



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 05:21 am BST

PDB ID : 8PJ2 / pdb_00008pj2
EMDB ID : EMD-17697
Title : Structure of human 48S translation initiation complex in AUG recognition state after eIF5-induced GTP hydrolysis by eIF2 (48S-2)
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on : 2023-06-22
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

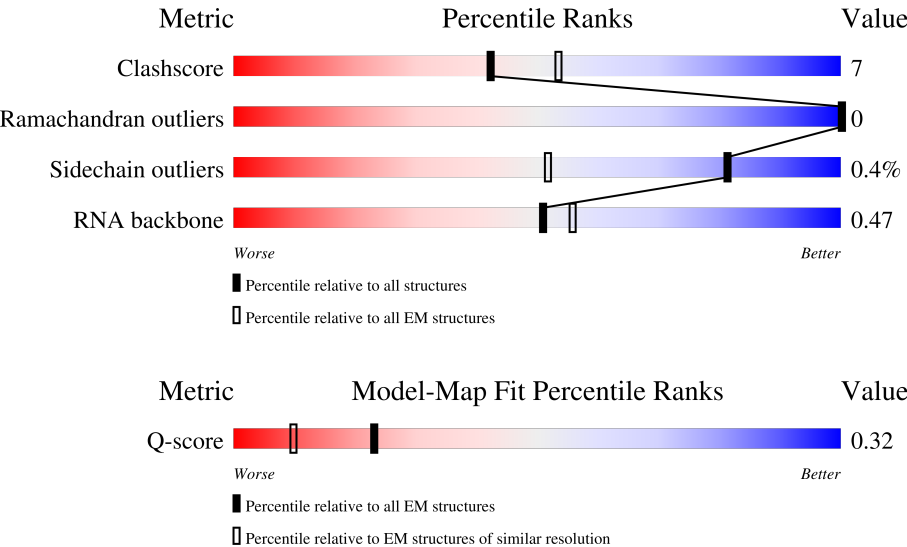
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 i

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	1	814	70% 67% 5% 28%
2	2	325	94% 93% 6%
3	3	218	78% 97% ..

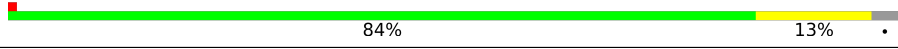
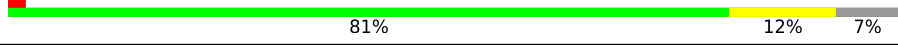
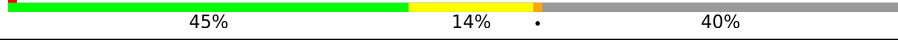
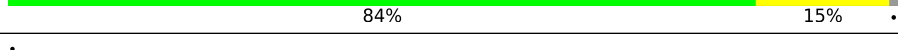
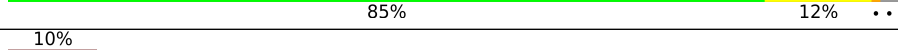
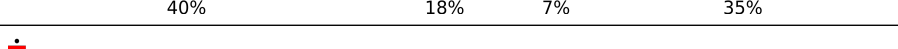
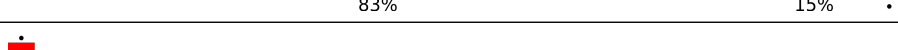
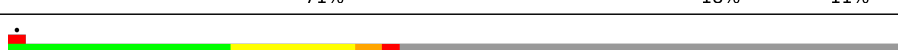
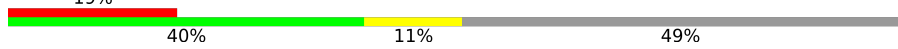
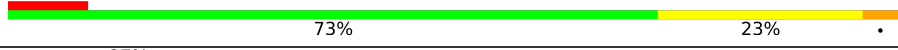
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Mol	Chain	Length	Quality of chain
4	4	357	
5	5	564	
6	6	374	
7	7	255	
8	8	352	
9	9	25	
10	A	1869	
11	B	158	
12	C	263	
13	D	194	
14	E	143	
15	F	59	
16	G	194	
17	H	84	
18	I	151	
19	J	130	
20	K	83	
21	L	293	
22	M	135	
23	N	295	
24	O	264	
25	P	151	
26	Q	115	
27	R	208	
28	S	249	

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Mol	Chain	Length	Quality of chain
29	T	133	
30	V	204	
31	Y	146	
32	Z	243	
33	a	165	
34	b	145	
35	c	317	
36	d	145	
37	e	125	
38	f	152	
39	h	119	
40	i	56	
41	k	156	
42	m	132	
43	n	69	
44	o	320	
45	q	144	
46	r	315	
47	t	472	
48	u	1382	
49	v	445	
50	w	75	
51	x	548	
52	y	913	
53	z	430	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 118707 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 Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	588	Total	C	N	O	S	0	0
			3258	1986	633	634	5		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	304	Total	C	N	O	0	0
			1493	885	304	304		

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	520	Total	C	N	O	S	0	0
			4347	2814	721	793	19		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	362	Total	C	N	O	S	0	0
			2196	1348	414	427	7		

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	57	Total	C	N	O	P	0	0
			1218	547	231	383	57		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	317	Total	C	N	O		0	0
			1574	937	318	319			

- Molecule 9 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 10 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1754	Total	C	N	O	P	0	0
			37429	16718	6714	12244	1753		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1248	B8N	U	conflict	GB NR_046235.3

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 12 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 13 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 15 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	59	Total	C	N	O	S	0	0
			468	290	102	75	1		

- Molecule 16 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 17 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 19 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 20 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 21 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 22 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 23 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 24 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 25 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 26 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 28 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 31 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 32 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 33 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 34 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 36 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	81	Total	C	N	O	S	0	0
			649	420	119	109	1		

- Molecule 38 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	149	Total	C	N	O	S	0	0
			1227	770	249	207	1		

- Molecule 39 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 40 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 41 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

- Molecule 42 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 43 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	77	Total	C	N	O	S	0	0
			616	389	111	116			

- Molecule 45 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	112	Total	C	N	O	S	0	0
			902	560	173	165	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	296	Total	C	N	O	S	0	0
			2138	1342	384	404	8		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	455	Total	C	N	O	S	0	0
			3439	2179	599	643	18		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	405	Total	C	N	O	S	0	0
			2740	1720	498	510	12		

- Molecule 50 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	422	Total	C	N	O	S	0	0
			2837	1749	522	556	10		

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	656	Total	C	N	O	S	0	0
			5263	3312	939	977	35		

- Molecule 53 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	145	Total	C	N	O	S	0	0
			1146	723	203	209	11		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	83	Total	Mg	0
			83	83	
54	V	1	Total	Mg	0
			1	1	
54	f	1	Total	Mg	0
			1	1	

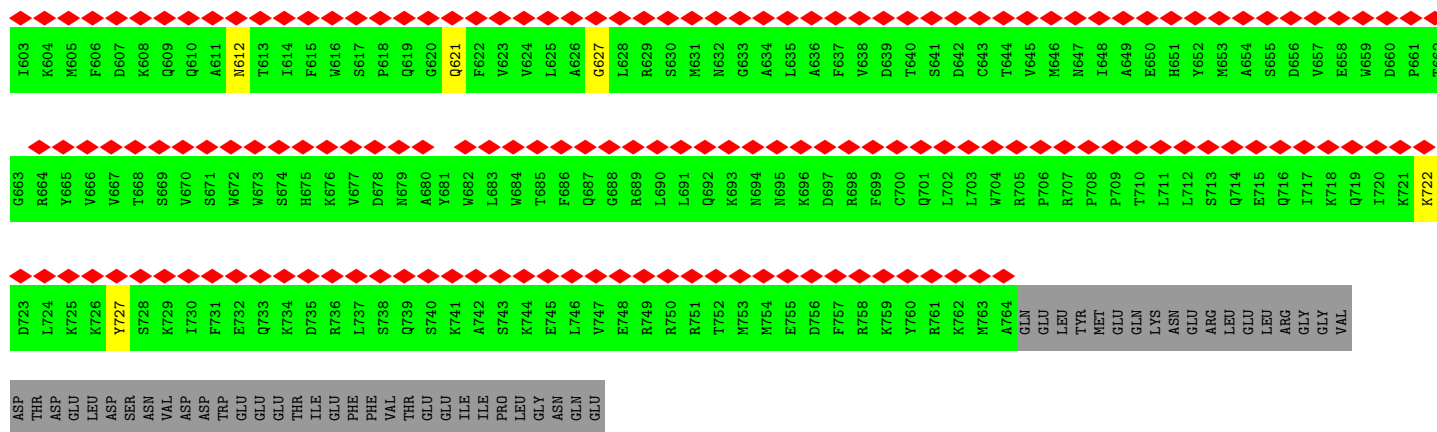
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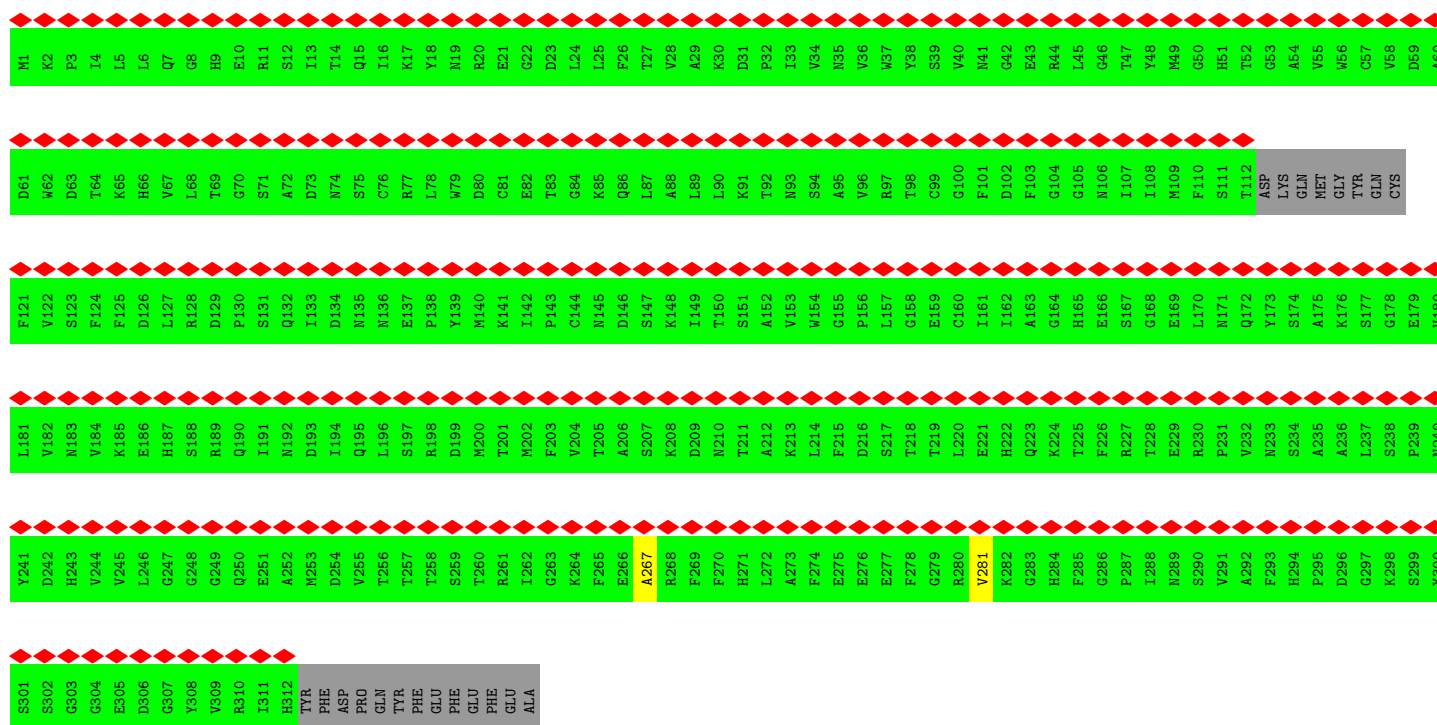
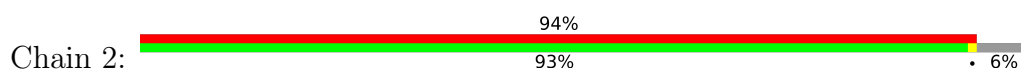
Mol	Chain	Residues	Atoms		AltConf
54	i	2	Total	Mg	0
			2	2	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

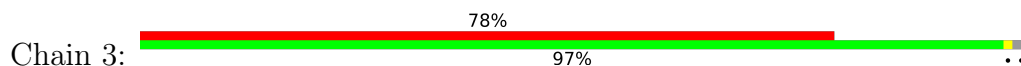
Mol	Chain	Residues	Atoms		AltConf
55	Q	1	Total	Zn	0
			1	1	
55	k	1	Total	Zn	0
			1	1	

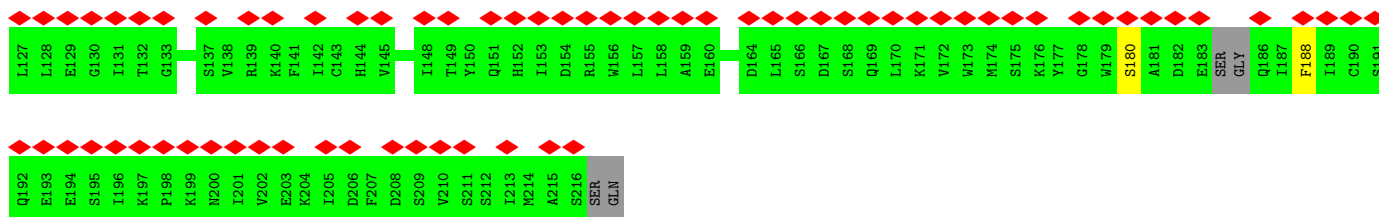


• Molecule 2: Eukaryotic translation initiation factor 3 subunit I

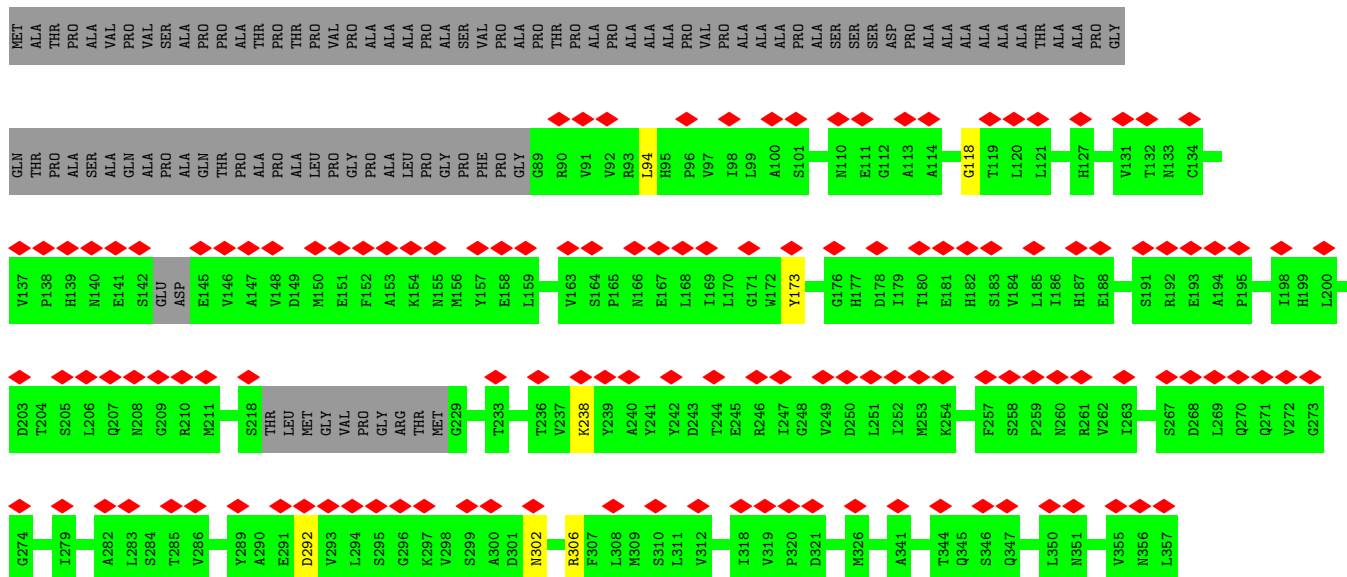


• Molecule 3: Eukaryotic translation initiation factor 3 subunit K

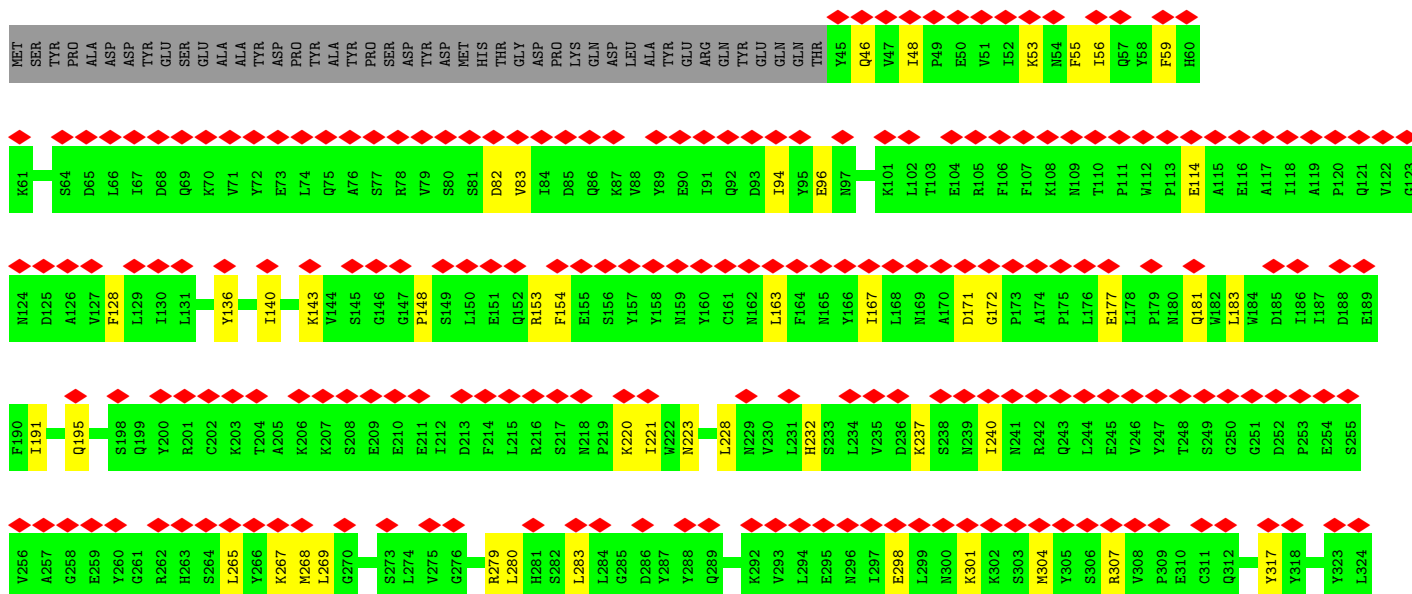
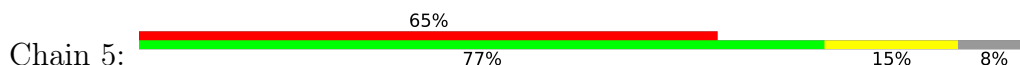


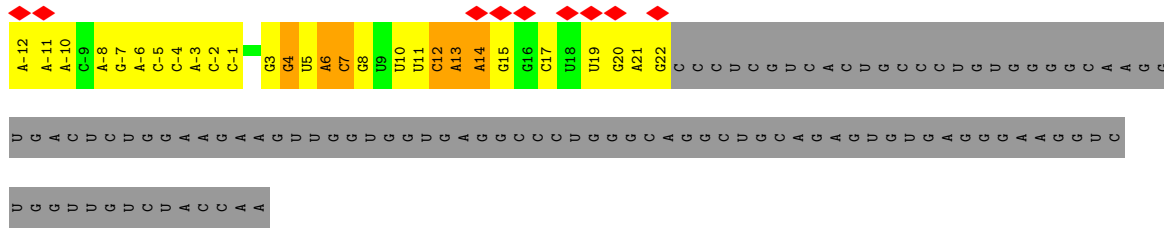


- Molecule 4: Eukaryotic translation initiation factor 3 subunit F

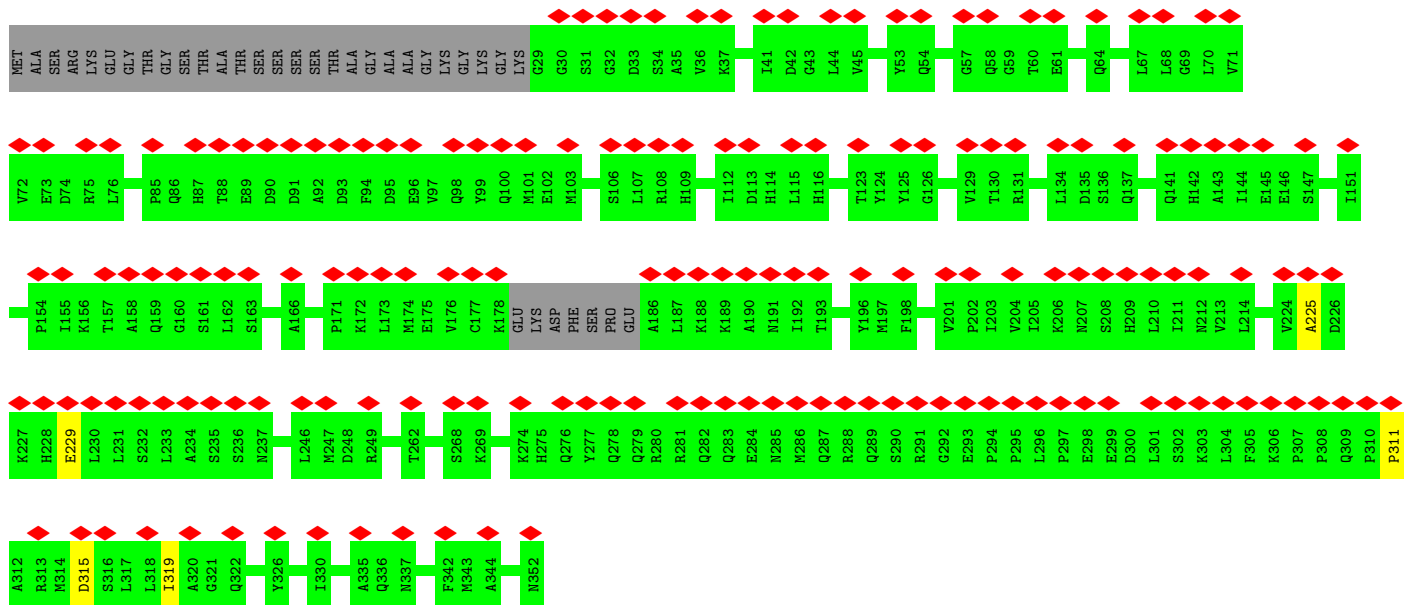
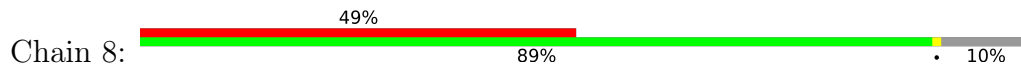


- Molecule 5: Eukaryotic translation initiation factor 3 subunit L





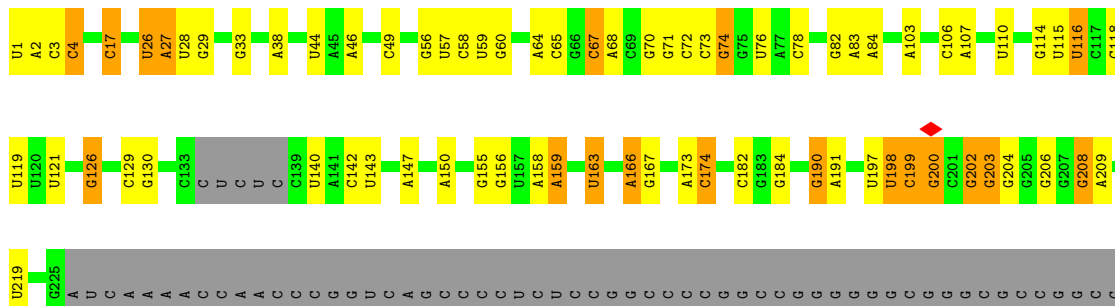
• Molecule 8: Eukaryotic translation initiation factor 3 subunit H



• Molecule 9: 60S ribosomal protein L41

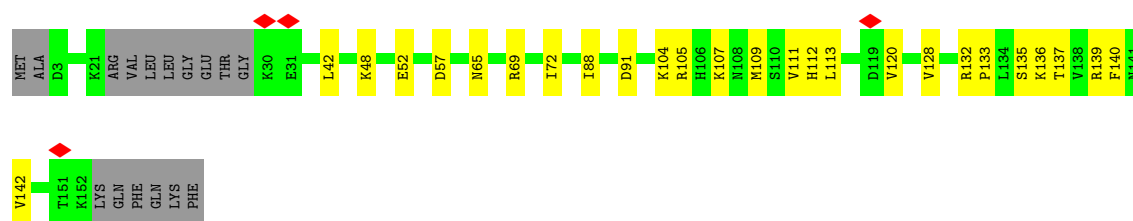
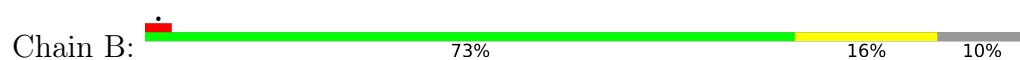


• Molecule 10: 18S rRNA

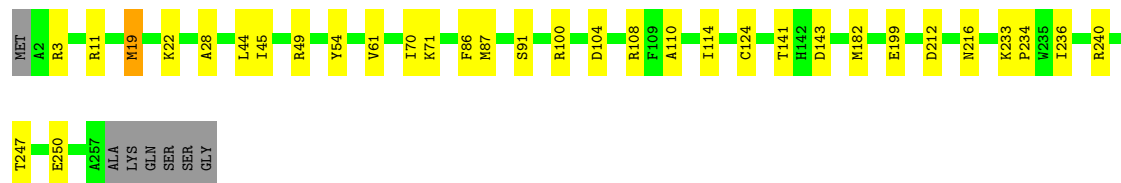
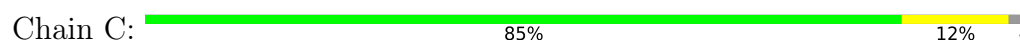




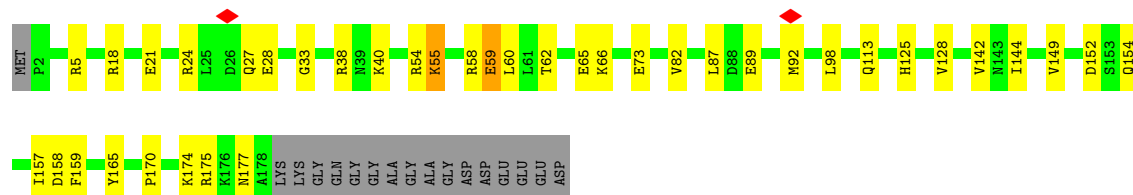
- Molecule 11: 40S ribosomal protein S11



- Molecule 12: 40S ribosomal protein S4, X isoform



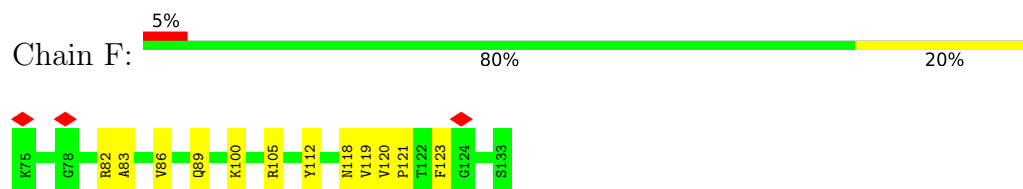
- Molecule 13: 40S ribosomal protein S9



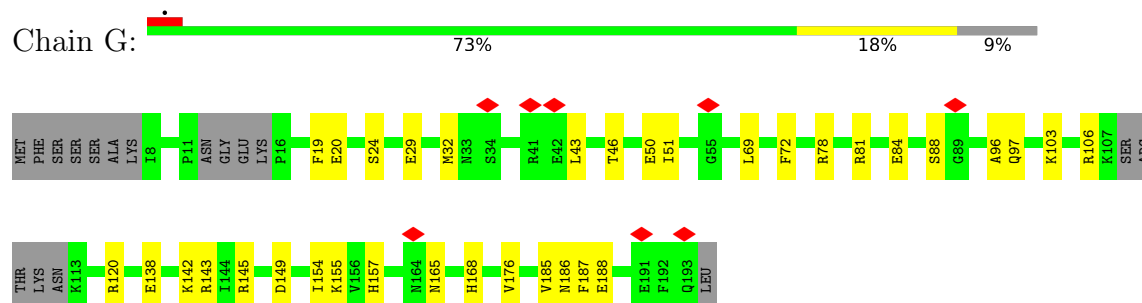
- Molecule 14: 40S ribosomal protein S23



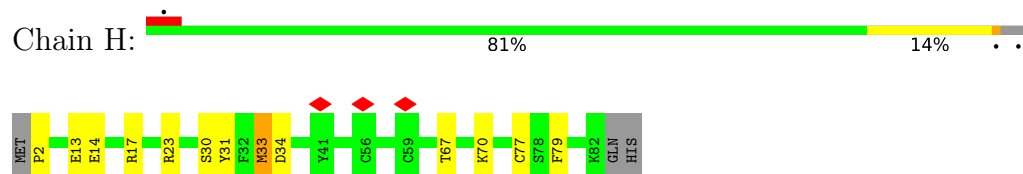
- Molecule 15: 40S ribosomal protein S30



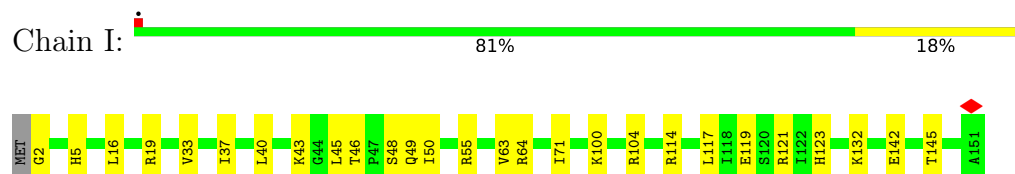
- Molecule 16: 40S ribosomal protein S7



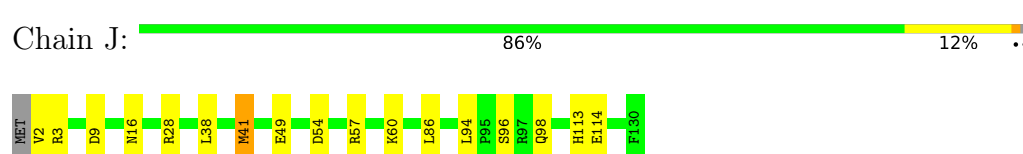
- Molecule 17: 40S ribosomal protein S27



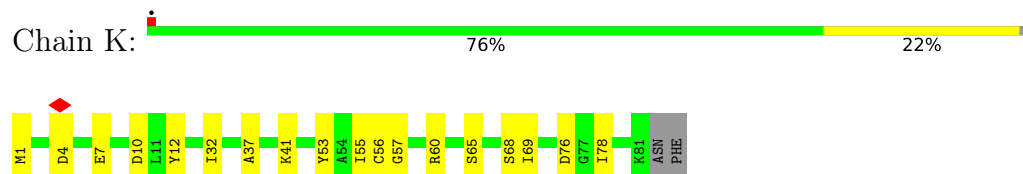
- Molecule 18: 40S ribosomal protein S13



- Molecule 19: 40S ribosomal protein S15a

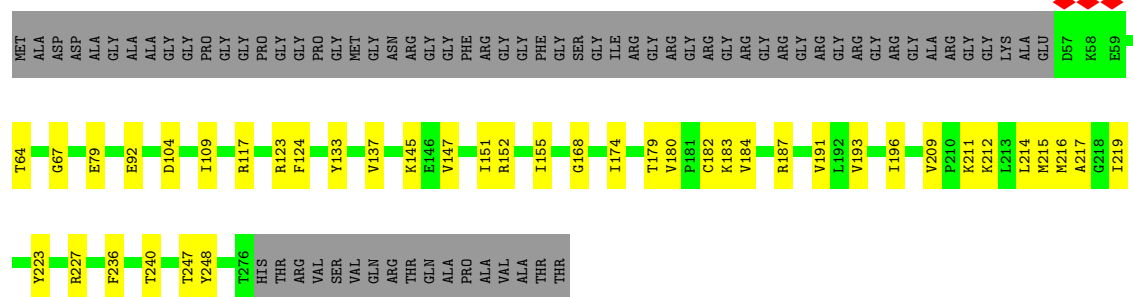


- Molecule 20: 40S ribosomal protein S21



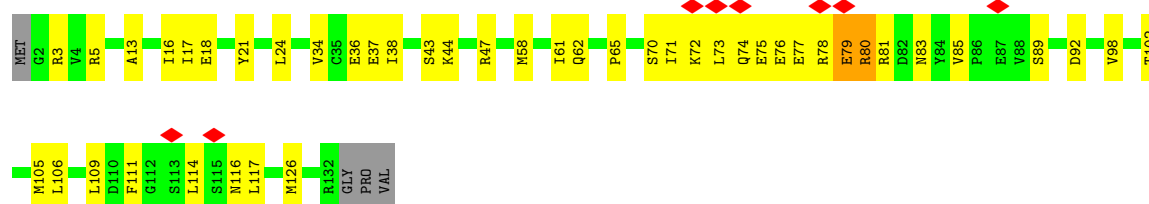
- Molecule 21: 40S ribosomal protein S2

Chain L: 



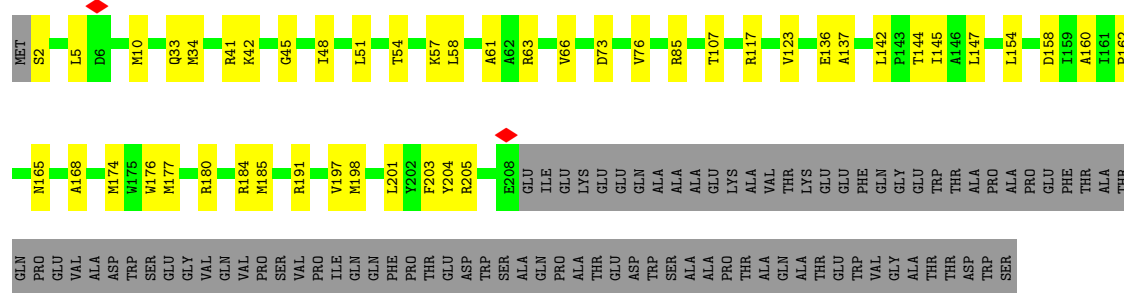
- Molecule 22: 40S ribosomal protein S17

Chain M: 



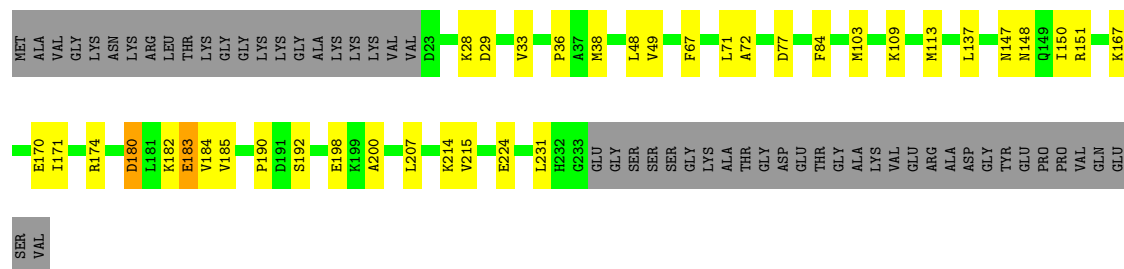
- Molecule 23: 40S ribosomal protein SA

Chain N: 



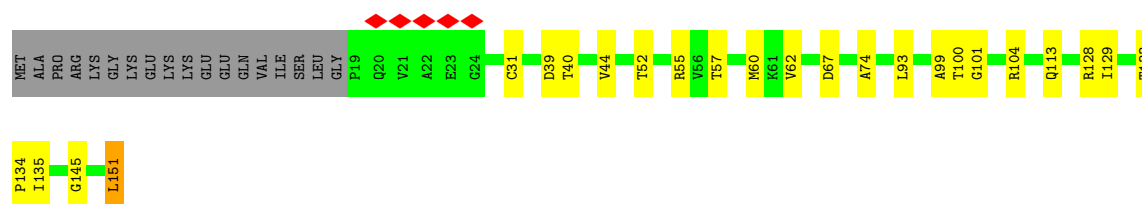
- Molecule 24: 40S ribosomal protein S3a

Chain O: 



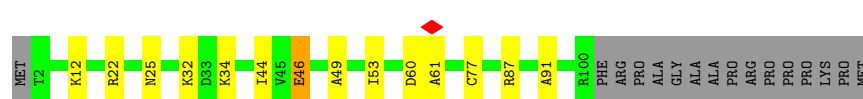
- Molecule 25: 40S ribosomal protein S14

Chain P:  72% 15% 12%



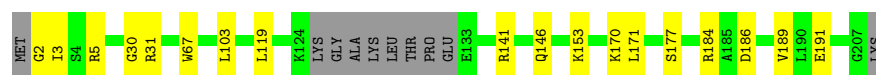
- Molecule 26: 40S ribosomal protein S26

Chain Q:  74% 11% 14%



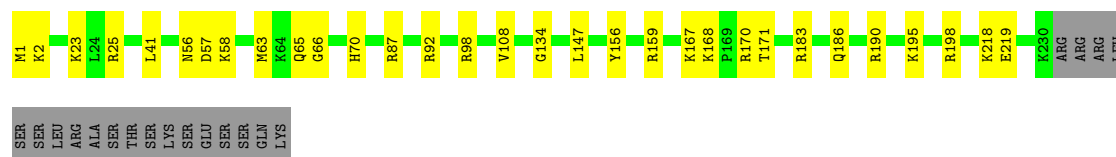
- Molecule 27: 40S ribosomal protein S8

Chain R:  87% 9% 5%



- Molecule 28: 40S ribosomal protein S6

Chain S:  80% 12% 8%



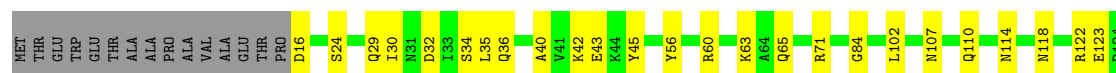
- Molecule 29: 40S ribosomal protein S24

Chain T:  81% 13% 6%



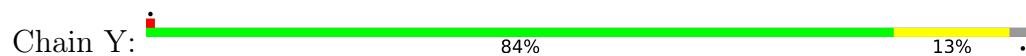
- Molecule 30: 40S ribosomal protein S5

Chain V:  73% 17% 10%

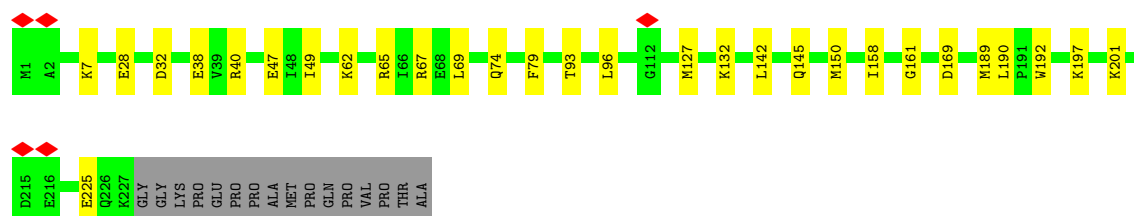
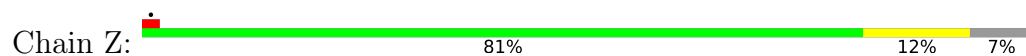




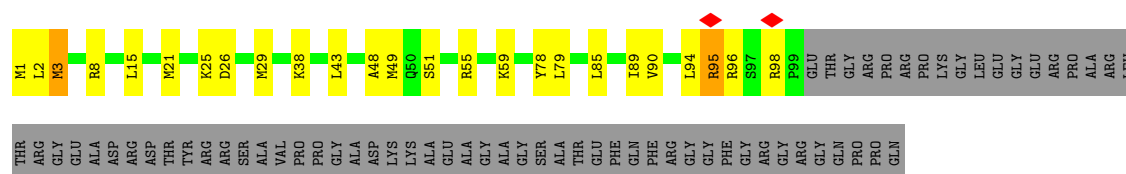
- Molecule 31: 40S ribosomal protein S16



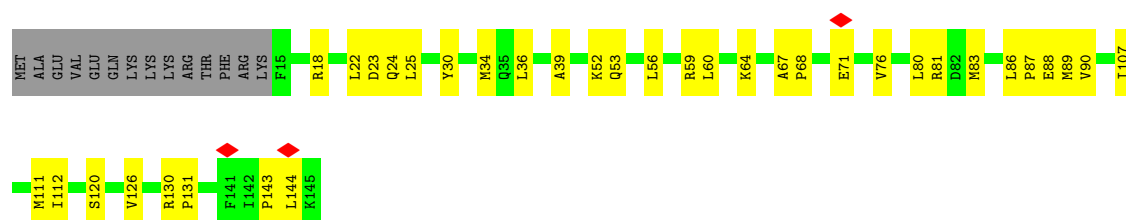
- Molecule 32: 40S ribosomal protein S3



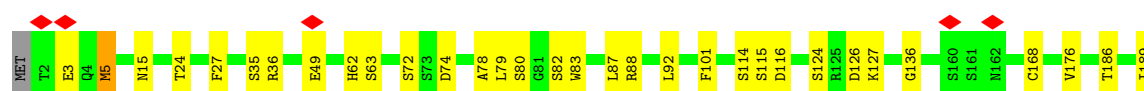
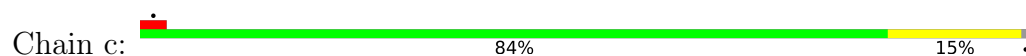
- Molecule 33: 40S ribosomal protein S10



- Molecule 34: 40S ribosomal protein S15

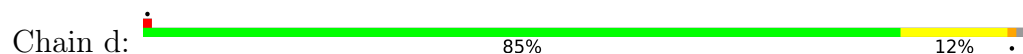


- Molecule 35: Receptor of activated protein C kinase 1

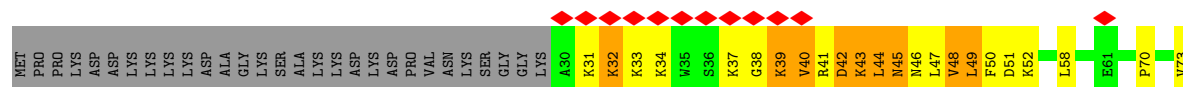




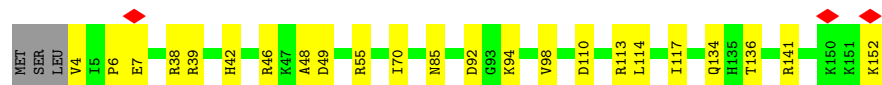
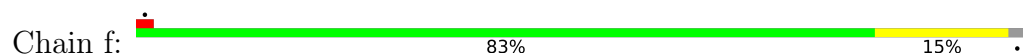
- Molecule 36: 40S ribosomal protein S19



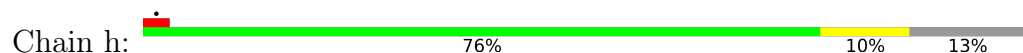
- Molecule 37: 40S ribosomal protein S25



- Molecule 38: 40S ribosomal protein S18



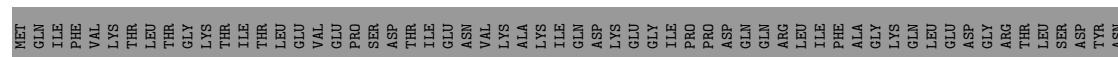
- Molecule 39: 40S ribosomal protein S20

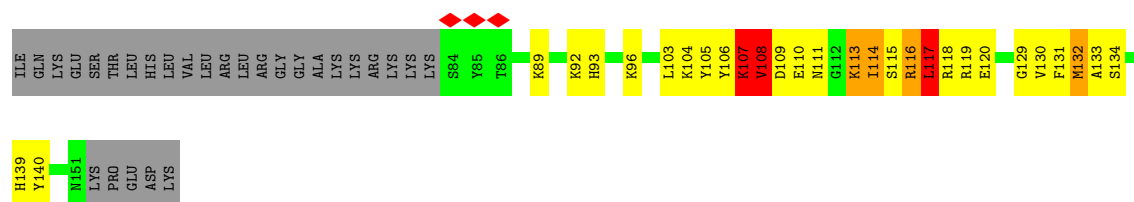


- Molecule 40: 40S ribosomal protein S29



- Molecule 41: Ubiquitin

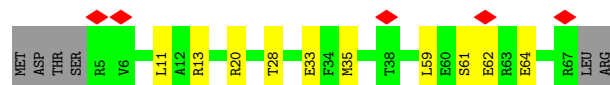
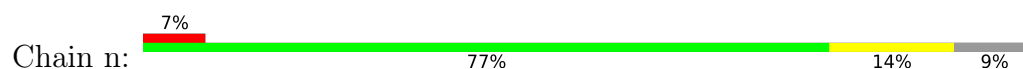




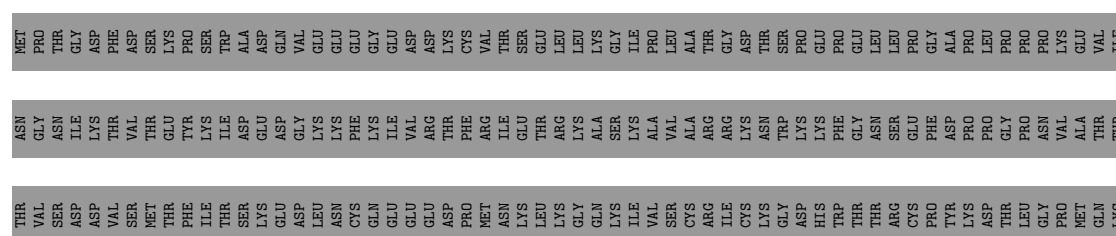
- Molecule 42: 40S ribosomal protein S12



- Molecule 43: 40S ribosomal protein S28

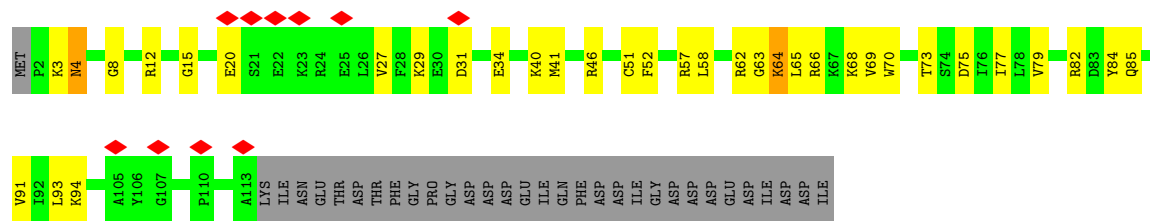


- Molecule 44: Eukaryotic translation initiation factor 3 subunit G

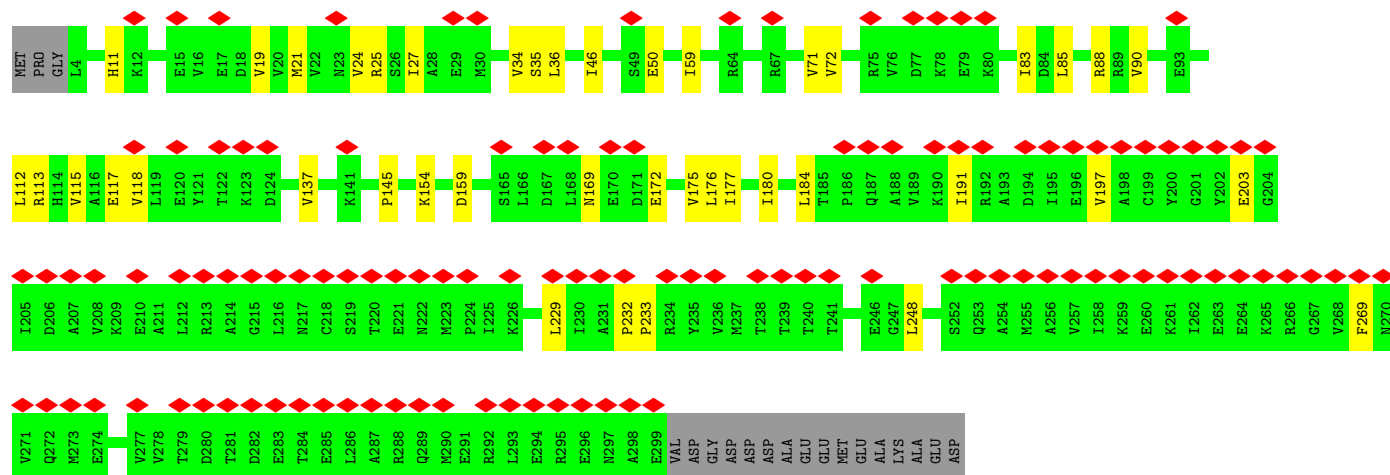
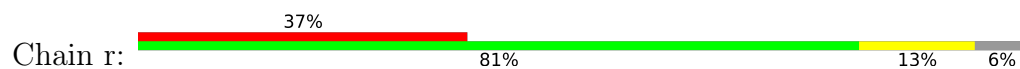


- Molecule 45: Eukaryotic translation initiation factor 1A, X-chromosomal

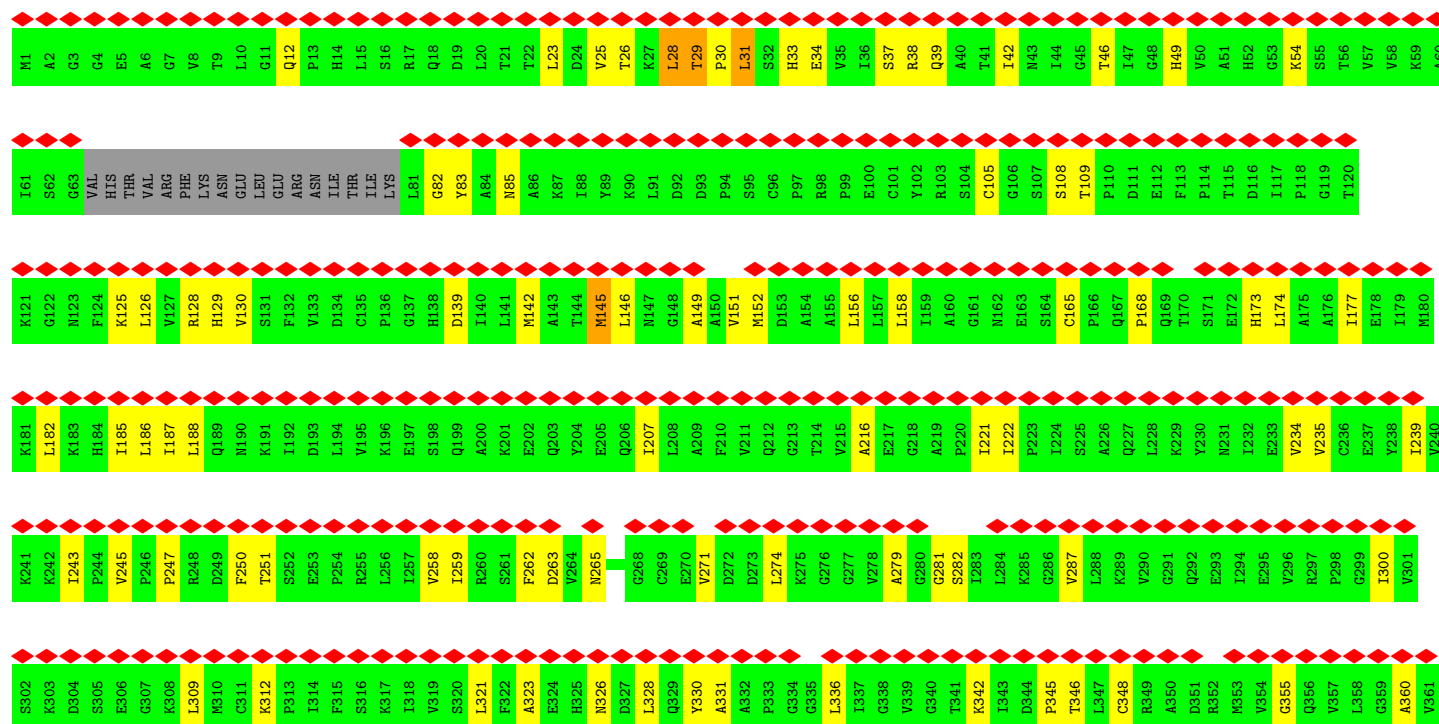
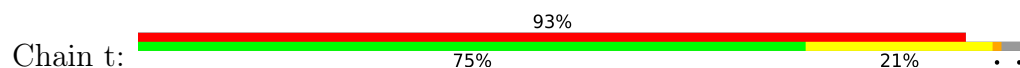


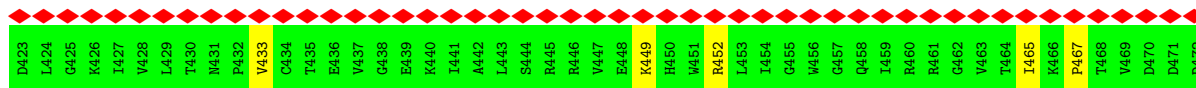
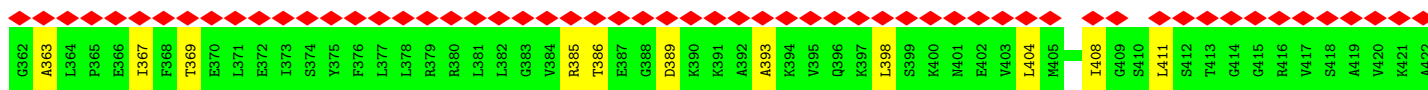


• Molecule 46: Eukaryotic translation initiation factor 2 subunit 1

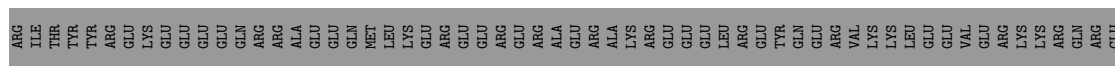
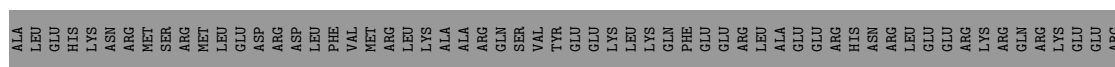
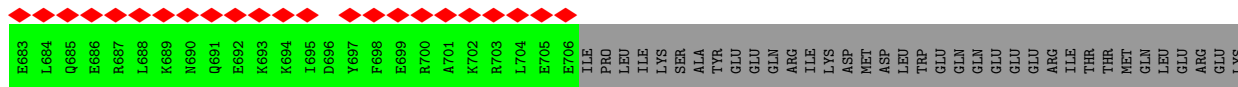
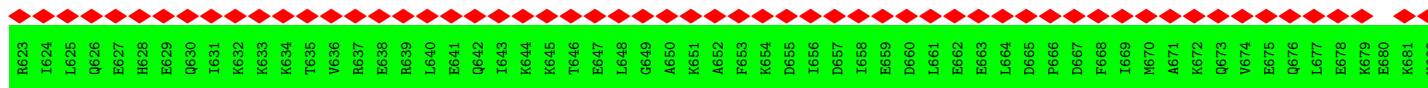
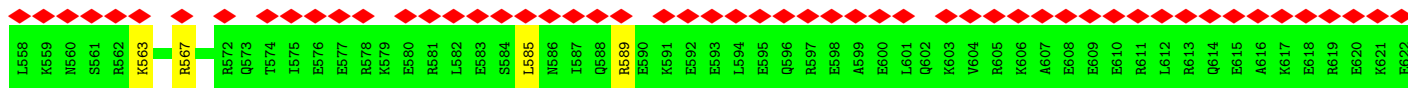
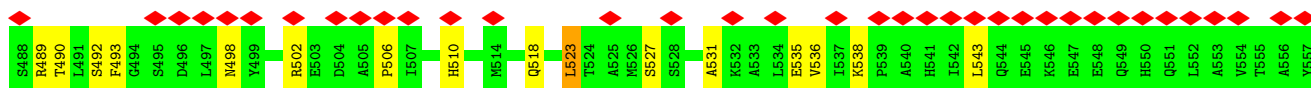
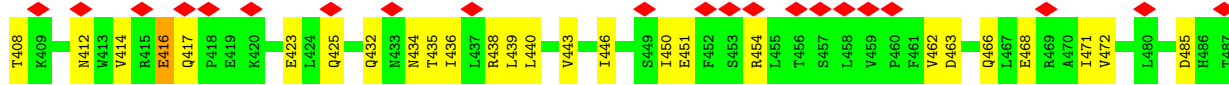
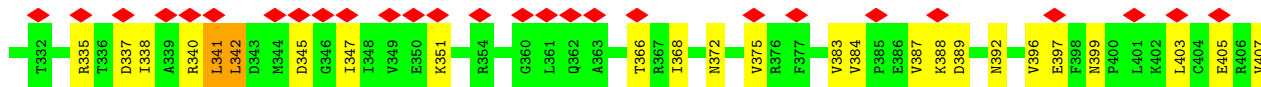
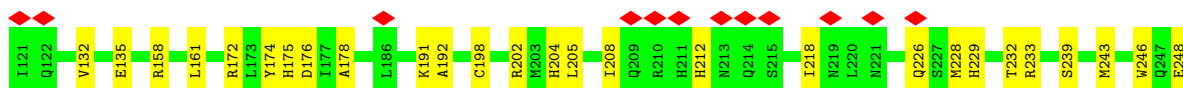
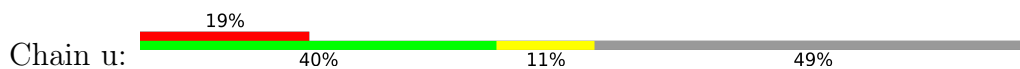


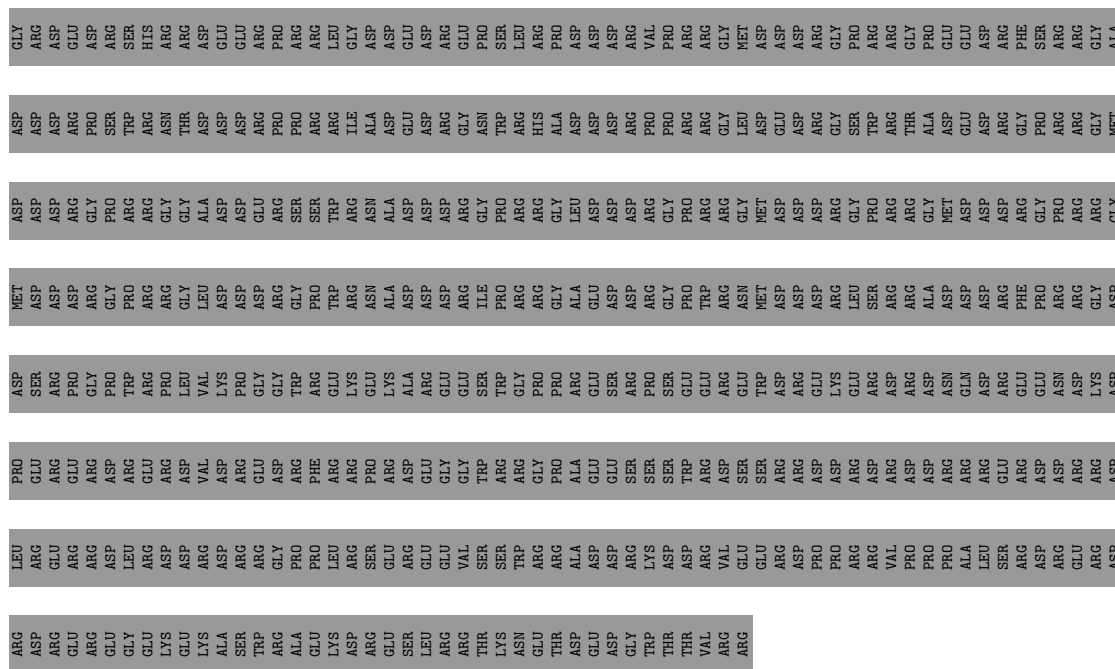
• Molecule 47: Eukaryotic translation initiation factor 2 subunit 3



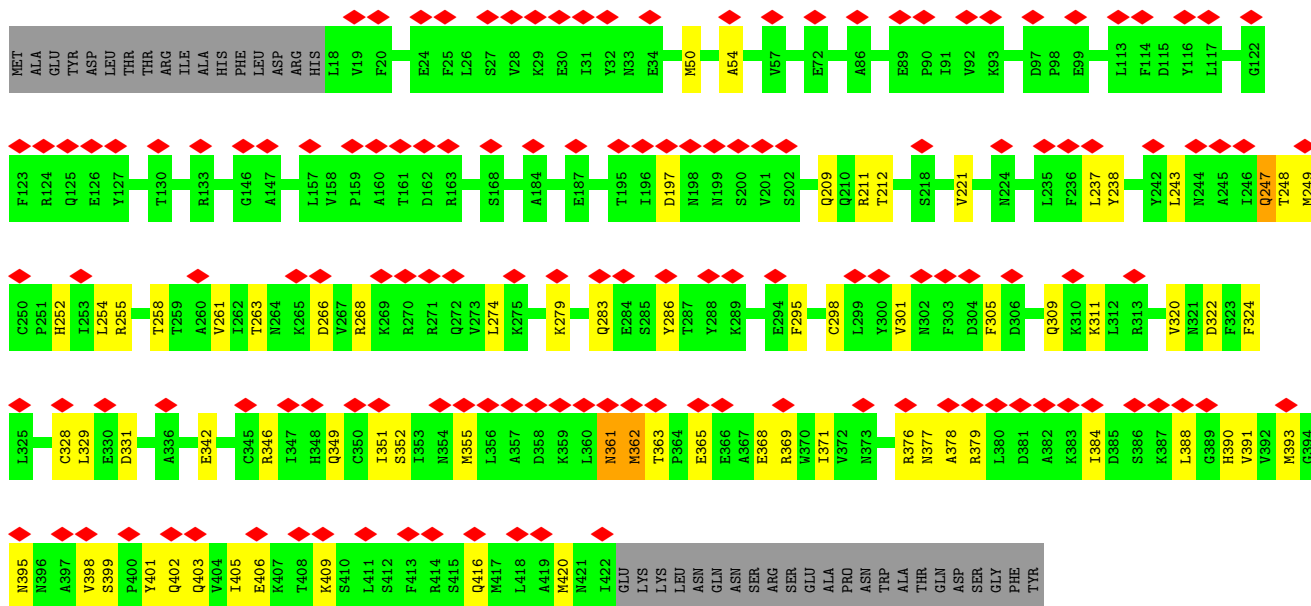
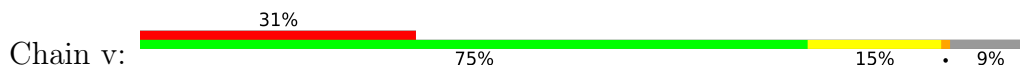


• Molecule 48: Eukaryotic translation initiation factor 3 subunit A

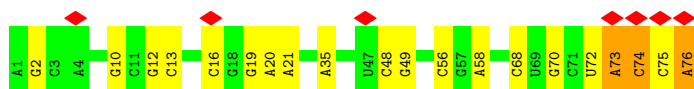




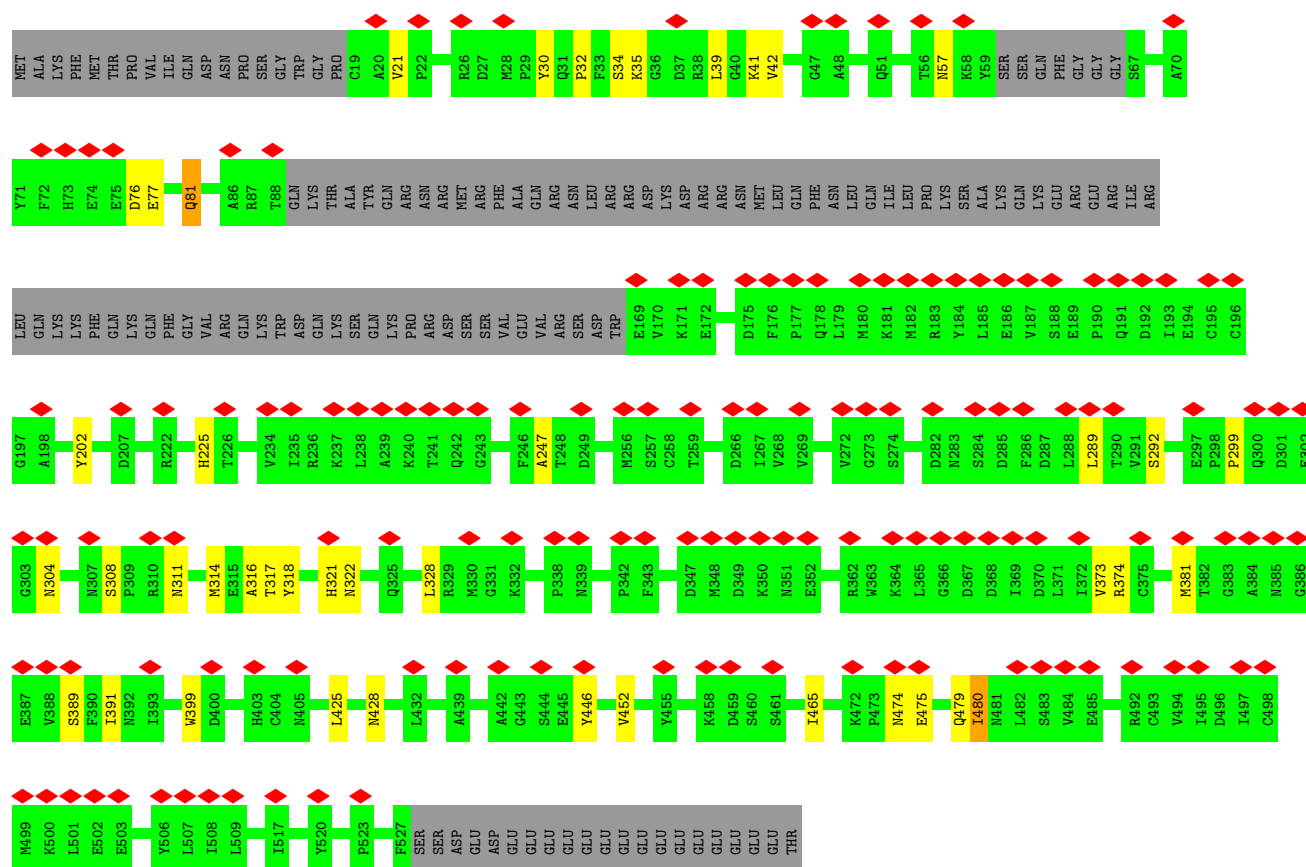
- Molecule 49: Eukaryotic translation initiation factor 3 subunit E



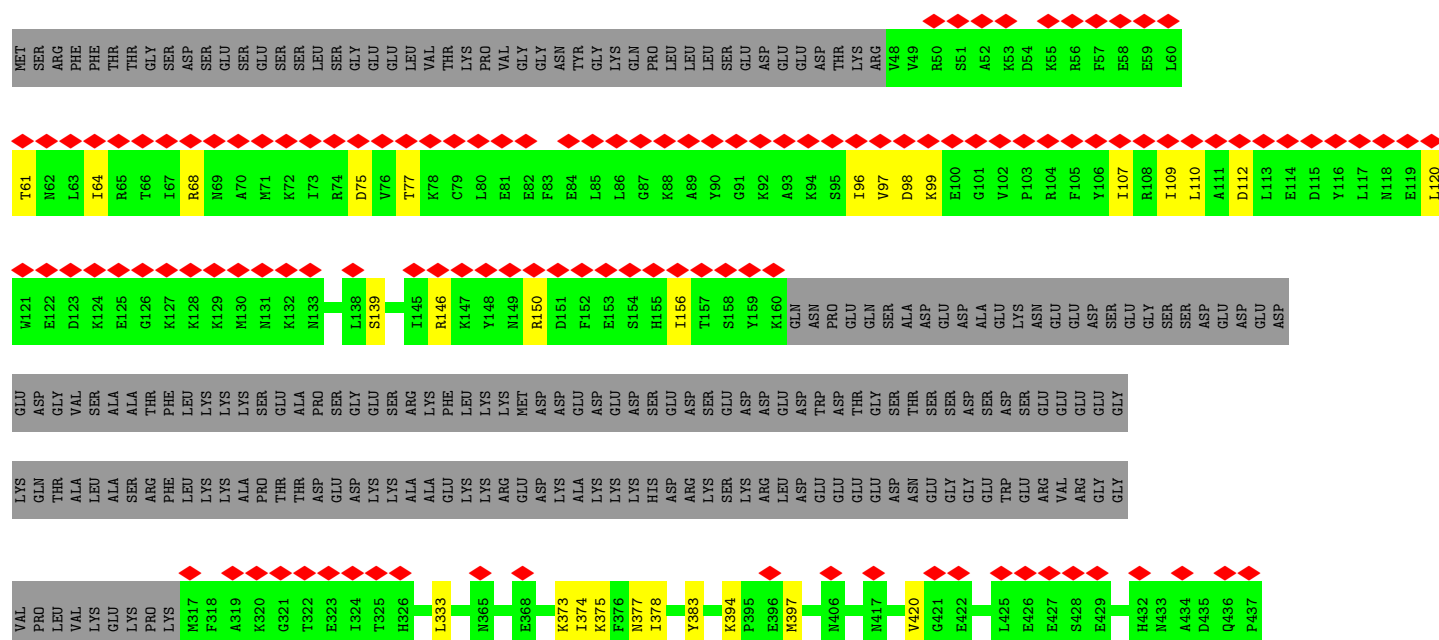
- Molecule 50: Initiator Met-tRNA-i

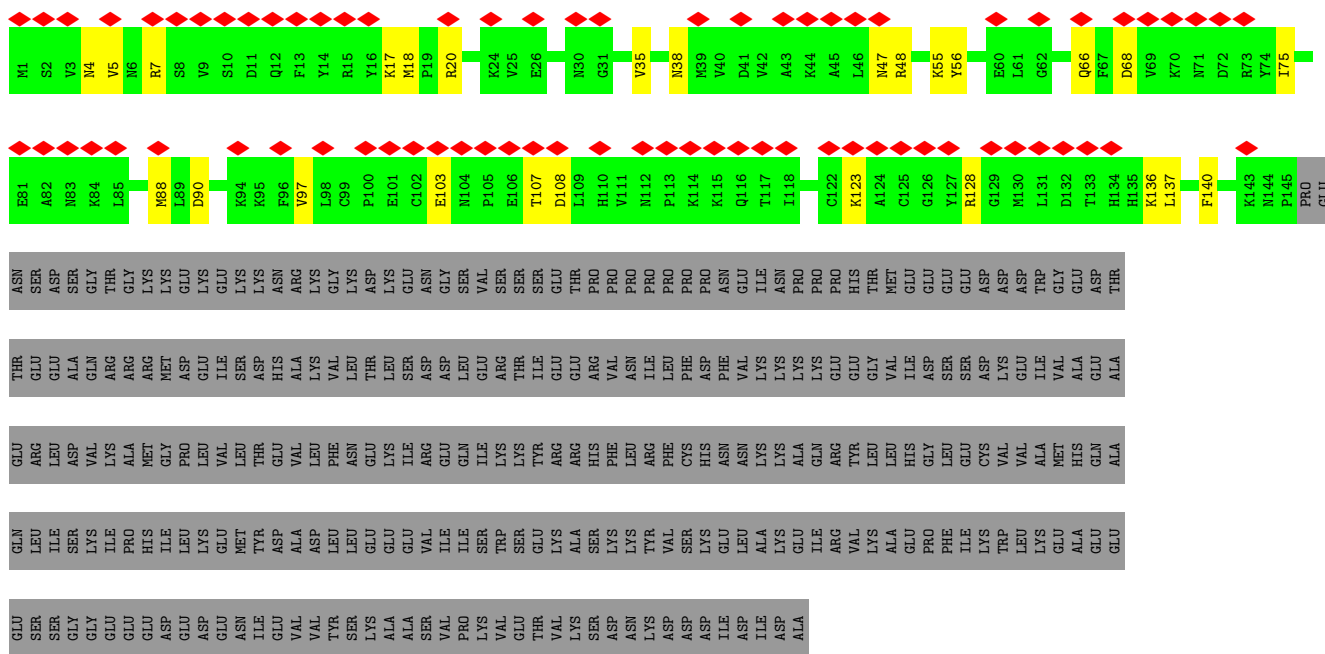


- Molecule 51: Eukaryotic translation initiation factor 3 subunit D



• Molecule 52: Eukaryotic translation initiation factor 3 subunit C





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61742	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	23.548	Depositor
Minimum map value	-8.712	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	417.74402, 417.74402, 417.74402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.96700007, 0.96700007, 0.96700007	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, MG, OMG, PSU, MA6, ZN, UR3, A2M, 6MZ, JMH, OMC, 5MU, OMU, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.20	0/3279	0.59	0/4534
2	2	0.11	0/1491	0.36	0/2068
3	3	0.13	0/1055	0.39	0/1469
4	4	0.12	0/1269	0.37	0/1762
5	5	0.19	0/4458	0.51	2/6027 (0.0%)
6	6	0.21	0/2212	0.60	1/3034 (0.0%)
7	7	0.21	0/1365	0.53	1/2124 (0.0%)
8	8	0.15	0/1572	0.46	0/2187
9	9	0.22	0/231	0.52	0/294
10	A	0.26	0/41130	0.44	6/64100 (0.0%)
11	B	0.21	0/1186	0.40	0/1585
12	C	0.24	0/2077	0.52	1/2796 (0.0%)
13	D	0.32	0/1502	0.65	1/2008 (0.0%)
14	E	0.26	0/1105	0.57	0/1476
15	F	0.28	0/474	0.72	0/623
16	G	0.23	0/1451	0.57	0/1942
17	H	0.34	0/644	0.79	3/864 (0.3%)
18	I	0.25	0/1232	0.57	0/1656
19	J	0.28	0/1051	0.58	1/1406 (0.1%)
20	K	0.27	0/623	0.59	0/833
21	L	0.28	0/1743	0.65	2/2354 (0.1%)
22	M	0.32	0/1078	0.68	2/1447 (0.1%)
23	N	0.25	0/1670	0.51	0/2271
24	O	0.27	0/1742	0.63	0/2330
25	P	0.33	0/1010	0.70	1/1353 (0.1%)
26	Q	0.25	0/805	0.61	1/1079 (0.1%)
27	R	0.20	0/1654	0.40	0/2203
28	S	0.20	0/1885	0.46	1/2510 (0.0%)
29	T	0.22	0/1032	0.53	0/1371
30	V	0.28	0/1481	0.66	1/1988 (0.1%)
31	Y	0.22	0/1142	0.57	2/1528 (0.1%)
32	Z	0.23	0/1793	0.53	2/2414 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.27	0/859	0.71	2/1159 (0.2%)
34	b	0.28	0/1094	0.67	0/1464
35	c	0.21	0/2493	0.51	1/3394 (0.0%)
36	d	0.25	0/1123	0.54	1/1504 (0.1%)
37	e	0.53	0/657	0.77	0/878
38	f	0.22	0/1245	0.51	0/1665
39	h	0.25	0/827	0.60	1/1110 (0.1%)
40	i	0.24	0/429	0.53	0/568
41	k	0.37	0/566	0.90	4/753 (0.5%)
42	m	0.20	0/960	0.50	0/1286
43	n	0.26	0/500	0.63	1/669 (0.1%)
44	o	0.21	0/628	0.58	0/846
45	q	0.52	2/913 (0.2%)	0.79	2/1213 (0.2%)
46	r	0.21	0/2167	0.53	1/2943 (0.0%)
47	t	0.23	0/3494	0.60	3/4726 (0.1%)
48	u	0.28	0/5475	0.73	10/7432 (0.1%)
49	v	0.31	2/2778 (0.1%)	0.67	1/3797 (0.0%)
50	w	0.23	0/1795	0.43	0/2798
51	x	0.19	0/2880	0.54	3/3933 (0.1%)
52	y	0.26	0/5350	0.72	2/7215 (0.0%)
53	z	0.21	0/1169	0.61	1/1575 (0.1%)
All	All	0.25	4/123844 (0.0%)	0.54	61/176564 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	q	3	LYS	C-N	8.95	1.44	1.33
45	q	4	ASN	C-N	-7.65	1.23	1.33
49	v	361	ASN	C-N	7.54	1.44	1.33
49	v	362	MET	C-N	-5.04	1.25	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	t	247	PRO	CA-N-CD	-9.45	98.77	112.00
48	u	96	MET	CB-CG-SD	8.30	137.61	112.70
53	z	103	GLU	CA-CB-CG	8.22	130.53	114.10
17	H	2	PRO	CA-N-CD	-7.90	100.94	112.00
30	V	43	GLU	CA-CB-CG	7.67	129.43	114.10
51	x	81	GLN	CA-CB-CG	7.45	129.00	114.10
10	A	644	OMG	O3'-P-O5'	7.36	115.04	104.00
47	t	145	MET	CA-CB-CG	7.30	128.70	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	h	82	MET	CA-CB-CG	7.06	128.22	114.10
10	A	509	OMG	O3'-P-O5'	6.88	114.31	104.00
45	q	73	THR	N-CA-C	6.87	118.77	111.28
51	x	480	ILE	N-CA-C	-6.66	105.98	111.91
48	u	506	PRO	CA-N-CD	-6.46	102.96	112.00
41	k	117	LEU	N-CA-C	-6.33	104.38	111.28
35	c	5	MET	CB-CG-SD	6.29	131.59	112.70
52	y	653	ARG	N-CA-CB	-6.24	102.54	111.84
36	d	88	MET	CA-CB-CG	6.19	126.48	114.10
48	u	342	LEU	N-CA-C	-6.12	98.41	108.76
48	u	96	MET	CA-CB-CG	6.12	126.34	114.10
43	n	64	GLU	CA-CB-CG	6.11	126.33	114.10
10	A	517	OMC	P-O3'-C3'	-6.04	111.14	120.20
5	5	398	MET	CA-CB-CG	6.03	126.17	114.10
21	L	214	LEU	CA-C-N	-5.90	110.64	120.68
21	L	214	LEU	C-N-CA	-5.90	110.64	120.68
33	a	95	ARG	CA-CB-CG	5.90	125.89	114.10
48	u	341	LEU	CA-C-N	5.88	131.80	122.74
48	u	341	LEU	C-N-CA	5.88	131.80	122.74
17	H	33	MET	CB-CG-SD	5.87	130.30	112.70
12	C	19	MET	CG-SD-CE	-5.85	88.03	100.90
31	Y	41	MET	CB-CG-SD	-5.81	95.27	112.70
48	u	96	MET	N-CA-CB	5.80	119.28	110.28
31	Y	41	MET	CA-CB-CG	5.79	125.68	114.10
32	Z	169	ASP	N-CA-C	-5.79	101.45	110.42
51	x	81	GLN	CB-CG-CD	5.77	122.41	112.60
6	6	297	MET	CA-CB-CG	5.67	125.44	114.10
46	r	137	VAL	N-CA-C	-5.65	108.00	113.53
33	a	21	MET	CB-CG-SD	5.63	129.60	112.70
25	P	151	LEU	CA-CB-CG	5.62	135.96	116.30
28	S	1	MET	N-CA-C	-5.60	95.31	111.00
13	D	27	GLN	CA-CB-CG	5.58	125.27	114.10
17	H	2	PRO	N-CD-CG	-5.57	94.85	103.20
26	Q	46	GLU	CA-CB-CG	5.56	125.22	114.10
48	u	523	LEU	CA-CB-CG	5.52	135.63	116.30
19	J	41	MET	N-CA-CB	5.48	118.27	110.16
48	u	228	MET	CA-CB-CG	5.46	125.03	114.10
5	5	367	MET	CA-CB-CG	5.40	124.90	114.10
49	v	247	GLN	CA-CB-CG	5.38	124.87	114.10
32	Z	197	LYS	CB-CG-CD	5.38	123.66	111.30
41	k	132	MET	CA-CB-CG	5.35	124.80	114.10
52	y	653	ARG	CA-CB-CG	5.33	124.76	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	k	108	VAL	N-CA-C	5.21	115.94	110.62
41	k	107	LYS	N-CA-C	-5.20	104.72	111.74
10	A	731	G	P-O3'-C3'	5.20	127.99	120.20
7	7	-21	A	P-O3'-C3'	5.18	127.97	120.20
10	A	694	G	C2'-C3'-O3'	5.17	121.46	113.70
45	q	29	LYS	CA-CB-CG	5.16	124.43	114.10
47	t	247	PRO	N-CA-C	5.14	118.57	110.50
48	u	416	GLU	CA-CB-CG	5.13	124.37	114.10
22	M	109	LEU	CA-C-N	5.07	131.23	123.47
22	M	109	LEU	C-N-CA	5.07	131.23	123.47
10	A	1703	OMC	O3'-P-O5'	5.04	111.56	104.00

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	1	3258	0	1917	29	0
2	2	1493	0	677	1	0
3	3	1057	0	475	1	0
4	4	1272	0	564	4	0
5	5	4347	0	4294	58	0
6	6	2196	0	1547	21	0
7	7	1218	0	620	14	0
8	8	1574	0	687	3	0
9	9	230	0	276	9	0
10	A	37429	0	18908	352	0
11	B	1166	0	1233	17	0
12	C	2035	0	2138	24	0
13	D	1477	0	1589	33	0
14	E	1087	0	1154	5	0
15	F	468	0	516	8	0
16	G	1430	0	1520	21	0
17	H	631	0	657	9	0
18	I	1208	0	1294	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	1034	0	1080	13	0
20	K	617	0	622	14	0
21	L	1707	0	1794	30	0
22	M	1064	0	1118	46	0
23	N	1633	0	1640	33	0
24	O	1715	0	1785	31	0
25	P	997	0	1021	19	0
26	Q	792	0	843	10	0
27	R	1627	0	1706	12	0
28	S	1862	0	2018	25	0
29	T	1015	0	1086	12	0
30	V	1461	0	1511	25	0
31	Y	1124	0	1193	11	0
32	Z	1765	0	1865	18	0
33	a	834	0	861	19	0
34	b	1072	0	1121	24	0
35	c	2436	0	2393	31	0
36	d	1105	0	1138	17	0
37	e	649	0	723	60	0
38	f	1227	0	1298	25	0
39	h	817	0	882	8	0
40	i	419	0	415	8	0
41	k	554	0	556	62	0
42	m	950	0	987	23	0
43	n	498	0	525	8	0
44	o	616	0	600	5	0
45	q	902	0	925	30	0
46	r	2138	0	1930	27	0
47	t	3439	0	3578	76	0
48	u	5383	0	5085	104	0
49	v	2740	0	2251	44	0
50	w	1604	0	816	4	0
51	x	2837	0	2207	29	0
52	y	5263	0	5219	96	0
53	z	1146	0	1158	16	0
54	A	83	0	0	0	0
54	V	1	0	0	0	0
54	f	1	0	0	0	0
54	i	2	0	0	0	0
55	Q	1	0	0	0	0
55	k	1	0	0	0	0
All	All	118707	0	94016	1374	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 7.

All (1374) 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)
10:A:814:5MU:C4	10:A:814:5MU:C5	1.79	1.64
37:e:44:LEU:HG	37:e:46:ASN:ND2	1.29	1.44
37:e:44:LEU:O	37:e:44:LEU:CD1	1.74	1.36
37:e:44:LEU:CD1	37:e:46:ASN:H	1.41	1.33
37:e:44:LEU:CG	37:e:46:ASN:ND2	1.91	1.30
37:e:44:LEU:HD13	37:e:44:LEU:C	1.43	1.27
37:e:44:LEU:O	37:e:44:LEU:HD13	1.33	1.20
37:e:44:LEU:HD21	37:e:46:ASN:CG	1.73	1.13
37:e:44:LEU:HD13	37:e:46:ASN:H	1.14	1.12
37:e:43:LYS:NZ	37:e:44:LEU:H	1.51	1.09
37:e:44:LEU:HD21	37:e:46:ASN:OD1	1.51	1.09
37:e:44:LEU:O	37:e:44:LEU:HD12	1.51	1.06
37:e:44:LEU:CD1	37:e:46:ASN:N	2.20	1.04
37:e:44:LEU:HD11	37:e:46:ASN:H	1.19	1.04
37:e:44:LEU:CD1	37:e:46:ASN:ND2	2.20	1.03
37:e:44:LEU:CD1	37:e:44:LEU:C	2.15	1.03
37:e:44:LEU:HD11	37:e:46:ASN:CB	1.88	1.02
41:k:109:ASP:HB2	41:k:115:SER:HB2	1.46	0.94
10:A:1033:G:H1	10:A:1080:A:HO2'	1.16	0.94
41:k:119:ARG:HH11	41:k:132:MET:HE2	1.33	0.94
37:e:44:LEU:CD2	37:e:46:ASN:CG	2.41	0.93
37:e:44:LEU:HD11	37:e:46:ASN:N	1.82	0.92
10:A:191:A:H62	10:A:208:G:H21	1.13	0.90
37:e:44:LEU:HD13	37:e:46:ASN:N	1.82	0.90
37:e:43:LYS:HZ2	37:e:44:LEU:N	1.70	0.89
37:e:43:LYS:HZ2	37:e:44:LEU:H	0.90	0.89
15:F:119:VAL:HG12	15:F:121:PRO:HD3	1.55	0.87
37:e:44:LEU:HD11	37:e:46:ASN:CG	1.99	0.87
10:A:1314:U:H2'	33:a:2:LEU:HG	1.56	0.87
41:k:104:LYS:HZ1	41:k:110:GLU:HG2	1.40	0.84
37:e:44:LEU:CG	37:e:46:ASN:CG	2.49	0.84
41:k:116:ARG:HE	41:k:131:PHE:HE2	1.26	0.82
37:e:44:LEU:HD11	37:e:46:ASN:ND2	1.96	0.81
41:k:109:ASP:HB2	41:k:115:SER:CB	2.10	0.81
48:u:205:LEU:HD11	48:u:233:ARG:HH12	1.46	0.80
41:k:105:TYR:HD2	41:k:117:LEU:HD11	1.47	0.79
37:e:44:LEU:HG	37:e:46:ASN:HD21	0.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:y:110:LEU:HD22	52:y:156:ILE:HD13	1.65	0.77
10:A:509:OMG:HM22	10:A:510:G:C8	2.20	0.76
49:v:405:ILE:HG22	49:v:409:LYS:HE2	1.67	0.76
37:e:44:LEU:CD1	37:e:46:ASN:HD22	1.97	0.75
10:A:878:G:H1	10:A:908:A:H61	1.31	0.75
10:A:191:A:H62	10:A:208:G:N2	1.84	0.75
52:y:548:MET:HE1	52:y:572:HIS:HA	1.68	0.75
37:e:44:LEU:HD11	37:e:46:ASN:HB2	1.68	0.75
41:k:118:ARG:HB2	41:k:131:PHE:HB3	1.69	0.74
10:A:1091:C:HO2'	19:J:2:VAL:N	1.86	0.73
7:7:7:C:H42	45:q:64:LYS:HE2	1.53	0.73
10:A:925:G:H1	10:A:1017:U:H3	1.33	0.73
48:u:340:ARG:NH2	48:u:345:ASP:O	2.20	0.73
10:A:888:U:H3	10:A:900:C:H42	1.34	0.73
41:k:104:LYS:NZ	41:k:110:GLU:HG2	2.02	0.73
48:u:407:VAL:HG21	48:u:435:THR:HG21	1.71	0.73
48:u:472:VAL:HG23	52:y:798:VAL:HG11	1.72	0.72
49:v:243:LEU:HA	49:v:247:GLN:HB3	1.71	0.72
10:A:191:A:N6	10:A:208:G:H21	1.88	0.71
37:e:44:LEU:HD11	37:e:46:ASN:CA	2.21	0.71
33:a:95:ARG:O	33:a:95:ARG:NE	2.23	0.71
49:v:342:GLU:HG3	49:v:346:ARG:HH22	1.54	0.71
22:M:61:ILE:HG23	22:M:73:LEU:HD13	1.71	0.70
49:v:406:GLU:HA	49:v:409:LYS:HD2	1.72	0.70
10:A:1703:OMC:HM22	10:A:1704:C:O4'	1.92	0.70
37:e:50:PHE:H	38:f:4:VAL:HG12	1.56	0.70
37:e:44:LEU:CD2	37:e:46:ASN:OD1	2.33	0.69
5:5:478:PHE:O	49:v:369:ARG:NH1	2.25	0.69
48:u:338:ILE:HG23	52:y:745:LYS:HD3	1.72	0.69
10:A:1550:G:H3'	10:A:1579:A:H61	1.58	0.69
22:M:73:LEU:O	22:M:76:GLU:HG3	1.93	0.69
37:e:50:PHE:HE2	37:e:87:ALA:HB2	1.57	0.68
37:e:44:LEU:HD13	37:e:45:ASN:N	2.05	0.68
6:6:249:LEU:HD23	6:6:277:MET:HE1	1.74	0.68
52:y:758:ASN:HB3	52:y:761:MET:HG2	1.76	0.68
48:u:397:GLU:OE1	48:u:399:ASN:ND2	2.27	0.68
41:k:118:ARG:HD2	41:k:133:ALA:HA	1.75	0.68
41:k:107:LYS:NZ	42:m:68:LEU:HG	2.10	0.67
10:A:1396:A:O2'	10:A:1398:G:N7	2.28	0.67
37:e:50:PHE:HB2	38:f:4:VAL:HG12	1.76	0.67
26:Q:87:ARG:NH1	26:Q:91:ALA:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Z:132:LYS:NZ	32:Z:190:LEU:O	2.28	0.67
47:t:177:ILE:HG21	47:t:185:ILE:HD11	1.77	0.67
37:e:44:LEU:CD1	37:e:46:ASN:CG	2.61	0.67
47:t:28:LEU:HD12	47:t:287:VAL:HG21	1.77	0.67
10:A:528:A:N1	10:A:557:U:O2'	2.27	0.66
5:5:560:MET:HE3	5:5:561:GLY:H	1.59	0.66
48:u:523:LEU:HG	48:u:527:SER:HB3	1.76	0.66
49:v:279:LYS:O	49:v:283:GLN:NE2	2.28	0.66
5:5:183:LEU:HD22	5:5:269:LEU:HD13	1.78	0.66
13:D:54:ARG:HH21	13:D:98:LEU:HD22	1.61	0.66
47:t:449:LYS:HZ3	53:z:128:ARG:HH22	1.44	0.66
1:1:505:ARG:NH1	1:1:554:VAL:O	2.27	0.66
33:a:3:MET:SD	33:a:8:ARG:HB2	2.36	0.66
34:b:53:GLN:HG3	34:b:83:MET:HE1	1.78	0.66
52:y:832:MET:HE1	52:y:843:VAL:HG22	1.78	0.66
7:7:7:C:N4	45:q:64:LYS:HE2	2.10	0.65
36:d:85:ASN:HB2	36:d:88:MET:HB2	1.77	0.65
5:5:167:ILE:O	5:5:237:LYS:NZ	2.29	0.65
41:k:117:LEU:HD12	41:k:118:ARG:HG2	1.78	0.65
46:r:72:VAL:HG13	46:r:90:VAL:HG22	1.78	0.65
5:5:556:THR:OG1	49:v:416:GLN:NE2	2.29	0.65
10:A:1288:U:O4	10:A:1311:C:N3	2.29	0.65
17:H:77:CYS:O	51:x:81:GLN:NE2	2.24	0.65
41:k:109:ASP:HB3	41:k:113:LYS:O	1.97	0.65
41:k:119:ARG:O	41:k:132:MET:HB3	1.97	0.65
22:M:70:SER:HA	22:M:74:GLN:HG2	1.78	0.65
22:M:74:GLN:O	22:M:78:ARG:HG2	1.97	0.65
36:d:9:VAL:HG21	36:d:138:VAL:HG13	1.79	0.64
6:6:283:MET:HE3	6:6:320:MET:HG2	1.79	0.64
11:B:104:LYS:O	14:E:11:ARG:NH2	2.30	0.64
36:d:36:THR:O	38:f:39:ARG:NH2	2.31	0.64
51:x:30:TYR:HA	52:y:591:MET:HE1	1.78	0.64
10:A:956:G:H4'	25:P:60:MET:HE1	1.80	0.64
37:e:42:ASP:O	37:e:43:LYS:HB2	1.97	0.64
5:5:394:TYR:HB3	5:5:397:LYS:HB2	1.80	0.64
10:A:615:C:OP1	45:q:62:ARG:NH1	2.30	0.64
34:b:64:LYS:NZ	34:b:90:VAL:O	2.29	0.64
49:v:352:SER:HB3	49:v:355:MET:HE2	1.78	0.64
5:5:48:ILE:HB	5:5:53:LYS:HE3	1.80	0.64
10:A:925:G:OP1	18:I:121:ARG:NH2	2.31	0.63
23:N:34:MET:HE1	23:N:162:PRO:HB3	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:509:OMG:N3	10:A:509:OMG:HM23	2.13	0.63
41:k:104:LYS:NZ	41:k:108:VAL:O	2.27	0.63
46:r:19:VAL:HG22	46:r:72:VAL:HG12	1.81	0.63
5:5:402:GLN:OE1	49:v:379:ARG:NH1	2.29	0.63
12:C:100:ARG:HB2	12:C:114:ILE:HD13	1.81	0.63
12:C:87:MET:HE1	12:C:236:ILE:HG21	1.79	0.62
18:I:63:VAL:HG11	18:I:71:ILE:HG13	1.81	0.62
47:t:263:ASP:OD1	47:t:265:ASN:ND2	2.32	0.62
52:y:504:LEU:HD11	52:y:567:CYS:HB3	1.81	0.62
10:A:838:G:O6	29:T:21:LYS:NZ	2.33	0.62
10:A:878:G:H1	10:A:908:A:N6	1.97	0.62
13:D:58:ARG:O	13:D:62:THR:HG23	1.99	0.62
47:t:222:ILE:HD13	47:t:235:VAL:HA	1.81	0.62
10:A:1760:G:H21	10:A:1772:C:H5'	1.64	0.62
24:O:77:ASP:OD2	48:u:14[B]:ARG:NH1	2.33	0.62
10:A:1273:C:O2'	10:A:1506:A:N1	2.30	0.62
10:A:1524:G:N7	38:f:141:ARG:NH1	2.48	0.62
49:v:298:CYS:HA	49:v:301:VAL:HG12	1.80	0.62
6:6:312:VAL:HG11	6:6:325:ILE:HD13	1.81	0.62
23:N:51:LEU:HA	23:N:54:THR:HG22	1.82	0.62
47:t:30:PRO:HD3	47:t:250:PHE:HZ	1.64	0.62
10:A:1507:G:H1'	41:k:89:LYS:HG3	1.82	0.62
12:C:11:ARG:HA	12:C:28:ALA:HB2	1.81	0.62
29:T:117:VAL:HG21	29:T:125:VAL:HG21	1.80	0.62
10:A:919:A:OP2	18:I:64:ARG:NH2	2.33	0.61
51:x:391:ILE:HG22	51:x:446:TYR:HB2	1.82	0.61
10:A:888:U:O4	10:A:900:C:N3	2.33	0.61
10:A:814:5MU:OP1	12:C:22:LYS:NZ	2.33	0.61
10:A:1064:C:H5'	25:P:151:LEU:HD12	1.81	0.61
38:f:85:ASN:ND2	38:f:98:VAL:O	2.33	0.61
20:K:12:TYR:O	21:L:248:TYR:OH	2.17	0.61
22:M:36:GLU:OE1	22:M:47:ARG:NH1	2.34	0.61
13:D:170:PRO:O	13:D:175:ARG:NH1	2.33	0.61
22:M:58:MET:O	22:M:62:GLN:NE2	2.33	0.61
10:A:494:C:H41	10:A:509:OMG:HN22	1.49	0.61
22:M:17:ILE:HG22	22:M:71:ILE:HG21	1.83	0.61
22:M:18:GLU:HA	22:M:71:ILE:HG22	1.83	0.61
47:t:31:LEU:HD22	47:t:31:LEU:H	1.65	0.61
37:e:50:PHE:CE2	37:e:87:ALA:HB2	2.35	0.61
52:y:627:LYS:HA	52:y:693:LEU:HD21	1.83	0.61
1:1:508:ASN:ND2	13:D:165:TYR:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:327:ARG:HH22	5:5:496:LYS:HG2	1.65	0.61
6:6:243:ILE:O	6:6:340:ARG:NH1	2.34	0.61
24:O:182:LYS:O	24:O:185:VAL:HG12	2.00	0.61
10:A:801:U:O4	16:G:106:ARG:NH1	2.34	0.60
48:u:405:GLU:HA	48:u:408:THR:HG22	1.81	0.60
30:V:40:ALA:HB1	30:V:45:TYR:HD2	1.66	0.60
10:A:1669:G:OP1	39:h:79:ARG:NH1	2.34	0.60
25:P:99:ALA:H	25:P:133:THR:HG22	1.66	0.60
52:y:788:LEU:HD11	52:y:818:VAL:HG23	1.83	0.60
48:u:414:VAL:O	48:u:425:GLN:NE2	2.33	0.60
10:A:156:G:OP1	28:S:2:LYS:NZ	2.32	0.60
35:c:256:ILE:HB	35:c:270:LEU:HB2	1.83	0.60
41:k:107:LYS:HZ3	42:m:67:ALA:HB3	1.66	0.60
10:A:1497:G:N7	33:a:25:LYS:NZ	2.41	0.60
49:v:416:GLN:HG2	49:v:420:MET:HE1	1.84	0.60
28:S:159:ARG:NH2	28:S:171:THR:O	2.35	0.60
10:A:450:C:OP1	12:C:3:ARG:NH1	2.35	0.60
47:t:128:ARG:NH1	47:t:243:ILE:O	2.35	0.60
10:A:1086:G:OP2	26:Q:12:LYS:NZ	2.35	0.60
10:A:1597:C:OP2	37:e:85:ARG:NH2	2.35	0.60
10:A:1605:G:OP1	36:d:84:ARG:NH2	2.34	0.60
12:C:54:TYR:O	29:T:15:ASN:ND2	2.35	0.60
28:S:23:LYS:HB3	28:S:41:LEU:HD23	1.84	0.60
34:b:143:PRO:HB2	45:q:70:TRP:CG	2.36	0.60
47:t:49:HIS:O	47:t:54:LYS:NZ	2.34	0.59
10:A:70:G:OP2	28:S:167:LYS:NZ	2.35	0.59
10:A:319:C:N4	28:S:186:GLN:OE1	2.36	0.59
49:v:401:TYR:H	52:y:846:ARG:HH22	1.49	0.59
10:A:1488:C:O2'	10:A:1490:G:OP2	2.19	0.59
29:T:53:ASP:OD1	29:T:53:ASP:N	2.33	0.59
30:V:32:ASP:OD1	30:V:34:SER:OG	2.21	0.59
38:f:48:ALA:HB2	38:f:70:ILE:HG13	1.84	0.59
47:t:23:LEU:HD11	47:t:28:LEU:HD11	1.84	0.59
10:A:4:C:H1'	13:D:18:ARG:HH22	1.67	0.59
30:V:71:ARG:NH2	30:V:148:ASN:OD1	2.36	0.59
41:k:105:TYR:HB2	41:k:117:LEU:HD21	1.85	0.59
5:5:183:LEU:HD12	5:5:268:MET:HG3	1.84	0.59
6:6:325:ILE:HG12	48:u:446:ILE:HG13	1.83	0.59
6:6:344:LYS:HA	6:6:347:TRP:HD1	1.66	0.59
46:r:203:GLU:HG2	47:t:342:LYS:HD2	1.85	0.59
6:6:278:ARG:HD3	6:6:311:PHE:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:614:C:P	45:q:62:ARG:HH22	2.25	0.59
12:C:45:ILE:HA	12:C:61:VAL:HG11	1.84	0.59
30:V:156:THR:HG23	30:V:188:TYR:HE2	1.67	0.59
47:t:185:ILE:HD12	47:t:216:ALA:HB2	1.84	0.59
21:L:64:THR:HG23	21:L:67:GLY:H	1.67	0.59
10:A:922:A:OP2	19:J:28:ARG:NH1	2.36	0.58
22:M:73:LEU:HA	22:M:76:GLU:HG3	1.84	0.58
34:b:81:ARG:NH2	34:b:120:SER:O	2.36	0.58
10:A:379:C:O2	27:R:5:ARG:NE	2.36	0.58
10:A:496:C:OP1	12:C:49:ARG:NH2	2.30	0.58
10:A:643:A:OP1	13:D:38:ARG:NH1	2.36	0.58
10:A:1703:OMC:HM23	10:A:1703:OMC:O2	2.03	0.58
49:v:212:THR:OG1	49:v:247:GLN:NE2	2.32	0.58
49:v:398:VAL:HA	52:y:846:ARG:HH21	1.67	0.58
10:A:560:A:OP2	13:D:177:ASN:ND2	2.36	0.58
49:v:320:VAL:HG12	49:v:329:LEU:HD11	1.84	0.58
10:A:641:A:OP1	13:D:40:LYS:NZ	2.32	0.58
10:A:839:C:H41	29:T:10:ARG:HA	1.68	0.58
10:A:1688:C:OP1	21:L:117:ARG:NH1	2.37	0.58
10:A:1825:A:N6	45:q:69:VAL:O	2.36	0.58
48:u:108:SER:O	48:u:111:MET:HG3	2.03	0.58
26:Q:25:ASN:ND2	26:Q:77:CYS:SG	2.76	0.58
29:T:78:SER:OG	29:T:80:ASP:OD1	2.19	0.58
37:e:44:LEU:CD2	37:e:46:ASN:ND2	2.59	0.58
49:v:209:GLN:NE2	51:x:21:VAL:O	2.36	0.58
10:A:614:C:H5	10:A:626:G:OP2	1.87	0.58
10:A:1829:G:H1'	10:A:1850:MA6:H2	1.84	0.58
10:A:1589:A:N3	10:A:1653:U:O2'	2.35	0.58
9:9:11:ARG:NH2	10:A:1844:U:OP1	2.36	0.58
48:u:132:VAL:O	52:y:678:ASN:ND2	2.34	0.58
5:5:544:ILE:HA	5:5:547:ILE:HD12	1.86	0.58
10:A:517:OMC:H2'	10:A:518:G:O4'	2.03	0.58
25:P:31:CYS:HB2	25:P:93:LEU:HD12	1.85	0.58
52:y:61:THR:HA	52:y:64:ILE:HD12	1.86	0.58
30:V:45:TYR:OH	30:V:65:GLN:OE1	2.22	0.58
41:k:117:LEU:CD1	41:k:118:ARG:HG2	2.34	0.58
48:u:372:ASN:HA	48:u:375:VAL:HG22	1.85	0.58
10:A:838:G:O2'	10:A:840:C:OP2	2.22	0.57
10:A:1658:G:OP2	10:A:1660:C:N4	2.37	0.57
11:B:135:SER:O	11:B:139:ARG:NH1	2.37	0.57
38:f:92:ASP:O	38:f:94:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:r:197:VAL:HG12	46:r:269:PHE:HA	1.87	0.57
22:M:83:ASN:HB2	23:N:201:LEU:HD11	1.85	0.57
32:Z:62:LYS:O	32:Z:67:ARG:NH2	2.37	0.57
48:u:347:ILE:HG12	52:y:723:ARG:HA	1.86	0.57
7:7:-21:A:H62	48:u:192:ALA:HB1	1.70	0.57
10:A:1013:U:OP1	10:A:1129:G:O2'	2.22	0.57
29:T:81:TYR:O	29:T:85:ASN:ND2	2.35	0.57
45:q:31:ASP:OD1	45:q:31:ASP:N	2.35	0.57
52:y:394:LYS:HB3	52:y:397:MET:HG2	1.87	0.57
6:6:327:GLN:O	6:6:330:ARG:NH2	2.37	0.57
53:z:47:ASN:O	53:z:48:ARG:NH1	2.37	0.57
6:6:327:GLN:HE21	48:u:450:ILE:HA	1.69	0.57
7:7:4:G:H1'	45:q:70:TRP:NE1	2.18	0.57
10:A:71:G:O6	28:S:170:ARG:NH1	2.37	0.57
10:A:126:G:OP2	28:S:195:LYS:NZ	2.36	0.57
10:A:71:G:OP2	28:S:168:LYS:NZ	2.33	0.57
10:A:1285:G:OP2	42:m:61:TYR:OH	2.18	0.57
13:D:152:ASP:N	13:D:152:ASP:OD1	2.35	0.57
22:M:102:THR:HA	22:M:105:MET:HB3	1.86	0.57
10:A:734:C:O2'	10:A:736:C:N4	2.38	0.57
52:y:651:LEU:HD11	52:y:667:ARG:HD2	1.86	0.57
53:z:108:ASP:OD1	53:z:123:LYS:NZ	2.38	0.57
5:5:195:GLN:HG2	5:5:421:LEU:HD21	1.86	0.57
10:A:380:G:OP1	27:R:31:ARG:NH1	2.35	0.57
10:A:1756:C:H42	10:A:1776:G:H2'	1.69	0.57
23:N:147:LEU:O	23:N:165:ASN:ND2	2.37	0.57
48:u:268:LYS:NZ	48:u:269:PRO:O	2.32	0.57
10:A:1021:U:OP1	18:I:132:LYS:NZ	2.38	0.56
10:A:1274:G:H5'	33:a:1:MET:HE3	1.87	0.56
33:a:90:VAL:O	33:a:96:ARG:NH1	2.38	0.56
34:b:52:LYS:HG3	34:b:80:LEU:HD11	1.86	0.56
41:k:117:LEU:HD13	41:k:118:ARG:HE	1.70	0.56
10:A:72:C:O2'	10:A:74:G:N2	2.38	0.56
20:K:41:LYS:HA	23:N:5:LEU:HD12	1.87	0.56
41:k:118:ARG:HB3	41:k:132:MET:O	2.05	0.56
47:t:105:CYS:HB3	47:t:109:THR:HG21	1.87	0.56
10:A:750:C:H41	10:A:793:G:H1'	1.71	0.56
10:A:1171:G:O2'	10:A:1187:G:O6	2.23	0.56
10:A:1579:A:OP1	32:Z:7:LYS:NZ	2.38	0.56
43:n:61:SER:OG	43:n:62:GLU:N	2.37	0.56
10:A:350:C:O2'	10:A:383:G:N1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1752:C:O2'	10:A:1782:G:N2	2.39	0.56
47:t:46:THR:HG22	47:t:156:LEU:HD12	1.86	0.56
10:A:924:G:H1	10:A:1018:U:H3	1.53	0.56
11:B:91:ASP:OD1	11:B:104:LYS:NZ	2.30	0.56
18:I:45:LEU:HA	18:I:49:GLN:HE21	1.70	0.56
45:q:4:ASN:HD21	45:q:8:GLY:H	1.53	0.56
48:u:315:MET:HA	48:u:318:MET:HG3	1.87	0.56
1:1:381:PHE:HA	1:1:388:LEU:HA	1.87	0.56
47:t:386:THR:HB	47:t:389:ASP:HB2	1.88	0.56
48:u:172:ARG:HH21	48:u:176:ASP:HB2	1.70	0.56
10:A:614:C:C5	10:A:626:G:H5'	2.41	0.56
28:S:57:ASP:OD1	28:S:58:LYS:N	2.39	0.56
32:Z:74:GLN:NE2	32:Z:79:PHE:O	2.38	0.56
49:v:255:ARG:NH2	49:v:322:ASP:OD2	2.39	0.56
10:A:1398:G:O2'	35:c:88:ARG:NH2	2.38	0.56
35:c:168:CYS:HB2	35:c:195:LEU:HD13	1.88	0.56
5:5:298:GLU:HB3	5:5:301:LYS:HG2	1.88	0.56
10:A:1310:U:OP1	42:m:36:ARG:NH2	2.39	0.56
15:F:86:VAL:O	15:F:89:GLN:C	2.48	0.56
25:P:101:GLY:HA3	25:P:134:PRO:HG2	1.88	0.56
37:e:46:ASN:HB3	37:e:79:ILE:C	2.31	0.56
16:G:165:ASN:O	16:G:168:HIS:NE2	2.38	0.56
49:v:363:THR:OG1	49:v:365:GLU:OE1	2.22	0.56
5:5:148:PRO:HG2	5:5:153:ARG:HE	1.71	0.55
10:A:1273:C:O2	10:A:1508:A:N6	2.38	0.55
35:c:282:GLU:N	35:c:282:GLU:OE2	2.40	0.55
41:k:105:TYR:CD2	41:k:117:LEU:HD11	2.35	0.55
41:k:107:LYS:HG3	41:k:114:ILE:HG22	1.87	0.55
53:z:66:GLN:HB3	53:z:75:ILE:HB	1.87	0.55
5:5:364:ASN:O	5:5:368:HIS:ND1	2.38	0.55
5:5:380:MET:SD	5:5:380:MET:N	2.79	0.55
10:A:65:C:N4	28:S:134:GLY:O	2.34	0.55
10:A:752:G:N2	10:A:793:G:O2'	2.40	0.55
10:A:1017:U:OP2	18:I:55:ARG:NH1	2.40	0.55
22:M:37:GLU:OE2	35:c:127:LYS:NZ	2.40	0.55
23:N:58:LEU:HD21	23:N:177:MET:HG3	1.87	0.55
47:t:142:MET:HA	47:t:145:MET:HG3	1.89	0.55
10:A:1738:C:OP1	28:S:92:ARG:NH1	2.39	0.55
46:r:233:PRO:HB3	47:t:346:THR:HG23	1.89	0.55
48:u:109:GLN:O	48:u:112:VAL:HG22	2.06	0.55
48:u:135:GLU:OE2	52:y:465:HIS:ND1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:485:ASP:OD1	52:y:801:SER:OG	2.24	0.55
10:A:198:U:H1'	10:A:202:G:H1	1.71	0.55
10:A:1606:G:O2'	10:A:1632:G:N2	2.39	0.55
13:D:55:LYS:HA	13:D:58:ARG:HE	1.70	0.55
47:t:108:SER:HA	47:t:326:ASN:HD21	1.71	0.55
51:x:289:LEU:HD23	51:x:316:ALA:HB1	1.88	0.55
52:y:673:PHE:HA	52:y:676:HIS:CD2	2.41	0.55
10:A:1114:U:O2'	10:A:1119:A:N6	2.39	0.55
11:B:88:ILE:HD11	11:B:109:MET:HE3	1.89	0.55
22:M:85:VAL:HG23	23:N:198:MET:HG2	1.89	0.55
30:V:123:GLU:HB2	43:n:59:LEU:HD22	1.89	0.55
47:t:156:LEU:HD13	47:t:188:LEU:HD11	1.89	0.55
1:1:507:ARG:HD3	1:1:556:VAL:HG11	1.88	0.55
10:A:943:U:O2'	25:P:135:ILE:O	2.23	0.55
48:u:208:ILE:O	48:u:212:HIS:ND1	2.35	0.55
48:u:321:ARG:HE	48:u:423:GLU:HG3	1.72	0.55
10:A:114:G:N7	11:B:69:ARG:NH2	2.55	0.55
10:A:166:A2M:H2'	10:A:167:G:H8	1.72	0.55
10:A:929:G:N2	10:A:1013:U:O2	2.39	0.55
47:t:152:MET:HE3	47:t:182:LEU:HD12	1.87	0.55
52:y:745:LYS:HA	52:y:790:THR:HG21	1.87	0.55
53:z:4:ASN:OD1	53:z:17:LYS:NZ	2.37	0.55
10:A:3:C:O2'	13:D:18:ARG:NH2	2.40	0.55
10:A:26:U:H2'	10:A:27:A2M:H8	1.88	0.55
52:y:64:ILE:HG23	52:y:109:ILE:HD11	1.87	0.55
35:c:124:SER:OG	35:c:126:ASP:OD1	2.25	0.55
38:f:7:GLU:OE1	38:f:7:GLU:N	2.40	0.55
46:r:21:MET:SD	46:r:21:MET:N	2.80	0.55
46:r:118:VAL:HG21	46:r:175:VAL:HG21	1.88	0.55
48:u:563:LYS:HA	48:u:567:ARG:HB2	1.87	0.55
52:y:75:ASP:OD1	52:y:77:THR:OG1	2.24	0.55
52:y:375:LYS:HA	52:y:378:ILE:HD12	1.89	0.55
1:1:500:THR:HG23	1:1:502:GLN:H	1.71	0.54
19:J:3:ARG:NH1	19:J:9:ASP:OD2	2.40	0.54
33:a:96:ARG:HD3	33:a:98:ARG:HH22	1.72	0.54
42:m:18:LEU:HD21	42:m:51:VAL:HG21	1.88	0.54
10:A:482:G:N1	10:A:485:A:OP2	2.39	0.54
10:A:1533:A:OP2	30:V:164:ARG:NH1	2.39	0.54
7:7:-19:G:O3'	48:u:158:ARG:NH2	2.40	0.54
16:G:154:ILE:HB	16:G:185:VAL:HG12	1.88	0.54
25:P:40:THR:HG21	25:P:74:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:89:GLU:OE2	13:D:89:GLU:N	2.40	0.54
32:Z:40:ARG:NH1	32:Z:47:GLU:OE1	2.39	0.54
48:u:468:GLU:HA	48:u:471:ILE:HD12	1.88	0.54
52:y:420:VAL:HG13	52:y:440:VAL:HG13	1.89	0.54
52:y:596:ASP:OD1	52:y:596:ASP:N	2.41	0.54
34:b:23:ASP:OD1	34:b:24:GLN:N	2.41	0.54
10:A:64:A:N6	10:A:83:A:OP2	2.41	0.54
10:A:1358:U:OP2	21:L:123:ARG:NH2	2.41	0.54
12:C:44:LEU:HD21	12:C:70:ILE:HG21	1.88	0.54
18:I:119:GLU:OE2	18:I:123:HIS:NE2	2.41	0.54
41:k:103:LEU:HB3	41:k:106:TYR:CE2	2.42	0.54
41:k:116:ARG:HG3	41:k:118:ARG:O	2.07	0.54
48:u:48:GLU:OE2	48:u:85:SER:OG	2.23	0.54
10:A:1285:G:N1	42:m:57:ASP:OD2	2.38	0.54
28:S:63:MET:SD	28:S:63:MET:N	2.81	0.54
10:A:57:U:OP1	10:A:504:G:O2'	2.23	0.54
10:A:509:OMG:HM23	10:A:509:OMG:C4	2.43	0.54
19:J:113:HIS:NE2	19:J:114:GLU:OE1	2.40	0.54
41:k:106:TYR:HB2	41:k:131:PHE:CD2	2.42	0.54
48:u:191:LYS:NZ	48:u:248:GLU:OE2	2.41	0.54
10:A:67:C:N4	28:S:168:LYS:O	2.40	0.53
32:Z:158:ILE:HG12	32:Z:189:MET:HE3	1.89	0.53
45:q:77:ILE:HG22	45:q:94:LYS:HA	1.89	0.53
12:C:233:LYS:NZ	12:C:234:PRO:O	2.41	0.53
18:I:40:LEU:HD23	18:I:43:LYS:HD3	1.91	0.53
46:r:229:LEU:HD23	47:t:271:VAL:HG22	1.89	0.53
10:A:734:C:O2	10:A:735:C:N4	2.31	0.53
47:t:271:VAL:HA	47:t:274:LEU:HD13	1.89	0.53
10:A:1124:C:H5''	24:O:150:ILE:HG12	1.91	0.53
12:C:71:LYS:HB2	12:C:91:SER:HB2	1.91	0.53
48:u:440:LEU:HD21	48:u:471:ILE:HG12	1.90	0.53
10:A:588:G:OP2	10:A:588:G:N2	2.35	0.53
10:A:1593:C:O2	36:d:12:GLN:NE2	2.41	0.53
10:A:1702:G:O6	10:A:1836:G:N2	2.42	0.53
11:B:65:ASN:O	11:B:132:ARG:NH2	2.42	0.53
35:c:116:ASP:OD1	35:c:116:ASP:N	2.36	0.53
46:r:191:ILE:HG21	46:r:248:LEU:HA	1.91	0.53
49:v:351:ILE:HB	49:v:391:VAL:HB	1.89	0.53
10:A:84:A:N3	10:A:150:A:O2'	2.39	0.53
10:A:1007:C:O2'	18:I:104:ARG:NH2	2.42	0.53
42:m:79:VAL:HG21	42:m:85:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:r:24:VAL:HA	46:r:34:VAL:HG12	1.91	0.53
17:H:67:THR:OG1	17:H:70:LYS:O	2.26	0.53
47:t:82:GLY:HA2	50:w:76:A:H2'	1.91	0.53
10:A:323:C:O2'	10:A:328:U:O4	2.26	0.53
10:A:1825:A:N6	45:q:65:LEU:O	2.42	0.53
5:5:59:PHE:HD1	5:5:94:ILE:HD13	1.74	0.53
6:6:258:ASN:OD1	6:6:259:ASN:N	2.42	0.53
7:7:4:G:H1'	45:q:70:TRP:HE1	1.74	0.53
10:A:1389:C:OP1	22:M:43:SER:OG	2.26	0.53
10:A:1446:A:H5''	39:h:58:THR:HG23	1.91	0.53
10:A:1757:G:H8	10:A:1777:G:H22	1.55	0.53
35:c:79:LEU:HD11	35:c:87:LEU:HD23	1.90	0.53
48:u:161:LEU:HD11	48:u:178:ALA:HB2	1.91	0.53
52:y:656:GLN:OE1	52:y:658:ARG:NH1	2.34	0.53
10:A:553:U:O4	10:A:555:A:N6	2.42	0.52
46:r:50:GLU:HA	46:r:88:ARG:HD2	1.91	0.52
48:u:281:THR:OG1	48:u:285:LYS:NZ	2.41	0.52
9:9:17:ARG:NH1	10:A:1173:A:OP1	2.41	0.52
32:Z:192:TRP:NE1	32:Z:201:LYS:O	2.38	0.52
47:t:29:THR:OG1	47:t:30:PRO:HD2	2.08	0.52
48:u:246:TRP:NE1	52:y:731:GLU:OE2	2.42	0.52
10:A:1825:A:OP2	45:q:66:ARG:NH2	2.33	0.52
41:k:110:GLU:CD	42:m:63:LYS:HG3	2.34	0.52
47:t:345:PRO:HA	47:t:348:CYS:HB2	1.92	0.52
52:y:448:VAL:HG11	52:y:486:VAL:HG21	1.91	0.52
4:4:118:GLY:N	4:4:173:TYR:O	2.42	0.52
6:6:312:VAL:HG11	6:6:325:ILE:HG21	1.92	0.52
10:A:546:G:N2	10:A:547:G:O6	2.41	0.52
48:u:233:ARG:NH1	48:u:255:ASP:OD2	2.42	0.52
51:x:311:ASN:HA	51:x:314:MET:HG3	1.91	0.52
34:b:130:ARG:NH1	38:f:152:LYS:O	2.35	0.52
52:y:626:THR:HG21	52:y:692:LEU:HD12	1.91	0.52
12:C:247:THR:OG1	12:C:250:GLU:OE1	2.27	0.52
51:x:35:LYS:HA	52:y:590:LEU:HD13	1.92	0.52
51:x:42:VAL:HG11	52:y:636:ILE:HB	1.91	0.52
51:x:304:ASN:OD1	51:x:311:ASN:ND2	2.41	0.52
29:T:114:MET:O	29:T:122:LYS:NZ	2.43	0.52
10:A:110:U:O2	10:A:351:G:N2	2.38	0.52
10:A:1348:G:OP1	21:L:145:LYS:NZ	2.38	0.52
10:A:1458:G:OP1	35:c:276:SER:OG	2.27	0.52
24:O:224:GLU:OE1	24:O:224:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:18:ARG:NH1	34:b:36:LEU:O	2.43	0.52
45:q:51:CYS:SG	45:q:57:ARG:NH1	2.79	0.52
48:u:502:ARG:HD2	52:y:850:THR:HG21	1.92	0.52
5:5:432:HIS:HB3	5:5:435:TYR:HB2	1.92	0.51
7:7:12:C:H4'	21:L:147:VAL:HG11	1.92	0.51
32:Z:28:GLU:OE2	33:a:59:LYS:NZ	2.42	0.51
10:A:517:OMC:HM23	10:A:517:OMC:O2	2.11	0.51
10:A:1204:A:O2'	10:A:1700:C:OP2	2.23	0.51
10:A:1378:A:N6	23:N:136:GLU:OE2	2.44	0.51
13:D:142:VAL:HG12	13:D:144:ILE:H	1.74	0.51
22:M:92:ASP:OD1	22:M:92:ASP:N	2.35	0.51
10:A:126:G:OP1	28:S:198:ARG:NE	2.40	0.51
10:A:1275:G:N2	10:A:1506:A:OP2	2.38	0.51
10:A:1844:U:H3	10:A:1855:G:H1	1.58	0.51
12:C:212:ASP:OD1	12:C:216:ASN:N	2.44	0.51
41:k:103:LEU:HB3	41:k:106:TYR:CZ	2.45	0.51
22:M:98:VAL:HG21	22:M:117:LEU:HB3	1.91	0.51
25:P:44:VAL:HG23	25:P:93:LEU:HD11	1.92	0.51
39:h:20:ILE:HD12	39:h:98:VAL:HG21	1.92	0.51
47:t:28:LEU:HD12	47:t:287:VAL:HG11	1.92	0.51
10:A:484:A2M:O5'	10:A:484:A2M:H8	2.10	0.51
30:V:102:LEU:HD11	37:e:100:VAL:HG21	1.92	0.51
4:4:302:ASN:O	4:4:306:ARG:N	2.44	0.51
10:A:303:C:O2	27:R:184:ARG:NH1	2.44	0.51
35:c:35:SER:OG	35:c:36:ARG:N	2.44	0.51
37:e:40:VAL:HG12	37:e:41:ARG:H	1.76	0.51
37:e:50:PHE:H	38:f:4:VAL:CG1	2.22	0.51
41:k:111:ASN:C	41:k:113:LYS:HZ2	2.19	0.51
49:v:402:GLN:O	49:v:406:GLU:HG2	2.10	0.51
10:A:163:U:OP2	28:S:87:ARG:NH2	2.44	0.51
47:t:187:ILE:HG21	47:t:207:ILE:HG21	1.92	0.51
48:u:272:MET:HA	48:u:275:TYR:HB3	1.92	0.51
51:x:41:LYS:HB2	52:y:595:GLN:HG3	1.93	0.51
10:A:1228:A:H2'	10:A:1229:G:C8	2.46	0.51
10:A:1580:A:OP1	39:h:86:LYS:NZ	2.44	0.51
16:G:69:LEU:HD22	16:G:96:ALA:HB2	1.92	0.51
30:V:29:GLN:N	30:V:110:GLN:OE1	2.44	0.51
10:A:617:G:H4'	14:E:88:ASP:HB2	1.92	0.51
10:A:639:C:H2'	10:A:640:A:H8	1.75	0.51
10:A:1129:G:H3'	10:A:1130:G:H21	1.76	0.51
10:A:1416:C:OP1	36:d:133:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:70:SER:HA	22:M:74:GLN:CG	2.39	0.51
27:R:171:LEU:HD23	27:R:189:VAL:HG11	1.93	0.51
42:m:54:SER:HB2	42:m:80:ASP:HA	1.93	0.51
42:m:72:HIS:HB2	42:m:74:ILE:HD11	1.93	0.51
47:t:386:THR:HG21	47:t:393:ALA:HB2	1.91	0.51
10:A:1710:C:O2	45:q:46:ARG:NH2	2.44	0.51
25:P:145:GLY:O	26:Q:22:ARG:NH2	2.44	0.51
34:b:86:LEU:H	34:b:89:MET:HE3	1.76	0.51
9:9:15:ARG:NH1	10:A:1183:A:OP1	2.44	0.50
10:A:664:A:O2'	10:A:670:A:N1	2.43	0.50
10:A:1332:A:O2'	32:Z:145:GLN:O	2.29	0.50
11:B:135:SER:OG	11:B:136:LYS:N	2.44	0.50
23:N:85:ARG:NH1	23:N:203:PHE:O	2.45	0.50
34:b:68:PRO:HG2	34:b:71:GLU:HG2	1.93	0.50
36:d:141:ALA:HA	36:d:144:LYS:HE3	1.93	0.50
47:t:367:ILE:HD12	47:t:467:PRO:HG3	1.93	0.50
47:t:369:THR:HG21	47:t:465:ILE:HD12	1.93	0.50
5:5:191:ILE:HG21	5:5:279:ARG:HE	1.76	0.50
10:A:624:C:H2'	10:A:625:G:H5'	1.92	0.50
10:A:1256:G:N2	40:i:30:LEU:O	2.40	0.50
47:t:33:HIS:NE2	47:t:37:SER:HB2	2.24	0.50
48:u:17:GLU:HA	48:u:20:GLU:HG3	1.93	0.50
48:u:440:LEU:HA	48:u:443:VAL:HG12	1.93	0.50
10:A:531:A:N1	10:A:552:G:C6	2.79	0.50
17:H:30:SER:OG	17:H:31:TYR:N	2.45	0.50
48:u:498:ASN:HA	48:u:518:GLN:HE22	1.77	0.50
7:7:6:A:N7	45:q:12:ARG:NH1	2.60	0.50
10:A:1108:G:H21	22:M:126:MET:HE1	1.76	0.50
10:A:1650:A:H5''	31:Y:139:ALA:HB2	1.93	0.50
24:O:180:ASP:H	24:O:183:GLU:HG3	1.74	0.50
28:S:70:HIS:O	28:S:98:ARG:NH1	2.45	0.50
30:V:35:LEU:HD21	30:V:146:ARG:HH11	1.75	0.50
52:y:801:SER:HA	52:y:842:VAL:HA	1.93	0.50
1:1:516:LYS:HG3	1:1:518:HIS:CD2	2.46	0.50
5:5:96:GLU:OE2	5:5:181:GLN:NE2	2.43	0.50
31:Y:19:ALA:HB2	31:Y:75:GLY:HA3	1.93	0.50
41:k:120:GLU:CD	41:k:129:GLY:H	2.20	0.50
47:t:186:LEU:HG	47:t:243:ILE:HD11	1.92	0.50
5:5:457:LEU:HD11	5:5:492:VAL:HG12	1.94	0.50
10:A:326:C:N4	10:A:327:G:N7	2.59	0.50
48:u:340:ARG:C	48:u:342:LEU:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:174:OMC:O2	10:A:174:OMC:HM23	2.12	0.50
10:A:847:A:OP1	12:C:108:ARG:NH1	2.44	0.50
10:A:940:U:H3	10:A:1002:U:H3	1.59	0.50
47:t:174:LEU:HA	47:t:177:ILE:HD12	1.94	0.50
48:u:416:GLU:OE2	48:u:417:GLN:HG3	2.12	0.50
49:v:261:VAL:HG11	49:v:274:LEU:HD13	1.94	0.50
53:z:56:TYR:HB2	53:z:137:LEU:HD22	1.94	0.50
10:A:1757:G:O2'	10:A:1776:G:N1	2.45	0.50
24:O:36:PRO:HB2	24:O:38:MET:HE1	1.93	0.50
41:k:107:LYS:HD3	42:m:64:LEU:HD11	1.94	0.50
47:t:30:PRO:HD3	47:t:250:PHE:CZ	2.47	0.50
48:u:174:TYR:OH	48:u:204:HIS:ND1	2.41	0.50
1:l:292:ASN:C	1:l:294:ARG:H	2.20	0.50
5:5:398:MET:HE3	5:5:402:GLN:NE2	2.27	0.50
10:A:1094:C:O2	19:J:16:ASN:ND2	2.44	0.50
10:A:1283:C:O2'	10:A:1313:A:N1	2.36	0.50
17:H:23:ARG:O	19:J:60:LYS:NZ	2.45	0.50
20:K:41:LYS:HE2	20:K:41:LYS:N	2.27	0.50
46:r:113:ARG:NH1	46:r:117:GLU:OE2	2.45	0.50
10:A:1037:G:H4'	10:A:1845:A:H4'	1.94	0.49
10:A:1142:G:OP1	21:L:187:ARG:NH1	2.45	0.49
20:K:7:GLU:OE1	20:K:7:GLU:N	2.45	0.49
34:b:22:LEU:HA	34:b:25:LEU:HD12	1.94	0.49
10:A:1722:G:N2	10:A:1812:U:O2	2.40	0.49
22:M:65:PRO:HB3	22:M:77:GLU:CD	2.37	0.49
33:a:1:MET:HE1	33:a:43:LEU:HD21	1.94	0.49
48:u:38:LYS:HD3	48:u:41:ARG:HE	1.77	0.49
10:A:796:G:N2	10:A:798:G:OP2	2.45	0.49
27:R:3:ILE:O	27:R:30:GLY:N	2.45	0.49
51:x:32:PRO:O	52:y:593:HIS:NE2	2.32	0.49
52:y:476:GLU:OE2	52:y:509:HIS:ND1	2.33	0.49
10:A:928:G:H2'	10:A:929:G:C8	2.47	0.49
10:A:1550:G:O2'	10:A:1558:C:O2	2.26	0.49
25:P:39:ASP:OD1	25:P:40:THR:N	2.45	0.49
9:9:9:ARG:NH1	10:A:1851:MA6:OP1	2.46	0.49
10:A:973:C:N3	25:P:55:ARG:NH2	2.60	0.49
22:M:78:ARG:NE	22:M:78:ARG:HA	2.27	0.49
32:Z:142:LEU:HD13	32:Z:150:MET:HE3	1.94	0.49
45:q:63:GLY:O	45:q:64:LYS:C	2.55	0.49
10:A:751:G:H22	10:A:789:G:H5''	1.78	0.49
13:D:82:VAL:HG21	13:D:92:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:65:PRO:HB3	22:M:77:GLU:OE2	2.13	0.49
22:M:105:MET:HE1	23:N:51:LEU:H	1.76	0.49
43:n:13:ARG:NH2	43:n:33:GLU:OE2	2.45	0.49
48:u:108:SER:O	48:u:112:VAL:HG13	2.13	0.49
48:u:329:ILE:O	48:u:434:ASN:ND2	2.45	0.49
48:u:462:VAL:HG13	48:u:466:GLN:HG2	1.95	0.49
53:z:35:VAL:HG22	53:z:75:ILE:HG13	1.95	0.49
13:D:24:ARG:NE	13:D:28:GLU:OE2	2.46	0.49
19:J:86:LEU:HD21	19:J:113:HIS:HB2	1.93	0.49
21:L:184:VAL:HG21	21:L:247:THR:HG22	1.93	0.49
28:S:65:GLN:OE1	28:S:66:GLY:N	2.45	0.49
48:u:51:MET:HB3	48:u:89:VAL:HG21	1.95	0.49
2:2:267:ALA:N	2:2:281:VAL:O	2.43	0.49
29:T:74:MET:HE3	29:T:74:MET:HA	1.94	0.49
46:r:232:PRO:HD3	50:w:73:A:H4'	1.94	0.49
47:t:33:HIS:CE1	47:t:37:SER:HB2	2.48	0.49
4:4:292:ASP:HA	6:6:344:LYS:HE2	1.94	0.49
10:A:535:G:N2	10:A:536:A:N7	2.61	0.49
10:A:614:C:H3'	45:q:62:ARG:HH12	1.78	0.49
10:A:846:G:N3	12:C:19:MET:HE1	2.27	0.49
10:A:926:A:H61	10:A:1015:U:H3	1.61	0.49
10:A:1677:U:O4	10:A:1678:A2M:N6	2.46	0.49
42:m:71:GLU:O	42:m:73:GLN:NE2	2.46	0.49
48:u:175:HIS:HB3	48:u:232:THR:HG21	1.95	0.49
1:1:520:GLN:HE22	1:1:570:TRP:CD1	2.31	0.49
34:b:64:LYS:NZ	34:b:88:GLU:O	2.34	0.49
35:c:3:GLU:HB3	35:c:247:TRP:HH2	1.78	0.49
41:k:114:ILE:HG12	41:k:115:SER:H	1.78	0.49
45:q:84:TYR:HD1	45:q:85:GLN:HG2	1.77	0.49
10:A:317:C:OP2	28:S:183:ARG:NH2	2.45	0.48
10:A:476:A:N3	10:A:488:U:O2'	2.35	0.48
10:A:516:A:N1	10:A:643:A:O2'	2.41	0.48
22:M:72:LYS:HA	22:M:75:GLU:HG3	1.95	0.48
36:d:133:ARG:HG2	36:d:137:GLN:HE22	1.78	0.48
41:k:117:LEU:HD12	41:k:118:ARG:H	1.78	0.48
47:t:12:GLN:HB2	47:t:38:ARG:HH12	1.78	0.48
48:u:198:CYS:HG	48:u:202:ARG:HH21	1.61	0.48
51:x:452:VAL:HG22	51:x:465:ILE:HG22	1.95	0.48
53:z:56:TYR:HE1	53:z:88:MET:HB3	1.78	0.48
5:5:228:LEU:O	5:5:232:HIS:ND1	2.46	0.48
10:A:591:U:OP1	15:F:100:LYS:NZ	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:489:ARG:HH12	52:y:806:THR:HG21	1.78	0.48
5:5:56:ILE:HG23	5:5:128:PHE:HZ	1.77	0.48
10:A:789:G:OP2	10:A:789:G:N2	2.42	0.48
16:G:142:LYS:HB3	19:J:54:ASP:OD1	2.12	0.48
41:k:107:LYS:HZ1	42:m:68:LEU:HG	1.78	0.48
48:u:347:ILE:HG13	48:u:351:LYS:HG3	1.94	0.48
52:y:719:ARG:HG2	52:y:723:ARG:HH12	1.77	0.48
10:A:790:C:OP1	10:A:791:C:O2'	2.30	0.48
19:J:96:SER:OG	19:J:98:GLN:OE1	2.31	0.48
37:e:32:LYS:O	37:e:33:LYS:HB2	2.13	0.48
41:k:109:ASP:H	41:k:115:SER:HB2	1.78	0.48
41:k:119:ARG:HD3	41:k:132:MET:CE	2.43	0.48
48:u:114:ASP:O	48:u:115:ILE:C	2.56	0.48
48:u:239:SER:O	48:u:243:MET:HG2	2.13	0.48
10:A:545:A:O2'	10:A:546:G:O4'	2.31	0.48
10:A:952:G:H21	25:P:52:THR:HG21	1.77	0.48
45:q:34:GLU:OE2	45:q:52:PHE:N	2.46	0.48
49:v:377:ASN:OD1	49:v:378:ALA:N	2.46	0.48
10:A:517:OMC:HM22	10:A:518:G:O4'	2.12	0.48
10:A:1512:C:O2'	40:i:7:TYR:O	2.24	0.48
23:N:76:VAL:HG12	23:N:123:VAL:HB	1.95	0.48
37:e:43:LYS:NZ	37:e:44:LEU:N	2.36	0.48
44:o:243:VAL:HB	44:o:283:ALA:HB3	1.95	0.48
48:u:384:VAL:HB	48:u:387:VAL:HG22	1.96	0.48
53:z:66:GLN:NE2	53:z:68:ASP:OD2	2.47	0.48
5:5:154:PHE:HD1	5:5:221:ILE:HG21	1.78	0.48
10:A:28:U:H2'	10:A:29:G:H8	1.79	0.48
10:A:199:C:O2	10:A:200:G:N2	2.46	0.48
10:A:562:U:H2'	10:A:563:G:C8	2.48	0.48
10:A:719:G:H5''	10:A:719:G:H8	1.78	0.48
10:A:996:A:OP1	18:I:114:ARG:NH2	2.43	0.48
10:A:1064:C:H2'	10:A:1065:G:H8	1.78	0.48
17:H:33:MET:HE3	17:H:79:PHE:CD1	2.48	0.48
22:M:76:GLU:HA	22:M:79:GLU:OE1	2.13	0.48
46:r:46:ILE:HG12	46:r:85:LEU:HB2	1.94	0.48
47:t:262:PHE:HB2	50:w:74:C:H4'	1.94	0.48
48:u:451:GLU:HA	48:u:490:THR:HA	1.95	0.48
13:D:158:ASP:OD1	13:D:159:PHE:N	2.47	0.48
31:Y:32:ILE:HD12	31:Y:39:LEU:HD22	1.96	0.48
46:r:154:LYS:HD2	46:r:184:LEU:HD21	1.96	0.48
52:y:68:ARG:HH12	52:y:112:ASP:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:56:LEU:HD23	34:b:83:MET:HE3	1.94	0.48
52:y:373:LYS:O	52:y:377:ASN:ND2	2.46	0.48
10:A:919:A:H5''	18:I:16:LEU:HD12	1.96	0.48
10:A:1217:A:H2'	10:A:1218:C:H6	1.79	0.48
14:E:45:SER:OG	14:E:46:HIS:ND1	2.40	0.48
21:L:104:ASP:OD1	21:L:104:ASP:N	2.46	0.48
41:k:133:ALA:N	41:k:140:TYR:O	2.46	0.48
49:v:351:ILE:N	49:v:391:VAL:O	2.43	0.48
10:A:368:U:H2'	52:y:139:SER:HB3	1.94	0.47
10:A:1291:A:O2'	41:k:140:TYR:OH	2.17	0.47
10:A:1593:C:OP1	37:e:103:HIS:NE2	2.36	0.47
22:M:81:ARG:HH12	23:N:205:ARG:HD3	1.79	0.47
51:x:308:SER:OG	51:x:311:ASN:ND2	2.42	0.47
5:5:82:ASP:OD1	5:5:83:VAL:N	2.46	0.47
6:6:283:MET:HE1	6:6:337:SER:HB2	1.97	0.47
6:6:352:ASP:OD1	6:6:353:THR:N	2.47	0.47
8:8:315:ASP:O	8:8:319:ILE:N	2.46	0.47
10:A:334:C:OP2	28:S:190:ARG:NH2	2.42	0.47
10:A:1665:G:N7	36:d:88:MET:HE1	2.29	0.47
10:A:1729:U:H3	10:A:1805:G:H1	1.61	0.47
12:C:141:THR:OG1	12:C:143:ASP:OD1	2.28	0.47
23:N:42:LYS:HZ3	23:N:48:ILE:HD11	1.79	0.47
23:N:85:ARG:NH2	23:N:201:LEU:O	2.46	0.47
32:Z:28:GLU:HG2	32:Z:69:LEU:HD21	1.96	0.47
41:k:118:ARG:NH1	41:k:134:SER:O	2.46	0.47
45:q:46:ARG:HB3	45:q:58:LEU:HD11	1.96	0.47
45:q:75:ASP:OD1	45:q:75:ASP:N	2.45	0.47
10:A:1562:C:H5''	36:d:71:GLY:HA3	1.97	0.47
30:V:125:SER:O	30:V:136:ARG:NH2	2.35	0.47
52:y:771:GLU:HB3	52:y:774:LYS:HD3	1.96	0.47
10:A:1754:G:P	10:A:1780:G:H22	2.36	0.47
19:J:94:LEU:O	21:L:183:LYS:NZ	2.45	0.47
47:t:139:ASP:HB2	47:t:452:ARG:HH12	1.79	0.47
49:v:50:MET:O	49:v:54:ALA:N	2.48	0.47
1:1:722:LYS:HA	1:1:727:TYR:HA	1.95	0.47
5:5:59:PHE:HD2	5:5:128:PHE:HE1	1.61	0.47
10:A:614:C:C6	10:A:626:G:H5'	2.49	0.47
24:O:171:ILE:HG12	24:O:174:ARG:HH12	1.80	0.47
41:k:107:LYS:CG	41:k:114:ILE:HG22	2.44	0.47
52:y:641:ARG:HA	52:y:652:LEU:HD21	1.96	0.47
52:y:667:ARG:HH22	52:y:668:ARG:NH2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:y:701:HIS:CE1	52:y:702:GLU:HG2	2.49	0.47
5:5:547:ILE:HA	5:5:550:PHE:CE1	2.49	0.47
10:A:1705:C:H2'	10:A:1706:G:C8	2.49	0.47
38:f:110:ASP:OD1	38:f:113:ARG:NH2	2.48	0.47
40:i:47:ALA:O	40:i:52:PHE:N	2.46	0.47
47:t:54:LYS:HG2	47:t:158:LEU:HD22	1.96	0.47
5:5:462:SER:OG	49:v:376:ARG:NH1	2.48	0.47
10:A:199:C:H2'	10:A:200:G:H21	1.79	0.47
10:A:393:U:OP2	52:y:146:ARG:NH2	2.48	0.47
10:A:644:OMG:H2'	10:A:645:C:C6	2.50	0.47
10:A:1096:G:H1	10:A:1136:U:H3	1.60	0.47
10:A:1308:U:O2'	41:k:118:ARG:NH1	2.48	0.47
10:A:1326:U:O4	40:i:28:HIS:ND1	2.47	0.47
10:A:1398:G:H22	10:A:1448:A:H2	1.63	0.47
10:A:1568:C:H2'	10:A:1569:A:C8	2.49	0.47
13:D:149:VAL:HG11	13:D:157:ILE:HD11	1.96	0.47
20:K:1:MET:HB2	20:K:10:ASP:HB2	1.95	0.47
22:M:74:GLN:O	22:M:78:ARG:N	2.40	0.47
23:N:144:THR:N	23:N:158:ASP:OD2	2.45	0.47
24:O:109:LYS:O	24:O:113:MET:HG3	2.14	0.47
24:O:137:LEU:HG	24:O:215:VAL:HG22	1.96	0.47
35:c:49:GLU:OE1	35:c:49:GLU:N	2.41	0.47
35:c:87:LEU:HB2	35:c:101:PHE:HB2	1.97	0.47
41:k:107:LYS:NZ	42:m:67:ALA:HB3	2.30	0.47
41:k:109:ASP:HB3	41:k:113:LYS:HB2	1.97	0.47
46:r:71:VAL:HG21	46:r:85:LEU:HD13	1.96	0.47
48:u:335:ARG:HH22	52:y:742:LYS:HG3	1.80	0.47
49:v:399:SER:HA	49:v:403:GLN:HB2	1.96	0.47
51:x:34:SER:OG	51:x:57:ASN:OD1	2.25	0.47
1:1:520:GLN:HG2	1:1:525:TYR:H	1.80	0.47
10:A:38:A:H5''	13:D:5:ARG:HB3	1.97	0.47
25:P:57:THR:HB	25:P:60:MET:HE3	1.97	0.47
25:P:62:VAL:HG11	25:P:67:ASP:HB2	1.97	0.47
37:e:50:PHE:N	38:f:4:VAL:HG12	2.24	0.47
51:x:425:LEU:HD13	51:x:480:ILE:HD12	1.97	0.47
10:A:1451:G:N7	22:M:44:LYS:NZ	2.58	0.47
19:J:38:LEU:HA	19:J:41:MET:HE3	1.97	0.47
20:K:37:ALA:O	23:N:63:ARG:NH1	2.48	0.47
22:M:72:LYS:HA	22:M:75:GLU:CG	2.44	0.47
24:O:72:ALA:HB3	25:P:128:ARG:HH12	1.79	0.47
25:P:113:GLN:HG3	26:Q:46:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:o:245:ASN:ND2	44:o:309:ILE:O	2.48	0.47
52:y:757:ILE:HD11	52:y:776:ARG:HD2	1.97	0.47
5:5:541:ASP:O	5:5:545:ARG:HG2	2.15	0.47
10:A:1513:C:H2'	10:A:1514:G:H8	1.78	0.47
10:A:1667:U:O2'	10:A:1668:U:H5'	2.15	0.47
12:C:250:GLU:OE1	12:C:250:GLU:N	2.48	0.47
21:L:180:VAL:HG22	21:L:219:ILE:HD13	1.95	0.47
21:L:211:LYS:HG2	21:L:215:MET:HE1	1.96	0.47
40:i:17:GLY:O	40:i:27:ARG:NH1	2.48	0.47
41:k:113:LYS:HB2	41:k:113:LYS:HZ3	1.80	0.47
46:r:177:ILE:HA	46:r:180:ILE:HG22	1.97	0.47
47:t:29:THR:HA	47:t:250:PHE:CZ	2.50	0.47
6:6:297:MET:HB3	6:6:303:ILE:HD11	1.97	0.46
10:A:1722:G:H1	10:A:1812:U:H3	1.61	0.46
11:B:42:LEU:HD13	11:B:72:ILE:HD11	1.97	0.46
17:H:33:MET:CE	17:H:79:PHE:CD1	2.98	0.46
51:x:39:LEU:HD22	52:y:589:MET:HE2	1.97	0.46
52:y:753:HIS:O	52:y:757:ILE:HG22	2.15	0.46
5:5:183:LEU:HD13	5:5:269:LEU:HB2	1.96	0.46
10:A:1520:G:H21	34:b:126:VAL:HG11	1.81	0.46
30:V:30:ILE:O	51:x:479:GLN:NE2	2.48	0.46
35:c:62:HIS:NE2	35:c:80:SER:OG	2.32	0.46
37:e:46:ASN:HB3	37:e:80:ARG:N	2.29	0.46
5:5:191:ILE:HD13	5:5:279:ARG:HE	1.80	0.46
10:A:1010:G:H2'	10:A:1011:A:C8	2.50	0.46
13:D:33:GLY:HA3	15:F:112:TYR:CG	2.50	0.46
18:I:5:HIS:HB3	18:I:117:LEU:HD13	1.97	0.46
42:m:60:MET:SD	42:m:60:MET:N	2.73	0.46
5:5:136:TYR:CZ	5:5:140:ILE:HD11	2.50	0.46
8:8:311:PRO:O	8:8:315:ASP:N	2.42	0.46
10:A:834:C:H42	10:A:839:C:H42	1.62	0.46
10:A:1388:A:H61	32:Z:161:GLY:HA3	1.80	0.46
10:A:1636:G:N7	37:e:39:LYS:HB2	2.30	0.46
24:O:167:LYS:HD2	24:O:200:ALA:HB1	1.98	0.46
33:a:15:LEU:HD22	33:a:49:MET:HE2	1.97	0.46
35:c:82:SER:OG	35:c:83:TRP:N	2.49	0.46
47:t:165:CYS:SG	47:t:207:ILE:HG12	2.55	0.46
49:v:401:TYR:H	52:y:846:ARG:NH2	2.14	0.46
51:x:76:ASP:OD1	51:x:77:GLU:N	2.49	0.46
51:x:299:PRO:HB3	51:x:399:TRP:HH2	1.80	0.46
10:A:914:U:O3'	16:G:120:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1283:C:N3	42:m:93:LYS:NZ	2.56	0.46
10:A:1360:U:O2'	10:A:1379:A:OP2	2.29	0.46
13:D:54:ARG:NH2	13:D:98:LEU:HD22	2.29	0.46
24:O:38:MET:SD	24:O:38:MET:N	2.89	0.46
10:A:570:C:O2'	29:T:34:THR:O	2.34	0.46
16:G:29:GLU:HA	16:G:32:MET:SD	2.54	0.46
21:L:196:ILE:HB	21:L:223:TYR:HB2	1.97	0.46
30:V:122:ARG:HD2	43:n:59:LEU:HD11	1.96	0.46
41:k:109:ASP:HB2	41:k:115:SER:OG	2.15	0.46
41:k:110:GLU:OE1	42:m:63:LYS:HG3	2.16	0.46
47:t:300:ILE:HD12	47:t:300:ILE:HA	1.83	0.46
48:u:208:ILE:HD11	48:u:218:ILE:H	1.80	0.46
10:A:846:G:C4	12:C:19:MET:HE1	2.50	0.46
10:A:955:A:N1	10:A:968:U:O2'	2.45	0.46
30:V:16:ASP:OD1	30:V:16:ASP:N	2.48	0.46
44:o:250:THR:O	44:o:251:ARG:NH1	2.47	0.46
47:t:29:THR:HG23	47:t:31:LEU:N	2.30	0.46
48:u:292:HIS:O	48:u:295:THR:OG1	2.28	0.46
10:A:1231:C:O2'	10:A:1253:A:N6	2.48	0.46
10:A:1613:G:OP2	34:b:39:ALA:N	2.49	0.46
22:M:111:PHE:HB3	22:M:114:LEU:HD23	1.97	0.46
41:k:114:ILE:HG13	41:k:116:ARG:HD2	1.96	0.46
41:k:119:ARG:O	41:k:132:MET:N	2.45	0.46
46:r:27:ILE:HG21	46:r:59:ILE:HG21	1.98	0.46
52:y:146:ARG:O	52:y:150:ARG:NE	2.49	0.46
1:1:547:PHE:CD1	1:1:556:VAL:HG12	2.51	0.46
10:A:1228:A:O2'	10:A:1634:A:N3	2.41	0.46
22:M:58:MET:HA	22:M:61:ILE:HB	1.97	0.46
34:b:30:TYR:O	34:b:34:MET:HG2	2.16	0.46
43:n:20:ARG:HA	43:n:28:THR:HA	1.97	0.46
52:y:628:ASP:OD1	52:y:629:ALA:N	2.48	0.46
1:1:552:LYS:HA	1:1:552:LYS:HD2	1.74	0.46
10:A:712:G:H5''	10:A:712:G:H8	1.80	0.46
10:A:899:U:O2'	10:A:900:C:O4'	2.34	0.46
10:A:1679:A:OP1	30:V:60:ARG:NH2	2.49	0.46
25:P:100:THR:HG21	25:P:104:ARG:HD2	1.98	0.46
47:t:85:ASN:HB3	47:t:129:HIS:CE1	2.51	0.46
47:t:355:GLY:HA3	47:t:411:LEU:HD13	1.99	0.46
51:x:247:ALA:HB3	51:x:373:VAL:HG22	1.98	0.46
52:y:664:LYS:HD2	52:y:667:ARG:HH21	1.80	0.46
1:1:497:GLN:HB3	1:1:500:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:342:PHE:HD2	6:6:346:GLN:HB2	1.80	0.45
10:A:920:A:OP1	19:J:57:ARG:NH2	2.49	0.45
10:A:982:G:H2'	10:A:983:A:C8	2.51	0.45
13:D:65:GLU:OE1	13:D:66:LYS:N	2.49	0.45
17:H:13:GLU:N	17:H:13:GLU:OE1	2.49	0.45
18:I:100:LYS:O	18:I:104:ARG:NH1	2.49	0.45
21:L:109:ILE:HD11	21:L:124:PHE:HB3	1.97	0.45
36:d:71:GLY:O	36:d:75:MET:HB2	2.16	0.45
49:v:237:LEU:HD12	49:v:238:TYR:HB3	1.97	0.45
10:A:644:OMG:HM22	10:A:645:C:C6	2.51	0.45
10:A:1309:C:H5'	41:k:118:ARG:HG3	1.96	0.45
10:A:1473:G:OP1	35:c:15:ASN:ND2	2.49	0.45
10:A:1603:G:H4'	38:f:38:ARG:HE	1.81	0.45
37:e:51:ASP:O	37:e:52:LYS:C	2.58	0.45
48:u:585:LEU:O	48:u:589:ARG:N	2.46	0.45
10:A:367:U:H4'	10:A:371:A:C8	2.51	0.45
10:A:641:A:O2'	10:A:645:C:OP1	2.34	0.45
10:A:692:G:H2'	10:A:693:A:C4	2.51	0.45
10:A:923:G:OP1	18:I:2:GLY:N	2.49	0.45
10:A:1010:G:H2'	10:A:1011:A:H8	1.81	0.45
13:D:55:LYS:HB2	13:D:55:LYS:HE3	1.76	0.45
23:N:184:ARG:NH1	23:N:191:ARG:O	2.49	0.45
24:O:167:LYS:HD3	24:O:170:GLU:OE2	2.15	0.45
33:a:15:LEU:HD23	33:a:79:LEU:HD11	1.96	0.45
37:e:79:ILE:HB	37:e:83:LEU:HD23	1.99	0.45
39:h:20:ILE:HG12	39:h:116:ILE:HA	1.97	0.45
47:t:145:MET:HG2	47:t:173:HIS:NE2	2.31	0.45
48:u:19:LEU:HD11	48:u:53:LYS:HD2	1.98	0.45
10:A:197:U:H2'	10:A:203:G:H21	1.81	0.45
16:G:51:ILE:HD11	16:G:176:VAL:HG22	1.97	0.45
22:M:76:GLU:OE1	22:M:77:GLU:HG3	2.16	0.45
33:a:29:MET:HE3	33:a:29:MET:HB2	1.87	0.45
45:q:27:VAL:HG21	45:q:93:LEU:HD21	1.98	0.45
48:u:531:ALA:O	48:u:535:GLU:HB2	2.16	0.45
4:4:94:LEU:N	4:4:238:LYS:O	2.47	0.45
9:9:10:MET:HB3	9:9:10:MET:HE2	1.85	0.45
10:A:557:U:H5'	10:A:558:G:C8	2.52	0.45
10:A:1729:U:O4	10:A:1805:G:O6	2.34	0.45
21:L:191:VAL:HG11	21:L:236:PHE:HA	1.98	0.45
22:M:34:VAL:O	22:M:38:ILE:HG12	2.16	0.45
31:Y:116:ASP:OD1	31:Y:118:THR:OG1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:85:LEU:HB3	33:a:89:ILE:HD12	1.99	0.45
41:k:116:ARG:HD2	41:k:116:ARG:H	1.81	0.45
47:t:149:ALA:HA	47:t:152:MET:HG2	1.98	0.45
49:v:197:ASP:HA	49:v:211:ARG:HH21	1.82	0.45
10:A:525:A:O2'	15:F:105:ARG:NH2	2.50	0.45
10:A:701:G:H8	10:A:701:G:H5''	1.82	0.45
10:A:888:U:C4	10:A:900:C:N3	2.85	0.45
10:A:1563:G:H5''	36:d:115:LYS:HE2	1.97	0.45
10:A:1707:U:O2'	53:z:136:LYS:NZ	2.50	0.45
21:L:168:GLY:N	21:L:179:THR:O	2.41	0.45
22:M:106:LEU:HD12	22:M:111:PHE:HB2	1.97	0.45
37:e:34:LYS:HE2	37:e:34:LYS:HB2	1.78	0.45
47:t:360:ALA:HB3	47:t:363:ALA:HB3	1.97	0.45
48:u:229:HIS:O	48:u:232:THR:OG1	2.33	0.45
49:v:384:ILE:HG22	49:v:391:VAL:HG13	1.99	0.45
1:l:612:ASN:H	1:l:627:GLY:HA2	1.81	0.45
10:A:1190:A:N3	10:A:1714:U:O2'	2.48	0.45
10:A:1466:G:OP1	22:M:5:ARG:NH1	2.50	0.45
20:K:53:TYR:OH	20:K:76:ASP:OD2	2.29	0.45
23:N:57:LYS:NZ	23:N:160:ALA:O	2.48	0.45
31:Y:93:VAL:HA	31:Y:108:ILE:HD11	1.98	0.45
31:Y:97:GLN:HB2	31:Y:105:LYS:HE2	1.97	0.45
49:v:388:LEU:HG	49:v:390:HIS:ND1	2.32	0.45
52:y:548:MET:SD	52:y:572:HIS:ND1	2.89	0.45
10:A:693:A:H2'	10:A:694:G:C8	2.51	0.45
10:A:943:U:OP1	24:O:214:LYS:NZ	2.44	0.45
11:B:113:LEU:HD21	11:B:120:VAL:HG21	1.98	0.45
13:D:18:ARG:HB3	13:D:21:GLU:OE2	2.16	0.45
13:D:92:MET:SD	13:D:92:MET:N	2.88	0.45
48:u:392:ASN:HA	48:u:396:VAL:HB	1.99	0.45
52:y:333:LEU:HD13	52:y:374:ILE:HG22	1.98	0.45
10:A:1060:A:O2'	10:A:1062:A:N7	2.46	0.45
10:A:1674:G:N7	31:Y:17:LYS:NZ	2.60	0.45
22:M:80:ARG:NH1	22:M:81:ARG:HA	2.31	0.45
24:O:38:MET:HG3	24:O:185:VAL:HG11	1.99	0.45
42:m:82:ASN:ND2	42:m:107:SER:OG	2.40	0.45
43:n:35:MET:SD	43:n:35:MET:N	2.90	0.45
47:t:25:VAL:HG13	47:t:287:VAL:HB	1.97	0.45
47:t:30:PRO:HG2	47:t:31:LEU:HD22	1.99	0.45
48:u:42:THR:HG22	48:u:79:GLN:HE21	1.81	0.45
52:y:832:MET:HE2	52:y:832:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:571:GLU:HG2	1:1:621:GLN:HA	1.99	0.45
10:A:523:A:OP2	13:D:38:ARG:NE	2.49	0.45
10:A:987:A:OP1	26:Q:32:LYS:NZ	2.50	0.45
46:r:36:LEU:HD11	46:r:83:ILE:HD13	1.99	0.45
49:v:368:GLU:HA	49:v:371:ILE:HB	1.98	0.45
9:9:10:MET:HE1	10:A:1172:U:H4'	1.99	0.44
12:C:86:PHE:HE1	12:C:182:MET:HE2	1.81	0.44
18:I:37:ILE:HD13	18:I:71:ILE:HG12	1.98	0.44
30:V:36:GLN:OE1	51:x:479:GLN:NE2	2.50	0.44
37:e:70:PRO:HA	37:e:73:VAL:HG22	2.00	0.44
38:f:114:LEU:HA	38:f:117:ILE:HG22	1.99	0.44
52:y:445:LEU:HA	52:y:448:VAL:HG22	1.99	0.44
52:y:468:GLU:O	52:y:472:HIS:ND1	2.50	0.44
10:A:1331:C:H41	45:q:15:GLY:HA2	1.82	0.44
16:G:19:PHE:CE2	16:G:50:GLU:HB2	2.53	0.44
27:R:177:SER:HB3	27:R:186:ASP:HB2	2.00	0.44
32:Z:32:ASP:OD2	32:Z:65:ARG:NH1	2.51	0.44
34:b:143:PRO:HB2	45:q:70:TRP:CD2	2.51	0.44
40:i:48:LYS:HE2	40:i:48:LYS:H	1.83	0.44
47:t:300:ILE:HG22	47:t:312:LYS:HB2	1.99	0.44
48:u:337:ASP:HA	48:u:341:LEU:HB2	1.99	0.44
1:1:549:MET:HB2	1:1:550:ARG:CZ	2.47	0.44
10:A:190:G:O2'	10:A:209:A:N6	2.50	0.44
20:K:55:ILE:HG13	20:K:69:ILE:HD11	1.99	0.44
20:K:56:CYS:SG	20:K:57:GLY:N	2.90	0.44
32:Z:93:THR:HG21	32:Z:96:LEU:HD12	1.99	0.44
47:t:323:ALA:HB2	47:t:328:LEU:HD11	1.98	0.44
48:u:366:THR:C	48:u:368:ILE:H	2.24	0.44
52:y:687:LEU:HD12	52:y:733:MET:HE1	1.99	0.44
10:A:520:A:O2'	10:A:825:A:N3	2.46	0.44
10:A:1474:A:H5''	31:Y:121:VAL:HG13	1.98	0.44
12:C:104:ASP:HB3	12:C:110:ALA:HB2	1.99	0.44
15:F:118:ASN:HB2	15:F:120:VAL:HG13	1.99	0.44
22:M:79:GLU:C	22:M:81:ARG:N	2.74	0.44
30:V:56:TYR:HB3	30:V:63:LYS:HA	2.00	0.44
32:Z:225:GLU:HG2	35:c:189:ILE:HD11	2.00	0.44
41:k:103:LEU:HD23	42:m:35:ILE:HG23	2.00	0.44
52:y:835:LEU:HB2	52:y:840:GLN:O	2.17	0.44
10:A:373:G:OP1	11:B:137:THR:OG1	2.29	0.44
10:A:640:A:H2'	10:A:641:A:C8	2.52	0.44
22:M:89:SER:HB2	23:N:198:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:192:SER:HB2	48:u:23:LYS:NZ	2.33	0.44
26:Q:49:ALA:O	26:Q:53:ILE:HG12	2.18	0.44
33:a:48:ALA:O	33:a:51:SER:OG	2.29	0.44
47:t:408:ILE:HD13	47:t:433:VAL:HG21	1.99	0.44
48:u:109:GLN:HE22	48:u:110:GLN:HE21	1.64	0.44
5:5:383:ASP:HA	5:5:545:ARG:HH21	1.81	0.44
5:5:457:LEU:HD13	5:5:493:PHE:HA	1.99	0.44
5:5:560:MET:HE3	5:5:561:GLY:N	2.30	0.44
6:6:28:GLU:O	6:6:32:GLU:N	2.49	0.44
10:A:1438:A:H2'	10:A:1439:A:C8	2.53	0.44
10:A:1652:G:H1	10:A:1672:U:H3	1.64	0.44
20:K:12:TYR:HB3	21:L:79:GLU:OE2	2.17	0.44
22:M:24:LEU:HD23	22:M:34:VAL:HG11	1.99	0.44
32:Z:38:GLU:HB3	32:Z:49:ILE:HB	1.99	0.44
41:k:132:MET:HE1	41:k:139:HIS:ND1	2.33	0.44
51:x:225:HIS:O	51:x:374:ARG:NH2	2.46	0.44
51:x:317:THR:O	51:x:321:HIS:ND1	2.50	0.44
53:z:5:VAL:HA	53:z:18:MET:HG3	2.00	0.44
6:6:341:THR:O	6:6:341:THR:OG1	2.35	0.44
10:A:531:A:N1	10:A:552:G:O6	2.50	0.44
10:A:1277:C:H2'	10:A:1278:A:H8	1.82	0.44
13:D:125:HIS:HA	13:D:128:VAL:HG22	1.98	0.44
18:I:33:VAL:O	18:I:37:ILE:HG13	2.18	0.44
48:u:298:ARG:HA	48:u:301:HIS:CE1	2.53	0.44
5:5:177:GLU:HA	5:5:265:LEU:HD22	2.00	0.44
10:A:219:U:H1'	27:R:184:ARG:HD2	1.99	0.44
10:A:354:U:OP2	11:B:107:LYS:NZ	2.51	0.44
10:A:1448:A:OP1	39:h:30:LYS:NZ	2.37	0.44
10:A:1520:G:OP1	38:f:136:THR:N	2.51	0.44
10:A:1757:G:H1'	10:A:1776:G:H22	1.81	0.44
11:B:111:VAL:HG12	11:B:140:PHE:HB2	1.99	0.44
21:L:152:ARG:HA	21:L:155:ILE:HG22	2.00	0.44
24:O:71:LEU:HD13	24:O:84:PHE:CE1	2.53	0.44
47:t:151:VAL:HB	47:t:282:SER:HB3	2.00	0.44
9:9:2:ARG:NE	10:A:1842:C:OP2	2.49	0.44
10:A:981:A:H2'	10:A:982:G:C8	2.52	0.44
10:A:1102:G:OP1	24:O:151:ARG:NH2	2.51	0.44
20:K:32:ILE:HG12	20:K:60:ARG:HD2	2.00	0.44
33:a:55:ARG:NH1	33:a:78:TYR:OH	2.50	0.44
1:1:575:SER:O	1:1:575:SER:OG	2.35	0.43
5:5:367:MET:HA	5:5:370:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:536:A:H3'	10:A:537:C:H4'	1.98	0.43
10:A:649:U:H2'	10:A:650:A:H8	1.82	0.43
10:A:874:G:H2'	10:A:875:A:H8	1.83	0.43
10:A:982:G:H21	10:A:1045:U:H1'	1.83	0.43
10:A:1722:G:H2'	10:A:1723:G:C8	2.53	0.43
23:N:66:VAL:HG11	23:N:185:MET:HG3	2.00	0.43
37:e:48:VAL:HG13	38:f:55:ARG:HG3	2.00	0.43
47:t:259:ILE:HD12	47:t:281:GLY:HA2	2.00	0.43
48:u:324:LEU:O	48:u:328:SER:N	2.51	0.43
1:1:521:LYS:HE2	1:1:572:PRO:HG3	2.00	0.43
1:1:575:SER:OG	1:1:594:VAL:O	2.32	0.43
10:A:116:OMU:HM23	10:A:116:OMU:H1'	1.64	0.43
10:A:644:OMG:N3	10:A:644:OMG:HM23	2.34	0.43
10:A:1403:C:N4	10:A:1433:C:OP1	2.52	0.43
10:A:1673:U:O2'	30:V:84:GLY:O	2.32	0.43
16:G:149:ASP:OD1	16:G:149:ASP:N	2.50	0.43
20:K:4:ASP:OD2	21:L:174:ILE:HG12	2.18	0.43
24:O:180:ASP:O	24:O:184:VAL:HG23	2.18	0.43
36:d:75:MET:HE1	36:d:79:TYR:HE2	1.82	0.43
40:i:53:ILE:HG13	40:i:55:LEU:HD22	2.01	0.43
48:u:33:ASP:HA	48:u:36:LYS:HB2	1.99	0.43
48:u:536:VAL:HB	48:u:543:LEU:HD22	2.00	0.43
5:5:471:PRO:HG2	5:5:474:LYS:HB2	2.00	0.43
10:A:1017:U:O2'	18:I:48:SER:O	2.35	0.43
10:A:1588:A:H2'	10:A:1589:A:C8	2.53	0.43
13:D:60:LEU:HD11	13:D:73:GLU:HB3	2.00	0.43
24:O:180:ASP:H	24:O:183:GLU:CD	2.26	0.43
27:R:67:TRP:NE1	27:R:191:GLU:OE2	2.48	0.43
30:V:114:ASN:O	30:V:118:ASN:ND2	2.49	0.43
40:i:48:LYS:HE2	40:i:48:LYS:N	2.34	0.43
47:t:263:ASP:O	50:w:74:C:H5''	2.18	0.43
48:u:412:ASN:O	48:u:416:GLU:HG3	2.18	0.43
52:y:636:ILE:O	52:y:639:SER:OG	2.29	0.43
5:5:171:ASP:OD1	5:5:172:GLY:N	2.49	0.43
10:A:355:G:OP1	11:B:105:ARG:NH1	2.42	0.43
10:A:1759:G:N2	10:A:1772:C:OP2	2.51	0.43
11:B:128:VAL:HG12	11:B:142:VAL:HA	2.00	0.43
22:M:116:ASN:OD1	22:M:116:ASN:N	2.51	0.43
28:S:2:LYS:HB2	28:S:108:VAL:HG23	2.00	0.43
35:c:260:ASP:OD1	35:c:261:LEU:N	2.51	0.43
49:v:266:ASP:O	49:v:268:ARG:NE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:x:474:ASN:OD1	51:x:475:GLU:N	2.51	0.43
53:z:7:ARG:NE	53:z:90:ASP:OD2	2.52	0.43
5:5:317:TYR:HA	5:5:336:PHE:HE1	1.83	0.43
10:A:440:G:OP1	27:R:2:GLY:N	2.50	0.43
10:A:1755:C:O2'	10:A:1778:C:O2	2.34	0.43
24:O:171:ILE:HG23	24:O:174:ARG:HH22	1.83	0.43
30:V:24:SER:O	30:V:107:ASN:ND2	2.45	0.43
37:e:48:VAL:CG1	38:f:55:ARG:HG3	2.48	0.43
46:r:115:VAL:HA	46:r:118:VAL:HG22	2.01	0.43
48:u:226:GLN:HE22	48:u:267:PRO:HB3	1.83	0.43
52:y:738:VAL:O	52:y:741:SER:OG	2.24	0.43
10:A:683:OMG:N3	10:A:683:OMG:HM23	2.33	0.43
41:k:105:TYR:O	41:k:117:LEU:HG	2.18	0.43
46:r:25:ARG:NH2	46:r:35:SER:OG	2.45	0.43
48:u:19:LEU:HD21	48:u:57:LEU:HD21	2.00	0.43
5:5:555:ARG:HA	5:5:558:LYS:HB2	1.99	0.43
29:T:102:THR:HG23	29:T:107:ARG:HH11	1.84	0.43
34:b:60:LEU:HD13	34:b:89:MET:HB3	2.01	0.43
35:c:24:THR:HG23	35:c:27:PHE:H	1.84	0.43
41:k:92:LYS:HZ3	41:k:93:HIS:H	1.67	0.43
48:u:208:ILE:HG13	48:u:212:HIS:CE1	2.53	0.43
51:x:318:TYR:O	51:x:322:ASN:ND2	2.51	0.43
53:z:5:VAL:HG22	53:z:18:MET:HB3	2.01	0.43
6:6:327:GLN:HE22	48:u:454:ARG:HG2	1.82	0.43
10:A:656:G:N3	21:L:227:ARG:NH2	2.66	0.43
10:A:701:G:H5''	10:A:701:G:C8	2.54	0.43
10:A:1286:G:O2'	10:A:1312:G:N2	2.39	0.43
23:N:107:THR:O	23:N:117:ARG:N	2.51	0.43
23:N:137:ALA:HB1	23:N:142:LEU:HB2	2.00	0.43
38:f:113:ARG:O	38:f:117:ILE:HB	2.18	0.43
48:u:384:VAL:O	48:u:388:LYS:N	2.48	0.43
48:u:463:ASP:H	48:u:466:GLN:NE2	2.17	0.43
5:5:59:PHE:CD1	5:5:94:ILE:HG21	2.54	0.43
16:G:84:GLU:O	16:G:88:SER:HA	2.18	0.43
21:L:193:VAL:HG21	21:L:240:THR:HA	2.00	0.43
24:O:33:VAL:HG21	24:O:67:PHE:CE2	2.54	0.43
38:f:49:ASP:OD1	38:f:49:ASP:N	2.49	0.43
48:u:109:GLN:HA	48:u:112:VAL:HG22	2.00	0.43
52:y:464:PRO:HG2	52:y:465:HIS:CD2	2.54	0.43
5:5:327:ARG:NH2	5:5:496:LYS:HG2	2.32	0.43
6:6:325:ILE:HG22	6:6:332:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1274:G:C5'	33:a:1:MET:HE3	2.49	0.43
13:D:113:GLN:OE1	13:D:154:GLN:NE2	2.44	0.43
23:N:42:LYS:NZ	23:N:48:ILE:HD11	2.34	0.43
25:P:129:ILE:HG21	26:Q:44:ILE:HG21	2.01	0.43
35:c:114:SER:OG	35:c:115:SER:N	2.52	0.43
35:c:249:CYS:SG	35:c:291:TRP:NE1	2.85	0.43
45:q:41:MET:HE3	45:q:41:MET:HB3	1.83	0.43
46:r:112:LEU:HA	46:r:115:VAL:HG22	2.00	0.43
46:r:169:ASN:HB3	46:r:172:GLU:HG2	2.01	0.43
48:u:106:GLU:O	48:u:110:GLN:HG2	2.19	0.43
52:y:801:SER:HB2	52:y:842:VAL:HG12	2.01	0.43
5:5:143:LYS:HA	5:5:143:LYS:HD2	1.89	0.42
10:A:393:U:H3'	52:y:150:ARG:HH22	1.84	0.42
10:A:1560:U:H2'	10:A:1561:A:H8	1.84	0.42
10:A:1838:U:H5'	25:P:151:LEU:HD23	2.01	0.42
24:O:29:ASP:N	24:O:49:VAL:O	2.49	0.42
34:b:87:PRO:HA	34:b:112:ILE:HD11	2.01	0.42
38:f:38:ARG:O	38:f:42:HIS:ND1	2.51	0.42
10:A:60:G:N2	10:A:316:G:H21	2.16	0.42
10:A:600:G:H2'	10:A:601:G:H8	1.84	0.42
10:A:868:G:OP2	10:A:868:G:N2	2.33	0.42
10:A:1543:U:OP1	36:d:62:ARG:NH1	2.45	0.42
16:G:138:GLU:OE1	18:I:19:ARG:NH1	2.53	0.42
18:I:46:THR:H	18:I:49:GLN:NE2	2.17	0.42
46:r:172:GLU:HA	46:r:175:VAL:HG12	2.01	0.42
49:v:305:PHE:O	49:v:309:GLN:N	2.52	0.42
51:x:202:TYR:HA	51:x:328:LEU:HB2	2.01	0.42
5:5:240:ILE:HD11	5:5:267:LYS:HA	2.00	0.42
11:B:48:LYS:O	11:B:52:GLU:HG3	2.20	0.42
12:C:199:GLU:N	12:C:199:GLU:OE1	2.52	0.42
21:L:184:VAL:HG11	21:L:247:THR:HA	1.99	0.42
52:y:697:TYR:O	52:y:701:HIS:ND1	2.38	0.42
1:1:486:ASP:HB3	1:1:489:ILE:HB	2.01	0.42
1:1:547:PHE:HD1	1:1:556:VAL:HG12	1.84	0.42
7:7:-24:A:O2'	52:y:653:ARG:NH2	2.49	0.42
10:A:625:G:H4'	10:A:629:A:C4	2.54	0.42
10:A:1860:A:N7	26:Q:34:LYS:NZ	2.67	0.42
30:V:42:LYS:O	30:V:45:TYR:HB2	2.18	0.42
30:V:122:ARG:HG3	43:n:59:LEU:HD21	2.00	0.42
48:u:76:ASN:O	48:u:79:GLN:NE2	2.49	0.42
52:y:706:ARG:HH12	52:y:857:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:447:A:H4'	12:C:3:ARG:HB2	2.02	0.42
10:A:624:C:C2'	10:A:625:G:H5'	2.49	0.42
10:A:681:U:H4'	14:E:9:THR:HG22	2.01	0.42
17:H:34:ASP:N	17:H:34:ASP:OD1	2.53	0.42
18:I:142:GLU:OE1	18:I:145:THR:N	2.36	0.42
20:K:65:SER:O	20:K:68:SER:OG	2.28	0.42
22:M:21:TYR:HD2	22:M:72:LYS:HB2	1.84	0.42
42:m:18:LEU:HD22	42:m:77:ILE:HG21	2.00	0.42
52:y:98:ASP:OD1	52:y:99:LYS:N	2.53	0.42
10:A:844:U:OP1	12:C:240:ARG:NH1	2.49	0.42
16:G:46:THR:HG21	16:G:97:GLN:HG2	2.02	0.42
28:S:218:LYS:NZ	28:S:219:GLU:OE2	2.48	0.42
31:Y:53:GLU:OE2	31:Y:115:TYR:OH	2.29	0.42
35:c:101:PHE:CE1	35:c:136:GLY:HA2	2.55	0.42
35:c:232:GLY:HA3	35:c:252:THR:HG21	2.00	0.42
36:d:35:ASP:HB2	38:f:46:ARG:HG2	2.01	0.42
37:e:49:LEU:HD13	38:f:6:PRO:HD2	2.01	0.42
42:m:22:LEU:HD22	42:m:89:VAL:HG12	2.00	0.42
46:r:172:GLU:O	46:r:176:LEU:HB2	2.20	0.42
48:u:226:GLN:HG2	48:u:264:LYS:HE3	2.02	0.42
51:x:381:MET:O	51:x:389:SER:OG	2.31	0.42
6:6:287:VAL:HG23	6:6:288:GLU:OE1	2.19	0.42
21:L:182:CYS:SG	21:L:183:LYS:N	2.93	0.42
33:a:26:ASP:OD1	33:a:29:MET:N	2.53	0.42
37:e:38:GLY:O	37:e:39:LYS:HB3	2.19	0.42
42:m:69:CYS:SG	42:m:76:LEU:HD21	2.59	0.42
49:v:252:HIS:HB2	49:v:286:TYR:CZ	2.55	0.42
52:y:643:LYS:O	52:y:648:GLN:N	2.52	0.42
52:y:706:ARG:NH1	52:y:857:LEU:HA	2.34	0.42
1:1:478:ILE:HD12	1:1:478:ILE:H	1.85	0.42
5:5:220:LYS:O	5:5:223:ASN:ND2	2.37	0.42
5:5:383:ASP:HA	5:5:545:ARG:NH2	2.34	0.42
10:A:1113:A:O2'	10:A:1114:U:O4'	2.23	0.42
10:A:1154:U:O4	21:L:227:ARG:NH2	2.49	0.42
10:A:1604:G:OP2	38:f:38:ARG:NH2	2.53	0.42
24:O:198:GLU:OE2	24:O:207:LEU:HB2	2.20	0.42
26:Q:60:ASP:OD1	26:Q:61:ALA:N	2.53	0.42
32:Z:127:MET:HA	32:Z:127:MET:HE3	2.01	0.42
37:e:73:VAL:HA	37:e:76:ARG:HG2	2.02	0.42
47:t:26:THR:HG22	47:t:251:THR:HA	2.02	0.42
47:t:33:HIS:O	47:t:34:GLU:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:t:258:VAL:HG13	47:t:279:ALA:HB1	2.02	0.42
48:u:105:LYS:O	48:u:109:GLN:HG3	2.20	0.42
1:1:524:ASP:O	1:1:549:MET:HG2	2.20	0.42
3:3:180:SER:O	3:3:188:PHE:N	2.53	0.42
7:7:4:G:H1'	45:q:70:TRP:CE2	2.55	0.42
10:A:453:C:O2'	28:S:92:ARG:O	2.28	0.42
10:A:959:G:H2'	10:A:960:U:C6	2.55	0.42
16:G:145:ARG:NH2	19:J:49:GLU:HG2	2.35	0.42
27:R:103:LEU:HD22	27:R:170:LYS:HB3	2.01	0.42
28:S:25:ARG:HA	28:S:25:ARG:NH1	2.35	0.42
35:c:72:SER:OG	35:c:74:ASP:OD1	2.26	0.42
39:h:21:ARG:HD3	39:h:88:LEU:HD23	2.02	0.42
41:k:109:ASP:CG	41:k:113:LYS:HZ3	2.28	0.42
47:t:130:VAL:HG11	47:t:239:ILE:HG21	2.01	0.42
52:y:445:LEU:HD22	52:y:501:ARG:CZ	2.49	0.42
52:y:702:GLU:OE1	52:y:707:ARG:HG3	2.20	0.42
52:y:802:ILE:N	52:y:841:THR:O	2.52	0.42
5:5:381:ARG:NH1	5:5:537:ARG:H	2.17	0.42
10:A:687:C:O2'	16:G:103:LYS:NZ	2.49	0.42
10:A:830:A:OP2	10:A:846:G:N2	2.36	0.42
13:D:21:GLU:N	13:D:21:GLU:OE1	2.53	0.42
16:G:186:ASN:OD1	16:G:187:PHE:N	2.52	0.42
34:b:59:ARG:HE	34:b:76:VAL:HG13	1.84	0.42
47:t:168:PRO:HD3	47:t:385:ARG:HE	1.85	0.42
47:t:222:ILE:HG12	47:t:234:VAL:HG12	2.01	0.42
47:t:398:LEU:HD22	47:t:404:LEU:HD11	2.02	0.42
53:z:20:ARG:O	53:z:38:ASN:ND2	2.43	0.42
5:5:46:GLN:NE2	5:5:114:GLU:OE1	2.37	0.41
10:A:110:U:H3	10:A:351:G:H1	1.68	0.41
10:A:1398:G:H1'	35:c:63:SER:HB3	2.01	0.41
10:A:1543:U:OP1	31:Y:37:ARG:NH2	2.53	0.41
23:N:61:ALA:HB1	23:N:145:ILE:HD13	2.02	0.41
48:u:281:THR:O	48:u:285:LYS:NZ	2.51	0.41
49:v:263:THR:HG21	49:v:328:CYS:HB3	2.01	0.41
49:v:393:MET:HE3	49:v:395:ASN:HD21	1.84	0.41
52:y:383:TYR:HB3	52:y:450:ARG:NH1	2.34	0.41
5:5:55:PHE:CE1	5:5:94:ILE:HG23	2.55	0.41
7:7:4:G:H5''	34:b:144:LEU:HA	2.01	0.41
10:A:1216:C:H42	10:A:1342:U:P	2.43	0.41
10:A:1578:U:H5''	10:A:1579:A:O4'	2.20	0.41
16:G:78:ARG:HH11	16:G:81:ARG:HH12	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:133:TYR:CD1	21:L:216:MET:HA	2.55	0.41
22:M:71:ILE:N	22:M:74:GLN:HB2	2.34	0.41
22:M:73:LEU:C	22:M:76:GLU:HG3	2.46	0.41
22:M:76:GLU:O	22:M:79:GLU:HB2	2.20	0.41
23:N:73:ASP:OD1	23:N:73:ASP:N	2.53	0.41
30:V:128:ILE:HD12	30:V:137:GLN:HB3	2.01	0.41
33:a:94:LEU:HD23	33:a:95:ARG:HB3	2.02	0.41
35:c:191:HIS:CD2	35:c:195:LEU:HD21	2.54	0.41
45:q:40:LYS:HD3	45:q:40:LYS:HA	1.76	0.41
48:u:312:GLN:HA	48:u:315:MET:SD	2.61	0.41
48:u:535:GLU:HG3	48:u:538:LYS:HD2	2.01	0.41
49:v:254:LEU:O	49:v:258:THR:HG23	2.20	0.41
10:A:560:A:O5'	13:D:174:LYS:NZ	2.53	0.41
16:G:157:HIS:NE2	16:G:188:GLU:OE2	2.53	0.41
23:N:168:ALA:HB1	23:N:204:TYR:HB3	2.03	0.41
28:S:147:LEU:HD11	28:S:156:TYR:CG	2.55	0.41
36:d:74:SER:HA	36:d:77:LYS:HG2	2.02	0.41
45:q:79:VAL:HG22	45:q:91:VAL:HA	2.03	0.41
48:u:52:LEU:HD22	48:u:89:VAL:HG23	2.01	0.41
48:u:284:TRP:HB2	48:u:292:HIS:ND1	2.34	0.41
10:A:851:C:H5''	10:A:852:G:H5'	2.02	0.41
10:A:1232:U:H2'	10:A:1233:G:C8	2.55	0.41
10:A:1609:C:OP2	38:f:134:GLN:NE2	2.53	0.41
10:A:1636:G:O6	37:e:41:ARG:NH1	2.54	0.41
13:D:55:LYS:O	13:D:59:GLU:HG2	2.20	0.41
16:G:143:ARG:HB2	16:G:155:LYS:HB2	2.03	0.41
21:L:92:GLU:N	21:L:92:GLU:OE1	2.54	0.41
23:N:10:MET:HE3	23:N:10:MET:HA	2.03	0.41
23:N:176:TRP:CH2	23:N:180:ARG:HD2	2.55	0.41
29:T:56:PHE:HB2	29:T:74:MET:HB3	2.02	0.41
37:e:50:PHE:CZ	37:e:58:LEU:HD13	2.55	0.41
43:n:11:LEU:HB3	43:n:35:MET:HG2	2.02	0.41
47:t:39:GLN:HB3	47:t:328:LEU:HD21	2.01	0.41
47:t:83:TYR:CD1	47:t:336:LEU:HD13	2.56	0.41
48:u:307:ARG:NH1	48:u:315:MET:HG2	2.36	0.41
1:l:529:LYS:HD2	1:l:529:LYS:HA	1.78	0.41
21:L:147:VAL:O	21:L:151:ILE:HG12	2.20	0.41
24:O:190:PRO:HA	48:u:14[B]:ARG:HH21	1.86	0.41
24:O:190:PRO:HB2	48:u:18:PHE:CZ	2.55	0.41
47:t:139:ASP:OD2	47:t:452:ARG:NH2	2.43	0.41
52:y:448:VAL:O	52:y:451:MET:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:y:555:ILE:HG23	52:y:564:ILE:HG22	2.03	0.41
1:1:524:ASP:HA	1:1:550:ARG:HH11	1.86	0.41
1:1:561:MET:HE3	1:1:561:MET:HA	2.03	0.41
10:A:1179:G:N2	10:A:1182:A:OP2	2.51	0.41
12:C:124:CYS:HB3	12:C:141:THR:HB	2.02	0.41
15:F:82:ARG:HG3	15:F:83:ALA:H	1.86	0.41
18:I:46:THR:O	18:I:50:ILE:HG12	2.20	0.41
21:L:209:VAL:HA	21:L:212:LYS:HE2	2.01	0.41
23:N:41:ARG:HE	23:N:45:GLY:HA2	1.85	0.41
35:c:78:ALA:HB2	35:c:92:LEU:HD21	2.03	0.41
41:k:114:ILE:HG13	41:k:116:ARG:CD	2.50	0.41
44:o:248:GLU:O	44:o:251:ARG:NH1	2.51	0.41
47:t:145:MET:SD	47:t:146:LEU:HG	2.61	0.41
47:t:321:LEU:HD22	47:t:331:ALA:HB2	2.03	0.41
48:u:389:ASP:OD1	48:u:389:ASP:N	2.53	0.41
49:v:295:PHE:CD1	49:v:311:LYS:HE3	2.55	0.41
52:y:107:ILE:HG23	52:y:156:ILE:HG12	2.03	0.41
5:5:340:LEU:HA	5:5:340:LEU:HD23	1.78	0.41
10:A:1454:A:O4'	22:M:3:ARG:NH1	2.53	0.41
23:N:174:MET:HB3	23:N:174:MET:HE2	1.78	0.41
41:k:96:LYS:HA	41:k:96:LYS:HD2	1.95	0.41
48:u:266:PRO:HA	48:u:267:PRO:HD3	1.92	0.41
51:x:39:LEU:HD13	52:y:589:MET:SD	2.61	0.41
52:y:614:VAL:O	52:y:618:ILE:HG12	2.20	0.41
1:1:528:VAL:HB	1:1:545:GLU:HB3	2.01	0.41
10:A:118:C:H1'	10:A:445:A:C5	2.56	0.41
10:A:729:C:H6	10:A:729:C:H5''	1.86	0.41
10:A:1281:G:OP2	42:m:102:LYS:NZ	2.50	0.41
10:A:1286:G:N2	10:A:1312:G:O2'	2.45	0.41
10:A:1310:U:H5''	41:k:130:VAL:HG23	2.02	0.41
13:D:87:LEU:HD12	13:D:87:LEU:HA	1.94	0.41
14:E:56:GLY:O	45:q:82:ARG:NH1	2.52	0.41
28:S:56:ASN:HB2	28:S:108:VAL:HG12	2.03	0.41
35:c:217:MET:HG2	35:c:229:THR:HG23	2.03	0.41
41:k:119:ARG:HD3	41:k:132:MET:HE1	2.03	0.41
47:t:207:ILE:HB	47:t:221:ILE:HD13	2.03	0.41
47:t:408:ILE:HD12	47:t:433:VAL:HG11	2.03	0.41
53:z:55:LYS:HG2	53:z:140:PHE:CG	2.55	0.41
1:1:525:TYR:HE1	1:1:548:ARG:HG3	1.86	0.41
5:5:350:PHE:HB3	5:5:357:TYR:HD1	1.85	0.41
7:7:7:C:C4	10:A:626:G:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:225:ALA:O	8:8:229:GLU:N	2.54	0.41
10:A:49:C:H2'	10:A:472:C:H41	1.86	0.41
10:A:996:A:H2'	10:A:997:A:C8	2.55	0.41
10:A:1083:A:N7	10:A:1841:C:O2'	2.47	0.41
10:A:1236:G:O2'	34:b:131:PRO:O	2.35	0.41
27:R:119:LEU:HD21	27:R:153:LYS:HG2	2.03	0.41
34:b:64:LYS:HA	34:b:67:ALA:HB2	2.03	0.41
34:b:107:ILE:HA	34:b:111:MET:CE	2.51	0.41
35:c:5:MET:HG3	35:c:270:LEU:HD21	2.02	0.41
41:k:109:ASP:CB	41:k:113:LYS:HB2	2.50	0.41
41:k:114:ILE:HD13	41:k:114:ILE:H	1.86	0.41
41:k:118:ARG:CD	41:k:133:ALA:HA	2.48	0.41
46:r:11:HIS:HE1	46:r:145:PRO:HG3	1.86	0.41
47:t:23:LEU:HD22	47:t:330:TYR:CD2	2.56	0.41
47:t:42:ILE:HD12	47:t:245:VAL:HA	2.02	0.41
47:t:125:LYS:HD3	47:t:126:LEU:N	2.36	0.41
48:u:92:ALA:HA	48:u:95:LYS:HE3	2.02	0.41
48:u:403:LEU:HD23	48:u:439:LEU:HD13	2.02	0.41
48:u:492:SER:OG	48:u:493:PHE:N	2.54	0.41
49:v:331:ASP:N	49:v:331:ASP:OD1	2.53	0.41
49:v:361:ASN:OD1	49:v:362:MET:N	2.53	0.41
52:y:96:ILE:HG23	52:y:97:VAL:HG13	2.03	0.41
52:y:109:ILE:HD13	52:y:109:ILE:HA	1.93	0.41
52:y:633:LEU:HD11	52:y:682:LEU:HD11	2.02	0.41
52:y:694:GLU:O	52:y:698:MET:HG2	2.21	0.41
10:A:27:A2M:H1'	10:A:27:A2M:HM'3	1.89	0.41
10:A:383:G:O2'	11:B:133:PRO:O	2.34	0.41
10:A:1722:G:H2'	10:A:1723:G:H8	1.86	0.41
10:A:1757:G:HO2'	10:A:1776:G:H1	1.69	0.41
20:K:78:ILE:O	23:N:2:SER:N	2.54	0.41
21:L:137:VAL:HB	21:L:217:ALA:HA	2.03	0.41
24:O:231:LEU:HD12	24:O:231:LEU:HA	1.93	0.41
35:c:176:VAL:HB	35:c:186:THR:HB	2.03	0.41
37:e:43:LYS:HG3	37:e:44:LEU:N	2.36	0.41
41:k:92:LYS:HA	41:k:92:LYS:HD2	1.82	0.41
47:t:29:THR:HG23	47:t:31:LEU:H	1.86	0.41
51:x:292:SER:N	51:x:428:ASN:OD1	2.45	0.41
52:y:440:VAL:HG12	52:y:443:CYS:H	1.86	0.41
52:y:551:LEU:O	52:y:555:ILE:HG12	2.21	0.41
52:y:709:MET:HE3	52:y:710:ILE:H	1.84	0.41
1:1:472:TRP:HZ3	1:1:498:LEU:HD12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:7:LYS:HD3	9:9:11:ARG:HE	1.86	0.40
10:A:17:C:O2'	10:A:1194:A:N1	2.45	0.40
10:A:1036:A:N3	10:A:1844:U:O2'	2.51	0.40
10:A:1204:A:OP1	21:L:117:ARG:NE	2.46	0.40
10:A:1643:U:H2'	10:A:1644:C:C6	2.56	0.40
10:A:1665:G:C5	36:d:88:MET:HE1	2.56	0.40
11:B:57:ASP:OD2	11:B:112:HIS:NE2	2.47	0.40
23:N:33:GLN:HB3	23:N:154:LEU:HD12	2.02	0.40
24:O:147:ASN:OD1	24:O:148:ASN:N	2.54	0.40
27:R:141:ARG:O	27:R:146:GLN:NE2	2.54	0.40
38:f:117:ILE:HA	38:f:117:ILE:HD12	1.83	0.40
47:t:188:LEU:HD22	47:t:235:VAL:HG22	2.02	0.40
52:y:635:ASP:OD1	52:y:636:ILE:N	2.54	0.40
52:y:793:PHE:CZ	52:y:825:MET:HE3	2.57	0.40
53:z:97:VAL:O	53:z:107:THR:OG1	2.34	0.40
7:7:14:A:H1'	15:F:123:PHE:CE2	2.56	0.40
9:9:18:ARG:NH2	10:A:1182:A:OP1	2.54	0.40
10:A:106:C:H2'	10:A:107:A:H8	1.86	0.40
10:A:1528:G:O2'	10:A:1666:C:OP1	2.31	0.40
22:M:71:ILE:HG12	22:M:74:GLN:OE1	2.21	0.40
31:Y:96:TYR:HA	31:Y:100:VAL:HG22	2.02	0.40
33:a:38:LYS:HE2	33:a:38:LYS:HB3	1.89	0.40
49:v:349:GLN:OE1	49:v:393:MET:N	2.51	0.40
52:y:120:LEU:HD23	52:y:120:LEU:HA	1.96	0.40
52:y:504:LEU:O	52:y:507:ILE:HG12	2.21	0.40
52:y:698:MET:O	52:y:702:GLU:HB2	2.22	0.40
52:y:733:MET:SD	52:y:734:ARG:HG3	2.61	0.40
5:5:304:MET:HB2	5:5:307:ARG:HH21	1.87	0.40
5:5:328:ARG:HH21	5:5:500:LEU:HD23	1.86	0.40
7:7:13:A:O2'	7:7:14:A:OP1	2.37	0.40
16:G:20:GLU:OE2	16:G:24:SER:OG	2.38	0.40
16:G:43:LEU:HD13	16:G:72:PHE:HD1	1.86	0.40
24:O:28:LYS:HD3	24:O:48:LEU:HD13	2.03	0.40
35:c:5:MET:HE3	35:c:5:MET:HA	2.03	0.40
46:r:159:ASP:N	46:r:159:ASP:OD1	2.53	0.40
48:u:274:ASN:O	48:u:278:LYS:HG2	2.22	0.40
48:u:438:ARG:HD3	48:u:510:HIS:CE1	2.56	0.40
52:y:670:GLN:H	52:y:670:GLN:HG2	1.60	0.40
5:5:163:LEU:HD12	5:5:163:LEU:HA	1.95	0.40
10:A:159:A2M:H2	10:A:467:G:H21	1.86	0.40
10:A:725:C:H6	10:A:725:C:H5''	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1288:U:N3	10:A:1311:C:O2	2.54	0.40
10:A:1798:C:H2'	10:A:1799:G:O4'	2.21	0.40
13:D:55:LYS:HA	13:D:58:ARG:NE	2.36	0.40
22:M:13:ALA:HA	22:M:16:ILE:HG22	2.04	0.40
24:O:103:MET:HE2	24:O:103:MET:HA	2.03	0.40
24:O:180:ASP:H	24:O:183:GLU:CG	2.34	0.40
30:V:40:ALA:HB1	30:V:45:TYR:CD2	2.53	0.40
48:u:106:GLU:HG3	48:u:109:GLN:HE21	1.86	0.40
48:u:111:MET:HE2	48:u:111:MET:HB2	1.86	0.40
48:u:320:THR:HG22	48:u:383:VAL:HB	2.02	0.40
49:v:221:VAL:HB	49:v:324:PHE:HE1	1.85	0.40
5:5:280:LEU:HA	5:5:283:LEU:HD12	2.03	0.40
5:5:550:PHE:O	5:5:554:ASN:N	2.52	0.40
10:A:509:OMG:HM21	10:A:510:G:O4'	2.21	0.40
10:A:649:U:H2'	10:A:650:A:C8	2.57	0.40
10:A:1628:C:H2'	10:A:1629:C:C6	2.56	0.40
17:H:14:GLU:OE1	17:H:17:ARG:NH1	2.55	0.40
23:N:176:TRP:NE1	23:N:197:VAL:O	2.53	0.40
30:V:152:TRP:O	30:V:156:THR:HG22	2.21	0.40
32:Z:189:MET:HE2	32:Z:189:MET:HB3	1.91	0.40
39:h:51:LYS:HB2	39:h:90:ASP:HB2	2.02	0.40
44:o:266:SER:HB3	44:o:288:HIS:HB2	2.03	0.40
47:t:309:LEU:HD23	47:t:309:LEU:HA	1.95	0.40
48:u:432:GLN:O	48:u:436:ILE:HG12	2.22	0.40
49:v:248:THR:OG1	49:v:249:MET:HE3	2.21	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	1	584/814 (72%)	542 (93%)	42 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	300/325 (92%)	293 (98%)	7 (2%)	0	100	100
3	3	209/218 (96%)	201 (96%)	8 (4%)	0	100	100
4	4	251/357 (70%)	235 (94%)	16 (6%)	0	100	100
5	5	518/564 (92%)	501 (97%)	17 (3%)	0	100	100
6	6	360/374 (96%)	339 (94%)	21 (6%)	0	100	100
8	8	313/352 (89%)	290 (93%)	23 (7%)	0	100	100
9	9	22/25 (88%)	22 (100%)	0	0	100	100
11	B	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
12	C	254/263 (97%)	246 (97%)	8 (3%)	0	100	100
13	D	175/194 (90%)	168 (96%)	7 (4%)	0	100	100
14	E	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
15	F	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
16	G	171/194 (88%)	163 (95%)	8 (5%)	0	100	100
17	H	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
18	I	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
19	J	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
20	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
21	L	218/293 (74%)	215 (99%)	3 (1%)	0	100	100
22	M	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
23	N	205/295 (70%)	195 (95%)	10 (5%)	0	100	100
24	O	209/264 (79%)	201 (96%)	8 (4%)	0	100	100
25	P	131/151 (87%)	120 (92%)	11 (8%)	0	100	100
26	Q	97/115 (84%)	92 (95%)	5 (5%)	0	100	100
27	R	194/208 (93%)	192 (99%)	2 (1%)	0	100	100
28	S	228/249 (92%)	217 (95%)	11 (5%)	0	100	100
29	T	123/133 (92%)	123 (100%)	0	0	100	100
30	V	180/204 (88%)	171 (95%)	9 (5%)	0	100	100
31	Y	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
32	Z	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
33	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100
34	b	129/145 (89%)	123 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	c	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
36	d	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
37	e	79/125 (63%)	72 (91%)	7 (9%)	0	100	100
38	f	147/152 (97%)	135 (92%)	12 (8%)	0	100	100
39	h	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
40	i	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
41	k	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
42	m	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
43	n	61/69 (88%)	56 (92%)	5 (8%)	0	100	100
44	o	75/320 (23%)	73 (97%)	2 (3%)	0	100	100
45	q	110/144 (76%)	92 (84%)	18 (16%)	0	100	100
46	r	294/315 (93%)	269 (92%)	25 (8%)	0	100	100
47	t	451/472 (96%)	441 (98%)	10 (2%)	0	100	100
48	u	705/1382 (51%)	656 (93%)	49 (7%)	0	100	100
49	v	403/445 (91%)	367 (91%)	36 (9%)	0	100	100
51	x	416/548 (76%)	391 (94%)	25 (6%)	0	100	100
52	y	650/913 (71%)	619 (95%)	31 (5%)	0	100	100
53	z	143/430 (33%)	136 (95%)	7 (5%)	0	100	100
All	All	10547/13474 (78%)	10010 (95%)	537 (5%)	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	1	97/702 (14%)	97 (100%)	0	100	100
5	5	477/515 (93%)	477 (100%)	0	100	100
6	6	112/335 (33%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	8	1/310 (0%)	1 (100%)	0	100	100
9	9	23/24 (96%)	23 (100%)	0	100	100
11	B	129/142 (91%)	129 (100%)	0	100	100
12	C	220/225 (98%)	220 (100%)	0	100	100
13	D	158/168 (94%)	156 (99%)	2 (1%)	61	71
14	E	112/115 (97%)	112 (100%)	0	100	100
15	F	48/48 (100%)	48 (100%)	0	100	100
16	G	159/174 (91%)	159 (100%)	0	100	100
17	H	73/76 (96%)	73 (100%)	0	100	100
18	I	130/131 (99%)	130 (100%)	0	100	100
19	J	112/113 (99%)	112 (100%)	0	100	100
20	K	65/67 (97%)	65 (100%)	0	100	100
21	L	186/225 (83%)	186 (100%)	0	100	100
22	M	119/122 (98%)	117 (98%)	2 (2%)	53	67
23	N	173/243 (71%)	173 (100%)	0	100	100
24	O	192/231 (83%)	190 (99%)	2 (1%)	68	75
25	P	104/119 (87%)	104 (100%)	0	100	100
26	Q	86/98 (88%)	86 (100%)	0	100	100
27	R	172/180 (96%)	172 (100%)	0	100	100
28	S	200/218 (92%)	200 (100%)	0	100	100
29	T	107/115 (93%)	107 (100%)	0	100	100
30	V	156/170 (92%)	156 (100%)	0	100	100
31	Y	117/121 (97%)	117 (100%)	0	100	100
32	Z	190/202 (94%)	190 (100%)	0	100	100
33	a	90/136 (66%)	89 (99%)	1 (1%)	65	74
34	b	117/130 (90%)	117 (100%)	0	100	100
35	c	272/275 (99%)	272 (100%)	0	100	100
36	d	112/115 (97%)	112 (100%)	0	100	100
37	e	71/103 (69%)	59 (83%)	12 (17%)	2	9
38	f	129/132 (98%)	129 (100%)	0	100	100
39	h	94/107 (88%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	i	44/49 (90%)	44 (100%)	0	100	100
41	k	61/140 (44%)	55 (90%)	6 (10%)	7	27
42	m	104/108 (96%)	104 (100%)	0	100	100
43	n	56/62 (90%)	56 (100%)	0	100	100
44	o	64/277 (23%)	64 (100%)	0	100	100
45	q	94/123 (76%)	91 (97%)	3 (3%)	34	58
46	r	190/280 (68%)	190 (100%)	0	100	100
47	t	380/397 (96%)	377 (99%)	3 (1%)	73	77
48	u	528/1259 (42%)	527 (100%)	1 (0%)	87	85
49	v	206/406 (51%)	206 (100%)	0	100	100
51	x	207/494 (42%)	207 (100%)	0	100	100
52	y	562/811 (69%)	562 (100%)	0	100	100
53	z	129/388 (33%)	129 (100%)	0	100	100
All	All	7228/10981 (66%)	7196 (100%)	32 (0%)	81	83

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	D	55	LYS
13	D	59	GLU
22	M	79	GLU
22	M	80	ARG
24	O	180	ASP
24	O	183	GLU
33	a	3	MET
37	e	31	LYS
37	e	32	LYS
37	e	37	LYS
37	e	39	LYS
37	e	40	VAL
37	e	42	ASP
37	e	43	LYS
37	e	44	LEU
37	e	45	ASN
37	e	47	LEU
37	e	48	VAL
37	e	49	LEU

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Mol	Chain	Res	Type
41	k	107	LYS
41	k	108	VAL
41	k	113	LYS
41	k	114	ILE
41	k	116	ARG
41	k	117	LEU
45	q	20	GLU
45	q	64	LYS
45	q	68	LYS
47	t	28	LEU
47	t	29	THR
47	t	31	LEU
48	u	111	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
5	5	225	HIS
5	5	263	HIS
5	5	389	GLN
6	6	327	GLN
12	C	188	ASN
13	D	75	ASN
15	F	89	GLN
15	F	111	GLN
18	I	49	GLN
18	I	105	ASN
19	J	24	GLN
19	J	64	ASN
20	K	2	GLN
20	K	33	GLN
21	L	235	ASN
22	M	62	GLN
23	N	113	GLN
24	O	95	ASN
25	P	38	ASN
31	Y	29	ASN
33	a	39	ASN
33	a	66	HIS
34	b	32	GLN
38	f	11	HIS
41	k	151	ASN

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Mol	Chain	Res	Type
45	q	11	ASN
46	r	11	HIS
47	t	167	GLN
47	t	265	ASN
47	t	450	HIS
48	u	25	GLN
48	u	76	ASN
48	u	79	GLN
48	u	110	GLN
48	u	120	ASN
48	u	229	HIS
48	u	288	ASN
48	u	430	GLN
48	u	442	GLN
48	u	445	GLN
48	u	522	GLN
48	u	551	GLN
49	v	239	GLN
49	v	247	GLN
49	v	416	GLN
51	x	51	GLN
51	x	68	GLN
51	x	479	GLN
52	y	334	ASN
52	y	467	GLN
52	y	597	ASN
52	y	631	ASN
52	y	659	ASN
52	y	716	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1746/1869 (93%)	415 (23%)	13 (0%)
50	w	74/75 (98%)	20 (27%)	0
7	7	56/255 (21%)	43 (76%)	3 (5%)
All	All	1876/2199 (85%)	478 (25%)	16 (0%)

All (478) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	7	-34	C
7	7	-31	C
7	7	-30	A
7	7	-29	A
7	7	-28	C
7	7	-27	A
7	7	-26	A
7	7	-23	A
7	7	-22	C
7	7	-21	A
7	7	-20	A
7	7	-18	G
7	7	-17	A
7	7	-15	C
7	7	-13	A
7	7	-12	A
7	7	-11	A
7	7	-10	A
7	7	-8	A
7	7	-7	G
7	7	-6	A
7	7	-5	C
7	7	-4	C
7	7	-3	A
7	7	-2	C
7	7	-1	C
7	7	3	G
7	7	4	G
7	7	5	U
7	7	6	A
7	7	7	C
7	7	8	G
7	7	10	U
7	7	11	U
7	7	12	C
7	7	13	A
7	7	14	A
7	7	15	G
7	7	17	C
7	7	19	U
7	7	20	G
7	7	21	A
7	7	22	G

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Mol	Chain	Res	Type
10	A	2	A
10	A	4	C
10	A	17	C
10	A	26	U
10	A	33	G
10	A	44	U
10	A	46	A
10	A	56	G
10	A	58	C
10	A	59	U
10	A	67	C
10	A	68	A
10	A	73	C
10	A	74	G
10	A	76	U
10	A	78	C
10	A	82	G
10	A	103	A
10	A	115	U
10	A	126	G
10	A	129	C
10	A	130	G
10	A	140	U
10	A	142	C
10	A	143	U
10	A	147	A
10	A	155	G
10	A	158	A
10	A	163	U
10	A	173	A
10	A	182	C
10	A	184	G
10	A	190	G
10	A	198	U
10	A	199	C
10	A	200	G
10	A	202	G
10	A	203	G
10	A	204	G
10	A	206	G
10	A	208	G
10	A	288	G

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Mol	Chain	Res	Type
10	A	291	G
10	A	292	A
10	A	294	U
10	A	295	C
10	A	306	C
10	A	307	G
10	A	308	G
10	A	309	G
10	A	314	U
10	A	318	A
10	A	319	C
10	A	320	G
10	A	321	C
10	A	323	C
10	A	324	C
10	A	325	C
10	A	326	C
10	A	327	G
10	A	329	G
10	A	332	G
10	A	347	G
10	A	351	G
10	A	362	C
10	A	364	A
10	A	368	U
10	A	369	C
10	A	370	G
10	A	381	C
10	A	384	U
10	A	385	G
10	A	386	C
10	A	409	C
10	A	418	A
10	A	421	G
10	A	448	A
10	A	449	A
10	A	450	C
10	A	452	G
10	A	455	A
10	A	465	A
10	A	467	G
10	A	471	G

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Mol	Chain	Res	Type
10	A	472	C
10	A	473	A
10	A	474	G
10	A	482	G
10	A	487	U
10	A	492	C
10	A	502	C
10	A	508	A
10	A	509	OMG
10	A	517	OMC
10	A	525	A
10	A	534	G
10	A	536	A
10	A	537	C
10	A	538	U
10	A	539	C
10	A	540	U
10	A	541	U
10	A	542	U
10	A	543	C
10	A	544	G
10	A	545	A
10	A	546	G
10	A	547	G
10	A	550	C
10	A	553	U
10	A	554	A
10	A	556	U
10	A	557	U
10	A	558	G
10	A	563	G
10	A	564	A
10	A	566	U
10	A	568	C
10	A	576	A
10	A	589	G
10	A	590	A
10	A	591	U
10	A	598	G
10	A	606	G
10	A	607	U
10	A	614	C

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Mol	Chain	Res	Type
10	A	617	G
10	A	625	G
10	A	626	G
10	A	627	U
10	A	628	A
10	A	643	A
10	A	644	OMG
10	A	645	C
10	A	655	A
10	A	659	G
10	A	660	C
10	A	662	G
10	A	668	A2M
10	A	669	A
10	A	671	A
10	A	672	A
10	A	673	G
10	A	683	OMG
10	A	688	U
10	A	689	U
10	A	691	G
10	A	692	G
10	A	694	G
10	A	695	C
10	A	696	G
10	A	697	G
10	A	698	G
10	A	699	C
10	A	700	G
10	A	705	G
10	A	707	C
10	A	712	G
10	A	713	C
10	A	715	A
10	A	717	G
10	A	719	G
10	A	720	A
10	A	721	G
10	A	723	C
10	A	725	C
10	A	726	C
10	A	728	C

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Mol	Chain	Res	Type
10	A	729	C
10	A	731	G
10	A	732	U
10	A	733	C
10	A	734	C
10	A	738	C
10	A	739	C
10	A	748	C
10	A	749	U
10	A	751	G
10	A	752	G
10	A	753	C
10	A	791	C
10	A	798	G
10	A	800	U
10	A	801	U
10	A	810	A
10	A	811	A
10	A	821	G
10	A	822	PSU
10	A	827	A
10	A	830	A
10	A	836	G
10	A	837	A
10	A	838	G
10	A	839	C
10	A	840	C
10	A	841	G
10	A	845	G
10	A	847	A
10	A	870	A
10	A	872	A
10	A	873	G
10	A	880	G
10	A	886	A
10	A	888	U
10	A	890	U
10	A	891	G
10	A	895	G
10	A	896	U
10	A	897	U
10	A	898	U

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Mol	Chain	Res	Type
10	A	899	U
10	A	900	C
10	A	903	A
10	A	908	A
10	A	909	G
10	A	913	A
10	A	914	U
10	A	917	U
10	A	920	A
10	A	922	A
10	A	930	C
10	A	933	G
10	A	956	G
10	A	963	A
10	A	965	U
10	A	969	U
10	A	970	G
10	A	972	A
10	A	990	A
10	A	992	A
10	A	999	G
10	A	1002	U
10	A	1017	U
10	A	1023	A
10	A	1045	U
10	A	1047	C
10	A	1058	A
10	A	1061	U
10	A	1062	A
10	A	1078	C
10	A	1083	A
10	A	1085	C
10	A	1089	G
10	A	1109	C
10	A	1112	U
10	A	1113	A
10	A	1114	U
10	A	1115	U
10	A	1117	C
10	A	1119	A
10	A	1120	U
10	A	1123	C

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Mol	Chain	Res	Type
10	A	1133	A
10	A	1138	C
10	A	1139	C
10	A	1153	C
10	A	1154	U
10	A	1170	A
10	A	1195	A
10	A	1208	A
10	A	1209	A
10	A	1211	G
10	A	1215	C
10	A	1216	C
10	A	1217	A
10	A	1221	G
10	A	1224	G
10	A	1242	U
10	A	1249	C
10	A	1251	A
10	A	1253	A
10	A	1256	G
10	A	1257	G
10	A	1259	A
10	A	1274	G
10	A	1275	G
10	A	1283	C
10	A	1288	U
10	A	1290	G
10	A	1294	G
10	A	1295	A
10	A	1301	A
10	A	1302	G
10	A	1303	C
10	A	1308	U
10	A	1312	G
10	A	1318	G
10	A	1322	G
10	A	1326	U
10	A	1332	A
10	A	1333	U
10	A	1342	U
10	A	1354	G
10	A	1356	G

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Mol	Chain	Res	Type
10	A	1358	U
10	A	1371	U
10	A	1372	U
10	A	1378	A
10	A	1382	A
10	A	1397	U
10	A	1401	A
10	A	1402	A
10	A	1417	C
10	A	1418	C
10	A	1419	C
10	A	1420	G
10	A	1421	A
10	A	1422	G
10	A	1423	C
10	A	1424	G
10	A	1433	C
10	A	1435	C
10	A	1436	C
10	A	1437	C
10	A	1438	A
10	A	1442	U
10	A	1454	A
10	A	1463	U
10	A	1464	C
10	A	1487	A
10	A	1489	A
10	A	1490	G
10	A	1497	G
10	A	1498	A
10	A	1507	G
10	A	1508	A
10	A	1520	G
10	A	1521	C
10	A	1531	A
10	A	1533	A
10	A	1534	C
10	A	1544	C
10	A	1552	G
10	A	1553	C
10	A	1556	A
10	A	1558	C

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Mol	Chain	Res	Type
10	A	1560	U
10	A	1565	C
10	A	1570	G
10	A	1579	A
10	A	1580	A
10	A	1585	U
10	A	1587	G
10	A	1588	A
10	A	1594	A
10	A	1600	G
10	A	1601	A
10	A	1603	G
10	A	1606	G
10	A	1619	A
10	A	1621	U
10	A	1623	A
10	A	1624	U
10	A	1639	G
10	A	1648	G
10	A	1654	G
10	A	1661	A
10	A	1663	A
10	A	1665	G
10	A	1668	U
10	A	1671	G
10	A	1686	G
10	A	1687	C
10	A	1695	A
10	A	1699	A
10	A	1710	C
10	A	1712	A
10	A	1715	A
10	A	1719	A
10	A	1721	U
10	A	1722	G
10	A	1729	U
10	A	1744	G
10	A	1749	G
10	A	1750	C
10	A	1752	C
10	A	1753	C
10	A	1754	G

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Mol	Chain	Res	Type
10	A	1755	C
10	A	1756	C
10	A	1757	G
10	A	1758	G
10	A	1759	G
10	A	1760	G
10	A	1772	C
10	A	1773	C
10	A	1774	C
10	A	1775	U
10	A	1776	G
10	A	1777	G
10	A	1778	C
10	A	1779	G
10	A	1780	G
10	A	1781	A
10	A	1782	G
10	A	1783	C
10	A	1784	G
10	A	1805	G
10	A	1808	U
10	A	1813	A
10	A	1819	A
10	A	1822	A
10	A	1823	A
10	A	1824	A
10	A	1826	G
10	A	1829	G
10	A	1835	A
10	A	1839	U
10	A	1849	G
10	A	1851	MA6
10	A	1852	C
10	A	1861	G
10	A	1862	G
10	A	1863	A
10	A	1865	C
50	w	2	G
50	w	10	G
50	w	12	G
50	w	13	C
50	w	16	C

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Mol	Chain	Res	Type
50	w	19	G
50	w	20	A
50	w	21	A
50	w	35	A
50	w	48	C
50	w	49	G
50	w	56	C
50	w	58	A
50	w	68	C
50	w	70	G
50	w	72	U
50	w	73	A
50	w	74	C
50	w	75	C
50	w	76	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	7	-31	C
7	7	-21	A
7	7	13	A
10	A	1	U
10	A	291	G
10	A	368	U
10	A	606	G
10	A	644	OMG
10	A	688	U
10	A	694	G
10	A	716	G
10	A	731	G
10	A	797	C
10	A	912	C
10	A	1600	G
10	A	1836	G

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

29 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
10	OMC	A	174	10,54	19,22,23	3.20	8 (42%)	26,31,34	2.79	9 (34%)
10	OMC	A	1703	10	19,22,23	3.23	8 (42%)	26,31,34	2.83	9 (34%)
10	OMU	A	121	10	19,22,23	2.97	6 (31%)	26,31,34	1.73	5 (19%)
10	5MC	A	1374	10	18,22,23	0.62	0	26,32,35	0.56	0
10	A2M	A	159	10	22,25,26	3.90	10 (45%)	31,36,39	3.26	12 (38%)
10	A2M	A	166	10	22,25,26	3.91	11 (50%)	31,36,39	3.28	13 (41%)
10	PSU	A	822	10	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
10	OMG	A	509	10,54	23,26,27	2.54	8 (34%)	33,38,41	3.35	14 (42%)
10	PSU	A	1081	10	18,21,22	1.00	1 (5%)	22,30,33	1.74	3 (13%)
10	UR3	A	1830	10	19,22,23	2.77	8 (42%)	26,32,35	1.45	4 (15%)
10	A2M	A	668	10,54	22,25,26	3.90	11 (50%)	31,36,39	3.27	14 (45%)
10	OMG	A	644	10	23,26,27	2.34	6 (26%)	33,38,41	3.21	15 (45%)
10	6MZ	A	1832	10,54	22,25,26	2.34	6 (27%)	30,36,39	2.30	11 (36%)
10	PSU	A	612	10	18,21,22	1.00	1 (5%)	22,30,33	1.82	5 (22%)
10	PSU	A	119	10	18,21,22	1.00	1 (5%)	22,30,33	1.64	4 (18%)
10	OMC	A	517	10	19,22,23	2.95	8 (42%)	26,31,34	3.28	8 (30%)
10	MA6	A	1850	10	23,26,27	1.57	2 (8%)	34,38,41	3.05	11 (32%)
10	5MU	A	814	10	19,22,23	7.25	10 (52%)	28,32,35	3.91	19 (67%)
10	MA6	A	1851	10	23,26,27	1.56	2 (8%)	34,38,41	3.18	12 (35%)
10	PSU	A	823	10	18,21,22	1.12	1 (5%)	22,30,33	1.78	5 (22%)
10	A2M	A	484	10	22,25,26	3.86	12 (54%)	31,36,39	3.34	13 (41%)
10	OMU	A	116	10	19,22,23	2.98	6 (31%)	26,31,34	1.64	4 (15%)
10	PSU	A	1243	10	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
10	A2M	A	1031	10	22,25,26	3.98	10 (45%)	31,36,39	3.31	13 (41%)
10	OMG	A	683	10	23,26,27	1.27	3 (13%)	33,38,41	2.06	7 (21%)
10	A2M	A	27	10,54	22,25,26	3.89	11 (50%)	31,36,39	3.33	13 (41%)
10	A2M	A	1678	10,54	22,25,26	3.97	12 (54%)	31,36,39	3.38	13 (41%)
10	B8N	A	1248	10	24,29,30	3.02	6 (25%)	29,42,45	2.29	7 (24%)
10	JMH	A	1219	10	18,22,23	2.87	6 (33%)	21,32,35	1.62	4 (19%)

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
10	OMC	A	174	10,54	-	1/9/27/28	0/2/2/2
10	OMC	A	1703	10	-	2/9/27/28	0/2/2/2
10	OMU	A	121	10	-	0/9/27/28	0/2/2/2
10	5MC	A	1374	10	-	0/7/25/26	0/2/2/2
10	A2M	A	159	10	-	3/9/27/28	0/3/3/3
10	A2M	A	166	10	-	1/9/27/28	0/3/3/3
10	PSU	A	822	10	-	2/7/25/26	0/2/2/2
10	OMG	A	509	10,54	-	3/9/27/28	0/3/3/3
10	PSU	A	1081	10	-	1/7/25/26	0/2/2/2
10	UR3	A	1830	10	-	2/7/25/26	0/2/2/2
10	A2M	A	668	10,54	-	2/9/27/28	0/3/3/3
10	OMG	A	644	10	-	4/9/27/28	0/3/3/3
10	6MZ	A	1832	10,54	-	2/9/27/28	0/3/3/3
10	PSU	A	612	10	-	0/7/25/26	0/2/2/2
10	PSU	A	119	10	-	0/7/25/26	0/2/2/2
10	OMC	A	517	10	-	3/9/27/28	0/2/2/2
10	MA6	A	1850	10	-	1/11/29/30	0/3/3/3
10	5MU	A	814	10	-	0/7/25/26	0/2/2/2
10	MA6	A	1851	10	-	3/11/29/30	0/3/3/3
10	PSU	A	823	10	-	2/7/25/26	0/2/2/2
10	A2M	A	484	10	-	1/9/27/28	0/3/3/3
10	OMU	A	116	10	-	1/9/27/28	0/2/2/2
10	PSU	A	1243	10	-	0/7/25/26	0/2/2/2
10	A2M	A	1031	10	-	1/9/27/28	0/3/3/3
10	OMG	A	683	10	-	2/9/27/28	0/3/3/3
10	A2M	A	27	10,54	-	1/9/27/28	0/3/3/3
10	A2M	A	1678	10,54	-	1/9/27/28	0/3/3/3
10	B8N	A	1248	10	-	5/16/34/35	0/2/2/2
10	JMH	A	1219	10	-	2/7/25/26	0/2/2/2

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	814	5MU	C4-C5	20.88	1.79	1.44
10	A	814	5MU	C6-N1	15.31	1.64	1.38
10	A	1031	A2M	C3'-C2'	-13.11	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1678	A2M	C3'-C2'	-12.88	1.24	1.52
10	A	27	A2M	C3'-C2'	-12.84	1.24	1.52
10	A	166	A2M	C3'-C2'	-12.76	1.24	1.52
10	A	159	A2M	C3'-C2'	-12.68	1.24	1.52
10	A	484	A2M	C3'-C2'	-12.47	1.25	1.52
10	A	668	A2M	C3'-C2'	-12.42	1.25	1.52
10	A	814	5MU	C6-C5	-12.32	1.14	1.34
10	A	814	5MU	C4-N3	-11.30	1.17	1.38
10	A	1832	6MZ	C6-N6	8.70	1.43	1.34
10	A	1219	JMH	C2-N1	8.12	1.50	1.38
10	A	1248	B8N	C4-N3	-8.06	1.25	1.40
10	A	1248	B8N	C6-N1	7.40	1.54	1.36
10	A	1830	UR3	C2-N1	7.38	1.49	1.38
10	A	116	OMU	C2-N1	7.05	1.49	1.38
10	A	116	OMU	C2-N3	6.97	1.50	1.38
10	A	668	A2M	O4'-C4'	-6.95	1.29	1.45
10	A	121	OMU	C2-N3	6.95	1.50	1.38
10	A	121	OMU	C2-N1	6.85	1.49	1.38
10	A	1678	A2M	O4'-C4'	-6.74	1.29	1.45
10	A	509	OMG	C4-N3	6.69	1.50	1.34
10	A	1031	A2M	O4'-C4'	-6.59	1.30	1.45
10	A	159	A2M	O4'-C4'	-6.52	1.30	1.45
10	A	166	A2M	O4'-C4'	-6.40	1.30	1.45
10	A	484	A2M	O4'-C4'	-6.34	1.30	1.45
10	A	1703	OMC	C4-N4	6.30	1.48	1.33
10	A	27	A2M	O4'-C4'	-6.26	1.31	1.45
10	A	174	OMC	C4-N4	6.18	1.48	1.33
10	A	121	OMU	C6-C5	6.13	1.49	1.35
10	A	644	OMG	C4-N3	6.08	1.48	1.34
10	A	116	OMU	C6-C5	6.05	1.49	1.35
10	A	1830	UR3	C6-C5	6.01	1.49	1.35
10	A	1219	JMH	C6-C5	5.90	1.48	1.35
10	A	174	OMC	C2-N3	5.82	1.48	1.36
10	A	1703	OMC	C2-N3	5.63	1.47	1.36
10	A	517	OMC	C2-N3	5.47	1.47	1.36
10	A	1248	B8N	C6-C5	5.30	1.42	1.34
10	A	1219	JMH	C2-N3	5.17	1.49	1.39
10	A	509	OMG	C2-N3	5.15	1.45	1.33
10	A	1678	A2M	C3'-C4'	5.14	1.66	1.53
10	A	174	OMC	C2-N1	5.14	1.51	1.40
10	A	1703	OMC	C6-C5	5.12	1.46	1.35
10	A	174	OMC	C6-C5	5.10	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	517	OMC	C4-N4	5.08	1.45	1.33
10	A	484	A2M	C3'-C4'	5.08	1.66	1.53
10	A	1248	B8N	C2-N1	5.05	1.54	1.39
10	A	1830	UR3	C2-N3	5.03	1.48	1.39
10	A	509	OMG	C2-N2	5.01	1.46	1.34
10	A	1703	OMC	O2-C2	-4.99	1.14	1.23
10	A	1031	A2M	C3'-C4'	4.96	1.65	1.53
10	A	159	A2M	C3'-C4'	4.95	1.65	1.53
10	A	1850	MA6	C6-N6	4.92	1.51	1.36
10	A	1851	MA6	C6-N6	4.91	1.51	1.36
10	A	668	A2M	C3'-C4'	4.88	1.65	1.53
10	A	166	A2M	C3'-C4'	4.86	1.65	1.53
10	A	27	A2M	C3'-C4'	4.85	1.65	1.53
10	A	1703	OMC	C2-N1	4.82	1.50	1.40
10	A	517	OMC	C2-N1	4.77	1.50	1.40
10	A	517	OMC	C4-N3	4.74	1.44	1.34
10	A	174	OMC	O2-C2	-4.72	1.15	1.23
10	A	1678	A2M	C1'-N9	-4.61	1.33	1.46
10	A	644	OMG	C2-N2	4.60	1.45	1.34
10	A	174	OMC	C4-N3	4.57	1.43	1.34
10	A	644	OMG	C2-N3	4.55	1.44	1.33
10	A	1678	A2M	C6-N6	4.49	1.45	1.34
10	A	166	A2M	C6-N6	4.47	1.45	1.34
10	A	159	A2M	C6-N6	4.47	1.45	1.34
10	A	1031	A2M	C6-N6	4.47	1.45	1.34
10	A	484	A2M	C6-N6	4.47	1.45	1.34
10	A	27	A2M	C6-N6	4.44	1.45	1.34
10	A	668	A2M	C6-N6	4.43	1.45	1.34
10	A	1031	A2M	C1'-N9	-4.38	1.33	1.46
10	A	166	A2M	C1'-N9	-4.37	1.34	1.46
10	A	1703	OMC	C4-N3	4.33	1.43	1.34
10	A	517	OMC	O2-C2	-4.31	1.15	1.23
10	A	27	A2M	C1'-N9	-4.30	1.34	1.46
10	A	668	A2M	C1'-N9	-4.29	1.34	1.46
10	A	159	A2M	C1'-N9	-4.20	1.34	1.46
10	A	517	OMC	C6-C5	4.11	1.44	1.35
10	A	1031	A2M	O4'-C1'	4.09	1.51	1.42
10	A	484	A2M	C1'-N9	-4.07	1.34	1.46
10	A	814	5MU	C2-N3	4.07	1.45	1.38
10	A	159	A2M	O4'-C1'	4.05	1.51	1.42
10	A	116	OMU	C4-N3	4.01	1.45	1.38
10	A	121	OMU	C4-N3	4.00	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1678	A2M	O4'-C1'	3.98	1.51	1.42
10	A	27	A2M	O4'-C1'	3.95	1.51	1.42
10	A	166	A2M	O4'-C1'	3.95	1.51	1.42
10	A	484	A2M	O4'-C1'	3.93	1.51	1.42
10	A	1248	B8N	C1'-C5	3.77	1.58	1.50
10	A	644	OMG	C5-N7	-3.69	1.31	1.39
10	A	668	A2M	O4'-C1'	3.58	1.50	1.42
10	A	1248	B8N	O2-C2	-3.50	1.16	1.22
10	A	509	OMG	C5-N7	-3.47	1.32	1.39
10	A	484	A2M	O2'-C2'	3.45	1.51	1.42
10	A	1243	PSU	C6-C5	3.40	1.39	1.35
10	A	159	A2M	O2'-C2'	3.38	1.51	1.42
10	A	27	A2M	O2'-C2'	3.38	1.51	1.42
10	A	823	PSU	C6-C5	3.37	1.39	1.35
10	A	1678	A2M	O2'-C2'	3.35	1.51	1.42
10	A	668	A2M	O2'-C2'	3.32	1.51	1.42
10	A	119	PSU	C6-C5	3.31	1.39	1.35
10	A	166	A2M	O2'-C2'	3.31	1.51	1.42
10	A	1031	A2M	O2'-C2'	3.28	1.51	1.42
10	A	668	A2M	C2'-C1'	3.21	1.61	1.53
10	A	509	OMG	O6-C6	-3.15	1.17	1.23
10	A	1851	MA6	C5-C4	-3.14	1.33	1.39
10	A	1832	6MZ	C5-N7	-3.14	1.33	1.39
10	A	484	A2M	C2'-C1'	3.10	1.61	1.53
10	A	1850	MA6	C5-C4	-3.09	1.33	1.39
10	A	668	A2M	C5-C4	-3.09	1.33	1.39
10	A	822	PSU	C6-C5	3.07	1.38	1.35
10	A	27	A2M	C5-C4	-3.05	1.33	1.39
10	A	1031	A2M	C5-C4	-3.05	1.33	1.39
10	A	1081	PSU	C6-C5	3.04	1.38	1.35
10	A	166	A2M	C5-C4	-3.02	1.33	1.39
10	A	1678	A2M	C5-C4	-3.01	1.33	1.39
10	A	159	A2M	C2'-C1'	2.98	1.60	1.53
10	A	1830	UR3	C6-N1	2.95	1.45	1.38
10	A	166	A2M	C2'-C1'	2.94	1.60	1.53
10	A	1703	OMC	C5-C4	2.86	1.49	1.42
10	A	159	A2M	C5-C4	-2.85	1.33	1.39
10	A	174	OMC	C6-N1	2.83	1.44	1.38
10	A	612	PSU	C6-C5	2.82	1.38	1.35
10	A	644	OMG	O6-C6	-2.82	1.18	1.23
10	A	484	A2M	C5-C4	-2.80	1.33	1.39
10	A	683	OMG	C5-C4	2.80	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1031	A2M	C2'-C1'	2.79	1.60	1.53
10	A	1219	JMH	C6-N1	2.76	1.44	1.38
10	A	1703	OMC	C6-N1	2.76	1.44	1.38
10	A	484	A2M	C5-N7	-2.72	1.33	1.39
10	A	683	OMG	C6-N1	-2.72	1.33	1.38
10	A	174	OMC	C5-C4	2.71	1.49	1.42
10	A	166	A2M	C5-N7	-2.68	1.34	1.39
10	A	159	A2M	C5-N7	-2.66	1.34	1.39
10	A	668	A2M	C5-N7	-2.66	1.34	1.39
10	A	27	A2M	C2'-C1'	2.66	1.59	1.53
10	A	27	A2M	C5-N7	-2.62	1.34	1.39
10	A	1832	6MZ	C6-N1	-2.59	1.30	1.35
10	A	517	OMC	C6-N1	2.57	1.44	1.38
10	A	1832	6MZ	C5-C4	-2.56	1.34	1.39
10	A	1031	A2M	C5-N7	-2.56	1.34	1.39
10	A	121	OMU	C6-N1	2.56	1.44	1.38
10	A	1678	A2M	C5-N7	-2.50	1.34	1.39
10	A	116	OMU	C6-N1	2.49	1.44	1.38
10	A	1219	JMH	C5-C4	2.47	1.48	1.42
10	A	509	OMG	C5-C6	2.43	1.53	1.44
10	A	814	5MU	O2-C2	-2.40	1.18	1.23
10	A	1832	6MZ	C9-N6	-2.38	1.41	1.45
10	A	683	OMG	C5-N7	-2.38	1.34	1.39
10	A	814	5MU	O4-C4	-2.36	1.19	1.23
10	A	1678	A2M	C2'-C1'	2.36	1.59	1.53
10	A	1830	UR3	O4-C4	-2.24	1.18	1.23
10	A	121	OMU	C5-C4	2.22	1.48	1.43
10	A	509	OMG	O2'-C2'	-2.20	1.37	1.42
10	A	517	OMC	C5-C4	2.20	1.48	1.42
10	A	1830	UR3	C5-C4	2.18	1.49	1.43
10	A	1830	UR3	O2-C2	-2.18	1.18	1.22
10	A	484	A2M	O3'-C3'	2.16	1.48	1.43
10	A	644	OMG	C5-C6	2.15	1.52	1.44
10	A	1678	A2M	C8-N9	-2.13	1.33	1.37
10	A	116	OMU	C5-C4	2.12	1.48	1.43
10	A	166	A2M	O3'-C3'	2.10	1.47	1.43
10	A	1830	UR3	C4-N3	2.08	1.45	1.40
10	A	814	5MU	C2-N1	2.08	1.41	1.38
10	A	668	A2M	C8-N9	-2.07	1.33	1.37
10	A	509	OMG	C2-N1	2.06	1.42	1.37
10	A	1219	JMH	O2-C2	-2.05	1.18	1.22
10	A	27	A2M	C8-N9	-2.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1832	6MZ	C8-N9	-2.03	1.33	1.37
10	A	484	A2M	C8-N9	-2.03	1.33	1.37
10	A	814	5MU	C2'-C1'	-2.02	1.47	1.53
10	A	1678	A2M	O3'-C3'	2.02	1.47	1.43
10	A	814	5MU	O2'-C2'	-2.00	1.38	1.43

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1851	MA6	N1-C6-N6	-12.41	103.51	117.08
10	A	1850	MA6	N1-C6-N6	-11.60	104.40	117.08
10	A	814	5MU	C5-C4-N3	10.31	124.11	115.31
10	A	1678	A2M	C1'-N9-C8	-9.25	106.25	127.14
10	A	484	A2M	C1'-N9-C8	-8.77	107.33	127.14
10	A	1031	A2M	C1'-N9-C8	-8.76	107.34	127.14
10	A	27	A2M	C1'-N9-C8	-8.58	107.77	127.14
10	A	668	A2M	C1'-N9-C8	-8.57	107.78	127.14
10	A	814	5MU	C5-C6-N1	-8.54	114.55	123.34
10	A	159	A2M	C1'-N9-C8	-8.50	107.94	127.14
10	A	166	A2M	C1'-N9-C8	-8.39	108.18	127.14
10	A	509	OMG	C1'-N9-C8	-8.01	103.89	126.70
10	A	517	OMC	C1'-N1-C6	-7.97	103.46	120.84
10	A	644	OMG	C1'-N9-C8	-7.90	104.20	126.70
10	A	509	OMG	C1'-N9-C4	7.87	149.88	126.50
10	A	484	A2M	C4-N9-C1'	7.80	145.17	126.59
10	A	644	OMG	C1'-N9-C4	7.76	149.55	126.50
10	A	1678	A2M	C4-N9-C1'	7.56	144.61	126.59
10	A	517	OMC	C1'-N1-C2	7.54	135.24	118.42
10	A	1031	A2M	C4-N9-C1'	7.41	144.25	126.59
10	A	509	OMG	C5-C4-N3	-7.38	116.49	128.46
10	A	668	A2M	C4-N9-C1'	7.34	144.09	126.59
10	A	159	A2M	C4-N9-C1'	7.34	144.09	126.59
10	A	27	A2M	C4-N9-C1'	7.28	143.93	126.59
10	A	166	A2M	C4-N9-C1'	7.05	143.39	126.59
10	A	1703	OMC	CM2-O2'-C2'	6.93	132.71	114.52
10	A	814	5MU	C4-N3-C2	-6.92	118.39	127.35
10	A	174	OMC	O2'-C2'-C1'	6.81	122.37	109.08
10	A	517	OMC	O2'-C2'-C1'	6.80	122.35	109.08
10	A	1851	MA6	C5-C6-N6	6.56	136.72	125.30
10	A	644	OMG	C5-C4-N3	-6.40	118.08	128.46
10	A	1248	B8N	C32-C31-N3	6.40	123.99	112.00
10	A	1850	MA6	C5-C6-N6	6.17	136.05	125.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	517	OMC	O3'-C3'-C4'	6.14	128.80	111.05
10	A	174	OMC	C1'-N1-C2	6.14	132.11	118.42
10	A	509	OMG	C2-N3-C4	6.12	123.21	112.30
10	A	1703	OMC	O2'-C2'-C1'	6.06	120.89	109.08
10	A	683	OMG	C5-C4-N3	-5.85	118.97	128.46
10	A	166	A2M	N3-C2-N1	-5.81	119.51	128.60
10	A	1832	6MZ	N1-C2-N3	-5.80	119.53	128.60
10	A	644	OMG	O3'-C3'-C4'	5.72	127.59	111.05
10	A	644	OMG	O2'-C2'-C1'	5.70	120.21	109.08
10	A	668	A2M	N6-C6-N1	-5.70	105.88	118.35
10	A	27	A2M	N3-C2-N1	-5.68	119.72	128.60
10	A	1678	A2M	N3-C2-N1	-5.67	119.72	128.60
10	A	159	A2M	N3-C2-N1	-5.66	119.74	128.60
10	A	1031	A2M	N6-C6-N1	-5.66	105.95	118.35
10	A	1703	OMC	C1'-N1-C2	5.63	130.97	118.42
10	A	484	A2M	N6-C6-N1	-5.58	106.12	118.35
10	A	1031	A2M	N3-C2-N1	-5.55	119.92	128.60
10	A	1851	MA6	N1-C2-N3	-5.53	119.96	128.60
10	A	159	A2M	N6-C6-N1	-5.52	106.25	118.35
10	A	1678	A2M	N6-C6-N1	-5.52	106.26	118.35
10	A	166	A2M	N6-C6-N1	-5.51	106.28	118.35
10	A	484	A2M	N3-C2-N1	-5.48	120.03	128.60
10	A	27	A2M	N6-C6-N1	-5.45	106.42	118.35
10	A	668	A2M	N3-C2-N1	-5.43	120.11	128.60
10	A	509	OMG	O2'-C2'-C1'	5.42	119.66	109.08
10	A	121	OMU	C4-N3-C2	-5.36	119.51	126.58
10	A	484	A2M	C5-C4-N3	-5.32	119.81	126.75
10	A	1850	MA6	N1-C2-N3	-5.30	120.32	128.60
10	A	1248	B8N	C5-C4-N3	5.28	125.95	116.17
10	A	644	OMG	C2-N3-C4	5.27	121.68	112.30
10	A	814	5MU	O3'-C3'-C4'	5.18	126.03	111.05
10	A	1248	B8N	C4-N3-C2	-5.14	118.96	125.46
10	A	517	OMC	CM2-O2'-C2'	5.07	127.83	114.52
10	A	27	A2M	C5-C4-N3	-5.02	120.20	126.75
10	A	116	OMU	C4-N3-C2	-5.00	119.99	126.58
10	A	1832	6MZ	C5-C4-N3	-4.95	120.29	126.75
10	A	174	OMC	O3'-C3'-C4'	4.94	125.34	111.05
10	A	668	A2M	C5-C4-N3	-4.94	120.31	126.75
10	A	668	A2M	C5-C6-N6	4.93	134.16	123.43
10	A	1678	A2M	N9-C8-N7	-4.91	107.20	113.91
10	A	159	A2M	C5-C4-N3	-4.89	120.37	126.75
10	A	1031	A2M	C5-C6-N6	4.89	134.07	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	174	OMC	C1'-N1-C6	-4.88	110.21	120.84
10	A	509	OMG	N9-C4-N3	4.87	135.72	125.94
10	A	1219	JMH	C1'-N1-C2	4.86	125.20	116.99
10	A	814	5MU	C5M-C5-C6	-4.83	116.41	122.85
10	A	1031	A2M	C5-C4-N3	-4.80	120.48	126.75
10	A	484	A2M	C5-C6-N6	4.79	133.86	123.43
10	A	166	A2M	C5-C6-N6	4.79	133.86	123.43
10	A	159	A2M	C5-C6-N6	4.78	133.83	123.43
10	A	1678	A2M	C5-C6-N6	4.77	133.81	123.43
10	A	1851	MA6	N9-C8-N7	-4.76	107.40	113.91
10	A	823	PSU	C4-N3-C2	-4.75	119.49	126.34
10	A	166	A2M	C5-C4-N3	-4.75	120.55	126.75
10	A	1243	PSU	N1-C2-N3	4.73	120.49	115.13
10	A	822	PSU	C4-N3-C2	-4.71	119.55	126.34
10	A	27	A2M	O4'-C1'-N9	4.70	117.33	108.06
10	A	1850	MA6	C5-C4-N3	-4.69	120.63	126.75
10	A	509	OMG	O3'-C3'-C4'	4.69	124.61	111.05
10	A	683	OMG	C2-N3-C4	4.69	120.65	112.30
10	A	166	A2M	N9-C8-N7	-4.66	107.54	113.91
10	A	1678	A2M	C5-C4-N3	-4.63	120.71	126.75
10	A	822	PSU	N1-C2-N3	4.61	120.36	115.13
10	A	1031	A2M	N9-C8-N7	-4.59	107.63	113.91
10	A	27	A2M	C5-C6-N6	4.59	133.41	123.43
10	A	1703	OMC	O3'-C3'-C4'	4.58	124.30	111.05
10	A	1081	PSU	C4-N3-C2	-4.58	119.74	126.34
10	A	612	PSU	C4-N3-C2	-4.57	119.76	126.34
10	A	1851	MA6	C5-C4-N3	-4.56	120.80	126.75
10	A	1243	PSU	C4-N3-C2	-4.56	119.77	126.34
10	A	612	PSU	N1-C2-N3	4.54	120.27	115.13
10	A	683	OMG	N9-C4-N3	4.52	135.01	125.94
10	A	1832	6MZ	N9-C8-N7	-4.51	107.74	113.91
10	A	27	A2M	N9-C8-N7	-4.50	107.75	113.91
10	A	1830	UR3	C4-N3-C2	-4.50	120.33	124.56
10	A	1850	MA6	N9-C8-N7	-4.49	107.77	113.91
10	A	823	PSU	N1-C2-N3	4.47	120.19	115.13
10	A	1081	PSU	N1-C2-N3	4.41	120.12	115.13
10	A	668	A2M	N9-C8-N7	-4.32	108.00	113.91
10	A	814	5MU	O4'-C1'-N1	4.31	118.21	108.36
10	A	159	A2M	N9-C8-N7	-4.27	108.07	113.91
10	A	119	PSU	N1-C2-N3	4.26	119.96	115.13
10	A	1703	OMC	C1'-N1-C6	-4.24	111.60	120.84
10	A	166	A2M	O4'-C1'-N9	4.21	116.35	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	814	5MU	C5M-C5-C4	4.18	123.37	118.77
10	A	119	PSU	C4-N3-C2	-4.11	120.41	126.34
10	A	484	A2M	N9-C8-N7	-3.91	108.57	113.91
10	A	484	A2M	O4'-C1'-N9	3.91	115.76	108.06
10	A	121	OMU	N3-C2-N1	3.89	120.05	114.89
10	A	1678	A2M	O4'-C1'-N9	3.87	115.69	108.06
10	A	814	5MU	O4-C4-C5	-3.83	120.47	124.90
10	A	814	5MU	N3-C2-N1	3.80	119.93	114.89
10	A	1031	A2M	O4'-C1'-N9	3.75	115.45	108.06
10	A	116	OMU	N3-C2-N1	3.71	119.82	114.89
10	A	174	OMC	CM2-O2'-C2'	3.70	124.24	114.52
10	A	644	OMG	N9-C4-N3	3.68	133.33	125.94
10	A	159	A2M	O4'-C1'-N9	3.68	115.31	108.06
10	A	1248	B8N	C31-N3-C4	3.67	122.72	117.31
10	A	1851	MA6	C2-N1-C6	3.65	120.38	111.75
10	A	1832	6MZ	C2-N3-C4	3.61	120.27	111.75
10	A	1850	MA6	C4-C5-C6	3.61	119.92	115.88
10	A	814	5MU	O2-C2-N1	-3.57	118.04	122.79
10	A	1850	MA6	C2-N1-C6	3.56	120.17	111.75
10	A	484	A2M	C2-N3-C4	3.54	120.12	111.75
10	A	27	A2M	C2-N3-C4	3.54	120.10	111.75
10	A	1219	JMH	C6-N1-C2	-3.49	118.66	121.79
10	A	509	OMG	O3'-C3'-C2'	3.49	121.08	111.17
10	A	1248	B8N	N3-C2-N1	3.47	121.66	116.76
10	A	159	A2M	C2-N3-C4	3.46	119.93	111.75
10	A	166	A2M	C2-N3-C4	3.46	119.91	111.75
10	A	1832	6MZ	C5-N7-C8	3.45	108.41	103.51
10	A	1678	A2M	C2-N3-C4	3.40	119.79	111.75
10	A	683	OMG	C2'-C1'-N9	-3.39	107.64	114.22
10	A	644	OMG	O3'-C3'-C2'	3.39	120.80	111.17
10	A	121	OMU	C5-C4-N3	3.38	119.90	114.84
10	A	1703	OMC	C5'-C4'-C3'	3.38	127.85	115.18
10	A	1031	A2M	C2-N3-C4	3.37	119.72	111.75
10	A	1851	MA6	C2-N3-C4	3.37	119.71	111.75
10	A	668	A2M	C2-N3-C4	3.36	119.69	111.75
10	A	1830	UR3	C1'-N1-C2	3.33	122.60	116.99
10	A	174	OMC	C2'-C1'-N1	3.32	120.67	114.22
10	A	1850	MA6	C2-N3-C4	3.25	119.43	111.75
10	A	1703	OMC	O2-C2-N3	-3.24	117.06	122.33
10	A	509	OMG	C2-N1-C6	-3.24	119.19	125.10
10	A	1678	A2M	C5-N7-C8	3.22	108.08	103.51
10	A	116	OMU	C5-C4-N3	3.22	119.66	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1219	JMH	O2-C2-N3	-3.21	116.82	121.34
10	A	166	A2M	C5-N7-C8	3.18	108.02	103.51
10	A	683	OMG	C6-C5-N7	3.15	136.11	130.25
10	A	174	OMC	C5'-C4'-C3'	3.14	126.95	115.18
10	A	1851	MA6	C4-C5-C6	3.14	119.39	115.88
10	A	517	OMC	C5-C4-N4	-3.13	115.64	120.57
10	A	509	OMG	C5'-C4'-C3'	3.13	126.91	115.18
10	A	1851	MA6	C5-N7-C8	3.13	107.95	103.51
10	A	1832	6MZ	C4-N9-C1'	-3.12	119.16	126.59
10	A	1031	A2M	C5-N7-C8	3.12	107.94	103.51
10	A	668	A2M	C2'-C1'-N9	3.09	118.74	113.53
10	A	27	A2M	C5-N7-C8	3.09	107.90	103.51
10	A	1678	A2M	C4-N9-C8	3.07	109.06	105.73
10	A	484	A2M	N3-C4-N9	3.07	132.15	127.08
10	A	509	OMG	C5-C6-N1	3.07	120.98	113.19
10	A	27	A2M	N3-C4-N9	3.03	132.07	127.08
10	A	159	A2M	C5-N7-C8	3.01	107.78	103.51
10	A	1850	MA6	C5-N7-C8	2.98	107.75	103.51
10	A	668	A2M	C5-N7-C8	2.98	107.74	103.51
10	A	612	PSU	O2-C2-N1	-2.95	119.54	122.79
10	A	1678	A2M	N3-C4-N9	2.93	131.92	127.08
10	A	814	5MU	C1'-N1-C6	-2.93	116.25	121.12
10	A	1248	B8N	O4-C4-N3	-2.91	115.03	119.98
10	A	644	OMG	O5'-C5'-C4'	2.91	118.89	108.99
10	A	517	OMC	C5'-C4'-C3'	2.90	126.04	115.18
10	A	484	A2M	C5-N7-C8	2.90	107.62	103.51
10	A	814	5MU	O2'-C2'-C3'	2.90	121.19	111.82
10	A	668	A2M	N3-C4-N9	2.88	131.82	127.08
10	A	174	OMC	O3'-C3'-C2'	2.87	119.33	111.17
10	A	166	A2M	N3-C4-N9	2.87	131.82	127.08
10	A	159	A2M	N3-C4-N9	2.86	131.80	127.08
10	A	1851	MA6	C4-N9-C8	2.84	108.80	105.73
10	A	1832	6MZ	C4-C5-C6	2.81	118.99	116.81
10	A	1850	MA6	N3-C4-N9	2.81	131.72	127.08
10	A	1031	A2M	N3-C4-N9	2.81	131.71	127.08
10	A	1703	OMC	C2'-C1'-N1	2.77	119.61	114.22
10	A	121	OMU	O4-C4-C5	-2.76	120.30	125.16
10	A	174	OMC	O2-C2-N3	-2.76	117.84	122.33
10	A	116	OMU	O4-C4-C5	-2.74	120.34	125.16
10	A	517	OMC	O2-C2-N1	2.71	124.50	118.89
10	A	814	5MU	O3'-C3'-C2'	2.68	120.50	111.82
10	A	1850	MA6	C4-N9-C8	2.68	108.63	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	822	PSU	O2-C2-N1	-2.68	119.84	122.79
10	A	1851	MA6	N3-C4-N9	2.62	131.40	127.08
10	A	1832	6MZ	C1'-N9-C8	2.60	133.00	127.14
10	A	814	5MU	C5'-C4'-C3'	2.60	124.92	115.18
10	A	1832	6MZ	N3-C4-N9	2.58	131.33	127.08
10	A	814	5MU	C6-C5-C4	2.57	120.18	118.03
10	A	1243	PSU	O2-C2-N1	-2.52	120.02	122.79
10	A	119	PSU	O2-C2-N1	-2.51	120.03	122.79
10	A	814	5MU	O2'-C2'-C1'	2.50	118.37	110.02
10	A	166	A2M	C4-N9-C8	2.49	108.43	105.73
10	A	119	PSU	C6-N1-C2	-2.48	120.15	122.68
10	A	1031	A2M	C4-N9-C8	2.46	108.40	105.73
10	A	814	5MU	O4-C4-N3	-2.45	115.42	120.12
10	A	683	OMG	C4-C5-N7	-2.44	106.86	110.72
10	A	1832	6MZ	C4-C5-N7	-2.44	107.65	110.62
10	A	668	A2M	C3'-C2'-C1'	2.43	107.45	102.89
10	A	823	PSU	O2-C2-N1	-2.42	120.13	122.79
10	A	1678	A2M	C4'-O4'-C1'	-2.41	104.17	109.47
10	A	1830	UR3	C6-N1-C2	-2.39	119.65	121.79
10	A	27	A2M	C4-N9-C8	2.38	108.30	105.73
10	A	644	OMG	C2-N1-C6	-2.37	120.77	125.10
10	A	484	A2M	C3'-C2'-C1'	2.34	107.29	102.89
10	A	668	A2M	C4'-O4'-C1'	-2.33	104.33	109.47
10	A	1031	A2M	C4'-O4'-C1'	-2.30	104.39	109.47
10	A	822	PSU	O4'-C1'-C2'	2.30	108.39	105.14
10	A	27	A2M	O4'-C1'-C2'	-2.30	102.53	106.57
10	A	121	OMU	O2-C2-N1	-2.30	119.73	122.79
10	A	1243	PSU	C6-N1-C2	-2.29	120.34	122.68
10	A	644	OMG	C5-C6-N1	2.29	119.00	113.19
10	A	509	OMG	N1-C2-N3	-2.28	119.06	123.32
10	A	612	PSU	C6-N1-C2	-2.28	120.35	122.68
10	A	644	OMG	O6-C6-C5	-2.28	120.56	126.60
10	A	1081	PSU	O2-C2-N1	-2.28	120.29	122.79
10	A	1703	OMC	O3'-C3'-C2'	2.26	117.57	111.17
10	A	683	OMG	O6-C6-C5	-2.25	120.64	126.60
10	A	1832	6MZ	C5-C4-N9	2.23	108.38	105.78
10	A	1248	B8N	C32-C33-C34	-2.23	104.99	110.30
10	A	823	PSU	C6-N1-C2	-2.22	120.41	122.68
10	A	644	OMG	N1-C2-N3	-2.19	119.23	123.32
10	A	644	OMG	N2-C2-N1	2.18	121.35	116.71
10	A	822	PSU	C6-N1-C2	-2.17	120.47	122.68
10	A	814	5MU	C3'-C2'-C1'	2.17	105.55	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	814	5MU	O5'-C5'-C4'	-2.17	101.63	108.99
10	A	668	A2M	C4-N9-C8	2.16	108.07	105.73
10	A	509	OMG	O6-C6-C5	-2.16	120.86	126.60
10	A	1219	JMH	C1'-N1-C6	-2.16	116.14	120.84
10	A	509	OMG	O4'-C1'-N9	2.15	113.28	108.36
10	A	612	PSU	O4'-C1'-C2'	2.13	108.15	105.14
10	A	1851	MA6	C4-C5-N7	-2.11	108.05	110.62
10	A	484	A2M	C6-C5-C4	2.10	120.00	117.18
10	A	1830	UR3	O2-C2-N3	-2.10	118.39	121.34
10	A	159	A2M	C4-N9-C8	2.07	107.97	105.73
10	A	644	OMG	C5'-C4'-C3'	2.05	122.88	115.18
10	A	823	PSU	O4'-C1'-C2'	2.05	108.04	105.14
10	A	166	A2M	C4'-O4'-C1'	-2.03	105.00	109.47

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	27	A2M	C1'-C2'-O2'-CM'
10	A	116	OMU	C1'-C2'-O2'-CM2
10	A	159	A2M	C1'-C2'-O2'-CM'
10	A	166	A2M	C1'-C2'-O2'-CM'
10	A	174	OMC	C1'-C2'-O2'-CM2
10	A	484	A2M	C1'-C2'-O2'-CM'
10	A	509	OMG	C1'-C2'-O2'-CM2
10	A	517	OMC	C1'-C2'-O2'-CM2
10	A	644	OMG	C3'-C4'-C5'-O5'
10	A	644	OMG	C1'-C2'-O2'-CM2
10	A	1031	A2M	C1'-C2'-O2'-CM'
10	A	1678	A2M	C1'-C2'-O2'-CM'
10	A	1832	6MZ	N1-C6-N6-C9
10	A	1851	MA6	O4'-C4'-C5'-O5'
10	A	1248	B8N	N34-C33-C34-O35
10	A	1248	B8N	C31-C32-C33-C34
10	A	1248	B8N	C31-C32-C33-N34
10	A	1830	UR3	O4'-C1'-N1-C2
10	A	668	A2M	O4'-C4'-C5'-O5'
10	A	668	A2M	C3'-C4'-C5'-O5'
10	A	683	OMG	O4'-C4'-C5'-O5'
10	A	1851	MA6	C3'-C4'-C5'-O5'
10	A	159	A2M	C3'-C4'-C5'-O5'
10	A	517	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	A	517	OMC	O4'-C4'-C5'-O5'
10	A	644	OMG	O4'-C4'-C5'-O5'
10	A	683	OMG	C3'-C4'-C5'-O5'
10	A	1830	UR3	O4'-C1'-N1-C6
10	A	1248	B8N	N34-C33-C34-O36
10	A	1703	OMC	C3'-C4'-C5'-O5'
10	A	822	PSU	C3'-C4'-C5'-O5'
10	A	644	OMG	C4'-C5'-O5'-P
10	A	509	OMG	C3'-C4'-C5'-O5'
10	A	822	PSU	O4'-C4'-C5'-O5'
10	A	1703	OMC	O4'-C4'-C5'-O5'
10	A	1850	MA6	C5-C6-N6-C10
10	A	1832	6MZ	C5-C6-N6-C9
10	A	1081	PSU	C4'-C5'-O5'-P
10	A	1851	MA6	C4'-C5'-O5'-P
10	A	823	PSU	O4'-C1'-C5-C4
10	A	159	A2M	O4'-C4'-C5'-O5'
10	A	509	OMG	O4'-C4'-C5'-O5'
10	A	1248	B8N	C32-C33-C34-O36
10	A	823	PSU	O4'-C1'-C5-C6
10	A	1219	JMH	C2'-C1'-N1-C2
10	A	1219	JMH	C2'-C1'-N1-C6

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	174	OMC	1	0
10	A	1703	OMC	2	0
10	A	159	A2M	1	0
10	A	166	A2M	1	0
10	A	509	OMG	5	0
10	A	644	OMG	3	0
10	A	517	OMC	3	0
10	A	1850	MA6	1	0
10	A	814	5MU	2	0
10	A	1851	MA6	1	0
10	A	484	A2M	1	0
10	A	116	OMU	1	0
10	A	683	OMG	1	0
10	A	27	A2M	2	0
10	A	1678	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 89 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

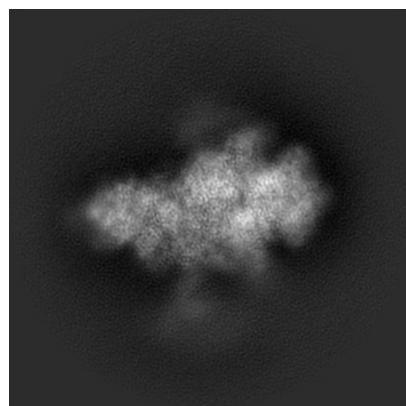
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17697. These allow visual inspection of the internal detail of the map and identification of artifacts.

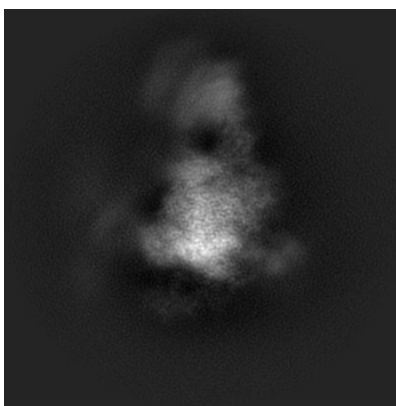
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

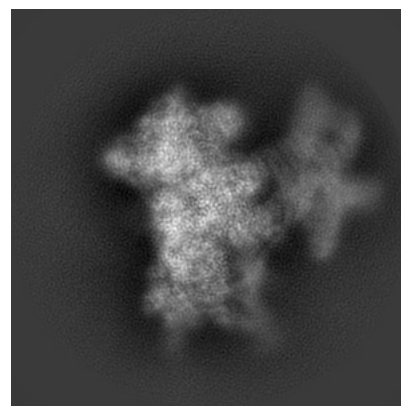
6.1.1 Primary map



X

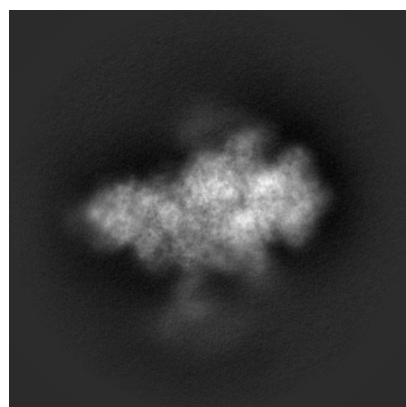


Y

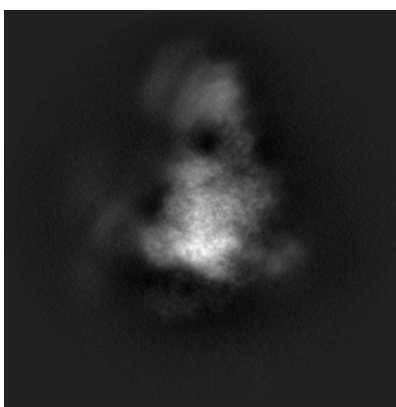


Z

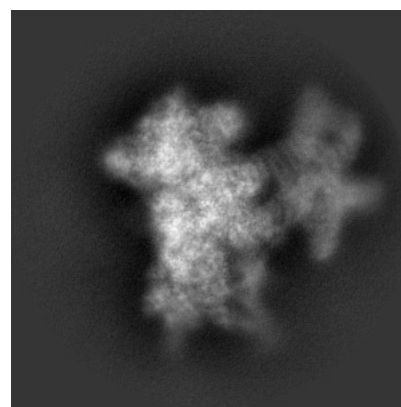
6.1.2 Raw map



X



Y

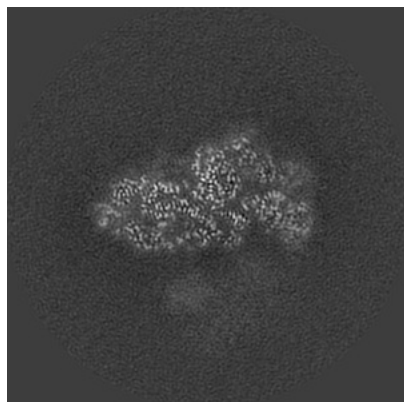


Z

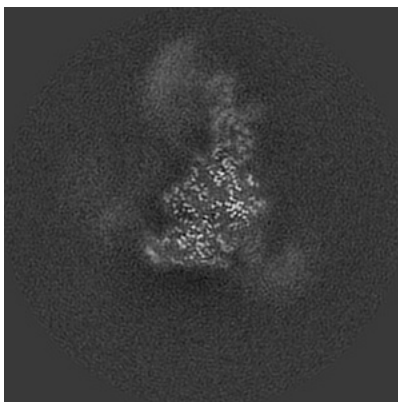
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

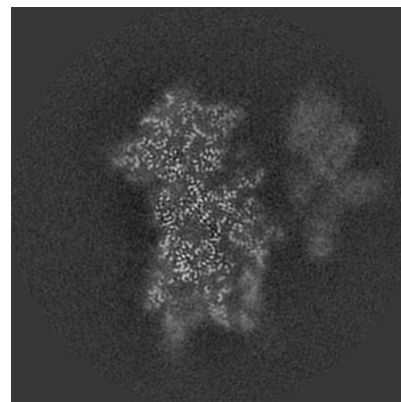
6.2.1 Primary map



X Index: 216

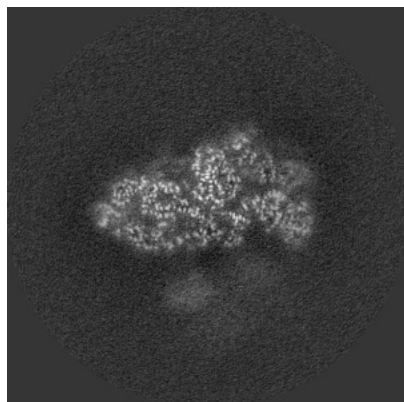


Y Index: 216

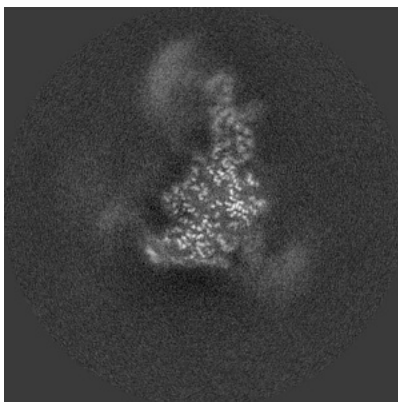


Z Index: 216

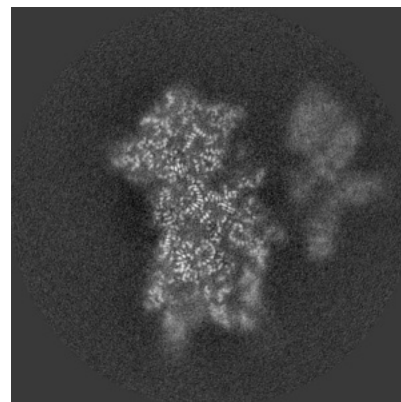
6.2.2 Raw map



X Index: 180



Y Index: 180

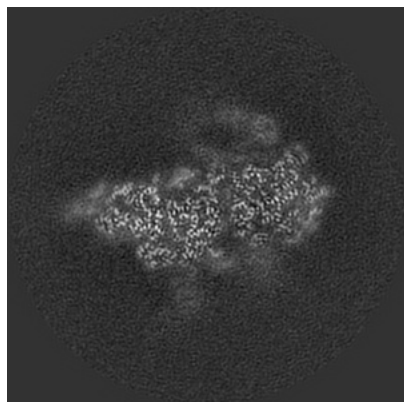


Z Index: 180

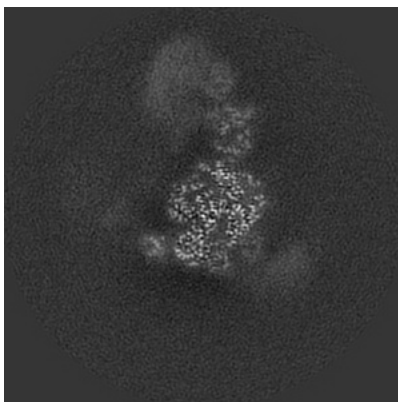
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

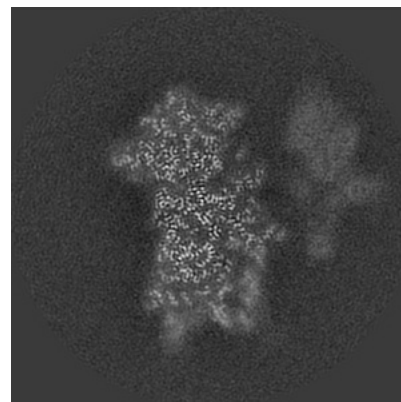
6.3.1 Primary map



X Index: 176

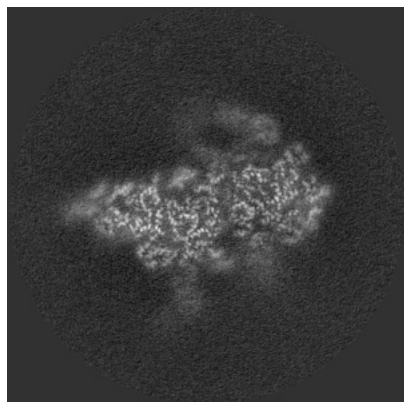


Y Index: 222

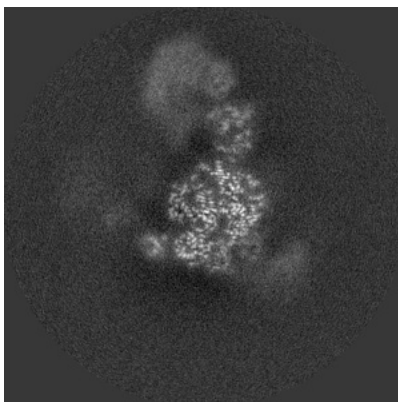


Z Index: 214

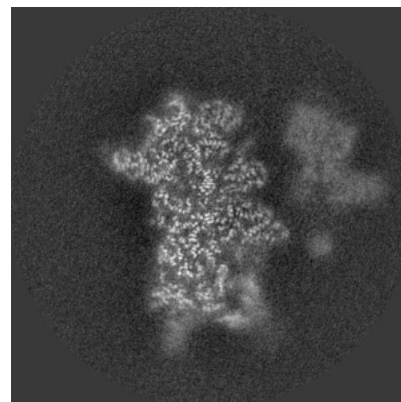
6.3.2 Raw map



X Index: 147



Y Index: 186

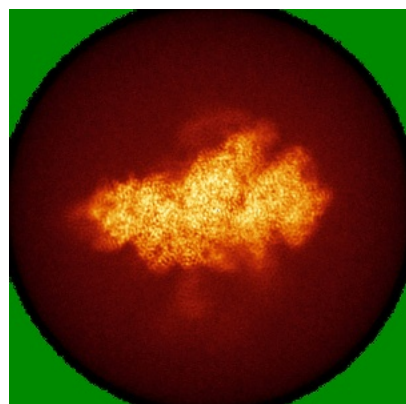


Z Index: 173

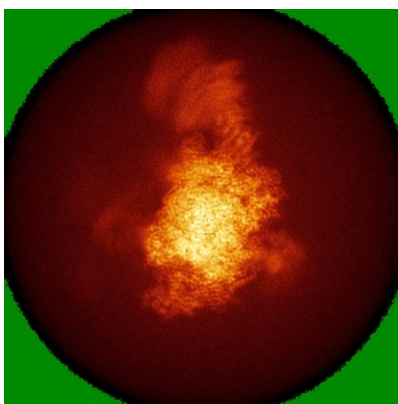
The images above show the largest variance slices of the map in three orthogonal directions.

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

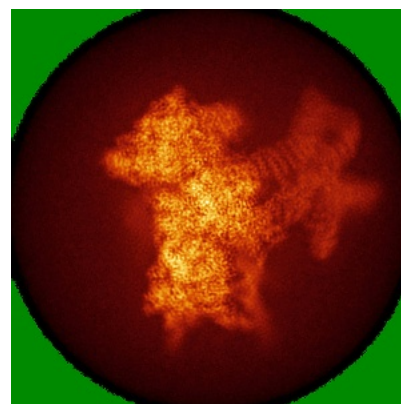
6.4.1 Primary map



X

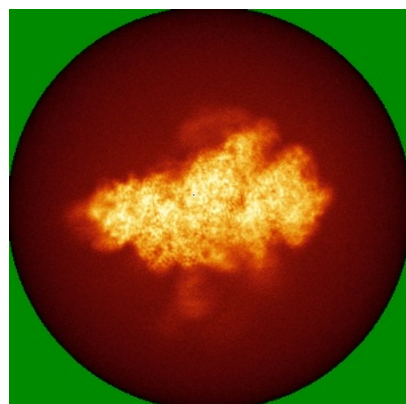


Y

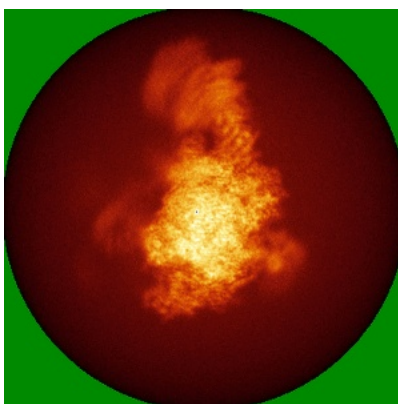


Z

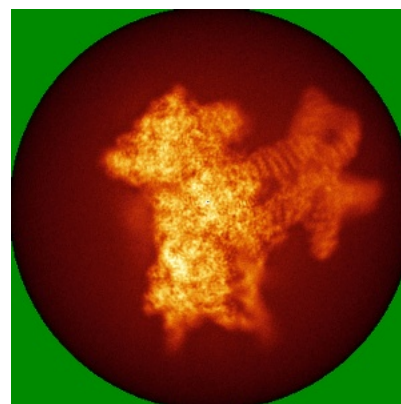
6.4.2 Raw map



X



Y

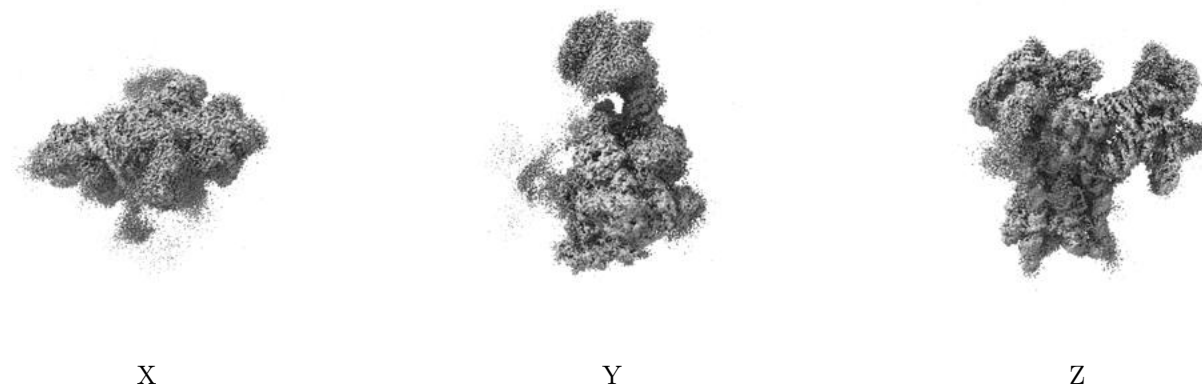


Z

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.

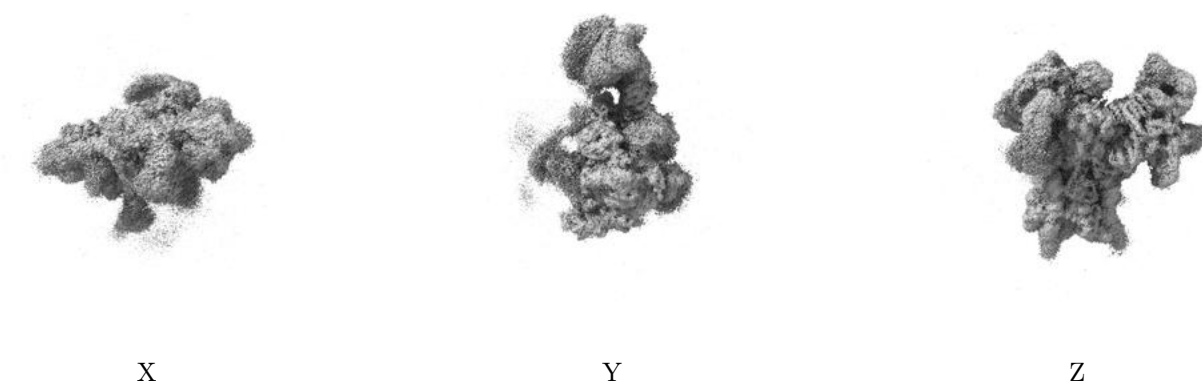
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

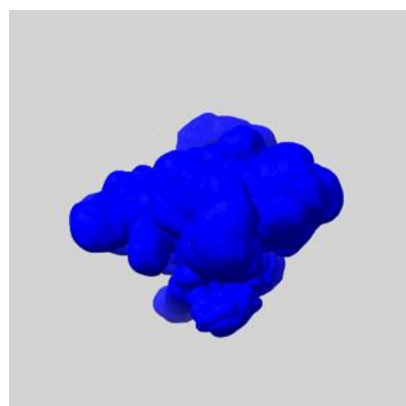
6.6 Mask visualisation [i](#)

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

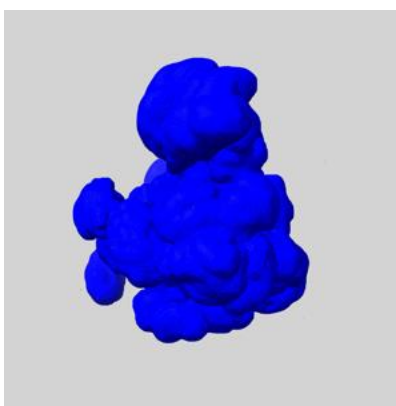
A mask typically either:

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

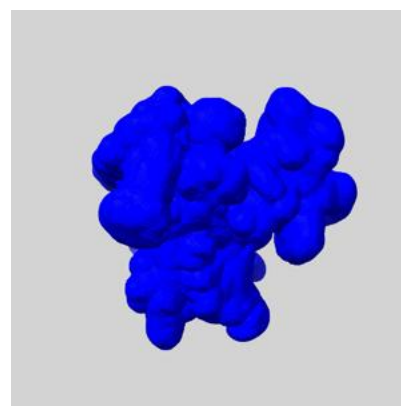
6.6.1 emd_17697_msk_1.map [i](#)



X



Y

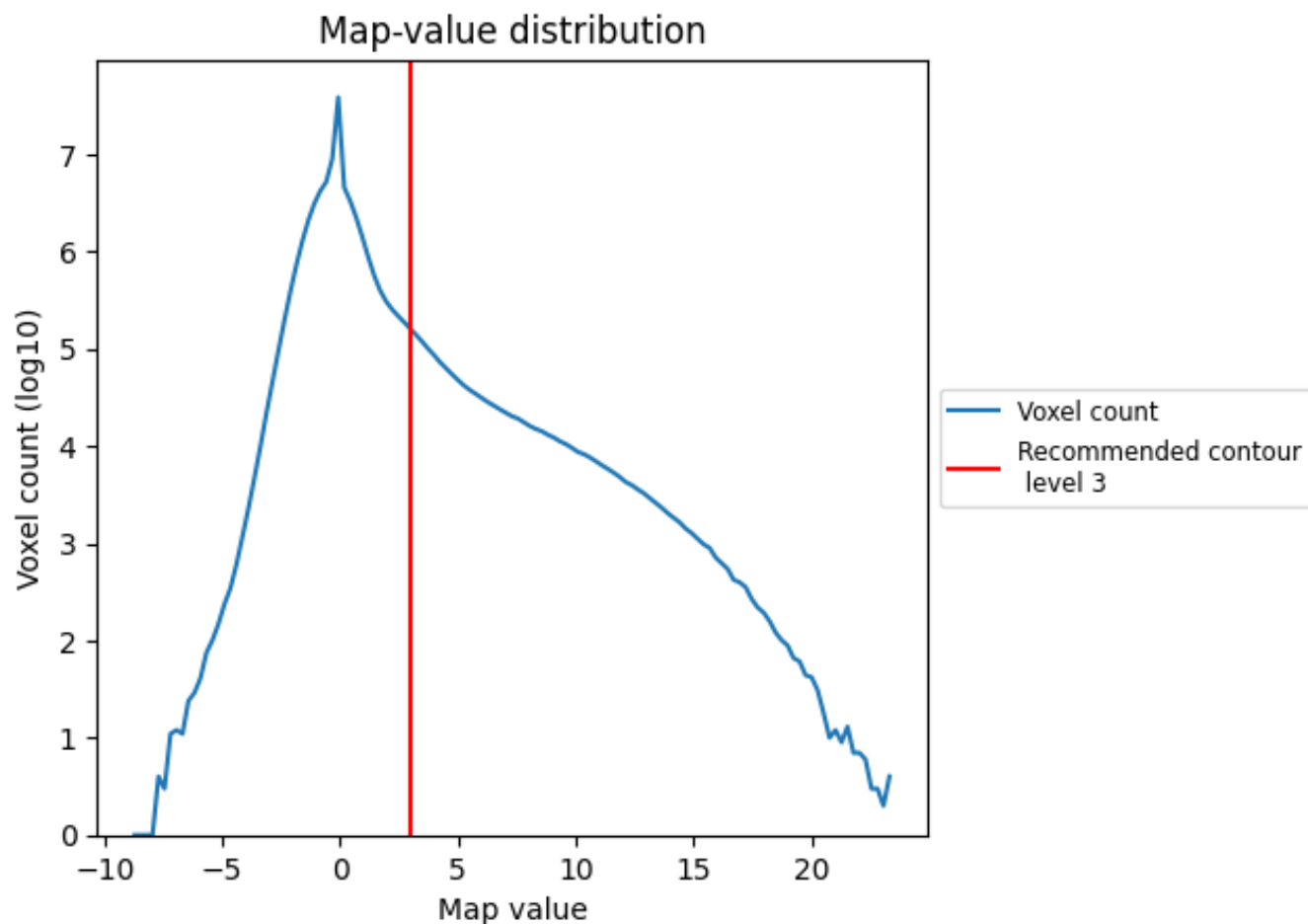


Z

7 Map analysis [i](#)

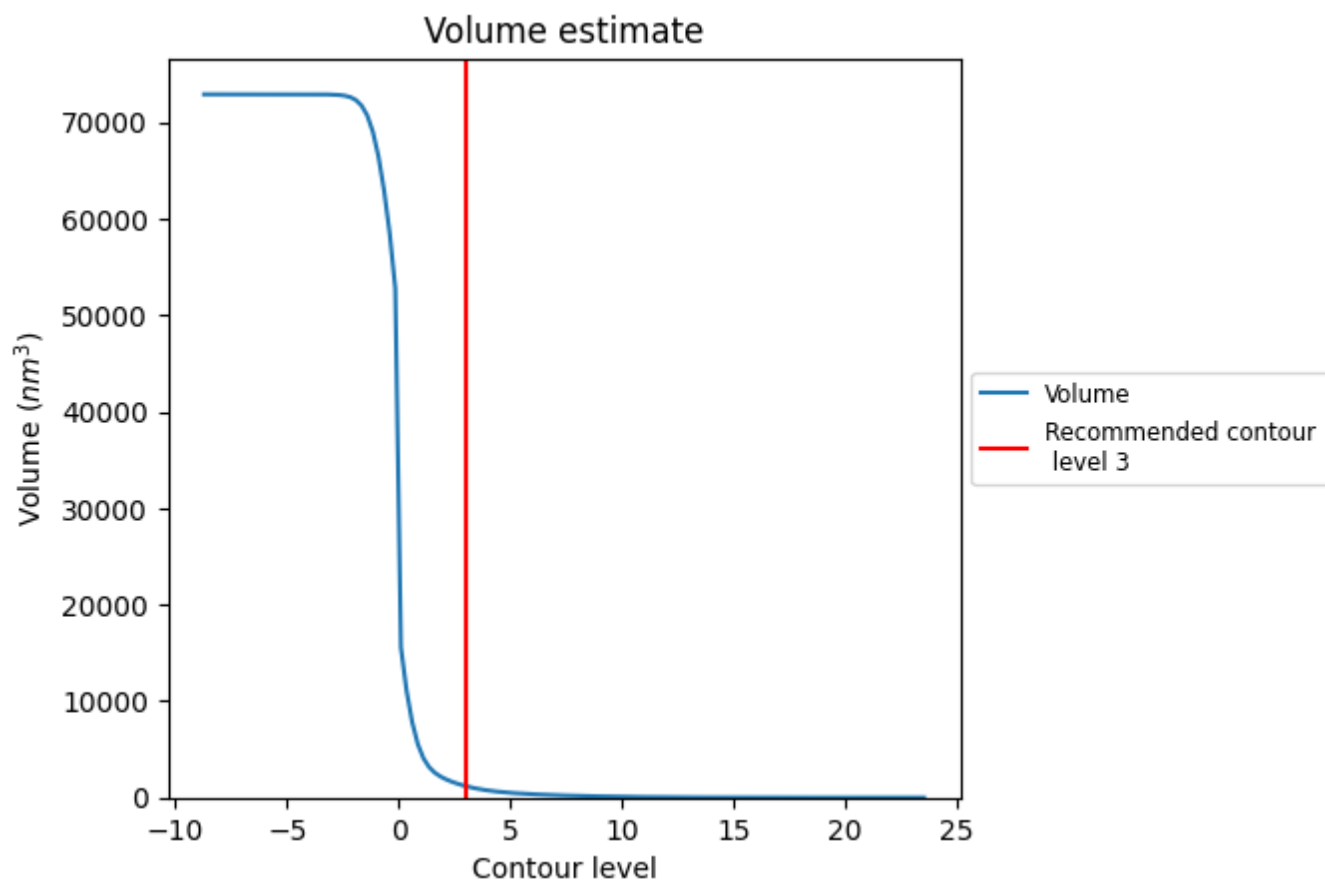
This section contains the results of statistical analysis of the map.

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.

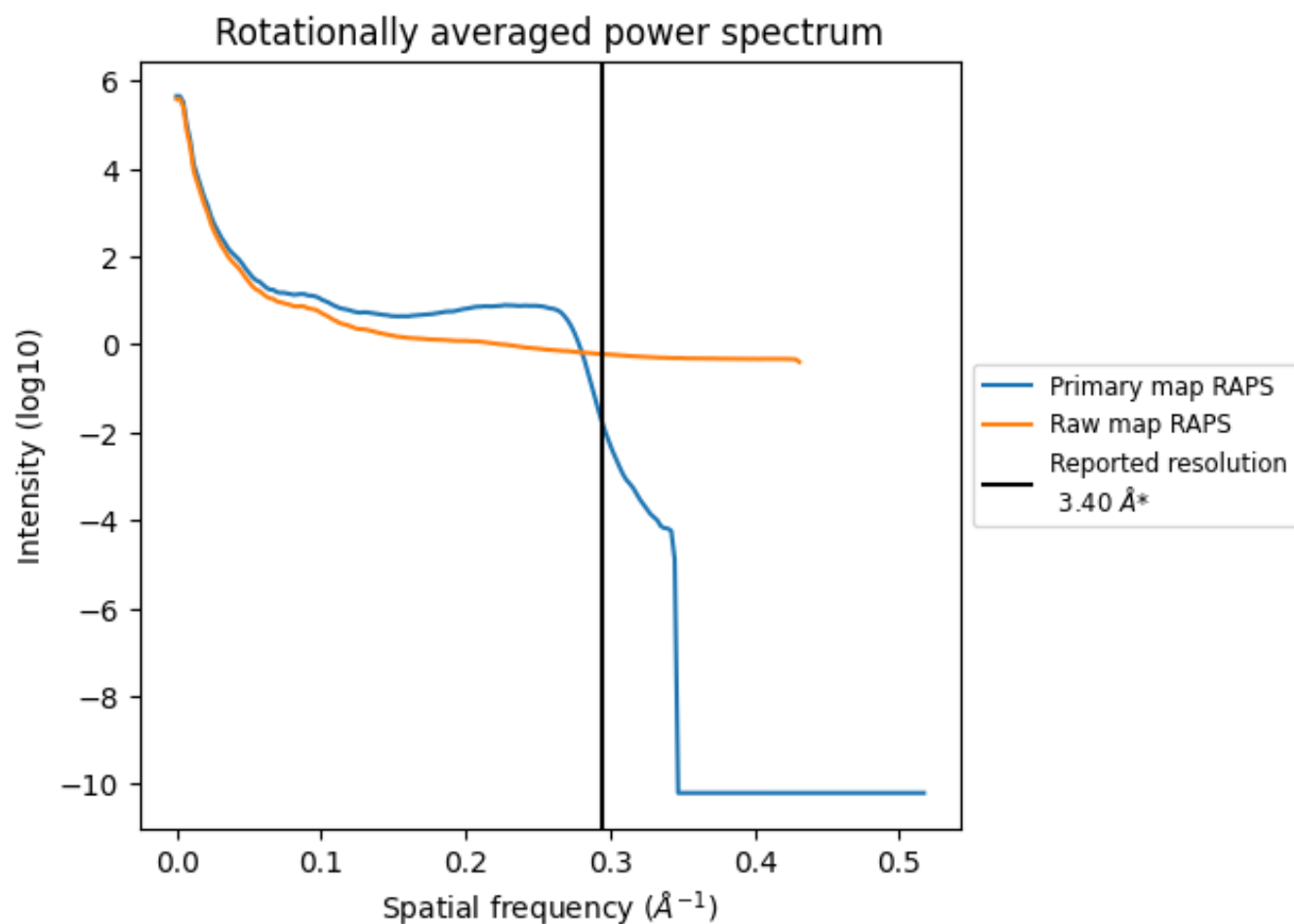
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1196 nm^3 ; this corresponds to an approximate mass of 1081 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

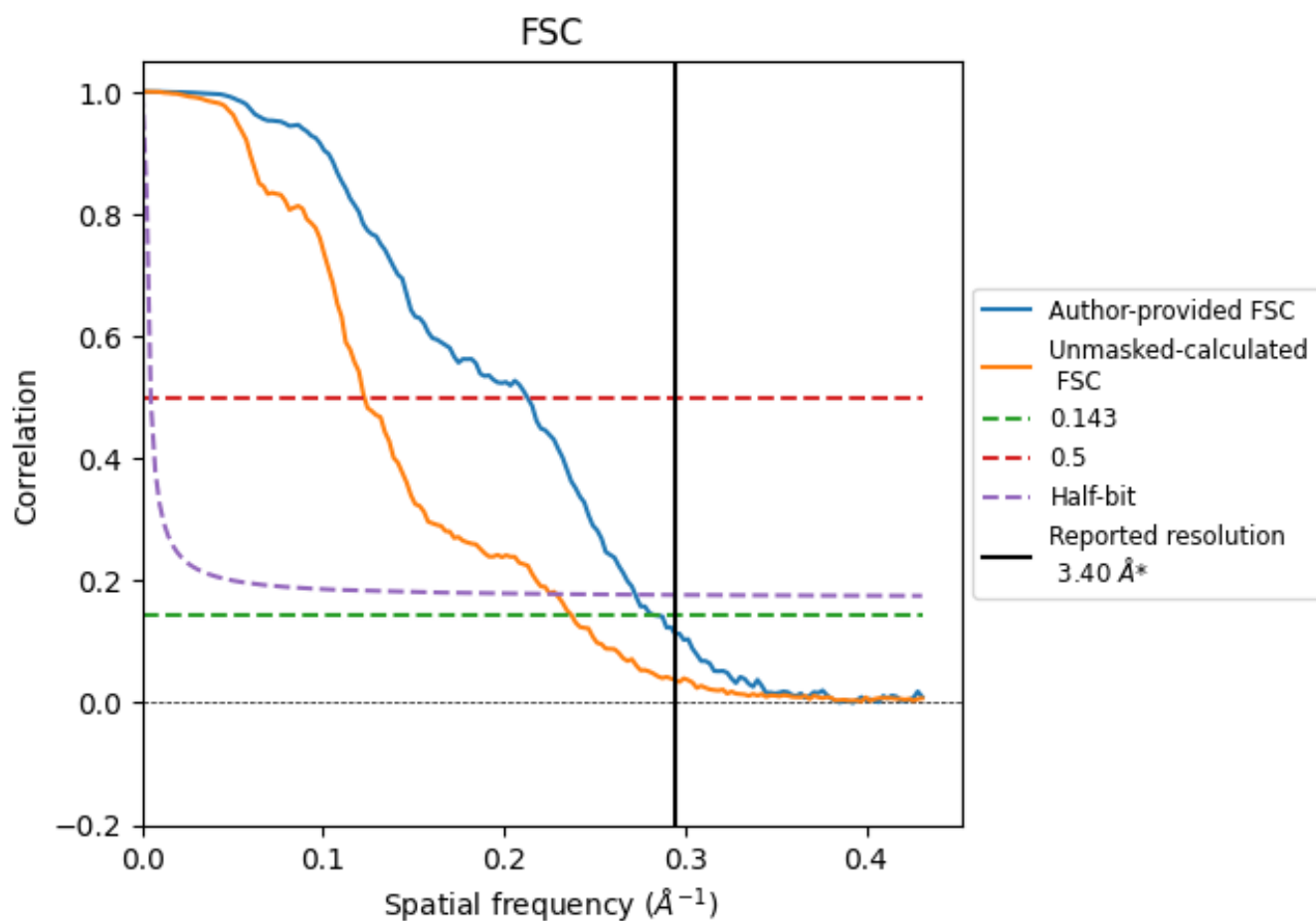


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

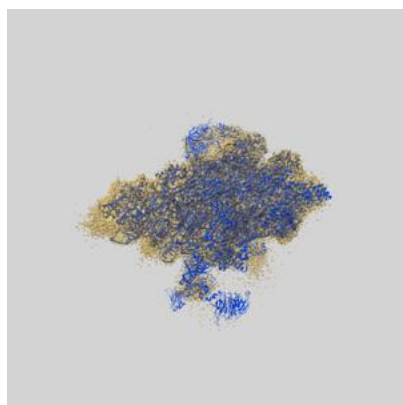
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.53	4.70	3.67
Unmasked-calculated*	4.22	8.15	4.37

*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 4.22 differs from the reported value 3.4 by more than 10 %

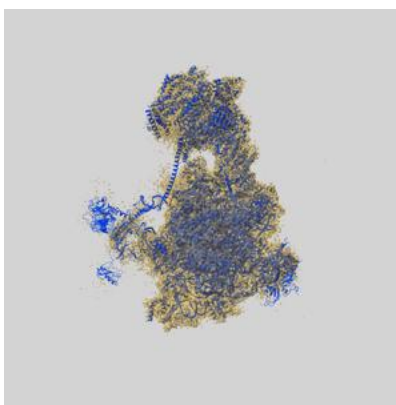
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17697 and PDB model 8PJ2. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

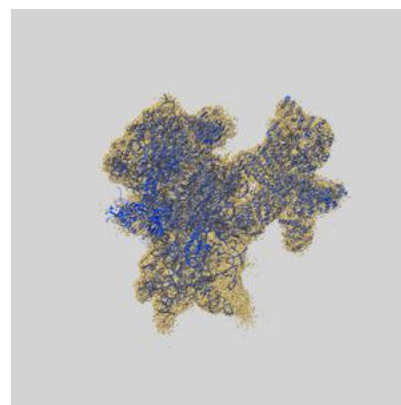
9.1 Map-model overlay [i](#)



X



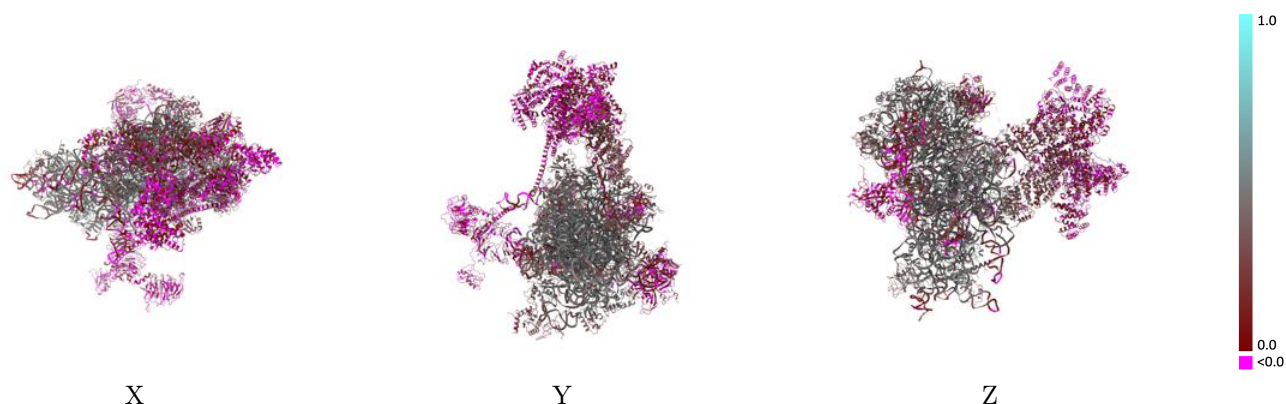
Y



Z

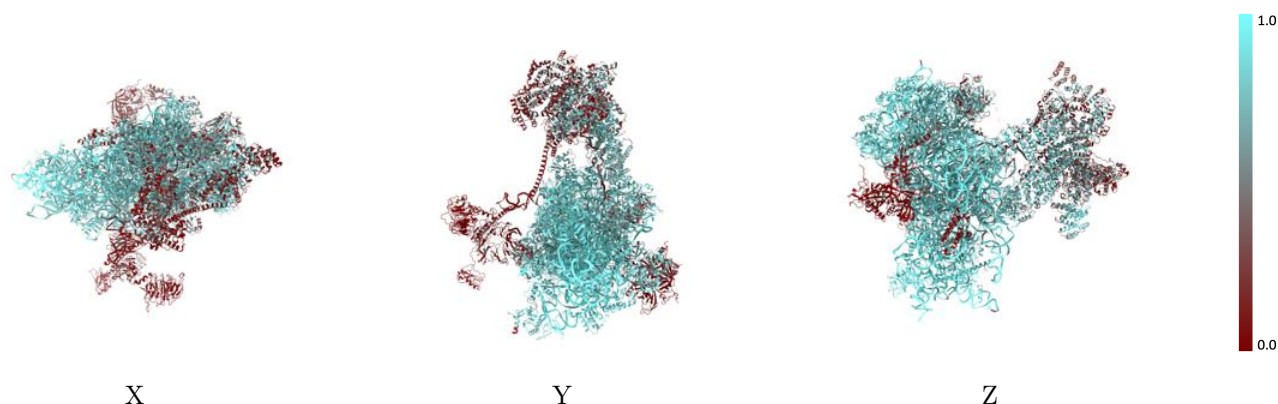
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



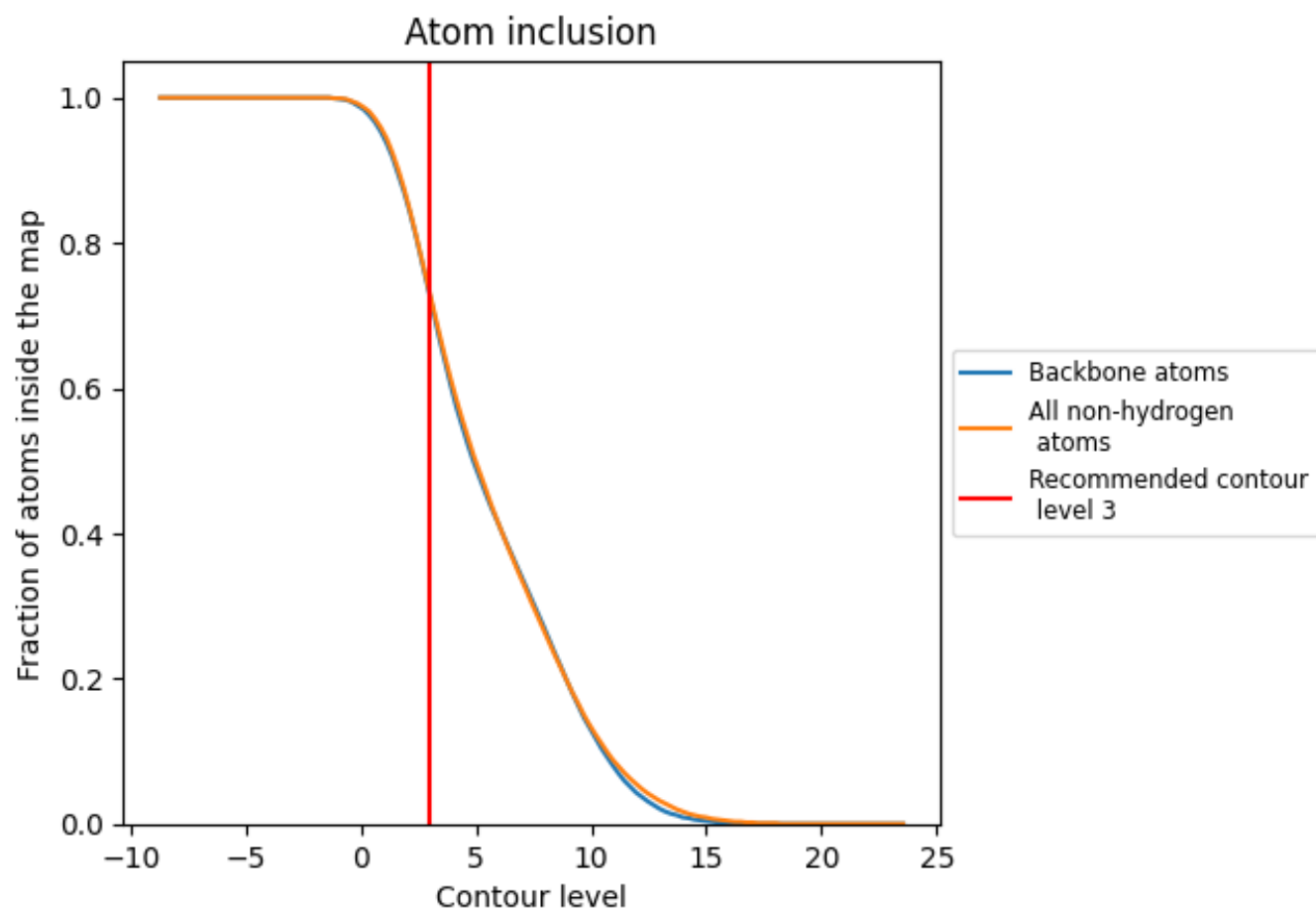
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 73% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.3200
1	 0.0660	 0.0560
2	 0.0030	 0.0270
3	 0.2680	 0.0420
4	 0.4680	 0.0680
5	 0.2880	 0.0140
6	 0.4120	 0.0450
7	 0.4450	 0.1710
8	 0.4440	 0.0950
9	 0.8130	 0.3960
A	 0.9550	 0.4200
B	 0.8770	 0.4630
C	 0.9170	 0.4800
D	 0.8830	 0.4620
E	 0.9000	 0.4850
F	 0.7810	 0.4060
G	 0.7900	 0.3880
H	 0.8420	 0.4310
I	 0.8670	 0.4410
J	 0.8900	 0.4870
K	 0.8230	 0.4450
L	 0.8350	 0.4600
M	 0.7810	 0.3970
N	 0.8590	 0.4560
O	 0.8670	 0.4260
P	 0.8470	 0.4250
Q	 0.9070	 0.4720
R	 0.9160	 0.4400
S	 0.9250	 0.4050
T	 0.9210	 0.4370
V	 0.8450	 0.4470
Y	 0.9070	 0.4670
Z	 0.8020	 0.4310
a	 0.8630	 0.4190
b	 0.8600	 0.4060



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Chain	Atom inclusion	Q-score
c	 0.8720	 0.4070
d	 0.9250	 0.4570
e	 0.7370	 0.3520
f	 0.8570	 0.4140
h	 0.8220	 0.4070
i	 0.9350	 0.4950
k	 0.7930	 0.2220
m	 0.7210	 0.2450
n	 0.7590	 0.4100
o	 0.4240	 0.1700
q	 0.7200	 0.3750
r	 0.5210	 0.2030
t	 0.0590	 0.0420
u	 0.5390	 0.1820
v	 0.5470	 0.1060
w	 0.8120	 0.2070
x	 0.5380	 0.2200
y	 0.5820	 0.2390
z	 0.3610	 0.2520