.79	0.46
2:1:1138:U:H2'	2:1:1139:G:H8	1.80	0.46
2:1:1301:A:O2'	2:1:1302:A:O4'	2.30	0.46
23:P:122:ALA:HB3	23:P:143:PRO:HB2	1.97	0.46
35:b:370:ASP:OD2	35:b:374:ARG:NH2	2.46	0.46
47:n:251:LYS:HA	47:n:254:LYS:HE3	1.96	0.46
57:x:255:SER:OG	57:x:257:ASP:OD1	2.25	0.46
57:x:378:SER:OG	57:x:379:ASP:N	2.48	0.46
2:1:798:G:H21	19:L:15:ARG:NH2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:23:VAL:HG12	33:Z:45:GLY:HA3	1.97	0.46
2:1:358:G:N2	2:1:361:A:OP2	2.42	0.46
2:1:3027:A:H62	35:b:162:SER:H	1.63	0.46
2:1:3283:U:O2'	2:1:3284:G:OP1	2.30	0.46
2:1:3302:U:H3	2:1:3312:U:H3	1.62	0.46
4:3:16:U:H2'	4:3:17:A:H8	1.79	0.46
37:d:36:ILE:HD12	37:d:59:ILE:HD11	1.97	0.46
43:j:14:LYS:HD3	45:l:51:ILE:HD11	1.97	0.46
55:v:112:ASP:HB3	55:v:240:PRO:HD3	1.96	0.46
57:x:187:ASN:HB3	57:x:206:MET:HB3	1.98	0.46
58:y:116:LEU:HG	58:y:177:LEU:HD21	1.97	0.46
2:1:1290:A:H2'	2:1:1291:A:C8	2.50	0.46
28:U:94:ARG:HB3	28:U:108:TYR:CZ	2.50	0.46
48:o:127:LYS:HA	48:o:182:ARG:HD3	1.96	0.46
2:1:2317:A:H5''	2:1:2318:U:H3'	1.96	0.46
2:1:2427:U:H3	2:1:2602:G:H1	1.63	0.46
2:1:2717:U:OP2	2:1:2753:G:O2'	2.27	0.46
4:3:23:A:HO2'	4:3:121:U:HO3'	1.57	0.46
16:I:127:LEU:O	16:I:131:LEU:HB2	2.15	0.46
55:v:143:PHE:HB2	56:w:29:PHE:HD1	1.81	0.46
2:1:2585:G:OP1	50:q:452:LYS:NZ	2.43	0.46
10:C:166:VAL:O	10:C:170:LYS:HG2	2.15	0.46
17:J:23:VAL:HG11	17:J:30:LEU:HB2	1.98	0.46
57:x:468:LEU:HD21	57:x:503:SER:HB3	1.98	0.46
1:A:9:ARG:NH2	2:1:912:G:OP2	2.42	0.46
1:A:128:ARG:HG3	2:1:2177:G:H2'	1.97	0.46
2:1:585:A:H2'	2:1:586:C:C6	2.50	0.46
2:1:1659:U:H2'	2:1:1660:C:C6	2.51	0.46
2:1:2871:G:OP1	35:b:117:LYS:NZ	2.41	0.46
51:r:205:GLN:HB2	51:r:209:TYR:HD2	1.81	0.46
60:4:325:SER:HB3	60:4:499:PRO:HG2	1.96	0.46
58:y:200:ASN:OD1	58:y:203:LEU:N	2.48	0.46
1:A:69:TYR:OH	2:1:2557:A:OP1	2.29	0.46
2:1:1300:G:H5''	2:1:1301:A:H5'	1.98	0.46
2:1:2108:C:H1'	2:1:3344:A:C8	2.51	0.46
29:V:15:LEU:HD23	29:V:53:SER:HB3	1.98	0.46
35:b:71:ILE:HD12	35:b:82:MET:HE3	1.98	0.46
37:d:96:VAL:HG12	37:d:98:VAL:HG13	1.98	0.46
48:o:211:LEU:HD22	48:o:216:ILE:HD12	1.98	0.46
56:w:13:VAL:HG11	56:w:56:ASP:HB3	1.97	0.46
2:1:422:A:N1	2:1:2362:C:O2'	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:728:G:H5'	24:Q:43:PRO:HB2	1.96	0.45
2:1:1838:G:H5''	2:1:1839:A:H5'	1.98	0.45
2:1:2094:C:H2'	2:1:2095:G:C8	2.51	0.45
2:1:2748:A:H1'	11:D:36:LEU:HD23	1.97	0.45
2:1:2883:U:H2'	2:1:2884:C:H6	1.81	0.45
12:E:52:VAL:HB	12:E:65:ILE:CG2	2.47	0.45
57:x:175:THR:OG1	57:x:177:THR:OG1	2.33	0.45
2:1:1615:C:H2'	2:1:1616:U:C6	2.51	0.45
2:1:2227:C:H2'	2:1:2228:A:C8	2.51	0.45
2:1:2433:U:H1'	21:N:125:SER:HB3	1.98	0.45
15:H:8:GLN:HB3	15:H:72:LYS:HD2	1.98	0.45
58:y:68:ARG:NH2	58:y:112:ASP:O	2.45	0.45
46:m:104:TYR:C	55:v:275:ILE:HG12	2.40	0.45
53:t:241:ASP:OD1	53:t:241:ASP:N	2.49	0.45
1:A:104:LEU:HD11	1:A:158:ILE:CD1	2.44	0.45
2:1:1497:C:O2'	2:1:1602:A:N3	2.47	0.45
2:1:1555:U:O2'	2:1:1556:C:H2'	2.17	0.45
2:1:1568:U:H4'	2:1:1569:U:O5'	2.16	0.45
2:1:2129:PSU:H2'	2:1:2130:G:C8	2.51	0.45
2:1:2609:A:H2'	2:1:2610:G:C8	2.52	0.45
2:1:2685:C:H2'	2:1:2686:A:H8	1.82	0.45
3:2:158:U:H1'	53:t:151:LEU:HD21	1.98	0.45
35:b:385:LEU:HD11	58:y:43:GLY:HA3	1.98	0.45
60:4:484:LYS:HE3	60:4:488:LEU:HD21	1.99	0.45
2:1:531:G:H2'	2:1:532:A:C8	2.51	0.45
2:1:1718:G:H2'	2:1:1719:G:H8	1.81	0.45
2:1:2318:U:O2	46:m:461:LYS:NZ	2.50	0.45
2:1:2681:U:H2'	2:1:2682:C:C6	2.51	0.45
2:1:2831:G:H2'	2:1:2832:C:C6	2.51	0.45
12:E:170:LYS:HB3	12:E:172:HIS:CE1	2.51	0.45
14:G:75:ILE:CD1	21:N:18:VAL:HG13	2.45	0.45
46:m:49:ARG:NH2	46:m:53:GLY:O	2.46	0.45
55:v:90:MET:HE2	55:v:90:MET:HB2	1.85	0.45
2:1:1718:G:H2'	2:1:1719:G:C8	2.52	0.45
2:1:3153:U:H3	2:1:3293:U:H3	1.64	0.45
11:D:208:MET:HG3	11:D:219:PHE:HE1	1.82	0.45
35:b:302:ARG:HA	35:b:305:LEU:HD12	1.99	0.45
2:1:664:U:H2'	2:1:665:A:C8	2.51	0.45
2:1:681:U:O4	10:C:118:LYS:NZ	2.42	0.45
2:1:2516:U:O2'	2:1:2595:A:N6	2.47	0.45
2:1:2616:C:H5''	2:1:2617:U:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:131:ALA:HB2	30:W:195:LEU:HD21	1.97	0.45
31:X:67:ILE:HD12	31:X:121:LYS:HG3	1.97	0.45
48:o:149:GLN:HG3	48:o:166:VAL:HG23	1.98	0.45
2:1:1096:U:OP2	27:T:116:ARG:NH2	2.50	0.45
2:1:1740:U:H1'	2:1:1741:A:H2	1.81	0.45
2:1:2565:U:H3	2:1:2576:G:H1	1.65	0.45
2:1:3322:A:H2'	2:1:3323:A:H8	1.82	0.45
51:r:24:LYS:NZ	51:r:28:GLU:OE2	2.36	0.45
2:1:1117:G:H2'	2:1:1118:C:C6	2.51	0.45
2:1:1176:C:H2'	2:1:1177:G:N2	2.31	0.45
2:1:1666:G:H2'	2:1:1667:A:C8	2.52	0.45
2:1:2403:G:H2'	2:1:2404:A:C8	2.51	0.45
24:Q:123:THR:OG1	24:Q:125:ASP:OD1	2.32	0.45
60:4:142:THR:HG23	60:4:155:SER:HB2	1.98	0.45
60:4:331:LYS:NZ	60:4:446:ASP:OD2	2.42	0.45
2:1:163:C:H2'	2:1:164:A:C8	2.52	0.45
2:1:297:G:OP2	2:1:297:G:N2	2.43	0.45
2:1:831:G:O2'	2:1:1864:A:N3	2.45	0.45
2:1:1624:G:O2'	2:1:1643:A:N1	2.40	0.45
2:1:3185:U:O2'	26:S:170:THR:OG1	2.30	0.45
15:H:21:LYS:HG3	20:M:8:LYS:HG3	1.99	0.45
46:m:244:GLU:HA	46:m:247:LYS:HG2	1.98	0.45
46:m:287:HIS:HB3	46:m:294:PHE:HB3	1.98	0.45
1:A:117:GLU:HG2	1:A:124:GLY:H	1.82	0.44
2:1:806:A:H2'	2:1:807:A2M:C8	2.47	0.44
2:1:1597:C:H2'	2:1:1598:G:C8	2.52	0.44
2:1:3296:A:H2'	2:1:3297:U:H6	1.82	0.44
6:6:9:A:H5'	53:t:97:LYS:NZ	2.32	0.44
18:K:279:ILE:HB	18:K:292:TYR:HB3	2.00	0.44
37:d:9:THR:OG1	37:d:111:GLU:OE2	2.30	0.44
51:r:5:ASP:OD1	51:r:5:ASP:N	2.49	0.44
1:A:101:VAL:HG22	1:A:165:VAL:HG22	1.99	0.44
2:1:2213:A:H2'	2:1:2214:A:C8	2.52	0.44
2:1:3379:C:H4'	9:B:315:GLY:HA2	2.00	0.44
11:D:31:TYR:HA	11:D:34:LYS:HE3	1.99	0.44
17:J:164:LYS:HE3	17:J:171:VAL:HG23	2.00	0.44
30:W:55:GLU:OE2	30:W:121:ARG:NH2	2.39	0.44
56:w:40:ASP:OD1	56:w:41:SER:N	2.50	0.44
60:4:48:ASP:HA	60:4:52:SER:HB2	1.99	0.44
60:4:211:LEU:HG	60:4:222:LEU:HD11	1.99	0.44
2:1:226:C:H2'	2:1:227:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:275:U:H2'	2:1:276:U:C6	2.52	0.44
2:1:671:U:H2'	2:1:672:A:H8	1.83	0.44
2:1:1340:G:H2'	2:1:1341:U:C6	2.53	0.44
7:8:126:ALA:HA	7:8:162:ILE:HG13	1.99	0.44
34:a:91:LEU:HD23	34:a:121:VAL:HG21	1.98	0.44
42:i:34:SER:H	42:i:37:THR:HG22	1.83	0.44
54:u:50:LYS:HG3	54:u:55:PHE:CE2	2.52	0.44
60:4:95:ILE:HG23	60:4:139:VAL:HG13	2.00	0.44
2:1:627:U:H2'	2:1:628:A:C8	2.52	0.44
2:1:1528:G:O2'	2:1:1588:A:N3	2.49	0.44
2:1:2880:PSU:H1'	9:B:250:ALA:HB3	2.00	0.44
26:S:112:ALA:O	26:S:115:ARG:NH1	2.50	0.44
47:n:176:VAL:O	47:n:177:ARG:NH1	2.48	0.44
2:1:3096:C:H2'	2:1:3097:C:C6	2.53	0.44
33:Z:50:PRO:HD3	33:Z:68:ILE:HG12	2.00	0.44
2:1:411:U:H2'	2:1:412:G:H8	1.83	0.44
2:1:2272:G:C6	46:m:471:LYS:HB3	2.52	0.44
4:3:45:A:H2'	4:3:46:A:H8	1.83	0.44
19:L:180:ARG:NE	19:L:184:GLU:OE2	2.44	0.44
2:1:541:U:H2'	2:1:542:G:C8	2.53	0.44
2:1:1568:U:H5'	50:q:437:LYS:HE3	2.00	0.44
2:1:1622:U:H2'	2:1:1623:G:H8	1.83	0.44
2:1:3162:C:H2'	2:1:3163:A:C8	2.53	0.44
2:1:3209:A:C4	20:M:106:ARG:HD3	2.52	0.44
18:K:43:GLU:OE2	48:o:217:GLU:N	2.51	0.44
29:V:15:LEU:HD13	29:V:51:ALA:HB3	1.98	0.44
2:1:507:U:H2'	2:1:508:U:C6	2.53	0.44
16:I:96:TYR:OH	54:u:2:ARG:NH2	2.51	0.44
58:y:114:VAL:CG1	58:y:177:LEU:HD23	2.47	0.44
4:3:7:G:OP2	11:D:22:ARG:NH2	2.51	0.44
11:D:43:LYS:HD2	55:v:168:GLU:HG2	2.00	0.44
19:L:179:PHE:HD1	19:L:182:ILE:HD12	1.83	0.44
21:N:9:GLU:HB3	42:i:44:VAL:HG11	1.99	0.44
57:x:170:ILE:HB	57:x:180:HIS:HB2	2.00	0.44
1:A:2:GLY:N	2:1:2608:G:OP1	2.51	0.43
2:1:87:U:H2'	2:1:88:A:H8	1.83	0.43
2:1:436:A:H2'	2:1:437:G:H8	1.82	0.43
2:1:532:A:H61	2:1:560:G:H1	1.66	0.43
2:1:629:U:H2'	2:1:630:A:C8	2.53	0.43
2:1:2372:A:O2'	2:1:2821:C:OP2	2.29	0.43
2:1:2843:U:O2'	2:1:2845:A:OP2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:3026:G:H4'	51:r:2:PRO:HD3	2.00	0.43
2:1:3347:A:H2'	2:1:3348:G:H8	1.82	0.43
62:1:3478:B3P:H71	62:1:3478:B3P:H31	1.75	0.43
7:8:124:THR:HG22	7:8:126:ALA:H	1.82	0.43
11:D:211:LEU:HD11	11:D:222:LEU:HD12	2.00	0.43
57:x:321:HIS:CG	57:x:379:ASP:HB3	2.53	0.43
60:4:453:ASN:OD1	60:4:453:ASN:N	2.51	0.43
2:1:2344:U:H2'	2:1:2345:A:H8	1.82	0.43
2:1:2813:A:H2'	2:1:2814:G:O4'	2.18	0.43
2:1:2969:A:H2'	2:1:2970:C:O4'	2.18	0.43
13:F:144:ILE:HD12	13:F:189:ILE:HD13	1.99	0.43
18:K:280:PHE:HB3	18:K:288:VAL:HB	1.99	0.43
26:S:110:MET:HB3	26:S:116:ALA:HB3	1.99	0.43
35:b:290:THR:HG21	35:b:319:THR:HB	2.00	0.43
2:1:1389:G:OP1	38:e:104:ASN:ND2	2.49	0.43
2:1:1688:U:H2'	2:1:1689:U:C6	2.53	0.43
13:F:189:ILE:HG23	13:F:190:THR:HG23	2.01	0.43
19:L:162:ASN:OD1	19:L:162:ASN:N	2.51	0.43
21:N:155:VAL:O	21:N:162:ARG:NH2	2.42	0.43
23:P:126:ARG:HA	23:P:140:GLU:HG2	2.00	0.43
27:T:91:LEU:HG	56:w:159:LEU:HD13	2.00	0.43
35:b:588:ARG:HG2	45:l:21:ARG:CZ	2.48	0.43
2:1:1276:U:O2'	2:1:1277:C:H5'	2.19	0.43
2:1:2716:U:C4	56:w:131:LYS:HB3	2.53	0.43
14:G:172:LYS:HE2	42:i:43:LEU:HD13	2.01	0.43
18:K:338:ASN:HB3	53:t:266:PHE:CG	2.53	0.43
23:P:33:ALA:CA	23:P:36:ILE:HG22	2.48	0.43
2:1:209:A:H4'	2:1:211:A:N7	2.33	0.43
2:1:616:G:H2'	2:1:617:G:C8	2.53	0.43
2:1:1746:U:O2'	44:k:4:GLU:OE1	2.31	0.43
2:1:2683:U:H2'	2:1:2684:C:H6	1.84	0.43
2:1:3013:U:H2'	2:1:3014:U:C6	2.54	0.43
2:1:3192:U:H2'	2:1:3193:C:C6	2.53	0.43
9:B:325:LYS:HE3	9:B:325:LYS:HB2	1.80	0.43
24:Q:76:ALA:HA	24:Q:79:LYS:HD2	2.00	0.43
33:Z:33:SER:OG	33:Z:35:SER:O	2.27	0.43
55:v:72:MET:HB3	55:v:110:ILE:HG13	2.00	0.43
2:1:897:U:H2'	2:1:898:OMU:H6	2.00	0.43
2:1:1064:A:N6	2:1:1093:A:N7	2.66	0.43
7:8:15:LEU:HD23	7:8:28:LEU:HD21	2.01	0.43
15:H:41:ILE:HD13	15:H:67:ALA:HB1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:57:VAL:HG23	15:H:68:LEU:HD13	2.01	0.43
17:J:36:VAL:HG11	17:J:120:ILE:HG23	2.00	0.43
17:J:59:ILE:HG21	17:J:65:ILE:HD11	2.00	0.43
23:P:36:ILE:HD11	23:P:95:LEU:HD21	2.01	0.43
35:b:214:LEU:HD11	58:y:239:THR:HA	2.00	0.43
60:4:80:TYR:HA	60:4:83:LYS:HE2	1.99	0.43
60:4:270:THR:OG1	60:4:273:HIS:ND1	2.40	0.43
2:1:158:G:H2'	2:1:159:A:H8	1.84	0.43
2:1:407:A:C2	3:2:17:A:H1'	2.53	0.43
2:1:925:A:N1	2:1:2414:G:H2'	2.33	0.43
2:1:991:G:H1	2:1:1058:U:H3	1.66	0.43
2:1:2724:OMU:H1'	2:1:2724:OMU:HM23	1.71	0.43
2:1:2768:U:H2'	2:1:2769:A:C8	2.54	0.43
2:1:3245:A:H61	59:z:78:SER:HA	1.84	0.43
3:2:26:U:H2'	3:2:27:U:C6	2.53	0.43
31:X:133:LEU:HD11	60:4:421:LEU:HB2	2.00	0.43
44:k:5:ILE:HD11	44:k:11:PHE:HD1	1.83	0.43
46:m:303:LEU:HD22	46:m:318:VAL:HG21	2.01	0.43
46:m:396:PRO:HA	46:m:399:TYR:HD2	1.83	0.43
58:y:114:VAL:CG1	58:y:115:ALA:N	2.81	0.43
2:1:808:A:H61	2:1:932:U:H3	1.64	0.43
2:1:1498:A:H2'	2:1:1499:C:C6	2.54	0.43
2:1:2684:C:H2'	2:1:2685:C:C6	2.53	0.43
2:1:3162:C:H2'	2:1:3163:A:H8	1.83	0.43
3:2:79:A:C6	3:2:80:A:H1'	2.53	0.43
4:3:106:U:H2'	4:3:107:C:C6	2.53	0.43
17:J:50:ALA:N	17:J:63:GLU:O	2.51	0.43
25:R:43:LYS:O	25:R:47:ASN:ND2	2.52	0.43
30:W:186:TYR:CD2	30:W:188:VAL:HG22	2.52	0.43
57:x:305:ASP:HB2	57:x:313:ILE:HG12	2.01	0.43
58:y:101:LEU:HD12	58:y:121:ILE:HG22	1.99	0.43
2:1:1223:A:H2'	2:1:1224:C:H6	1.84	0.43
2:1:1278:A:O2'	30:W:15:THR:O	2.32	0.43
2:1:1597:C:H2'	2:1:1598:G:H8	1.83	0.43
2:1:2784:G:H2'	2:1:2785:A:C8	2.53	0.43
2:1:3160:U:H2'	2:1:3161:C:C6	2.54	0.43
46:m:104:TYR:HB3	55:v:275:ILE:HG13	2.01	0.43
57:x:261:LYS:HG2	57:x:273:THR:HG23	2.01	0.43
2:1:708:G:N2	2:1:711:A:OP2	2.49	0.43
2:1:806:A:N6	2:1:936:A:O4'	2.52	0.43
2:1:815:G:OP2	43:j:31:LYS:NZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1828:A:H2'	2:1:1829:G:C8	2.54	0.43
2:1:2784:G:H2'	2:1:2785:A:H8	1.84	0.43
2:1:3218:A:H5''	2:1:3219:G:C5	2.54	0.43
9:B:238:LEU:HB2	9:B:246:LEU:HA	2.01	0.43
18:K:44:LEU:HD12	18:K:281:ILE:HG22	2.01	0.43
20:M:14:LEU:H	20:M:19:ARG:NH2	2.17	0.43
20:M:24:LYS:HD3	20:M:64:VAL:HG13	1.99	0.43
27:T:39:ILE:HG22	27:T:99:SER:HB3	2.01	0.43
35:b:18:LEU:HD11	35:b:137:ALA:HA	2.01	0.43
55:v:266:ASP:OD1	55:v:270:ASP:N	2.49	0.43
57:x:377:ALA:HA	57:x:383:MET:HG2	2.00	0.43
60:4:239:VAL:HB	60:4:322:LYS:HB2	2.01	0.43
2:1:179:C:H2'	2:1:180:C:H6	1.84	0.42
2:1:1201:C:OP2	2:1:1202:A:O2'	2.35	0.42
2:1:3233:C:H2'	2:1:3234:A:H8	1.83	0.42
2:1:3243:A:H4'	9:B:95:THR:HG22	2.01	0.42
10:C:282:SER:OG	24:Q:125:ASP:OD2	2.33	0.42
18:K:38:ILE:HG12	18:K:260:VAL:HG21	2.01	0.42
35:b:497:ARG:HH21	54:u:122:ARG:HE	1.67	0.42
2:1:1404:G:OP1	38:e:65:PHE:N	2.48	0.42
2:1:1620:U:H2'	2:1:1621:A:C8	2.54	0.42
2:1:1758:G:OP1	28:U:104:ARG:NH2	2.51	0.42
2:1:2213:A:H2'	2:1:2214:A:H8	1.84	0.42
4:3:106:U:H2'	4:3:107:C:H6	1.84	0.42
6:6:1:C:N4	14:G:85:ASN:OD1	2.52	0.42
17:J:37:LEU:HD23	17:J:37:LEU:HA	1.85	0.42
47:n:202:PRO:HG3	50:q:415:LEU:CD1	2.49	0.42
51:r:88:PRO:HD2	51:r:91:LEU:HB2	2.01	0.42
60:4:391:LYS:HE2	60:4:391:LYS:HB3	1.93	0.42
2:1:242:C:H2'	2:1:243:G:H8	1.85	0.42
2:1:928:C:H2'	2:1:929:A:C8	2.55	0.42
2:1:1153:A:N1	2:1:2371:G:O2'	2.42	0.42
6:6:20:U:H2'	6:6:21:G:C8	2.53	0.42
60:4:90:ALA:HB2	60:4:146:HIS:HB3	2.01	0.42
1:A:147:ARG:HG2	1:A:157:VAL:HG22	2.00	0.42
2:1:1920:U:O2'	2:1:1932:A:N7	2.48	0.42
2:1:1949:G:OP1	25:R:104:ARG:NH1	2.52	0.42
2:1:3015:G:OP2	59:z:2:ALA:N	2.52	0.42
7:8:15:LEU:HD13	7:8:17:ALA:HB2	2.00	0.42
14:G:81:THR:HG22	14:G:179:ILE:HG22	2.01	0.42
17:J:19:LEU:O	17:J:68:HIS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:33:PRO:HB2	18:K:36:ARG:HB3	2.02	0.42
19:L:57:VAL:HG22	19:L:147:ILE:HG23	2.00	0.42
21:N:183:THR:HG22	21:N:187:ARG:HB2	2.01	0.42
26:S:109:ASP:OD1	26:S:113:ARG:NH1	2.48	0.42
31:X:108:LEU:N	31:X:125:ARG:O	2.52	0.42
58:y:109:CYS:HB2	58:y:149:GLY:HA2	2.01	0.42
2:1:787:G:H2'	2:1:788:C:C6	2.54	0.42
2:1:1261:G:H4'	2:1:1278:A:C2	2.51	0.42
2:1:2160:G:H2'	2:1:2161:G:C8	2.50	0.42
12:E:40:LEU:HD11	12:E:54:TYR:HB2	2.00	0.42
15:H:92:TYR:HB3	15:H:179:ILE:HG12	2.01	0.42
20:M:19:ARG:HB3	20:M:35:ILE:HD12	2.00	0.42
40:g:76:TYR:HB3	40:g:80:ARG:HB2	2.01	0.42
58:y:62:MET:HE3	58:y:73:PRO:HG3	2.02	0.42
2:1:348:A:N3	2:1:352:A:O2'	2.53	0.42
2:1:2875:U:O2'	2:1:2876:C:O5'	2.37	0.42
2:1:2882:U:H2'	2:1:2883:U:C6	2.55	0.42
62:1:3479:B3P:H32	62:1:3479:B3P:H62	1.83	0.42
8:9:106:GLN:O	8:9:110:LEU:CD1	2.61	0.42
17:J:148:VAL:CG1	17:J:149:GLY:N	2.83	0.42
29:V:18:PRO:HA	29:V:51:ALA:HA	2.01	0.42
46:m:50:ASN:OD1	46:m:54:ASN:N	2.46	0.42
46:m:422:LYS:NZ	46:m:423:ASP:OD2	2.47	0.42
57:x:37:GLN:O	57:x:120:LEU:HA	2.20	0.42
57:x:282:SER:H	57:x:296:SER:HA	1.84	0.42
2:1:1913:A:N3	2:1:2120:A:H2'	2.34	0.42
28:U:54:VAL:HG22	28:U:67:SER:OG	2.20	0.42
47:n:25:LEU:HD12	47:n:32:PHE:HD1	1.85	0.42
2:1:2344:U:H2'	2:1:2345:A:C8	2.55	0.42
2:1:2367:A:H2'	2:1:2368:A:H8	1.85	0.42
2:1:2520:A:H2'	2:1:2521:U:C6	2.55	0.42
2:1:2577:C:H2'	2:1:2578:U:O4'	2.20	0.42
2:1:2898:G:H22	51:r:6:TYR:N	2.18	0.42
7:8:90:ARG:HB2	7:8:95:ASP:HB2	2.01	0.42
9:B:145:GLU:OE2	9:B:196:ARG:NH1	2.40	0.42
17:J:28:ASP:OD1	17:J:28:ASP:N	2.52	0.42
30:W:41:TRP:HH2	30:W:109:VAL:HG13	1.84	0.42
60:4:221:GLN:NE2	60:4:307:ASP:O	2.53	0.42
2:1:49:A:OP1	21:N:191:TRP:NE1	2.52	0.42
2:1:2418:G:O2'	46:m:10:ARG:NH1	2.52	0.42
3:2:57:C:H4'	3:2:63:G:N7	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:68:THR:HG22	11:D:70:THR:H	1.85	0.42
19:L:106:GLN:HB3	42:i:18:THR:HB	2.02	0.42
33:Z:22:LYS:NZ	33:Z:129:TRP:O	2.41	0.42
35:b:496:ILE:HD13	54:u:130:ASN:HB2	2.01	0.42
47:n:37:ILE:HD11	47:n:217:ILE:HG23	2.01	0.42
55:v:37:SER:OG	55:v:92:SER:O	2.38	0.42
2:1:289:A:H2'	2:1:290:G:H8	1.85	0.42
2:1:1259:A:C8	30:W:67:MET:HB2	2.54	0.42
2:1:2269:U:OP1	55:v:280:GLN:NE2	2.53	0.42
9:B:123:TYR:CZ	9:B:124:LYS:HG3	2.55	0.42
30:W:120:VAL:O	30:W:121:ARG:NH1	2.44	0.42
32:Y:51:ARG:HG2	32:Y:115:ARG:NH2	2.34	0.42
54:u:18:GLY:HA3	54:u:31:PHE:O	2.19	0.42
1:A:208:ASP:HB3	2:1:914:A:H2	1.85	0.41
2:1:436:A:H2'	2:1:437:G:C8	2.55	0.41
2:1:2547:A:O2'	2:1:2549:G:OP1	2.31	0.41
2:1:3199:G:H5''	20:M:6:ILE:HD13	2.02	0.41
62:1:3480:B3P:H101	62:1:3480:B3P:H21	1.79	0.41
4:3:112:G:H2'	4:3:113:C:C6	2.54	0.41
35:b:358:LEU:HA	35:b:361:ILE:HG22	2.02	0.41
46:m:395:HIS:O	46:m:398:GLN:HG2	2.20	0.41
50:q:392:GLU:HG3	50:q:421:ARG:CZ	2.50	0.41
53:t:132:LYS:HE3	53:t:308:PRO:HG3	2.02	0.41
56:w:19:VAL:CG2	56:w:30:ASP:HB3	2.50	0.41
2:1:426:G:OP1	38:e:15:LYS:NZ	2.43	0.41
2:1:571:U:H2'	2:1:572:A:H8	1.85	0.41
2:1:2150:G:O2'	2:1:2189:U:OP1	2.34	0.41
2:1:3138:U:OP2	9:B:30:LYS:HG3	2.20	0.41
62:1:3478:B3P:H21	62:1:3478:B3P:H112	1.71	0.41
11:D:180:PHE:HB3	11:D:195:LEU:HD13	2.01	0.41
22:O:127:LEU:HD22	26:S:156:VAL:HG13	2.02	0.41
35:b:583:LEU:CD1	60:4:465:THR:HG21	2.49	0.41
51:r:186:HIS:CE1	51:r:188:GLU:HB3	2.55	0.41
57:x:385:LEU:HB2	57:x:398:MET:HE1	2.02	0.41
60:4:488:LEU:O	60:4:492:THR:OG1	2.34	0.41
2:1:35:A:H2'	2:1:36:C:H6	1.85	0.41
2:1:1131:G:O2'	2:1:2822:U:O4	2.32	0.41
2:1:1813:A:OP2	50:q:380:LYS:NZ	2.45	0.41
2:1:2752:U:H2'	2:1:2753:G:C8	2.55	0.41
3:2:69:U:H2'	3:2:70:G:O4'	2.19	0.41
4:3:59:U:H2'	4:3:60:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:135:VAL:HG12	12:E:139:LYS:HE2	2.01	0.41
13:F:236:ILE:HD12	13:F:236:ILE:HA	1.90	0.41
21:N:20:ARG:O	21:N:23:GLN:HG3	2.20	0.41
23:P:33:ALA:C	23:P:36:ILE:HG22	2.44	0.41
47:n:374:ASP:OD1	47:n:374:ASP:N	2.52	0.41
2:1:126:U:OP1	21:N:144:ARG:NH1	2.49	0.41
2:1:656:A:H2'	2:1:657:A:C8	2.55	0.41
2:1:2138:A:C4	43:j:3:LYS:HB3	2.55	0.41
2:1:2220:A2M:H3'	2:1:2221:G:H8	1.85	0.41
4:3:110:G:H2'	4:3:111:U:C6	2.55	0.41
9:B:286:GLY:HA3	9:B:321:PHE:CZ	2.55	0.41
13:F:40:LYS:NZ	13:F:170:GLU:OE2	2.45	0.41
29:V:129:VAL:O	29:V:133:SER:OG	2.31	0.41
51:r:151:ILE:HD11	51:r:212:LEU:HD13	2.01	0.41
53:t:98:ASP:HB3	53:t:184:TYR:CZ	2.55	0.41
53:t:234:ILE:HA	53:t:237:GLU:HG2	2.02	0.41
53:t:244:ILE:HD12	53:t:253:GLU:HG3	2.01	0.41
2:1:867:OMG:H1'	2:1:867:OMG:HM23	1.82	0.41
2:1:2253:G:H2'	2:1:2254:U:C6	2.55	0.41
2:1:3252:G:H2'	2:1:3253:G:C8	2.56	0.41
11:D:59:ASP:OD1	11:D:60:ILE:N	2.53	0.41
18:K:44:LEU:HD23	18:K:44:LEU:HA	1.82	0.41
28:U:54:VAL:HG12	28:U:55:THR:N	2.35	0.41
46:m:21:ASN:OD1	46:m:21:ASN:N	2.51	0.41
2:1:651:G:O2'	2:1:1435:A:OP1	2.38	0.41
2:1:1083:G:H2'	2:1:1084:A:H8	1.85	0.41
2:1:1530:U:H3	47:n:2:ARG:CZ	2.34	0.41
2:1:1622:U:H2'	2:1:1623:G:C8	2.56	0.41
3:2:154:C:H4'	14:G:181:LYS:HB3	2.00	0.41
9:B:50:LYS:NZ	9:B:330:GLY:O	2.48	0.41
25:R:13:SER:OG	25:R:38:ARG:NH2	2.49	0.41
43:j:54:LYS:O	43:j:58:THR:HB	2.21	0.41
47:n:110:ASP:OD1	47:n:110:ASP:N	2.53	0.41
2:1:19:U:H2'	2:1:20:A:C8	2.56	0.41
2:1:562:C:H5''	26:S:71:LYS:HD2	2.01	0.41
2:1:717:C:OP1	2:1:751:A:O2'	2.30	0.41
2:1:1074:U:H3	2:1:1084:A:N6	2.17	0.41
2:1:1133:A2M:H1'	2:1:1133:A2M:HM'3	1.88	0.41
2:1:1260:A:H5''	30:W:18:LYS:HE2	2.03	0.41
2:1:1288:U:H2'	2:1:1289:G:C8	2.56	0.41
2:1:1452:A:N3	2:1:2346:C:O2'	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2413:A:H2'	2:1:2415:C:C6	2.56	0.41
2:1:2421:OMU:H3'	2:1:2422:C:H5''	2.02	0.41
2:1:3021:A:H2	2:1:3033:A:H62	1.69	0.41
3:2:21:C:OP1	10:C:193:LYS:NZ	2.39	0.41
9:B:261:MET:HB2	9:B:264:VAL:HG23	2.02	0.41
24:Q:100:THR:HG22	24:Q:120:GLU:CG	2.50	0.41
2:1:2683:U:H2'	2:1:2684:C:C6	2.56	0.41
3:2:6:U:H2'	3:2:7:U:C6	2.56	0.41
4:3:59:U:H2'	4:3:60:G:H8	1.86	0.41
19:L:108:ILE:HD13	19:L:108:ILE:HA	1.95	0.41
27:T:88:ARG:HB2	56:w:162:VAL:HB	2.03	0.41
30:W:217:VAL:HB	30:W:233:ILE:HB	2.02	0.41
35:b:596:GLY:HA3	60:4:460:TYR:CZ	2.56	0.41
51:r:188:GLU:HG2	51:r:189:LEU:HG	2.03	0.41
56:w:30:ASP:OD1	56:w:30:ASP:O	2.38	0.41
57:x:333:ALA:HA	57:x:336:ILE:HG22	2.02	0.41
2:1:80:G:H2'	2:1:81:C:H6	1.86	0.41
2:1:127:G:H2'	2:1:128:G:H8	1.85	0.41
2:1:1436:U:O5'	2:1:1437:OMC:H5'	2.21	0.41
2:1:1448:U:H2'	2:1:1449:A2M:H8	2.02	0.41
2:1:2533:G:H2'	2:1:2534:G:C8	2.56	0.41
2:1:2668:U:H2'	2:1:2669:G:H8	1.86	0.41
2:1:3315:G:P	9:B:116:ARG:HH22	2.44	0.41
2:1:3387:U:H2'	2:1:3388:C:C6	2.55	0.41
62:1:3480:B3P:O2	62:1:3480:B3P:O1	2.34	0.41
3:2:88:A:H2'	3:2:89:A:C8	2.56	0.41
3:2:134:G:H4'	50:q:192:LYS:HD3	2.03	0.41
6:6:21:G:HO2'	53:t:93:ILE:H	1.69	0.41
9:B:283:TYR:N	9:B:323:MET:O	2.46	0.41
11:D:135:VAL:HG21	55:v:175:VAL:HG21	2.03	0.41
12:E:70:LYS:HB3	12:E:146:ILE:HD11	2.02	0.41
24:Q:99:THR:O	24:Q:119:GLY:HA3	2.21	0.41
45:l:43:ASN:HB3	45:l:46:ARG:HD2	2.02	0.41
46:m:396:PRO:HG2	46:m:451:LYS:HG3	2.01	0.41
47:n:369:ARG:HG2	53:t:248:GLU:HB3	2.03	0.41
53:t:276:GLU:OE2	53:t:291:GLN:NE2	2.53	0.41
55:v:132:THR:HG22	55:v:226:ILE:HG23	1.88	0.41
57:x:169:ARG:HD3	57:x:181:THR:HG23	2.03	0.41
58:y:53:ILE:HG12	58:y:59:ILE:HG22	2.03	0.41
1:A:65:ASP:HB3	1:A:68:LYS:O	2.21	0.41
2:1:2421:OMU:H6	2:1:2421:OMU:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2717:U:C2'	2:1:2718:U:H5'	2.51	0.41
3:2:142:C:H2'	3:2:143:U:C6	2.56	0.41
7:8:88:PRO:HA	7:8:89:PRO:HD3	1.97	0.41
11:D:178:ASN:HA	11:D:183:TRP:CD2	2.56	0.41
21:N:158:HIS:HB3	21:N:161:ALA:HB3	2.02	0.41
23:P:141:SER:O	23:P:143:PRO:HD3	2.21	0.41
40:g:3:GLN:HB2	40:g:30:LEU:HD12	2.03	0.41
1:A:2:GLY:HA2	2:1:2414:G:H4'	2.02	0.40
2:1:294:U:H4'	42:i:77:LEU:HD23	2.04	0.40
2:1:2723:U:H2'	2:1:2724:OMU:H6	2.02	0.40
2:1:3388:C:H5''	2:1:3389:U:H5'	2.02	0.40
3:2:149:A:H2'	3:2:150:G:C8	2.56	0.40
4:3:4:U:H2'	4:3:5:G:C8	2.56	0.40
26:S:71:LYS:O	26:S:73:LYS:NZ	2.53	0.40
47:n:242:LEU:HD13	47:n:264:LEU:HD23	2.03	0.40
2:1:393:U:H2'	2:1:394:G:O4'	2.22	0.40
2:1:1067:U:H2'	2:1:1068:C:C6	2.56	0.40
2:1:1169:A:H5''	13:F:219:LYS:HD3	2.02	0.40
2:1:1277:C:C2	2:1:1278:A:C8	3.10	0.40
2:1:1597:C:H5'	2:1:1696:A:H1'	2.04	0.40
2:1:2883:U:H2'	2:1:2884:C:C6	2.56	0.40
2:1:3294:A:H2'	2:1:3295:A:O4'	2.22	0.40
4:3:16:U:H2'	4:3:17:A:C8	2.56	0.40
4:3:27:A:H4'	17:J:141:ARG:HH12	1.85	0.40
11:D:163:LEU:HD21	11:D:175:HIS:HB3	2.03	0.40
12:E:130:ILE:HD11	12:E:134:ARG:HB2	2.04	0.40
14:G:200:LEU:HD12	14:G:200:LEU:HA	1.91	0.40
46:m:227:HIS:CE1	46:m:239:CYS:H	2.38	0.40
47:n:380:ILE:O	47:n:383:CYS:O	2.39	0.40
57:x:176:GLN:HG3	57:x:512:LEU:HD12	2.03	0.40
57:x:424:ASN:N	57:x:424:ASN:OD1	2.53	0.40
60:4:33:GLN:HB3	60:4:575:MET:HE3	2.04	0.40
2:1:209:A:H4'	2:1:211:A:C8	2.57	0.40
2:1:307:A:H2'	2:1:308:A:C8	2.57	0.40
2:1:2389:C:H2'	2:1:2390:A:C8	2.56	0.40
2:1:3358:U:H2'	2:1:3359:A:H8	1.86	0.40
6:6:43:A:H2'	6:6:44:G:H8	1.87	0.40
23:P:33:ALA:O	23:P:36:ILE:CG2	2.68	0.40
35:b:283:VAL:HB	35:b:315:VAL:HG12	2.03	0.40
57:x:303:VAL:O	57:x:313:ILE:N	2.55	0.40
60:4:202:LEU:HD21	60:4:509:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:4:258:ILE:HG23	60:4:466:LEU:HD11	2.03	0.40
2:1:715:A:H5'	34:a:115:LYS:HA	2.03	0.40
2:1:2661:G:OP1	11:D:35:ARG:NH1	2.51	0.40
35:b:318:MET:HE3	35:b:318:MET:HB2	1.89	0.40
35:b:530:LYS:HA	35:b:533:GLU:HG2	2.04	0.40
48:o:149:GLN:HG2	48:o:164:VAL:HG12	2.04	0.40
59:z:82:ASP:OD1	59:z:82:ASP:N	2.54	0.40
2:1:1927:G:C8	49:p:16:VAL:HG12	2.57	0.40
3:2:18:U:H2'	3:2:19:C:C6	2.56	0.40
4:3:103:A:H2'	4:3:104:A:C8	2.55	0.40
11:D:260:PHE:HB2	11:D:265:TYR:CZ	2.56	0.40
14:G:162:LEU:HD23	21:N:7:LEU:HD11	2.03	0.40
16:I:35:LEU:HD23	16:I:35:LEU:HA	1.96	0.40
29:V:86:ARG:HB2	29:V:92:PHE:CE2	2.56	0.40
35:b:256:LEU:HD13	35:b:298:LEU:HD22	2.03	0.40
46:m:218:VAL:HG12	46:m:353:TRP:HE3	1.86	0.40
57:x:421:SER:OG	57:x:422:PHE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 ⓘ

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%)	86	91
10	C	288/289 (100%)	288 (100%)	0	100	100
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%)	155 (100%)	0	100	100
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%)	70	80
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%)	568 (100%)	0	100	100
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%)	411 (100%)	0	100	100
47	n	332/548 (61%)	331 (100%)	1 (0%)	86	91
48	o	118/199 (59%)	117 (99%)	1 (1%)	73	82
49	p	71/72 (99%)	71 (100%)	0	100	100
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%)	440 (100%)	2 (0%)	81	88
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%)	78	86
All	All	9306/11137 (84%)	9297 (100%)	9 (0%)	87	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	B	332	ARG
32	Y	74	TYR
47	n	427	ILE
48	o	102	PHE
57	x	208	ASN
57	x	424	ASN
60	4	200	CYS

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Mol	Chain	Res	Type
60	4	255	ASN
60	4	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	144	ASN
1	A	205	ASN
5	5	114	ASN
7	8	61	GLN
8	9	17	HIS
8	9	64	ASN
9	B	109	HIS
10	C	48	GLN
10	C	59	GLN
10	C	221	ASN
12	E	97	ASN
13	F	244	ASN
14	G	243	GLN
15	H	51	GLN
15	H	96	HIS
15	H	139	ASN
16	I	48	GLN
16	I	97	ASN
16	I	126	HIS
18	K	79	GLN
18	K	232	ASN
18	K	245	ASN
18	K	330	ASN
19	L	19	GLN
20	M	56	GLN
20	M	59	ASN
20	M	62	GLN
21	N	138	GLN
21	N	139	HIS
22	O	31	GLN
22	O	42	ASN
24	Q	136	ASN
25	R	141	HIS
27	T	66	ASN
27	T	90	ASN

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Mol	Chain	Res	Type
27	T	131	GLN
28	U	40	HIS
28	U	52	ASN
30	W	148	GLN
33	Z	106	GLN
35	b	208	HIS
35	b	217	GLN
35	b	384	ASN
35	b	394	ASN
35	b	540	HIS
35	b	546	GLN
37	d	21	HIS
38	e	21	HIS
38	e	49	ASN
38	e	98	HIS
40	g	3	GLN
41	h	99	GLN
44	k	28	ASN
45	l	32	ASN
46	m	90	GLN
46	m	227	HIS
46	m	287	HIS
47	n	160	GLN
48	o	199	ASN
51	r	20	HIS
51	r	49	GLN
51	r	68	HIS
51	r	154	HIS
51	r	179	GLN
51	r	211	GLN
52	s	26	HIS
52	s	53	ASN
55	v	26	ASN
55	v	144	GLN
55	v	238	HIS
55	v	299	GLN
56	w	25	ASN
56	w	57	ASN
56	w	91	GLN
56	w	201	ASN
57	x	31	ASN
57	x	44	ASN

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Mol	Chain	Res	Type
57	x	324	ASN
60	4	398	ASN
60	4	573	GLN
60	4	577	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	2976/3396 (87%)	510 (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%)	580 (17%)	4 (0%)

All (580) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	818	C
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	OMU	1	898	2	19,22,23	2.93	8 (42%)	25,31,34	1.79	5 (20%)
2	PSU	1	966	2	18,21,22	1.23	3 (16%)	21,30,33	1.52	4 (19%)
2	PSU	1	776	2	18,21,22	1.20	2 (11%)	21,30,33	1.57	5 (23%)
2	PSU	1	2349	61,2	18,21,22	1.13	1 (5%)	21,30,33	1.43	6 (28%)
2	OMU	1	1888	2	19,22,23	3.05	7 (36%)	25,31,34	2.05	8 (32%)
2	PSU	1	1110	2	18,21,22	1.17	1 (5%)	21,30,33	1.56	5 (23%)
2	OMU	1	2347	2	19,22,23	2.95	7 (36%)	25,31,34	1.78	4 (16%)
2	PSU	1	2826	61,2	18,21,22	1.09	1 (5%)	21,30,33	1.62	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1MA	1	2142	61,2	21,25,26	0.49	0	30,37,40	0.80	1 (3%)
2	5MC	1	2870	2	19,22,23	1.58	3 (15%)	26,32,35	1.12	2 (7%)
2	OMC	1	2959	2	19,22,23	0.56	0	25,31,34	0.76	0
2	OMG	1	2791	2	23,26,27	0.45	0	32,38,41	0.51	0
2	PSU	1	2923	2	18,21,22	1.26	2 (11%)	21,30,33	1.47	4 (19%)
2	OMC	1	663	2	19,22,23	0.53	0	25,31,34	0.66	0
2	OMG	1	908	2	23,26,27	0.45	0	32,38,41	0.48	0
2	PSU	1	2416	2	18,21,22	1.19	2 (11%)	21,30,33	1.59	5 (23%)
2	OMU	1	2729	2	19,22,23	2.97	8 (42%)	25,31,34	1.85	5 (20%)
2	PSU	1	2351	2	18,21,22	1.08	1 (5%)	21,30,33	1.55	4 (19%)
2	PSU	1	2975	2	18,21,22	1.13	1 (5%)	21,30,33	1.59	4 (19%)
2	PSU	1	990	2	18,21,22	1.17	1 (5%)	21,30,33	1.54	4 (19%)
2	PSU	1	2266	2	18,21,22	1.18	1 (5%)	21,30,33	1.50	5 (23%)
2	PSU	1	2880	2	18,21,22	1.20	2 (11%)	21,30,33	1.53	5 (23%)
2	OMC	1	2197	2	19,22,23	0.46	0	25,31,34	0.62	0
2	A2M	1	807	2	22,25,26	1.40	3 (13%)	30,36,39	0.90	0
2	A2M	1	876	2	22,25,26	1.34	2 (9%)	30,36,39	0.90	2 (6%)
2	A2M	1	1133	2	22,25,26	1.43	3 (13%)	30,36,39	0.96	2 (6%)
2	5MC	1	2278	2	19,22,23	1.64	3 (15%)	26,32,35	1.10	3 (11%)
2	PSU	1	2865	2	18,21,22	1.22	4 (22%)	21,30,33	1.53	4 (19%)
2	A2M	1	1449	61,2	22,25,26	1.35	2 (9%)	30,36,39	0.96	2 (6%)
2	OMG	1	2815	2	23,26,27	0.45	0	32,38,41	0.51	0
2	A2M	1	817	61,2	22,25,26	1.31	2 (9%)	30,36,39	1.00	2 (6%)
2	OMC	1	650	2	19,22,23	0.50	0	25,31,34	0.67	0
2	PSU	1	1124	2	18,21,22	1.21	1 (5%)	21,30,33	1.55	5 (23%)
2	OMC	1	1437	2	19,22,23	0.59	0	25,31,34	0.98	1 (4%)
2	OMC	1	2337	2	19,22,23	0.53	0	25,31,34	0.64	0
4	PSU	3	50	4	18,21,22	1.20	2 (11%)	21,30,33	1.60	4 (19%)
2	OMU	1	2724	2	19,22,23	2.95	8 (42%)	25,31,34	1.77	5 (20%)
2	A2M	1	649	2	22,25,26	1.37	2 (9%)	30,36,39	0.99	2 (6%)
2	A2M	1	2220	2	22,25,26	1.51	4 (18%)	30,36,39	1.06	3 (10%)
2	PSU	1	2735	2	18,21,22	1.11	1 (5%)	21,30,33	1.58	4 (19%)
2	PSU	1	2314	2	18,21,22	1.19	1 (5%)	21,30,33	1.54	4 (19%)
2	PSU	1	2129	2	18,21,22	1.20	2 (11%)	21,30,33	1.50	4 (19%)
2	OMG	1	2922	2	23,26,27	0.48	0	32,38,41	0.45	0
2	OMG	1	2793	2	23,26,27	0.45	0	32,38,41	0.59	0
2	PSU	1	960	2	18,21,22	1.20	3 (16%)	21,30,33	1.50	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	1	2264	2	18,21,22	1.22	3 (16%)	21,30,33	1.57	4 (19%)
3	PSU	2	73	3	18,21,22	1.11	1 (5%)	21,30,33	1.56	4 (19%)
2	OMG	1	805	2	23,26,27	0.46	0	32,38,41	0.57	0
2	PSU	1	986	2	18,21,22	1.12	1 (5%)	21,30,33	1.44	4 (19%)
2	OMU	1	2421	2	19,22,23	3.00	8 (42%)	25,31,34	1.82	5 (20%)
2	OMC	1	2948	2	19,22,23	0.51	0	25,31,34	0.77	0
2	PSU	1	2133	2	18,21,22	1.08	1 (5%)	21,30,33	1.58	4 (19%)
2	OMG	1	1450	2	23,26,27	0.48	0	32,38,41	0.44	0
2	OMU	1	2417	2	19,22,23	2.97	7 (36%)	25,31,34	1.74	4 (16%)
2	OMU	1	2921	2	19,22,23	2.99	8 (42%)	25,31,34	1.79	5 (20%)
2	PSU	1	2191	2	18,21,22	1.10	1 (5%)	21,30,33	1.54	4 (19%)
2	PSU	1	2340	2	18,21,22	1.04	1 (5%)	21,30,33	1.52	4 (19%)
2	OMG	1	867	2	23,26,27	0.47	0	32,38,41	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	1	898	2	-	0/9/27/28	0/2/2/2
2	PSU	1	966	2	-	0/7/25/26	0/2/2/2
2	PSU	1	776	2	-	2/7/25/26	0/2/2/2
2	PSU	1	2349	61,2	-	0/7/25/26	0/2/2/2
2	OMU	1	1888	2	-	2/9/27/28	0/2/2/2
2	PSU	1	1110	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2347	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2826	61,2	-	1/7/25/26	0/2/2/2
2	1MA	1	2142	61,2	-	2/7/25/26	0/3/3/3
2	5MC	1	2870	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2959	2	-	0/9/27/28	0/2/2/2
2	OMG	1	2791	2	-	3/9/27/28	0/3/3/3
2	PSU	1	2923	2	-	2/7/25/26	0/2/2/2
2	OMC	1	663	2	-	0/9/27/28	0/2/2/2
2	OMG	1	908	2	-	0/9/27/28	0/3/3/3
2	PSU	1	2416	2	-	3/7/25/26	0/2/2/2
2	OMU	1	2729	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2351	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2975	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	1	990	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2266	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2880	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2197	2	-	2/9/27/28	0/2/2/2
2	A2M	1	807	2	-	0/9/27/28	0/3/3/3
2	A2M	1	876	2	-	0/9/27/28	0/3/3/3
2	A2M	1	1133	2	-	0/9/27/28	0/3/3/3
2	5MC	1	2278	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2865	2	-	2/7/25/26	0/2/2/2
2	A2M	1	1449	61,2	-	0/9/27/28	0/3/3/3
2	OMG	1	2815	2	-	0/9/27/28	0/3/3/3
2	A2M	1	817	61,2	-	1/9/27/28	0/3/3/3
2	OMC	1	650	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	1437	2	-	4/9/27/28	0/2/2/2
2	OMC	1	2337	2	-	0/9/27/28	0/2/2/2
4	PSU	3	50	4	-	2/7/25/26	0/2/2/2
2	OMU	1	2724	2	-	1/9/27/28	0/2/2/2
2	A2M	1	649	2	-	3/9/27/28	0/3/3/3
2	A2M	1	2220	2	-	2/9/27/28	0/3/3/3
2	PSU	1	2735	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2314	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2129	2	-	0/7/25/26	0/2/2/2
2	OMG	1	2922	2	-	0/9/27/28	0/3/3/3
2	OMG	1	2793	2	-	0/9/27/28	0/3/3/3
2	PSU	1	960	2	-	2/7/25/26	0/2/2/2
2	PSU	1	2264	2	-	0/7/25/26	0/2/2/2
3	PSU	2	73	3	-	0/7/25/26	0/2/2/2
2	OMG	1	805	2	-	1/9/27/28	0/3/3/3
2	PSU	1	986	2	-	1/7/25/26	0/2/2/2
2	OMU	1	2421	2	-	2/9/27/28	0/2/2/2
2	OMC	1	2948	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2133	2	-	0/7/25/26	0/2/2/2
2	OMG	1	1450	2	-	2/9/27/28	0/3/3/3
2	OMU	1	2417	2	-	2/9/27/28	0/2/2/2
2	OMU	1	2921	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2191	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2340	2	-	3/7/25/26	0/2/2/2
2	OMG	1	867	2	-	0/9/27/28	0/3/3/3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	1888	OMU	C2-N1	7.77	1.50	1.38
2	1	2421	OMU	C2-N1	7.32	1.49	1.38
2	1	2921	OMU	C2-N1	7.30	1.49	1.38
2	1	2347	OMU	C2-N1	7.22	1.49	1.38
2	1	2417	OMU	C2-N1	7.17	1.49	1.38
2	1	2729	OMU	C2-N1	7.16	1.49	1.38
2	1	898	OMU	C2-N1	7.11	1.49	1.38
2	1	2724	OMU	C2-N1	7.06	1.49	1.38
2	1	2417	OMU	C2-N3	6.83	1.49	1.38
2	1	2421	OMU	C2-N3	6.80	1.49	1.38
2	1	2724	OMU	C2-N3	6.76	1.49	1.38
2	1	2921	OMU	C2-N3	6.75	1.49	1.38
2	1	2729	OMU	C2-N3	6.72	1.49	1.38
2	1	1888	OMU	C2-N3	6.68	1.49	1.38
2	1	2347	OMU	C2-N3	6.59	1.49	1.38
2	1	898	OMU	C2-N3	6.46	1.49	1.38
2	1	2278	5MC	C5-C4	5.99	1.48	1.44
2	1	2921	OMU	C6-C5	5.88	1.48	1.35
2	1	2421	OMU	C6-C5	5.87	1.48	1.35
2	1	2729	OMU	C6-C5	5.85	1.48	1.35
2	1	1888	OMU	C6-C5	5.83	1.48	1.35
2	1	898	OMU	C6-C5	5.81	1.48	1.35
2	1	2724	OMU	C6-C5	5.80	1.48	1.35
2	1	2417	OMU	C6-C5	5.80	1.48	1.35
2	1	2870	5MC	C5-C4	5.72	1.48	1.44
2	1	2347	OMU	C6-C5	5.70	1.48	1.35
2	1	807	A2M	O5'-C5'	-3.79	1.33	1.44
2	1	2220	A2M	O5'-C5'	-3.78	1.33	1.44
2	1	876	A2M	O5'-C5'	-3.73	1.33	1.44
2	1	2421	OMU	C4-N3	3.69	1.44	1.38
2	1	649	A2M	O5'-C5'	-3.67	1.33	1.44
2	1	1133	A2M	O5'-C5'	-3.65	1.33	1.44
2	1	817	A2M	O5'-C5'	-3.63	1.33	1.44
2	1	2921	OMU	C4-N3	3.62	1.44	1.38
2	1	1449	A2M	O5'-C5'	-3.61	1.33	1.44
2	1	2729	OMU	C4-N3	3.58	1.44	1.38
2	1	2417	OMU	C4-N3	3.57	1.44	1.38
2	1	2724	OMU	C4-N3	3.47	1.44	1.38
2	1	898	OMU	C4-N3	3.38	1.44	1.38
2	1	2347	OMU	C4-N3	3.38	1.44	1.38
2	1	2865	PSU	C2-N1	3.33	1.41	1.36
4	3	50	PSU	C2-N1	3.31	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	1888	OMU	C4-N3	3.29	1.44	1.38
2	1	2264	PSU	C2-N1	3.28	1.40	1.36
2	1	2129	PSU	C2-N1	3.27	1.40	1.36
2	1	2923	PSU	C2-N1	3.24	1.40	1.36
2	1	1110	PSU	C2-N1	3.22	1.40	1.36
2	1	1124	PSU	C2-N1	3.16	1.40	1.36
2	1	2975	PSU	C2-N1	3.16	1.40	1.36
2	1	2880	PSU	C2-N1	3.15	1.40	1.36
2	1	776	PSU	C2-N1	3.14	1.40	1.36
2	1	1888	OMU	O2-C2	-3.10	1.17	1.23
2	1	966	PSU	C2-N1	3.09	1.40	1.36
2	1	2314	PSU	C2-N1	3.08	1.40	1.36
2	1	990	PSU	C2-N1	3.07	1.40	1.36
2	1	2191	PSU	C2-N1	3.05	1.40	1.36
2	1	2351	PSU	C2-N1	3.04	1.40	1.36
2	1	2266	PSU	C2-N1	3.03	1.40	1.36
2	1	2416	PSU	C2-N1	3.03	1.40	1.36
2	1	2735	PSU	C2-N1	3.01	1.40	1.36
2	1	960	PSU	C2-N1	3.00	1.40	1.36
3	2	73	PSU	C2-N1	2.97	1.40	1.36
2	1	2133	PSU	C2-N1	2.93	1.40	1.36
2	1	2826	PSU	C2-N1	2.92	1.40	1.36
2	1	2349	PSU	C2-N1	2.92	1.40	1.36
2	1	2347	OMU	O4-C4	-2.89	1.18	1.24
2	1	898	OMU	O2-C2	-2.88	1.18	1.23
2	1	2347	OMU	O2-C2	-2.87	1.18	1.23
2	1	1888	OMU	O4-C4	-2.84	1.19	1.24
2	1	898	OMU	O4-C4	-2.80	1.19	1.24
2	1	2340	PSU	C2-N1	2.80	1.40	1.36
2	1	986	PSU	C2-N1	2.79	1.40	1.36
2	1	2278	5MC	C6-C5	2.75	1.39	1.34
2	1	2724	OMU	O4-C4	-2.73	1.19	1.24
2	1	2729	OMU	O2-C2	-2.72	1.18	1.23
2	1	2724	OMU	O2-C2	-2.70	1.18	1.23
2	1	2417	OMU	O2-C2	-2.66	1.18	1.23
2	1	2421	OMU	O4-C4	-2.65	1.19	1.24
2	1	2921	OMU	O2-C2	-2.64	1.18	1.23
2	1	2729	OMU	O4-C4	-2.64	1.19	1.24
2	1	2421	OMU	O2-C2	-2.63	1.18	1.23
2	1	2921	OMU	O4-C4	-2.62	1.19	1.24
2	1	2220	A2M	C5-C4	2.61	1.43	1.39
2	1	2417	OMU	O4-C4	-2.59	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2870	5MC	C6-C5	2.54	1.38	1.34
2	1	1133	A2M	C5-C4	2.36	1.43	1.39
2	1	2220	A2M	C8-N9	2.26	1.41	1.37
2	1	807	A2M	C5-C4	2.24	1.43	1.39
2	1	2870	5MC	C6-N1	-2.22	1.34	1.38
2	1	1888	OMU	C6-N1	2.18	1.43	1.38
2	1	2278	5MC	C6-N1	-2.18	1.34	1.38
2	1	649	A2M	C5-C4	2.18	1.43	1.39
2	1	966	PSU	C6-N1	2.14	1.39	1.36
2	1	2729	OMU	C5-C4	2.13	1.48	1.43
2	1	2421	OMU	C5-C4	2.12	1.48	1.43
2	1	876	A2M	C5-C4	2.11	1.42	1.39
2	1	2416	PSU	C6-N1	2.11	1.39	1.36
2	1	1449	A2M	C5-C4	2.11	1.42	1.39
2	1	960	PSU	C4-N3	2.10	1.42	1.38
4	3	50	PSU	C6-N1	2.09	1.39	1.36
2	1	1133	A2M	C8-N9	2.09	1.41	1.37
2	1	2921	OMU	C6-N1	2.08	1.43	1.38
2	1	2921	OMU	C5-C4	2.08	1.48	1.43
2	1	807	A2M	C8-N9	2.08	1.41	1.37
2	1	2865	PSU	C2-N3	2.08	1.40	1.37
2	1	2347	OMU	C6-N1	2.08	1.43	1.38
2	1	2729	OMU	C6-N1	2.07	1.43	1.38
2	1	2220	A2M	C4-N3	2.07	1.38	1.34
2	1	2880	PSU	C4-N3	2.07	1.42	1.38
2	1	2264	PSU	C4-N3	2.06	1.42	1.38
2	1	2865	PSU	C6-N1	2.06	1.39	1.36
2	1	898	OMU	C5-C4	2.06	1.48	1.43
2	1	2923	PSU	C6-N1	2.06	1.39	1.36
2	1	2421	OMU	C6-N1	2.05	1.43	1.38
2	1	2417	OMU	C5-C4	2.05	1.48	1.43
2	1	2724	OMU	C5-C4	2.05	1.48	1.43
2	1	817	A2M	C5-C4	2.04	1.42	1.39
2	1	898	OMU	C6-N1	2.04	1.43	1.38
2	1	2264	PSU	C6-N1	2.03	1.39	1.36
2	1	2724	OMU	C6-N1	2.02	1.42	1.38
2	1	960	PSU	C2-N3	2.02	1.40	1.37
2	1	2865	PSU	C4-N3	2.01	1.42	1.38
2	1	2129	PSU	C6-N1	2.00	1.39	1.36
2	1	776	PSU	C2-N3	2.00	1.40	1.37
2	1	966	PSU	C4-N3	2.00	1.42	1.38

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2729	OMU	C4-N3-C2	-5.81	119.39	126.61
2	1	2421	OMU	C4-N3-C2	-5.61	119.65	126.61
2	1	898	OMU	C4-N3-C2	-5.58	119.69	126.61
2	1	2921	OMU	C4-N3-C2	-5.57	119.70	126.61
2	1	2347	OMU	C4-N3-C2	-5.51	119.77	126.61
2	1	2724	OMU	C4-N3-C2	-5.44	119.86	126.61
2	1	2417	OMU	C4-N3-C2	-5.24	120.11	126.61
2	1	1888	OMU	C4-N3-C2	-5.05	120.35	126.61
2	1	2865	PSU	C6-C5-C4	4.57	121.26	118.17
4	3	50	PSU	C6-C5-C4	4.47	121.19	118.17
2	1	1888	OMU	C1'-N1-C2	4.43	125.55	117.59
2	1	2826	PSU	C6-C5-C4	4.42	121.16	118.17
2	1	2264	PSU	C6-C5-C4	4.38	121.13	118.17
2	1	2416	PSU	C6-C5-C4	4.38	121.13	118.17
2	1	2735	PSU	C6-C5-C4	4.30	121.08	118.17
2	1	776	PSU	C6-C5-C4	4.18	121.00	118.17
2	1	2975	PSU	C6-C5-C4	4.16	120.98	118.17
2	1	2314	PSU	C6-C5-C4	4.13	120.96	118.17
2	1	2351	PSU	C6-C5-C4	4.12	120.95	118.17
2	1	1110	PSU	C6-C5-C4	4.10	120.94	118.17
2	1	990	PSU	C6-C5-C4	4.10	120.94	118.17
3	2	73	PSU	C6-C5-C4	4.07	120.92	118.17
2	1	2729	OMU	N3-C2-N1	4.05	120.17	114.89
2	1	1888	OMU	N3-C2-N1	4.02	120.13	114.89
2	1	2129	PSU	C6-C5-C4	4.01	120.88	118.17
2	1	2880	PSU	C6-C5-C4	4.01	120.88	118.17
2	1	966	PSU	C6-C5-C4	4.00	120.88	118.17
2	1	2923	PSU	C6-C5-C4	4.00	120.87	118.17
2	1	898	OMU	N3-C2-N1	3.97	120.06	114.89
2	1	2421	OMU	N3-C2-N1	3.88	119.94	114.89
2	1	2340	PSU	C6-C5-C4	3.81	120.75	118.17
2	1	1124	PSU	C6-C5-C4	3.80	120.74	118.17
2	1	2191	PSU	C6-C5-C4	3.79	120.73	118.17
2	1	2921	OMU	N3-C2-N1	3.76	119.78	114.89
2	1	2724	OMU	N3-C2-N1	3.75	119.77	114.89
2	1	2347	OMU	N3-C2-N1	3.71	119.72	114.89
2	1	2347	OMU	C5-C4-N3	3.70	119.99	114.80
2	1	2266	PSU	C6-C5-C4	3.70	120.67	118.17
2	1	2133	PSU	C6-C5-C4	3.64	120.63	118.17
2	1	2729	OMU	C5-C4-N3	3.63	119.89	114.80
2	1	2421	OMU	C5-C4-N3	3.59	119.83	114.80
2	1	2921	OMU	C5-C4-N3	3.57	119.80	114.80
2	1	2724	OMU	C5-C4-N3	3.57	119.80	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2417	OMU	N3-C2-N1	3.53	119.49	114.89
2	1	2417	OMU	C5-C4-N3	3.50	119.70	114.80
2	1	898	OMU	C5-C4-N3	3.50	119.70	114.80
2	1	960	PSU	C6-C5-C4	3.48	120.53	118.17
2	1	1888	OMU	C5-C4-N3	3.40	119.56	114.80
2	1	2349	PSU	O4-C4-N3	-3.21	114.07	120.11
2	1	2870	5MC	C5-C6-N1	-3.18	119.86	123.31
2	1	986	PSU	C6-C5-C4	3.15	120.30	118.17
2	1	2865	PSU	C4-N3-C2	-3.15	122.03	126.37
2	1	2826	PSU	C4-N3-C2	-3.14	122.04	126.37
2	1	2133	PSU	C4-N3-C2	-3.11	122.09	126.37
2	1	2264	PSU	C4-N3-C2	-3.11	122.09	126.37
3	2	73	PSU	C4-N3-C2	-3.11	122.09	126.37
2	1	990	PSU	C4-N3-C2	-3.10	122.09	126.37
2	1	2735	PSU	C4-N3-C2	-3.09	122.11	126.37
2	1	2975	PSU	C4-N3-C2	-3.06	122.16	126.37
2	1	2880	PSU	C4-N3-C2	-3.05	122.17	126.37
4	3	50	PSU	C4-N3-C2	-3.04	122.19	126.37
2	1	2351	PSU	C4-N3-C2	-3.03	122.19	126.37
2	1	2416	PSU	C4-N3-C2	-3.02	122.21	126.37
2	1	776	PSU	C4-N3-C2	-3.01	122.22	126.37
2	1	2314	PSU	C4-N3-C2	-3.01	122.22	126.37
2	1	2133	PSU	O4-C4-N3	-3.00	114.47	120.11
2	1	1124	PSU	C4-N3-C2	-3.00	122.24	126.37
2	1	960	PSU	C4-N3-C2	-2.99	122.26	126.37
2	1	2278	5MC	C5-C6-N1	-2.99	120.07	123.31
2	1	2347	OMU	O4-C4-C5	-2.98	120.02	125.16
2	1	986	PSU	O4-C4-N3	-2.98	114.51	120.11
2	1	2266	PSU	C4-N3-C2	-2.98	122.27	126.37
2	1	2417	OMU	O4-C4-C5	-2.97	120.04	125.16
2	1	1110	PSU	C4-N3-C2	-2.97	122.28	126.37
2	1	966	PSU	C4-N3-C2	-2.95	122.31	126.37
2	1	2191	PSU	C4-N3-C2	-2.95	122.31	126.37
2	1	2129	PSU	C4-N3-C2	-2.94	122.32	126.37
2	1	2421	OMU	O4-C4-C5	-2.92	120.13	125.16
2	1	2340	PSU	C4-N3-C2	-2.91	122.36	126.37
2	1	2191	PSU	O4-C4-N3	-2.90	114.66	120.11
2	1	2923	PSU	C4-N3-C2	-2.90	122.38	126.37
2	1	2724	OMU	O4-C4-C5	-2.88	120.20	125.16
2	1	2921	OMU	O4-C4-C5	-2.86	120.23	125.16
2	1	2278	5MC	C5-C4-N3	-2.84	118.84	121.75
2	1	960	PSU	O4-C4-N3	-2.84	114.78	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2729	OMU	O4-C4-C5	-2.83	120.28	125.16
2	1	986	PSU	C4-N3-C2	-2.82	122.48	126.37
2	1	2340	PSU	O4-C4-N3	-2.78	114.88	120.11
2	1	2349	PSU	C6-C5-C4	2.76	120.04	118.17
2	1	1124	PSU	O4-C4-N3	-2.74	114.96	120.11
2	1	1437	OMC	C1'-N1-C2	2.73	124.46	118.44
2	1	2923	PSU	O4-C4-N3	-2.72	115.00	120.11
2	1	2266	PSU	O4-C4-N3	-2.70	115.03	120.11
2	1	2975	PSU	O4-C4-N3	-2.70	115.05	120.11
2	1	1888	OMU	O4-C4-C5	-2.68	120.55	125.16
2	1	2351	PSU	O4-C4-N3	-2.66	115.11	120.11
2	1	1110	PSU	O4-C4-N3	-2.65	115.14	120.11
3	2	73	PSU	O4-C4-N3	-2.63	115.18	120.11
2	1	966	PSU	O4-C4-N3	-2.62	115.18	120.11
2	1	898	OMU	O4-C4-C5	-2.60	120.67	125.16
2	1	2349	PSU	C4-N3-C2	-2.57	122.82	126.37
2	1	990	PSU	O4-C4-N3	-2.54	115.33	120.11
2	1	2220	A2M	N3-C4-N9	2.54	131.48	127.17
2	1	2826	PSU	O4-C4-N3	-2.53	115.35	120.11
4	3	50	PSU	O4-C4-N3	-2.53	115.36	120.11
2	1	2735	PSU	O4-C4-N3	-2.53	115.36	120.11
2	1	2880	PSU	O4-C4-N3	-2.52	115.37	120.11
2	1	2870	5MC	C5-C4-N3	-2.51	119.18	121.75
2	1	2133	PSU	N1-C2-N3	2.51	117.81	115.17
2	1	776	PSU	O4-C4-N3	-2.50	115.41	120.11
2	1	2129	PSU	O4-C4-N3	-2.49	115.42	120.11
2	1	2314	PSU	O4-C4-N3	-2.49	115.43	120.11
2	1	2142	1MA	N1-C6-N6	2.46	125.88	119.71
2	1	2416	PSU	O4-C4-N3	-2.44	115.52	120.11
2	1	649	A2M	N3-C4-N9	2.43	131.30	127.17
2	1	2264	PSU	O4-C4-N3	-2.41	115.58	120.11
2	1	2826	PSU	N1-C2-N3	2.40	117.70	115.17
2	1	1888	OMU	O2-C2-N3	-2.39	117.07	121.49
2	1	2729	OMU	O2-C2-N1	-2.39	119.68	122.80
2	1	1888	OMU	C6-N1-C2	-2.37	118.11	121.00
2	1	2865	PSU	O4-C4-N3	-2.37	115.66	120.11
3	2	73	PSU	N1-C2-N3	2.31	117.61	115.17
2	1	817	A2M	C3'-C2'-C1'	-2.29	98.42	102.81
2	1	2735	PSU	N1-C2-N3	2.28	117.57	115.17
2	1	2975	PSU	N1-C2-N3	2.28	117.57	115.17
4	3	50	PSU	N1-C2-N3	2.27	117.56	115.17
2	1	990	PSU	N1-C2-N3	2.27	117.56	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	1110	PSU	N1-C2-N3	2.26	117.55	115.17
2	1	960	PSU	N1-C2-N3	2.26	117.55	115.17
2	1	776	PSU	O4'-C1'-C2'	2.24	108.24	105.15
2	1	2191	PSU	N1-C2-N3	2.23	117.52	115.17
2	1	1124	PSU	O4'-C1'-C2'	2.22	108.23	105.15
2	1	2314	PSU	N1-C2-N3	2.22	117.51	115.17
2	1	2880	PSU	N1-C2-N3	2.22	117.51	115.17
2	1	1124	PSU	N1-C2-N3	2.22	117.50	115.17
2	1	2264	PSU	N1-C2-N3	2.21	117.50	115.17
2	1	2351	PSU	N1-C2-N3	2.21	117.50	115.17
2	1	776	PSU	N1-C2-N3	2.21	117.49	115.17
2	1	2416	PSU	O4'-C1'-C2'	2.20	108.20	105.15
2	1	1449	A2M	N3-C4-N9	2.20	130.91	127.17
2	1	2923	PSU	N1-C2-N3	2.20	117.49	115.17
2	1	2340	PSU	N1-C2-N3	2.19	117.48	115.17
2	1	2220	A2M	C5-C4-N3	-2.19	123.70	126.72
2	1	898	OMU	O2-C2-N1	-2.19	119.95	122.80
2	1	2865	PSU	N1-C2-N3	2.18	117.47	115.17
2	1	966	PSU	N1-C2-N3	2.17	117.46	115.17
2	1	986	PSU	N1-C2-N3	2.17	117.45	115.17
2	1	2421	OMU	O2-C2-N1	-2.16	119.98	122.80
2	1	1110	PSU	O4'-C1'-C2'	2.15	108.12	105.15
2	1	1449	A2M	C2-N1-C6	-2.15	115.20	118.73
2	1	817	A2M	C2-N1-C6	-2.15	115.21	118.73
2	1	1133	A2M	N3-C4-N9	2.14	130.81	127.17
2	1	2266	PSU	N1-C2-N3	2.14	117.42	115.17
2	1	2129	PSU	N1-C2-N3	2.14	117.42	115.17
2	1	2349	PSU	N1-C2-N3	2.13	117.41	115.17
2	1	2220	A2M	C2-N1-C6	-2.11	115.27	118.73
2	1	649	A2M	C2-N1-C6	-2.10	115.27	118.73
2	1	2278	5MC	O2-C2-N3	-2.09	119.03	122.33
2	1	2416	PSU	N1-C2-N3	2.09	117.37	115.17
2	1	1888	OMU	C1'-N1-C6	-2.09	116.32	120.78
2	1	2349	PSU	O4-C4-C5	2.08	129.18	124.01
2	1	876	A2M	N3-C4-N9	2.08	130.71	127.17
2	1	2921	OMU	O2-C2-N1	-2.07	120.10	122.80
2	1	1133	A2M	C2-N1-C6	-2.06	115.34	118.73
2	1	2880	PSU	O4'-C1'-C2'	2.06	108.00	105.15
2	1	876	A2M	C2-N1-C6	-2.02	115.41	118.73
2	1	2724	OMU	O2-C2-N1	-2.02	120.17	122.80
2	1	2349	PSU	O4'-C1'-C2'	2.01	107.94	105.15
2	1	2266	PSU	O4'-C1'-C2'	2.01	107.94	105.15

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	776	PSU	O4'-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	2724	OMU	C1'-C2'-O2'-CM2
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	O4'-C4'-C5'-O5'
4	3	50	PSU	O4'-C4'-C5'-O5'
2	1	649	A2M	O4'-C4'-C5'-O5'
2	1	649	A2M	C3'-C4'-C5'-O5'
2	1	776	PSU	C3'-C4'-C5'-O5'
2	1	960	PSU	C3'-C4'-C5'-O5'
2	1	2421	OMU	C3'-C4'-C5'-O5'
2	1	2421	OMU	O4'-C4'-C5'-O5'
2	1	2729	OMU	O4'-C4'-C5'-O5'
2	1	2948	OMC	C3'-C4'-C5'-O5'
4	3	50	PSU	C3'-C4'-C5'-O5'
2	1	1437	OMC	O4'-C4'-C5'-O5'
2	1	2142	1MA	C3'-C4'-C5'-O5'
2	1	2220	A2M	O4'-C4'-C5'-O5'
2	1	2340	PSU	C3'-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	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'

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Mol	Chain	Res	Type	Atoms
2	1	2826	PSU	O4'-C4'-C5'-O5'
2	1	2340	PSU	C4'-C5'-O5'-P
2	1	986	PSU	O4'-C4'-C5'-O5'
2	1	649	A2M	C4'-C5'-O5'-P
2	1	805	OMG	C3'-C2'-O2'-CM2
2	1	817	A2M	C4'-C5'-O5'-P
2	1	2791	OMG	C4'-C5'-O5'-P
2	1	2416	PSU	C4'-C5'-O5'-P
2	1	1437	OMC	C2'-C1'-N1-C2

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	898	OMU	1	0
2	1	663	OMC	1	0
2	1	2266	PSU	1	0
2	1	2880	PSU	1	0
2	1	807	A2M	1	0
2	1	1133	A2M	2	0
2	1	1449	A2M	1	0
2	1	1437	OMC	2	0
2	1	2724	OMU	3	0
2	1	2220	A2M	3	0
2	1	2129	PSU	1	0
2	1	2793	OMG	1	0
2	1	2421	OMU	2	0
2	1	867	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
65	GTP	m	501	61,66	33,34,34	0.96	1 (3%)	50,54,54	1.66	9 (18%)
62	B3P	1	3480	-	18,18,18	1.56	2 (11%)	23,23,23	1.90	6 (26%)
64	GDP	b	801	61	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
62	B3P	1	3479	-	18,18,18	1.59	3 (16%)	23,23,23	1.83	6 (26%)
62	B3P	1	3478	61	18,18,18	1.65	3 (16%)	23,23,23	1.76	6 (26%)

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
65	GTP	m	501	61,66	-	4/22/38/38	0/3/3/3
62	B3P	1	3480	-	-	7/28/28/28	-
64	GDP	b	801	61	-	3/16/32/32	0/3/3/3
62	B3P	1	3479	-	-	10/28/28/28	-
62	B3P	1	3478	61	-	13/28/28/28	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	1	3480	B3P	C6-C4	5.43	1.59	1.53
62	1	3478	B3P	C6-C4	5.13	1.59	1.53
62	1	3479	B3P	C6-C4	4.93	1.59	1.53
64	b	801	GDP	C5-C4	3.09	1.47	1.38
62	1	3479	B3P	C7-C4	2.75	1.56	1.53
62	1	3478	B3P	C7-C4	2.59	1.56	1.53
64	b	801	GDP	C6-N1	-2.45	1.34	1.38
62	1	3480	B3P	C7-C4	2.35	1.56	1.53
62	1	3478	B3P	C9-C8	2.22	1.56	1.53
62	1	3479	B3P	C11-C8	2.20	1.56	1.53
65	m	501	GTP	C5-N7	-2.07	1.34	1.39
64	b	801	GDP	C5-N7	-2.06	1.34	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	b	801	GDP	C5-C4-N3	-6.16	118.59	128.39
64	b	801	GDP	C2-N3-C4	5.06	121.02	112.30
62	1	3480	B3P	O5-C6-C4	5.05	121.96	111.68
62	1	3478	B3P	O5-C6-C4	4.98	121.80	111.68
62	1	3479	B3P	O5-C6-C4	4.97	121.80	111.68
65	m	501	GTP	C5-C4-N3	-4.78	120.78	128.39
64	b	801	GDP	N9-C4-N3	4.55	135.04	125.95
65	m	501	GTP	C2-N3-C4	4.48	120.02	112.30
62	1	3480	B3P	C2-N2-C8	-4.00	110.31	116.17
62	1	3479	B3P	C3-N1-C4	-3.86	110.51	116.17
62	1	3478	B3P	C3-N1-C4	-3.58	110.92	116.17
62	1	3480	B3P	C3-N1-C4	-3.51	111.02	116.17
64	b	801	GDP	C6-C5-N7	3.22	136.16	130.29
65	m	501	GTP	C2-N1-C6	-3.13	119.43	125.11
62	1	3479	B3P	C2-N2-C8	-3.10	111.63	116.17
65	m	501	GTP	N9-C8-N7	-3.04	107.77	113.40
65	m	501	GTP	N9-C4-N3	3.02	132.00	125.95
65	m	501	GTP	O2B-PB-O3B	3.00	115.38	107.27
62	1	3480	B3P	O6-C7-C4	-2.77	106.04	111.68
65	m	501	GTP	C8-N7-C5	2.72	109.11	104.26
62	1	3478	B3P	C2-N2-C8	-2.72	112.19	116.17
62	1	3479	B3P	O6-C7-C4	-2.68	106.23	111.68
62	1	3480	B3P	O3-C11-C8	-2.60	106.40	111.68
65	m	501	GTP	O6-C6-C5	-2.58	119.72	126.53
62	1	3479	B3P	O4-C5-C4	-2.58	106.44	111.68
64	b	801	GDP	C4-C5-N7	-2.57	106.59	110.67
65	m	501	GTP	C5-C6-N1	2.57	119.79	113.25
62	1	3478	B3P	O6-C7-C4	-2.54	106.52	111.68
62	1	3478	B3P	O4-C5-C4	-2.49	106.62	111.68
62	1	3479	B3P	O3-C11-C8	-2.41	106.78	111.68
62	1	3478	B3P	O3-C11-C8	-2.24	107.12	111.68
62	1	3480	B3P	O4-C5-C4	-2.10	107.42	111.68
64	b	801	GDP	O6-C6-C5	-2.05	121.12	126.53

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
62	1	3478	B3P	C7-C4-C6-O5
62	1	3478	B3P	N2-C8-C9-O1
62	1	3478	B3P	C10-C8-C9-O1

Continued on next page...

Continued from previous page...

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

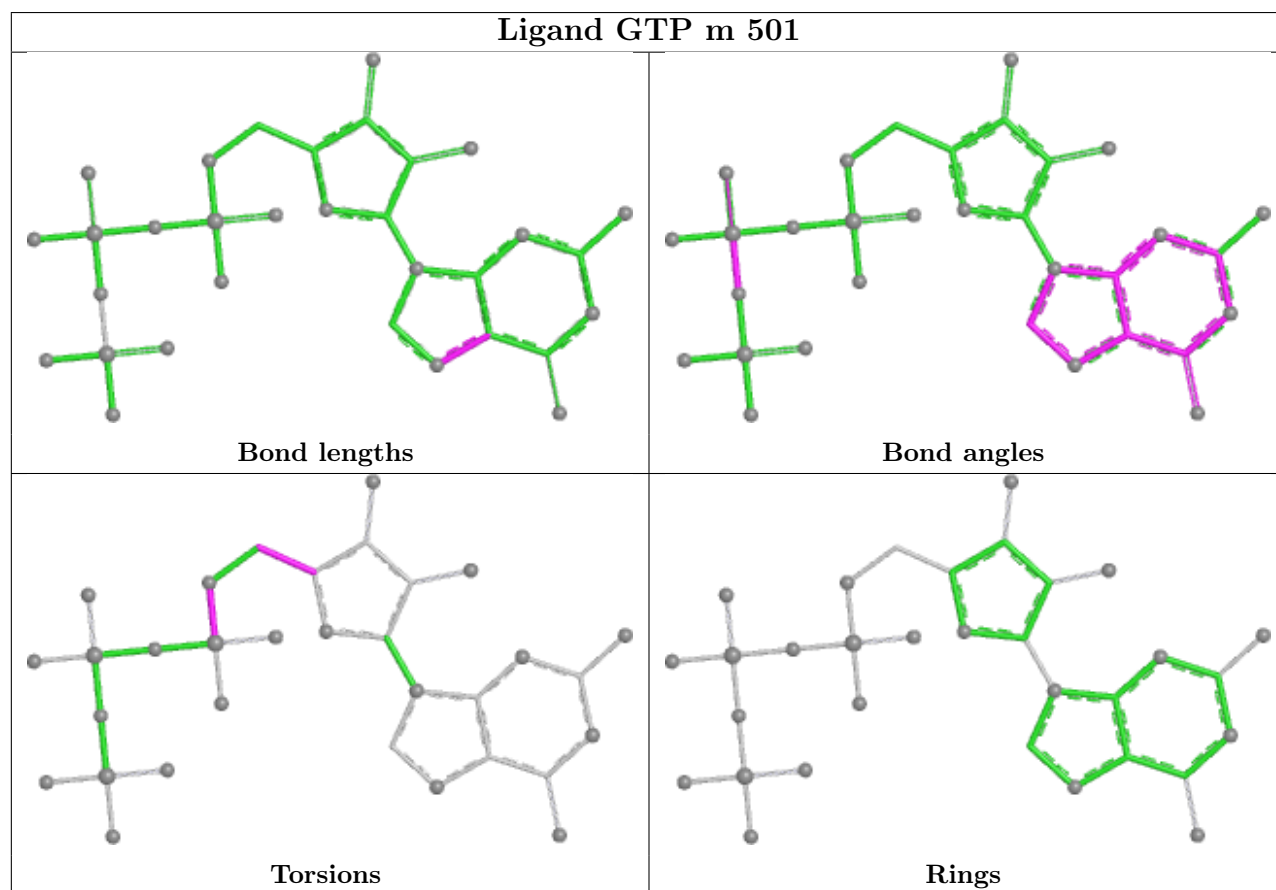
There are no ring outliers.

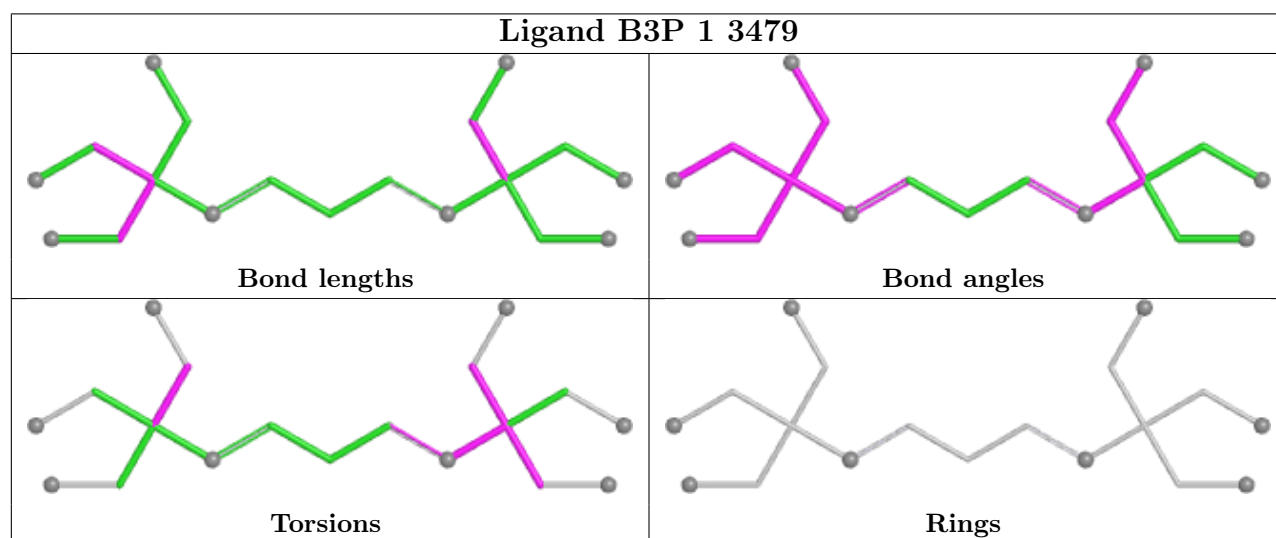
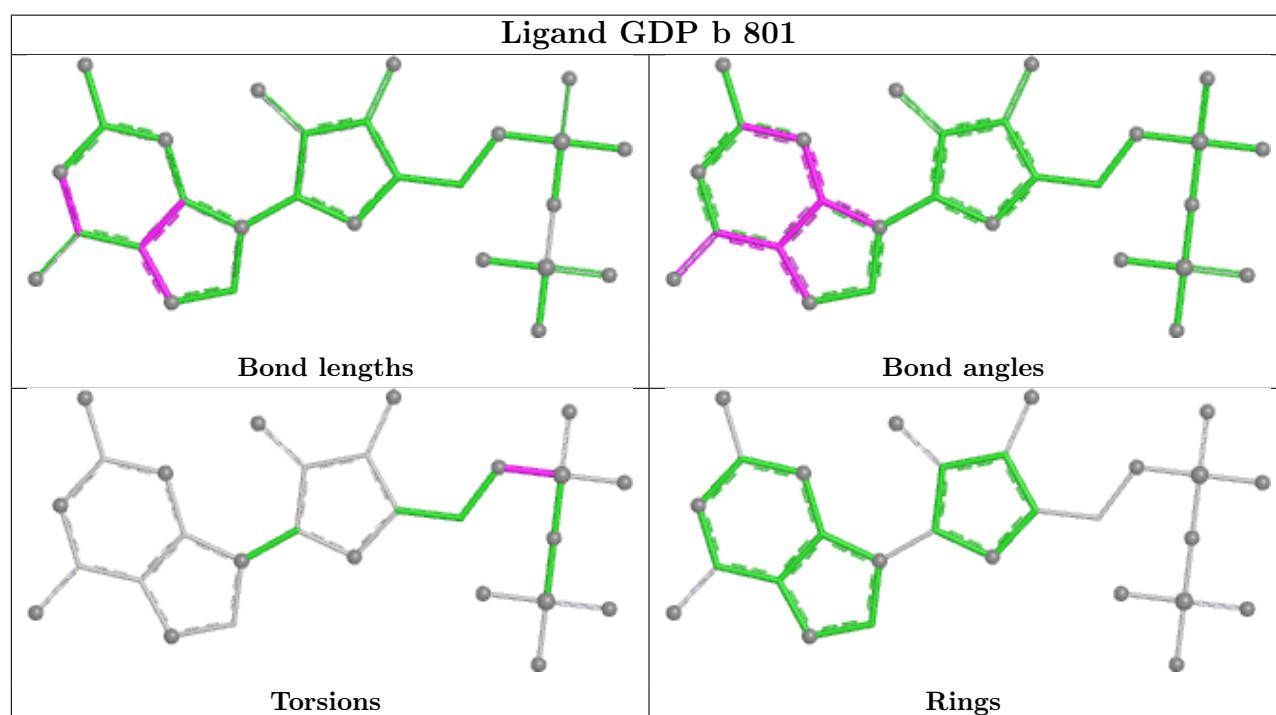
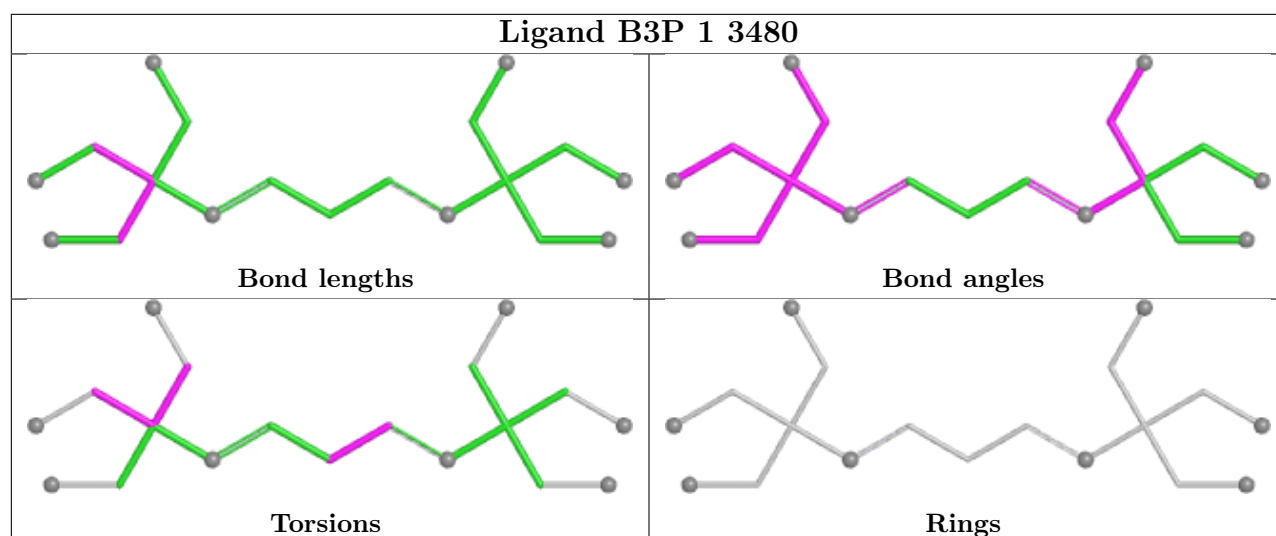
3 monomers are involved in 6 short contacts:

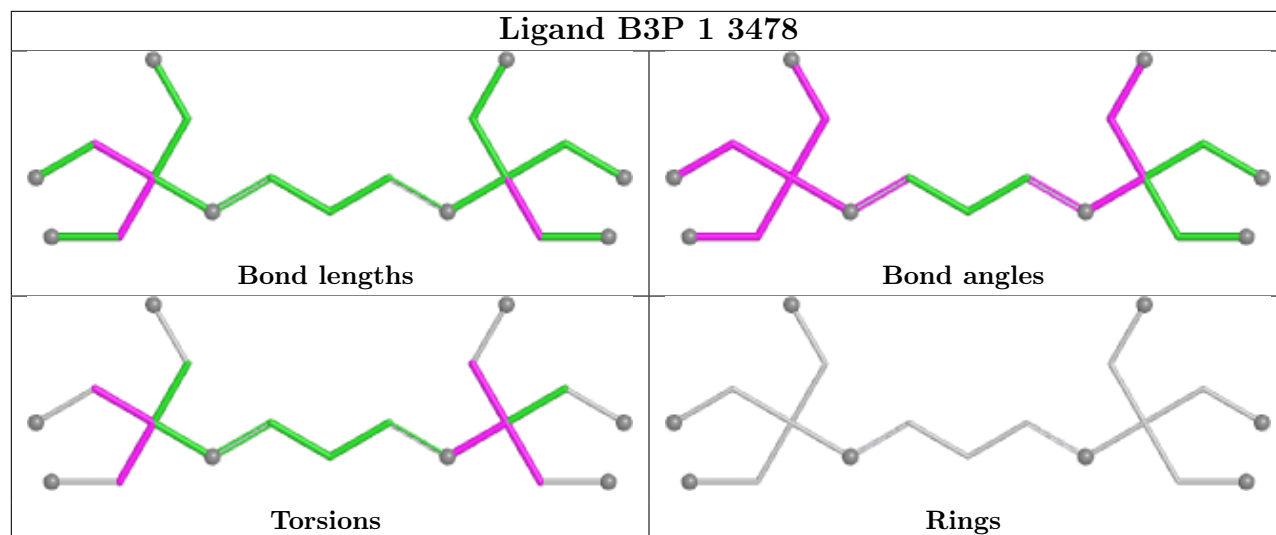
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	1	3480	B3P	2	0
62	1	3479	B3P	1	0
62	1	3478	B3P	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

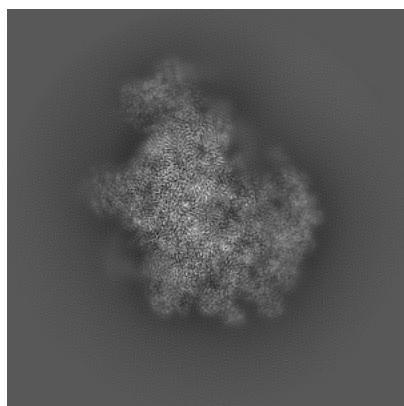
6 Map visualisation [i](#)

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.

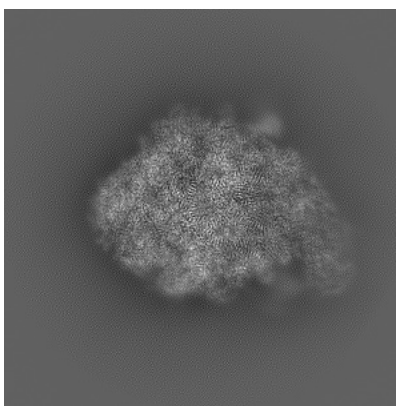
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

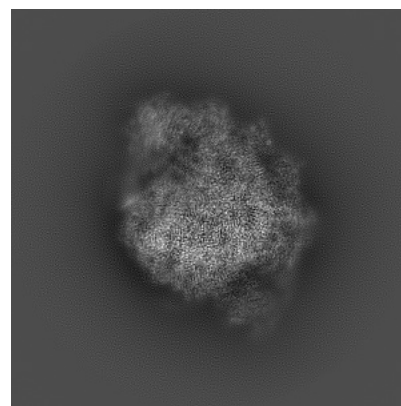
6.1.1 Primary map



X

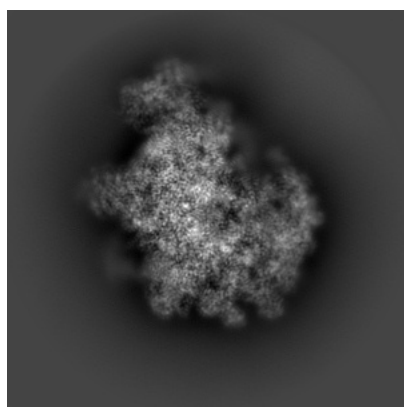


Y

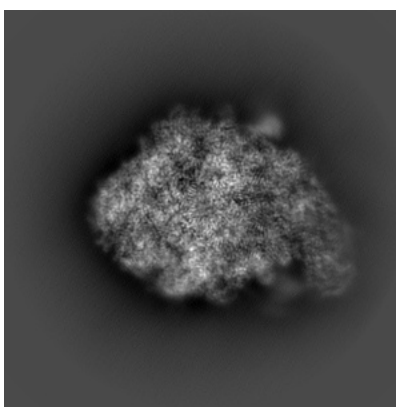


Z

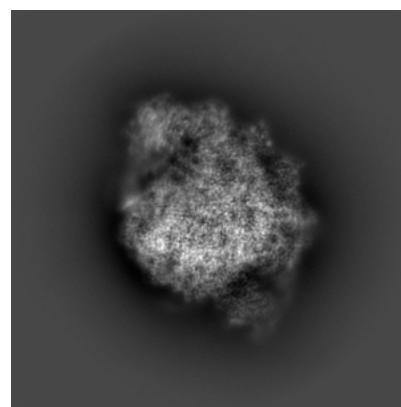
6.1.2 Raw map



X



Y

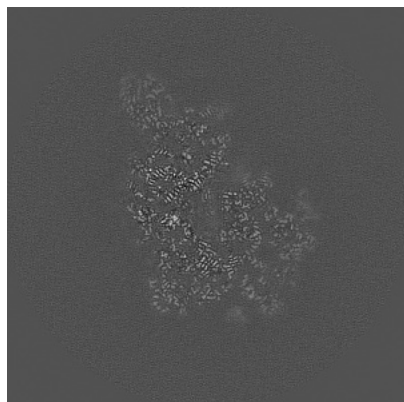


Z

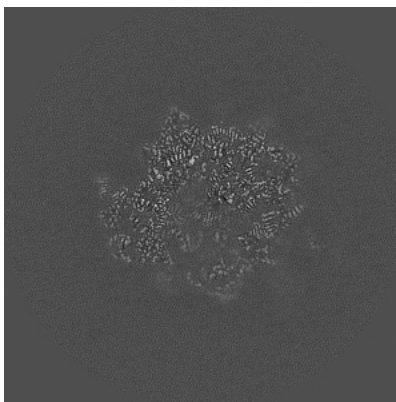
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

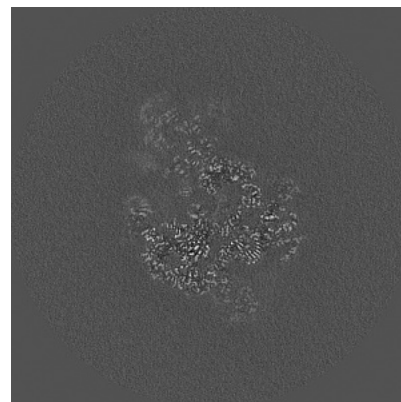
6.2.1 Primary map



X Index: 200

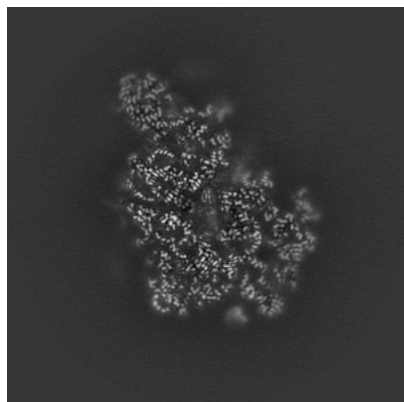


Y Index: 200

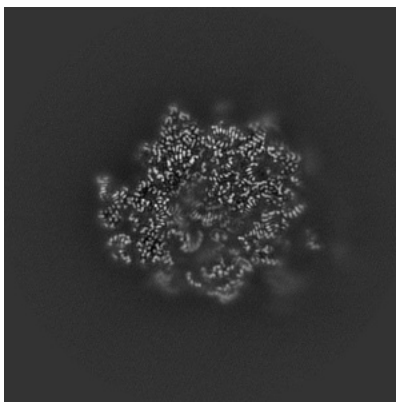


Z Index: 200

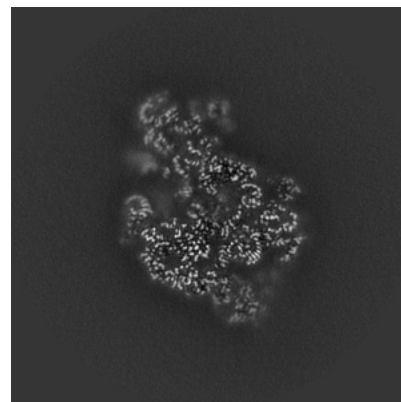
6.2.2 Raw map



X Index: 200



Y Index: 200

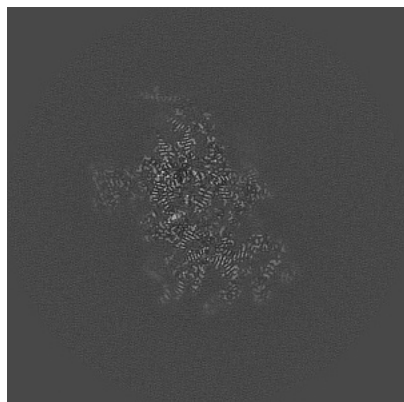


Z Index: 200

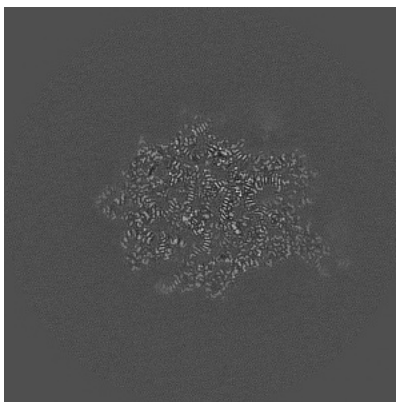
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

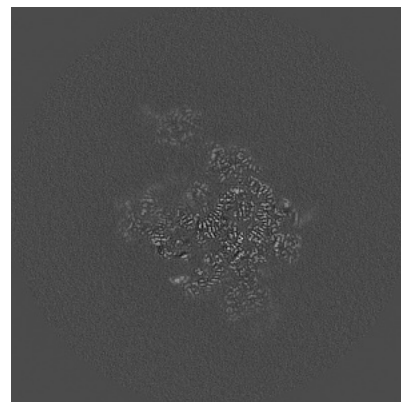
6.3.1 Primary map



X Index: 227

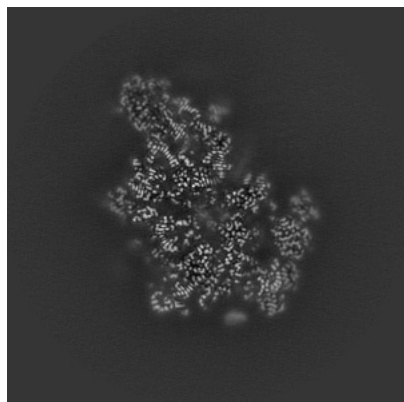


Y Index: 179

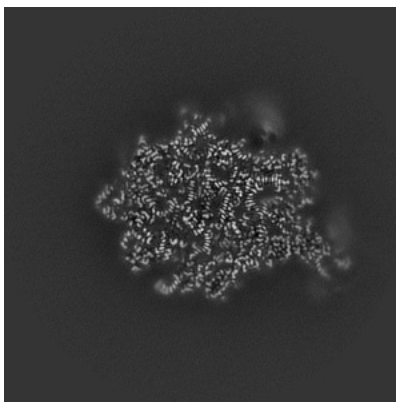


Z Index: 220

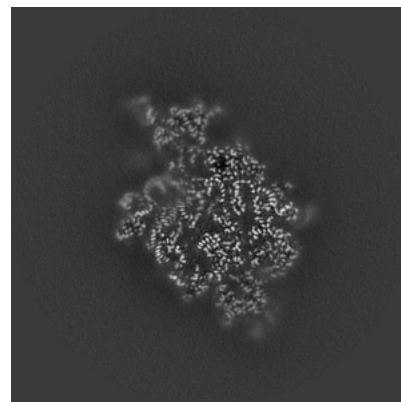
6.3.2 Raw map



X Index: 205



Y Index: 179

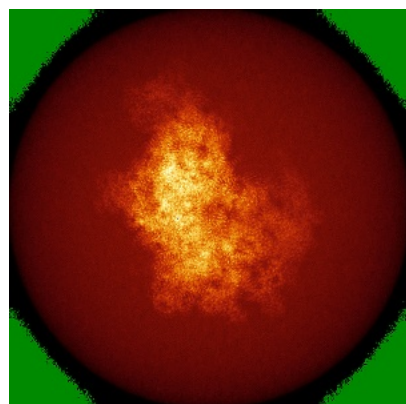


Z Index: 213

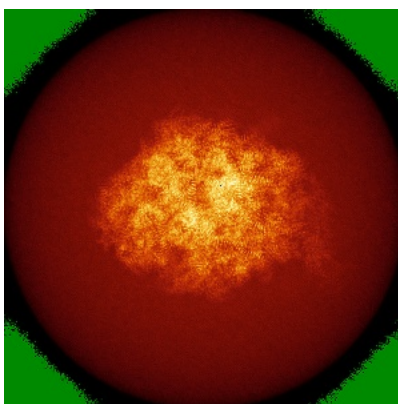
The images above show the largest variance slices of the map in three orthogonal directions.

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

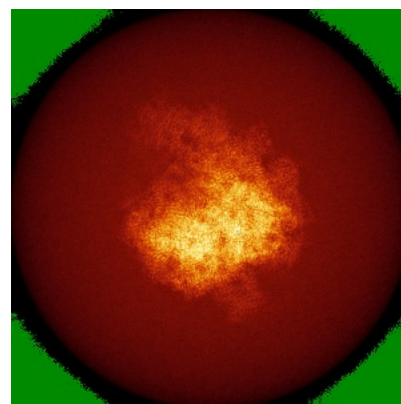
6.4.1 Primary map



X



Y



Z

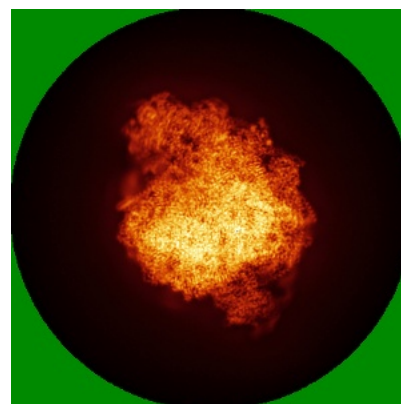
6.4.2 Raw map



X



Y

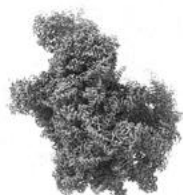


Z

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](#)

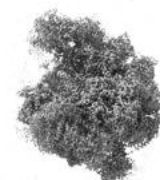
6.5.1 Primary map



X



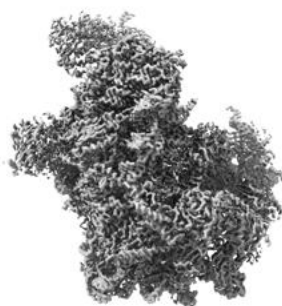
Y



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.

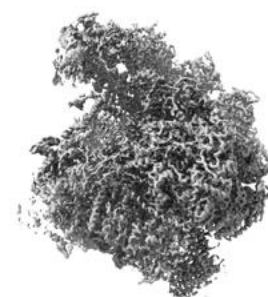
6.5.2 Raw map



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.

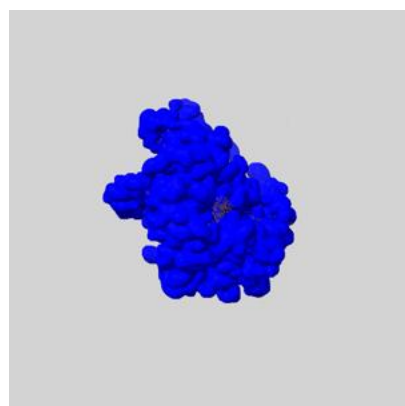
6.6 Mask visualisation [i](#)

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

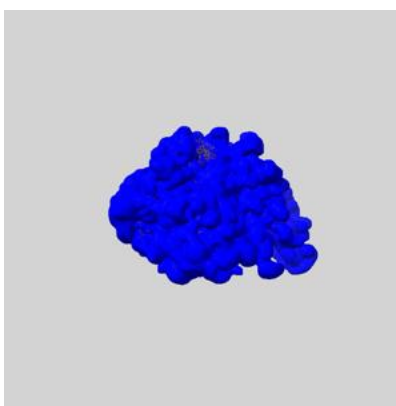
A mask typically either:

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

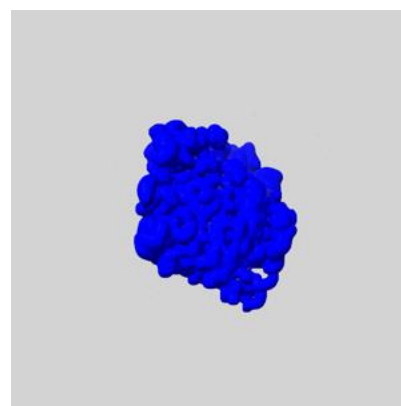
6.6.1 emd_26651_msk_1.map [i](#)



X



Y

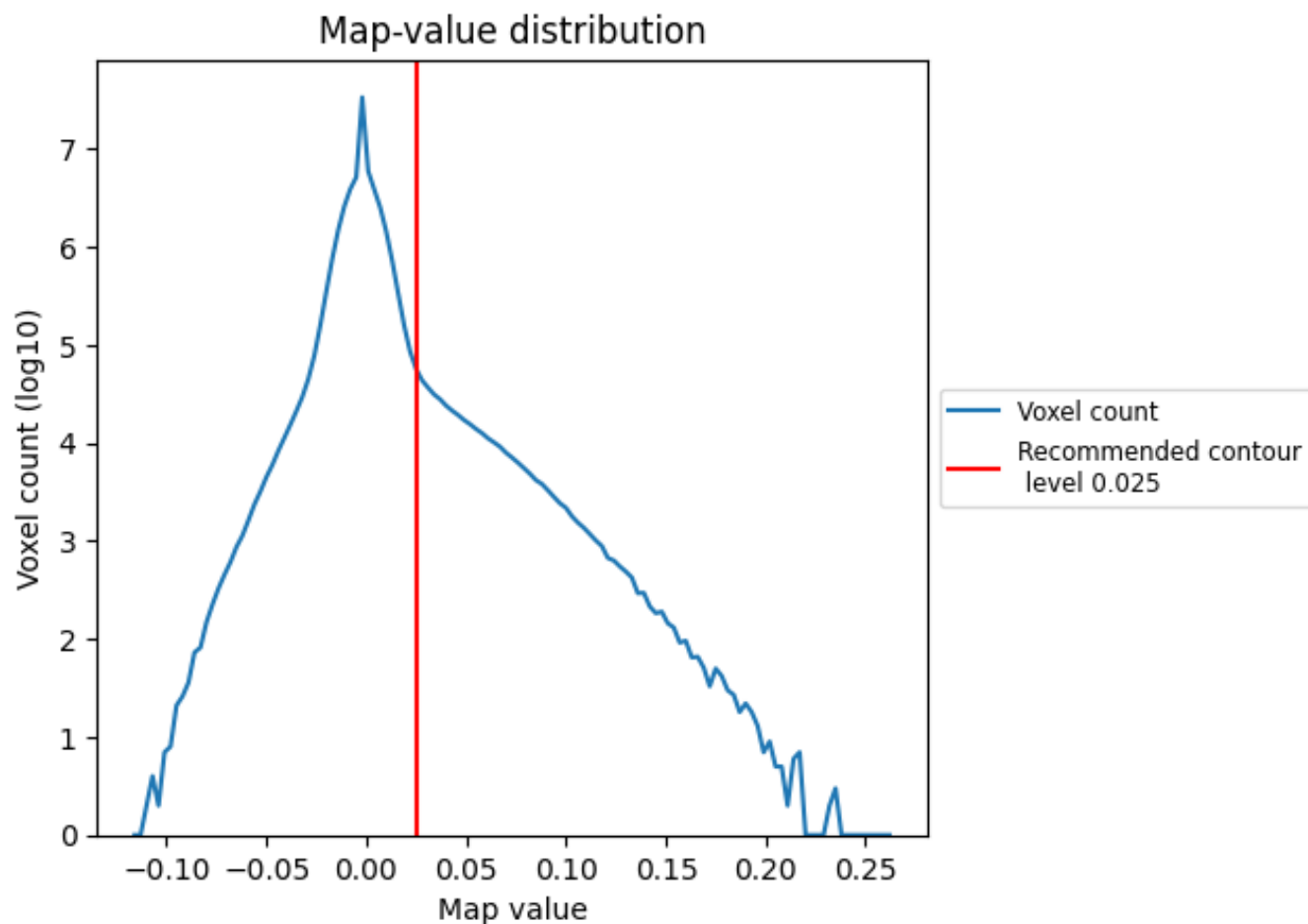


Z

7 Map analysis [i](#)

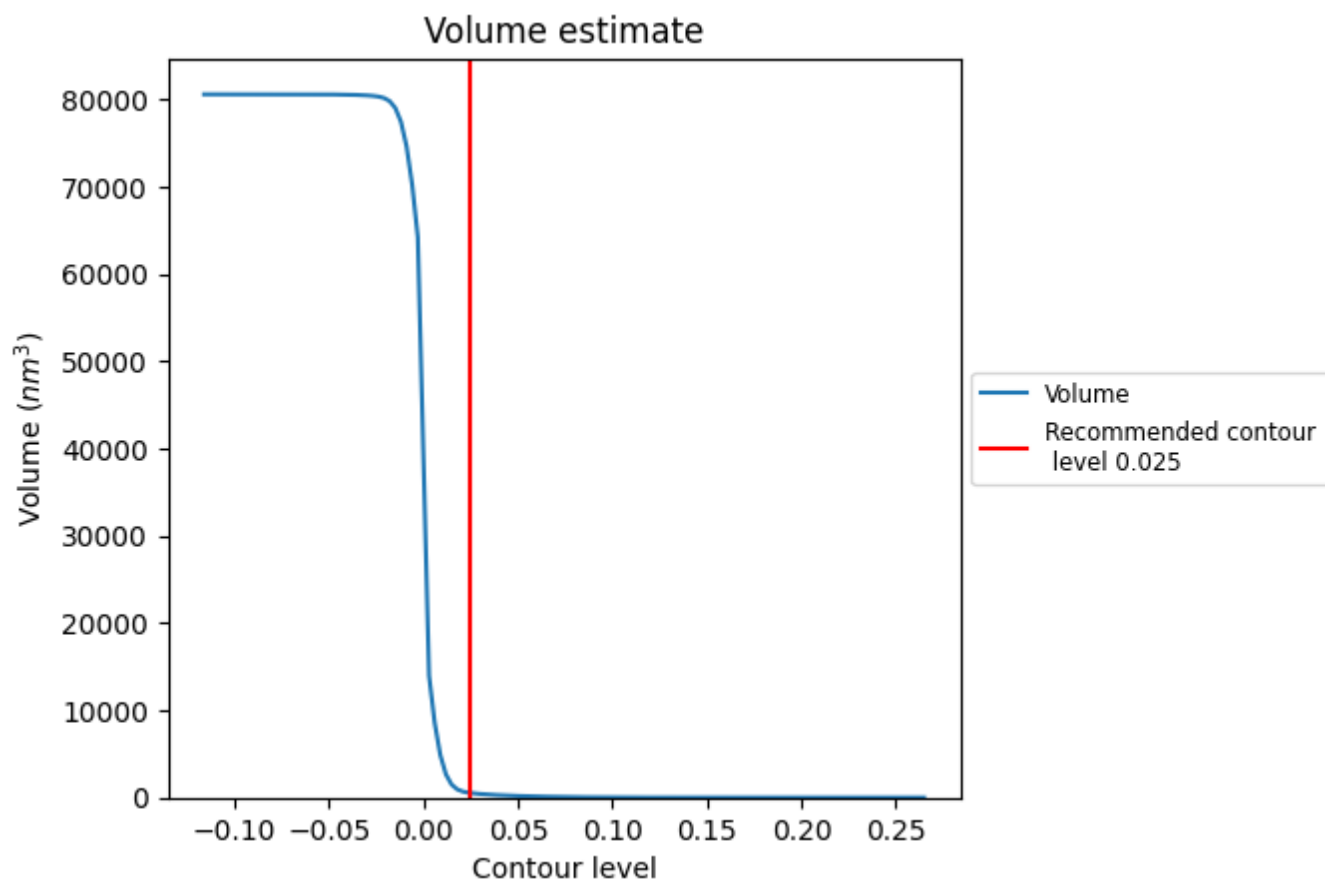
This section contains the results of statistical analysis of the map.

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.

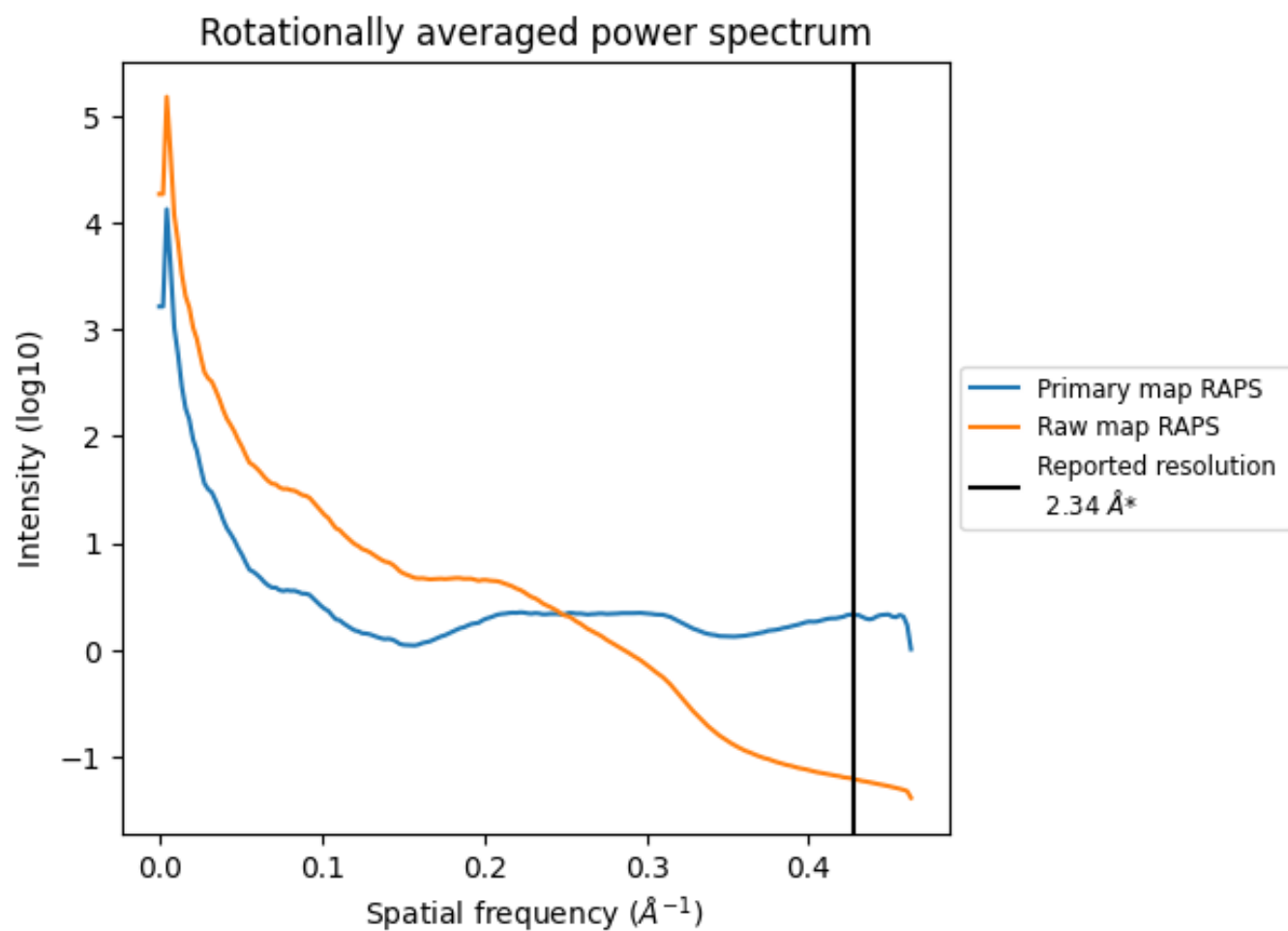
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 526 nm³; 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](#)

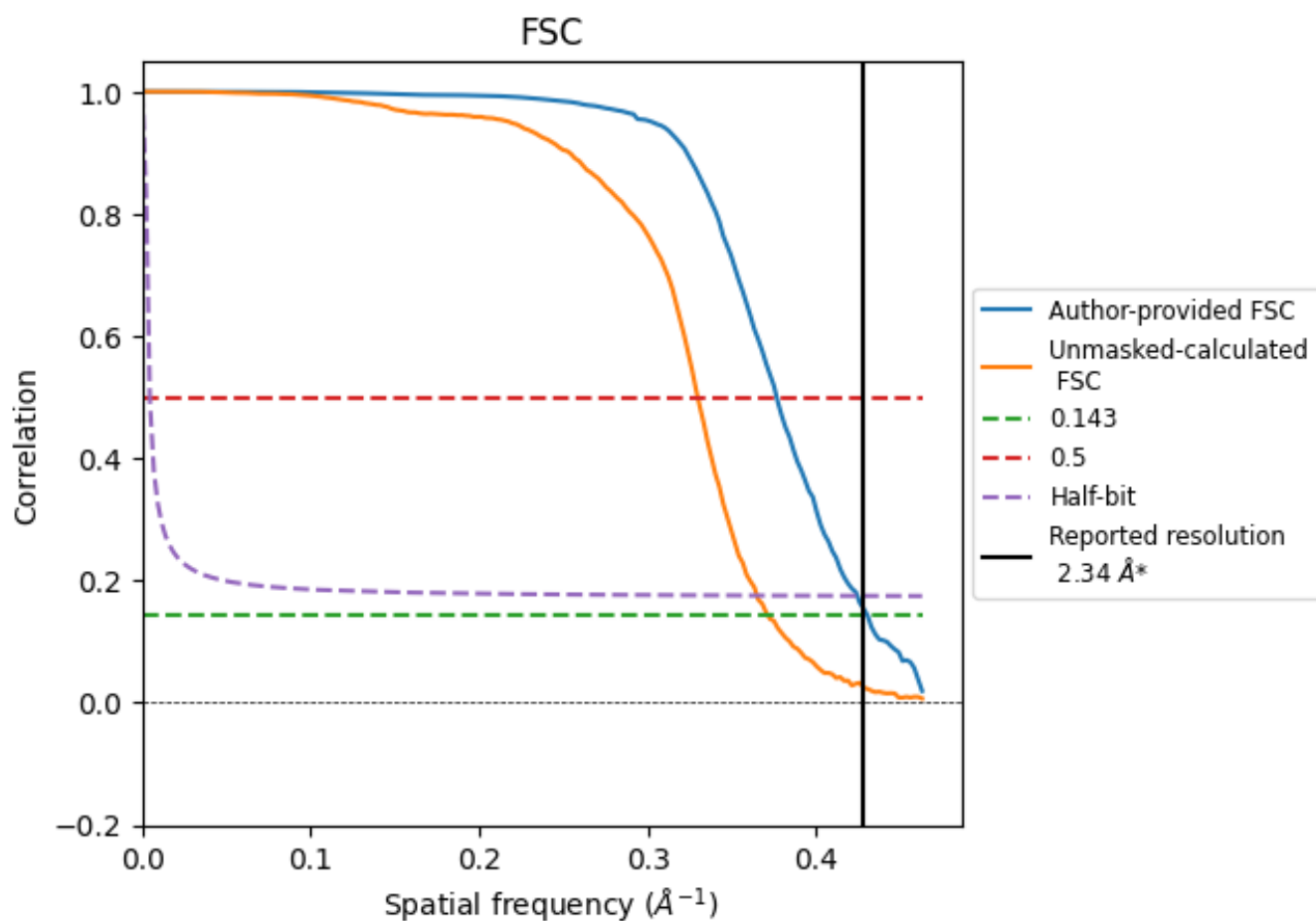


*Reported resolution corresponds to spatial frequency of 0.427 Å⁻¹

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](#)

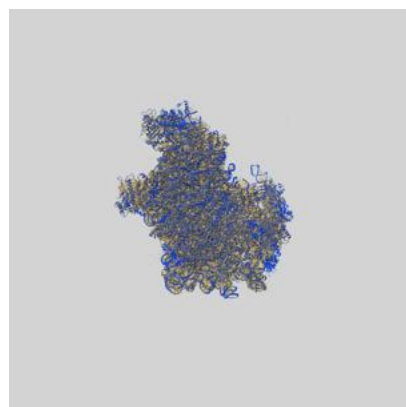
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.34	-	-
Author-provided FSC curve	2.32	2.66	2.36
Unmasked-calculated*	2.69	3.03	2.74

*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 %

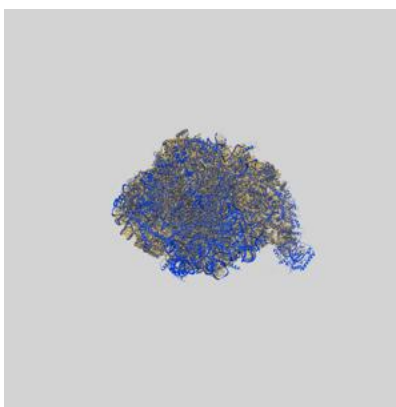
9 Map-model fit [i](#)

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](#).

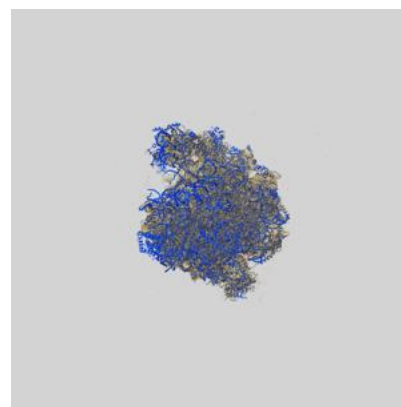
9.1 Map-model overlay [i](#)



X



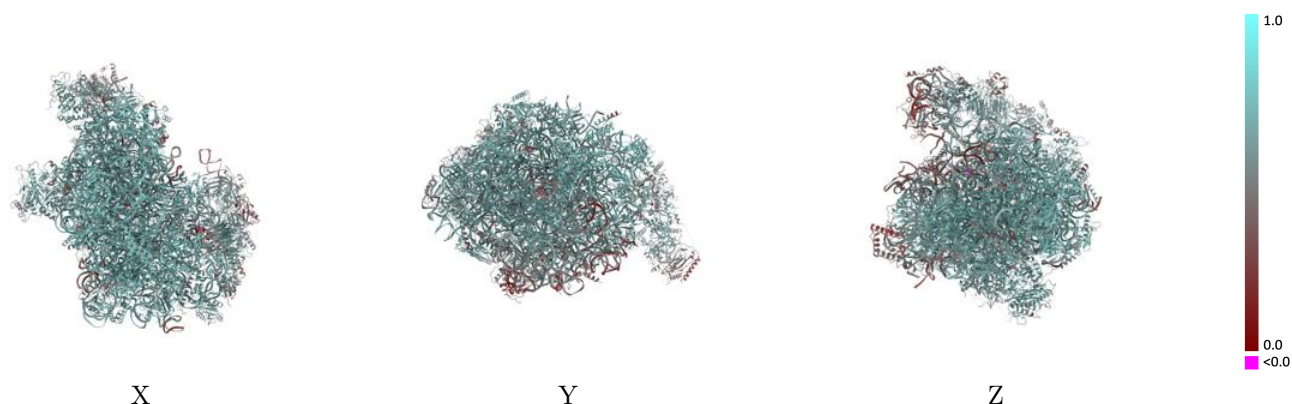
Y



Z

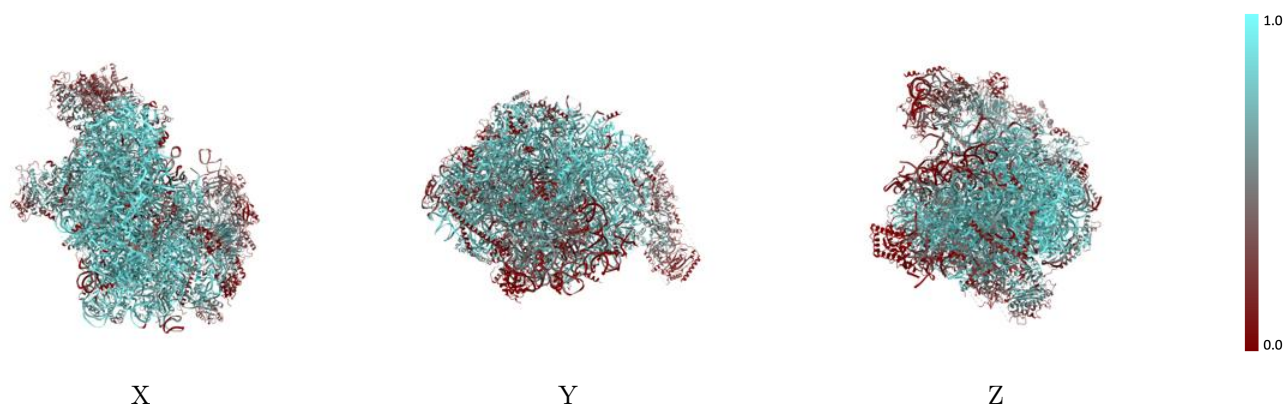
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



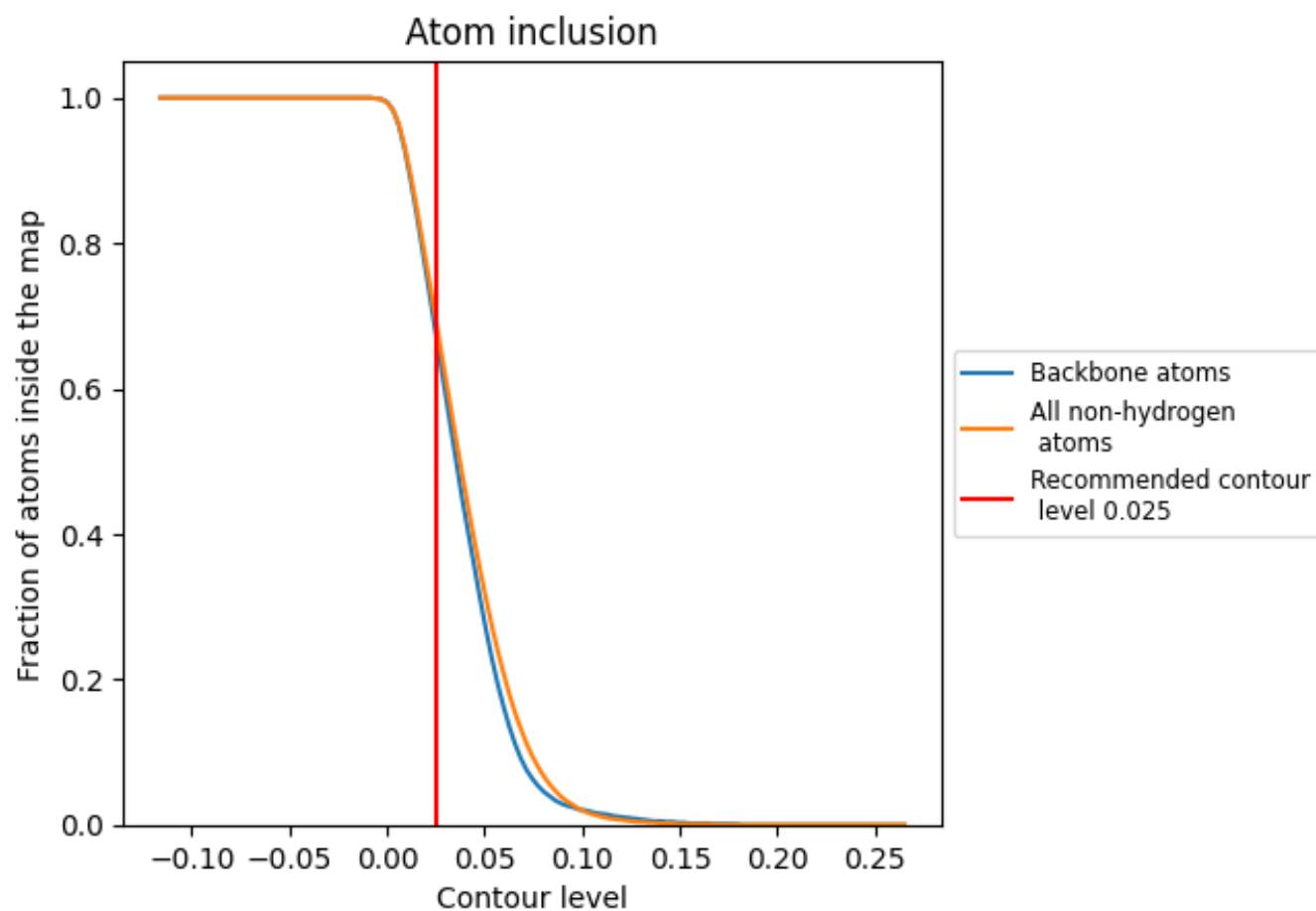
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

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 ⓘ

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