



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 01:37 am BST

PDB ID : 8PJ1 / pdb_00008pj1
EMDB ID : EMD-17696
Title : Structure of human 48S translation initiation complex in open codon scanning state (48S-1)
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:

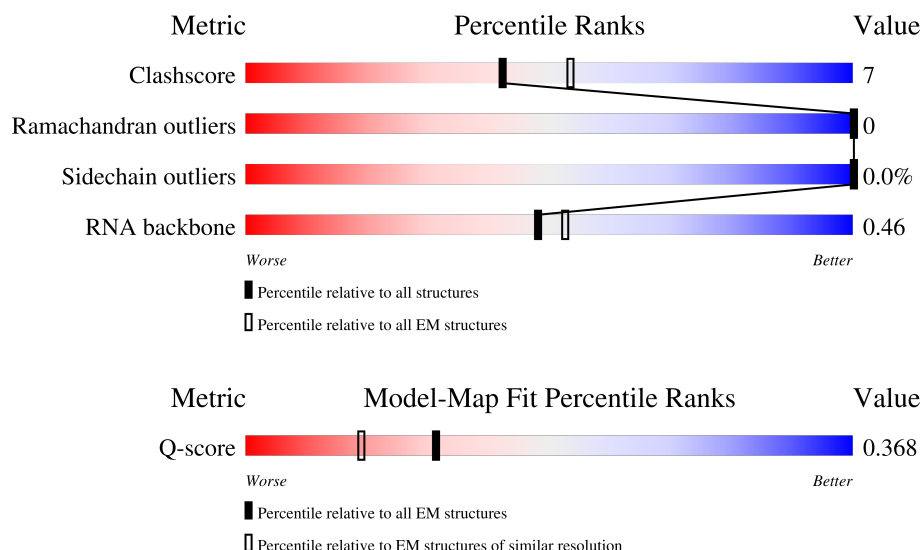
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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	
2	2	325	
3	3	218	

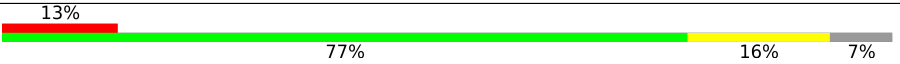
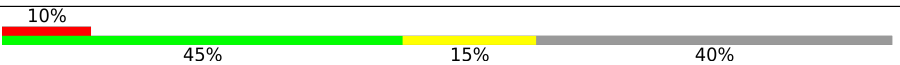
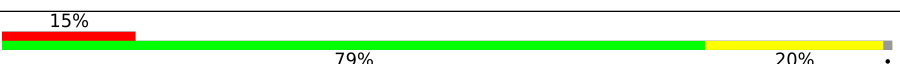
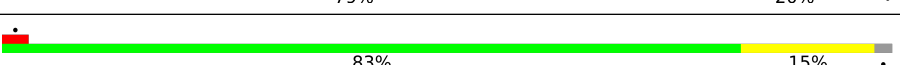
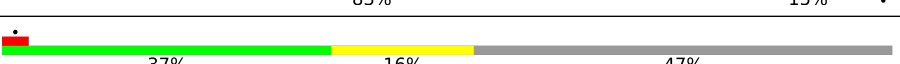
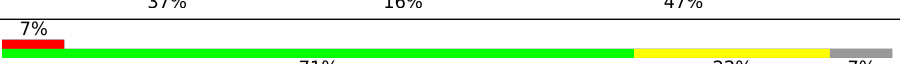
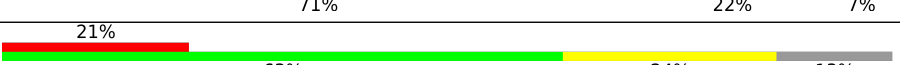
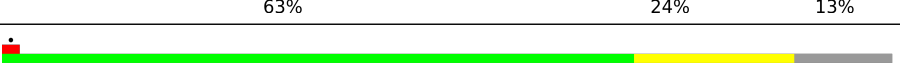
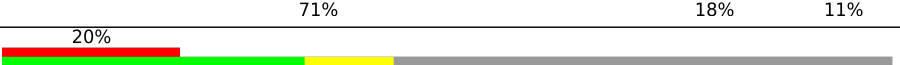
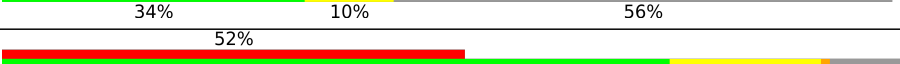
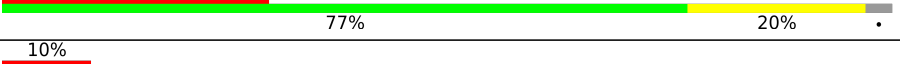
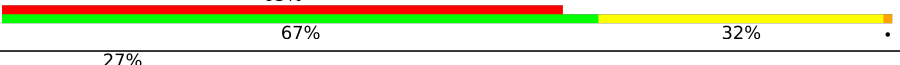
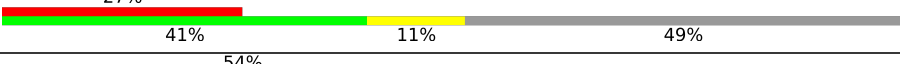
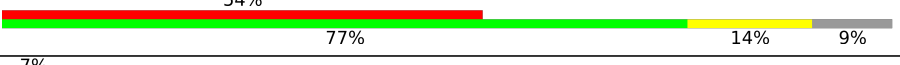
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Mol	Chain	Length	Quality of chain
4	4	357	
5	5	564	
6	6	374	
7	7	255	
8	8	352	
9	9	25	
10	A	1869	
11	B	158	
12	C	263	
13	D	194	
14	E	143	
15	F	59	
16	G	194	
17	H	84	
18	I	151	
19	J	130	
20	K	83	
21	L	293	
22	M	135	
23	N	295	
24	O	264	
25	P	151	
26	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	157	
42	m	132	
43	n	69	
44	o	320	
45	p	113	
46	q	144	
47	r	315	
48	s	333	
49	t	472	
50	u	1382	
51	v	445	
52	w	75	
53	x	548	

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Mol	Chain	Length	Quality of chain
54	y	913	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 119663 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	47	Total	C	N	O	P	0	0
			1003	453	199	304	47		

- 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	58	Total	C	N	O	S	0	0
			459	284	100	74	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	189	Total	C	N	O	S	0	0
			1495	934	284	270	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	121	Total	C	N	O	S	0	0
			989	628	185	169	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	66	Total	C	N	O	S	0	0
			523	338	93	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	142	Total	C	N	O	S	0	0
			1176	737	239	199	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	69	Total	C	N	O	S	0	0
			559	352	104	96	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	87	ALA	-	insertion	UNP P62979

- 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		0	0
			616	389	111	116			

- Molecule 45 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	110	Total	C	N	O	S	0	0
			830	524	150	154	2		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	93	Total	C	N	O	S	0	0
			754	476	137	137	4		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

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

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	159	Total	C	N	O	S	0	0
			1275	804	236	226	9		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	472	Total	C	N	O	S	0	0
			3586	2272	628	668	18		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit A.

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

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

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

- Molecule 52 is a RNA chain called Initiator Met-tRNA-i.

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

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	423	Total	C	N	O	S	0	0
			2842	1752	523	557	10		

- Molecule 54 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	731	Total	C	N	O	S	0	0
			5657	3547	1018	1057	35		

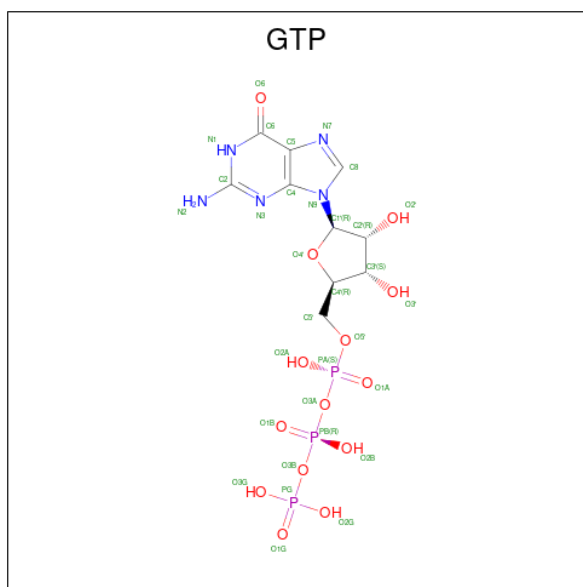
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	A	88	Total	Mg	0
			88	88	
55	f	1	Total	Mg	0
			1	1	
55	t	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

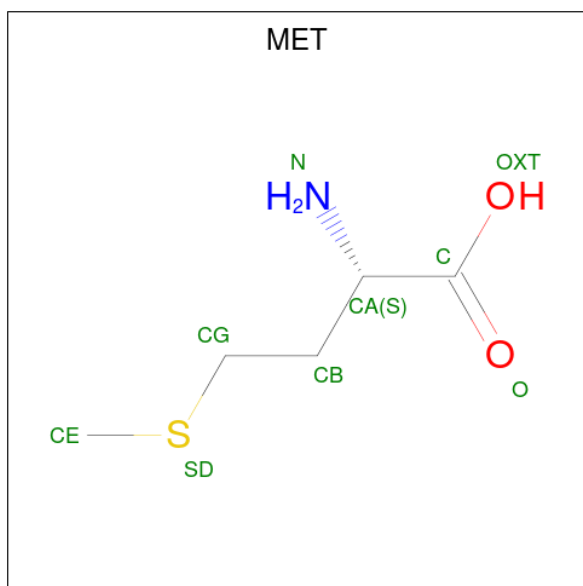
Mol	Chain	Residues	Atoms		AltConf
56	Q	1	Total	Zn	0
			1	1	
56	k	1	Total	Zn	0
			1	1	
56	s	1	Total	Zn	0
			1	1	

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

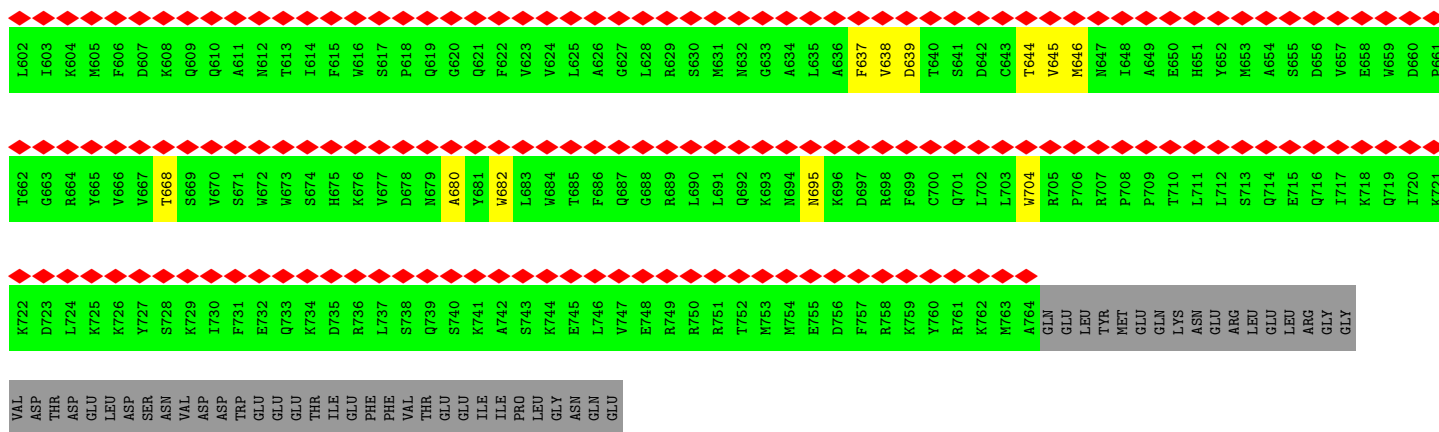


Mol	Chain	Residues	Atoms					AltConf
57	t	1	Total	C	N	O	P	0
			32	10	5	14	3	

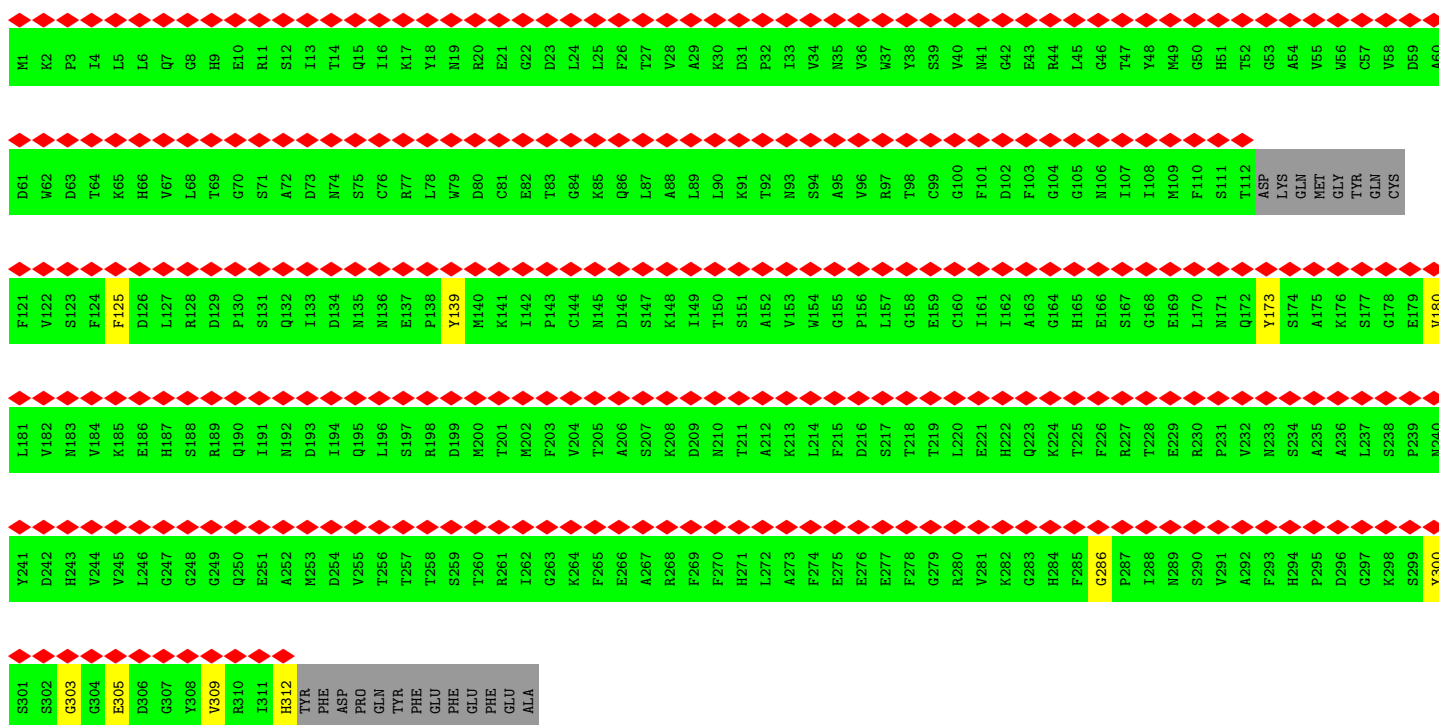
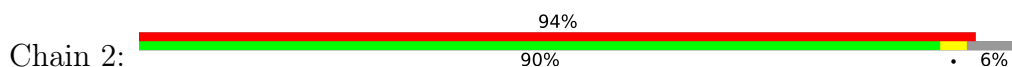
- Molecule 58 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



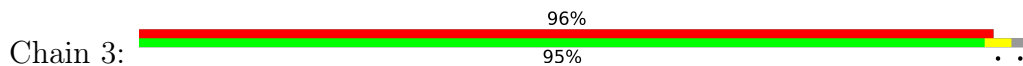
Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	S	0
			8	5	1	1	1	



• Molecule 2: Eukaryotic translation initiation factor 3 subunit I

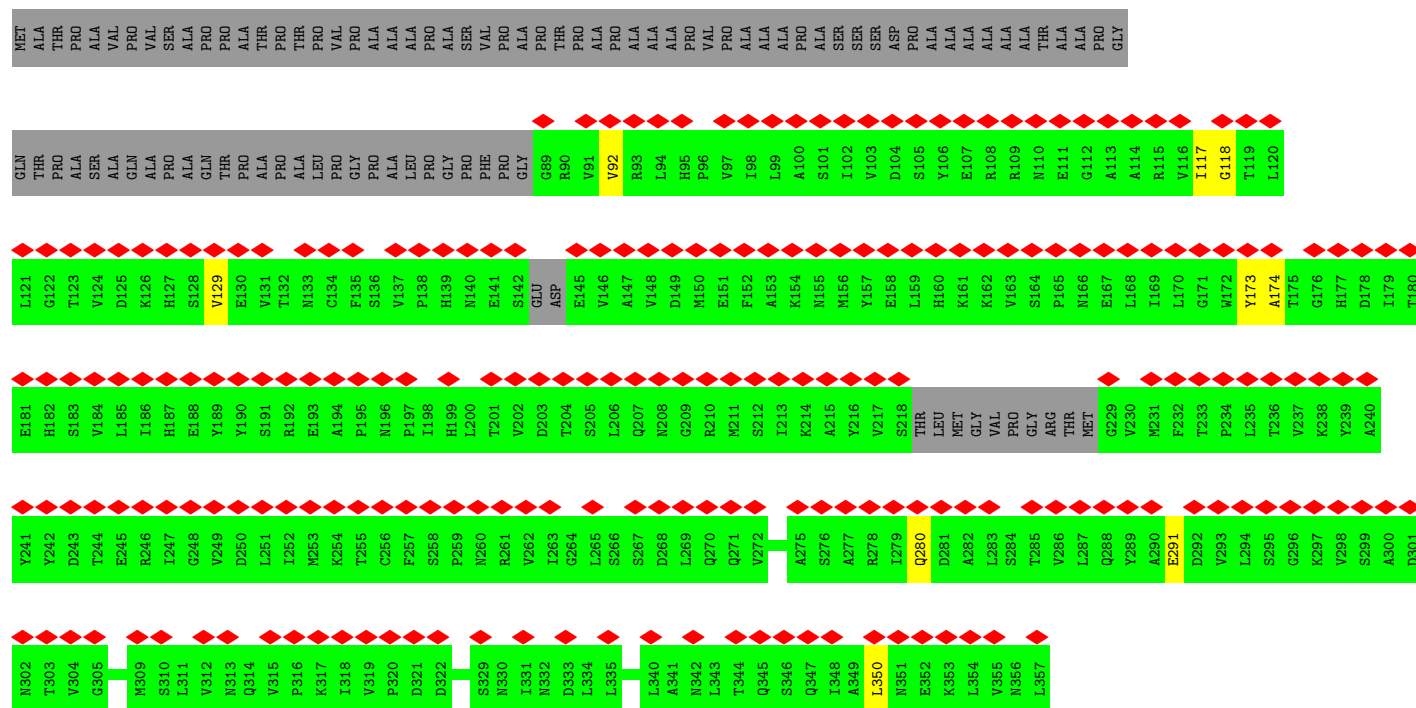


• Molecule 3: Eukaryotic translation initiation factor 3 subunit K

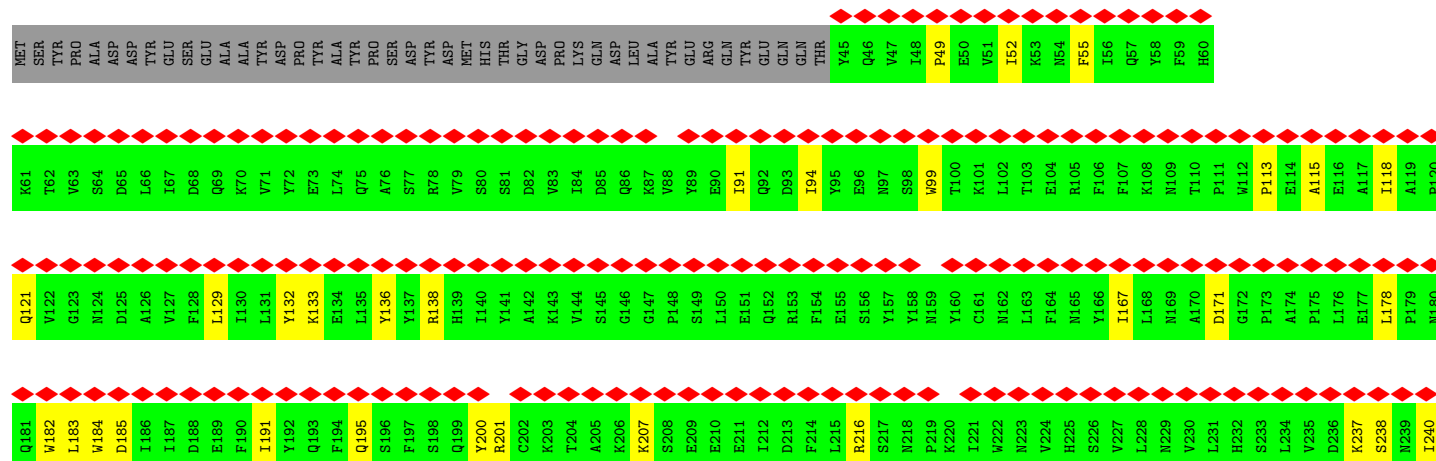
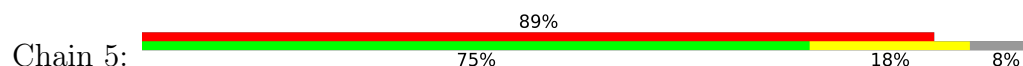


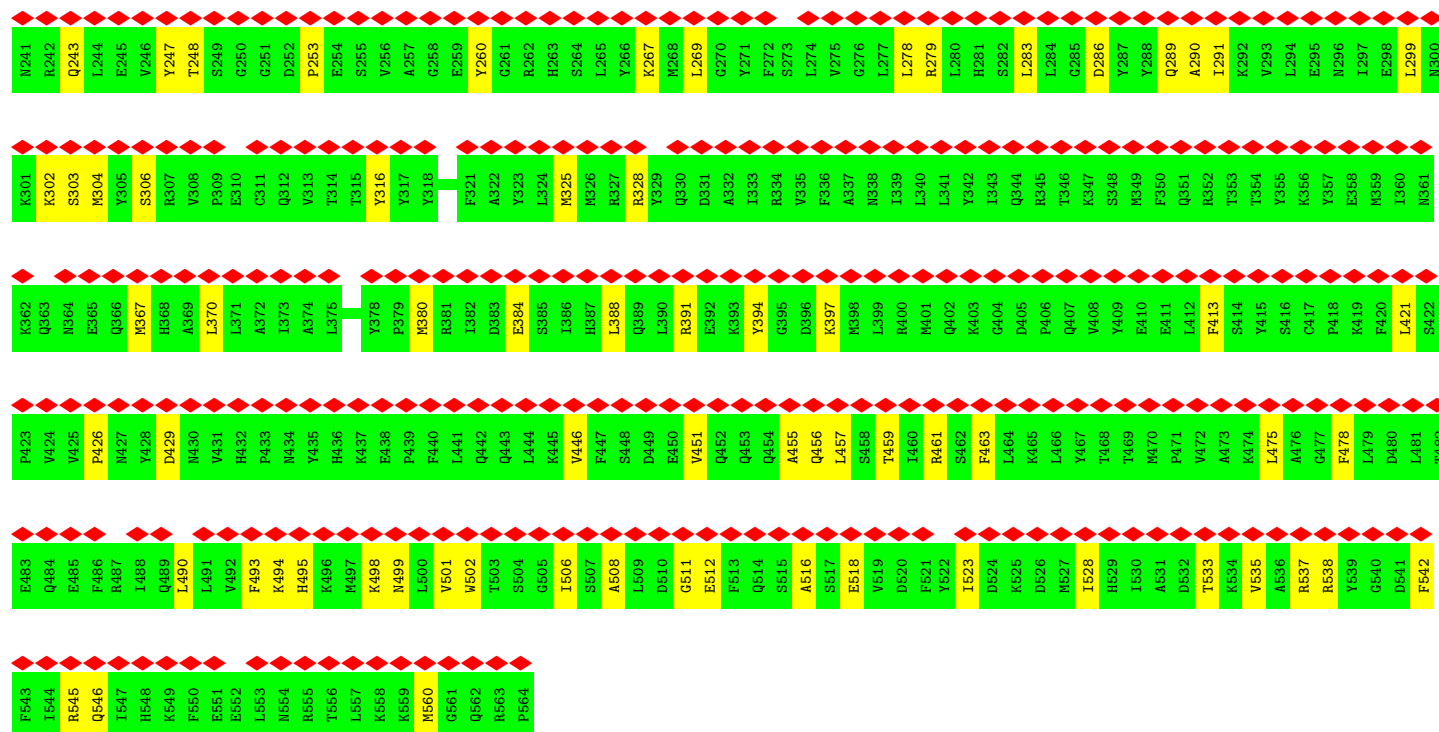


• Molecule 4: Eukaryotic translation initiation factor 3 subunit F

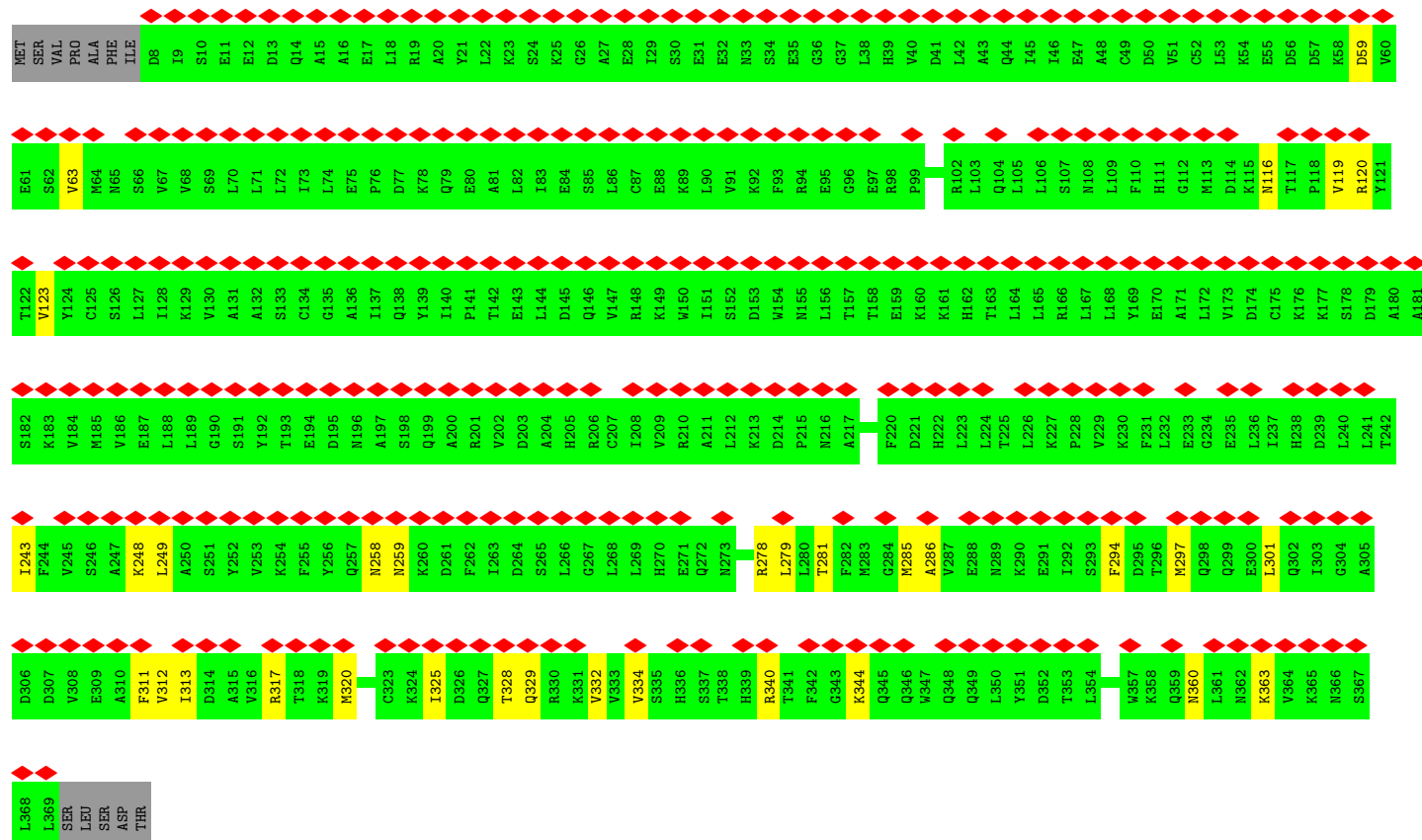
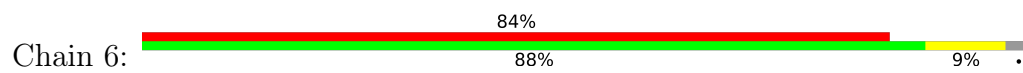


• Molecule 5: Eukaryotic translation initiation factor 3 subunit L





• Molecule 6: Eukaryotic translation initiation factor 3 subunit M



The diagram illustrates the assembly of a protein complex, likely a ribosome, showing the arrangement of various subunits and domains. The structure is represented by a large grey rectangular area, with specific regions highlighted in different colors (green, orange, yellow) and marked with red diamonds. Labels A6 through A19 and C1 through C19 are placed around the structure, corresponding to different subunits or domains. The diagram is divided into three main horizontal sections by thin lines.

Top Section: This section shows the arrangement of subunits A6 through A19 and C1 through C19. The subunits are arranged in a row, with A6 and A7 at the left end, followed by A8 through A19, and C1 through C19 at the right end. The subunits are color-coded: A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, and C19. The subunits A6 through A19 are arranged in a row, with A6 and A7 at the left end, followed by A8 through A19, and C1 through C19 at the right end. The subunits are color-coded: A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, and C19.

Middle Section: This section shows the arrangement of subunits A6 through A19 and C1 through C19. The subunits are arranged in a row, with A6 and A7 at the left end, followed by A8 through A19, and C1 through C19 at the right end. The subunits are color-coded: A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, and C19. The subunits A6 through A19 are arranged in a row, with A6 and A7 at the left end, followed by A8 through A19, and C1 through C19 at the right end. The subunits are color-coded: A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, and C19.

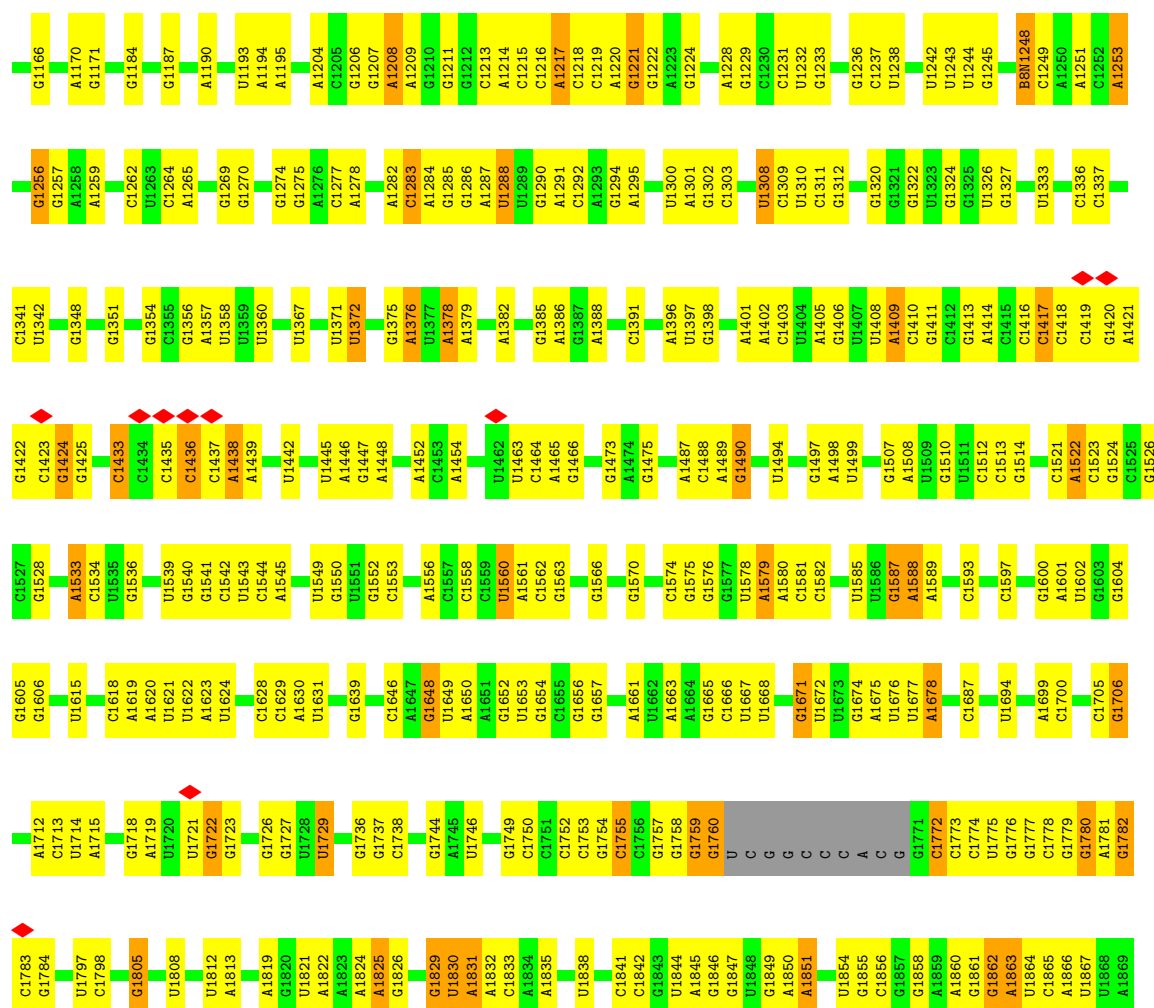
Bottom Section: This section shows the arrangement of subunits A6 through A19 and C1 through C19. The subunits are arranged in a row, with A6 and A7 at the left end, followed by A8 through A19, and C1 through C19 at the right end. The subunits are color-coded: A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, and C19. The subunits A6 through A19 are arranged in a row, with A6 and A7 at the left end, followed by A8 through A19, and C1 through C19 at the right end. The subunits are color-coded: A6, A7, A8, A9, A10, A11, A12, A13, A14, A15, A16, A17, A18, A19, C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, and C19.

P310	D248	L187	G126	V63	MET
P311	R249	K188	S127	V66	ALA
A312	V250	K189	F128	L67	SER
R313	D251	A190	V129	L68	ARG
M314	E252	M191	T130	O69	LYS
D315	M253	I192	R131	L70	GLU
S316	S254	T193	A132	L71	GLY
L317	Q255	F194	L133	V72	THR
L318	D256	E195	L134	E73	SER
I319	I257	Y196	D135	D74	ALA
A320	V258	M197	S136	R75	THR
G321	K259	F198	Q137	L76	SER
Q322	Y260	E199	F138	E77	SER
I323	M261	E200	S139	I78	THR
K331	T262	V201	Y140	I79	ALA
E332	M264	P202	Q141	N80	GLY
F333	Y267	T203	H142	C81	ALA
T334	T267	V204	A143	F82	LYS
L338	S268	T205	I144	P83	GLY
G339	K269	K206	E145	F84	LYS
K340	Q270	N207	E146	P85	LYS
L341	Q273	H209	S147	Q86	G29
F342	K274	L210	L150	H87	G30
M343	H275	T211	I151	T88	S31
A344	Q276	M212	Y152	E89	G32
Q345	Q277	V213	D153	D90	D33
A346	Q278	L214	P154	D91	D33
L347	Q279	M215	K156	A92	S34
Q348	R280	W216	T157	D93	A35
E349	R281	E219	A158	F94	V36
Y350	Q282	K220	Q159	D95	K37
N351	Q283	K221	G160	E96	Q38
N352	E284	S222	S161	V97	V39
	M285	L182	L162	Q98	Q40
	Q287	V224	S163	Y99	T41
	R288	A225	L164	Q100	D42
	Q289	D226	K165	M101	G43
	S290	K227	A166	E102	L44
	R291	H228	Y167	M103	V45
	E292	E229	R168	M104	V46
	E293	L230	L169	R105	L47
	P294	L231	T170	S106	K48
	P295	S232	P171	L107	L49
	L296	L233	K172	R108	
	P297	A234	L173	H109	V53
	E298	S235	M174	V110	Q54
	E299	S236	E175	M111	E55
	D300	W237	V176	I112	E56
	L301	H238	C177	D113	Q57
	S302	L239	K178	H114	Q58
	K303	G240	GLU	L115	Q59
	L304	K241	LYS	H116	T60
	F305	N242	ASP	V117	E61
	K306	L243	PHE	G118	V62
	P307	Q244	SER		
	P308	L245	PRO	S122	
	Q309	L246	GLU	T123	
			A186	Y124	
				V125	

Diagram illustrating a protein structure with residues M1, R2, R11, R12, R18, K19, M20, R21, Q22, R23, S24, and LYS. Red diamonds are positioned above residues K19, M20, R21, Q22, and R23.

Chain A:





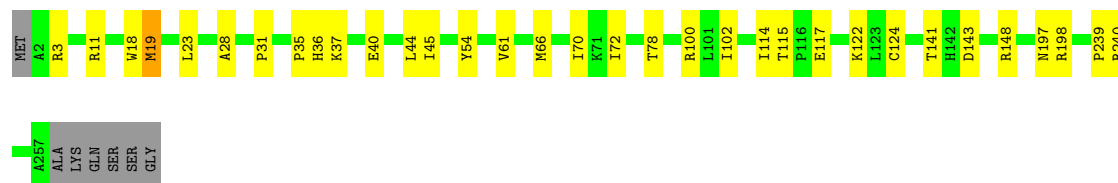
- Molecule 11: 40S ribosomal protein S11

Chain B: 78% 12% 10%



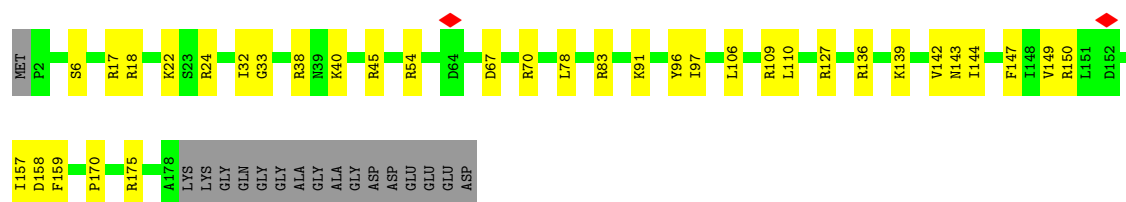
- Molecule 12: 40S ribosomal protein S4, X isoform

Chain C: 85% 12% 3%

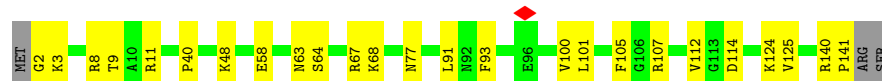
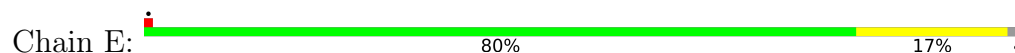


- Molecule 13: 40S ribosomal protein S9

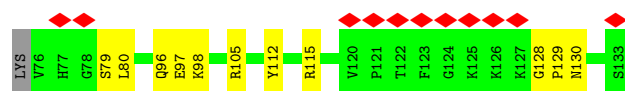
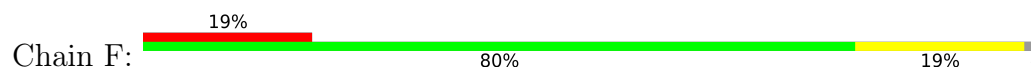
Chain D: 73% 18% 9%



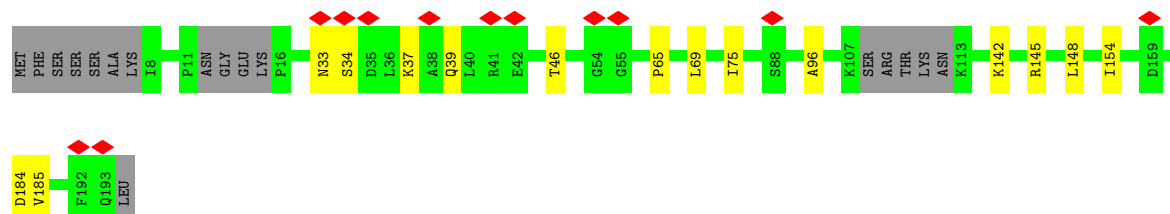
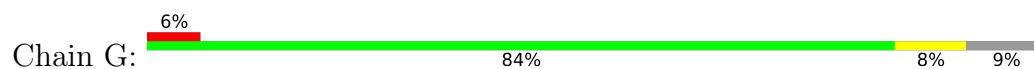
- Molecule 14: 40S ribosomal protein S23



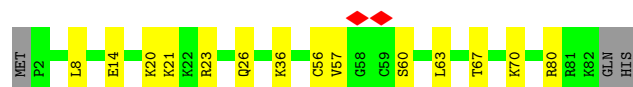
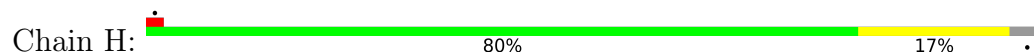
- Molecule 15: 40S ribosomal protein S30



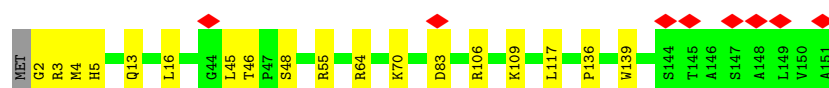
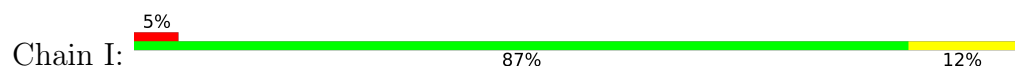
- Molecule 16: 40S ribosomal protein S7



- Molecule 17: 40S ribosomal protein S27



- Molecule 18: 40S ribosomal protein S13



- Molecule 19: 40S ribosomal protein S15a

- Molecule 20: 40S ribosomal protein S21

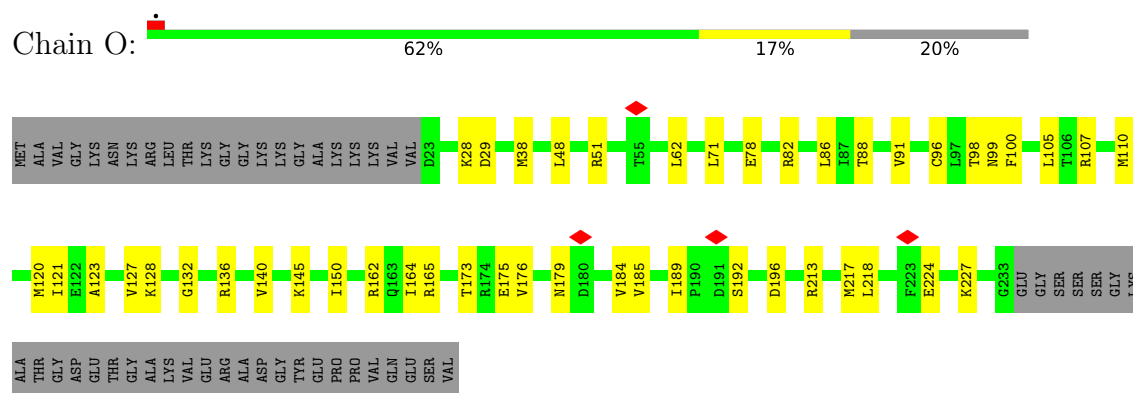
- Molecule 21: 40S ribosomal protein S2

- Molecule 22: 40S ribosomal protein S17

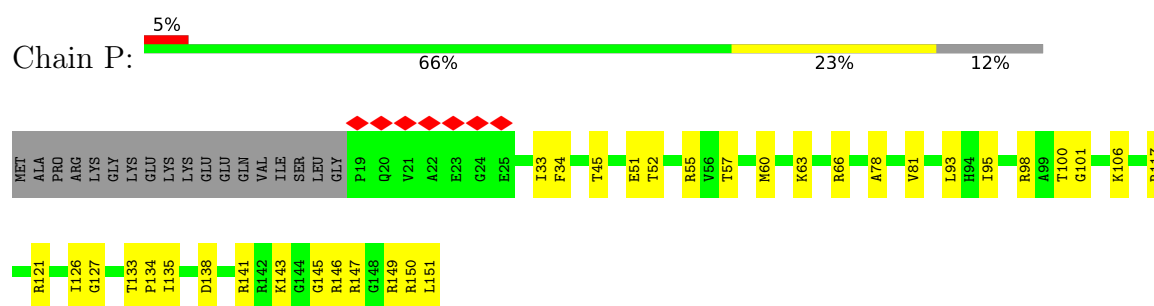
- Molecule 23: 40S ribosomal protein SA

PRO	GLU	VAL	ALA	ASP	TRP	SER	GLY	VAL	GLN	GLN	PRO	SER	SER	VAL	PRO	ILE	GLN	GLN	PHE	PRO	THR	GLU	ASP	TRP	SER	SER	ALA	GLN	GLN	PRO	THR	GLU	ASP	TRP	SER	SER	ALA	ALA	ALA	ALA	PRO	THR	THR	GLN	THR	THR	THR	THR	ASP	TRP	SER	TRP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

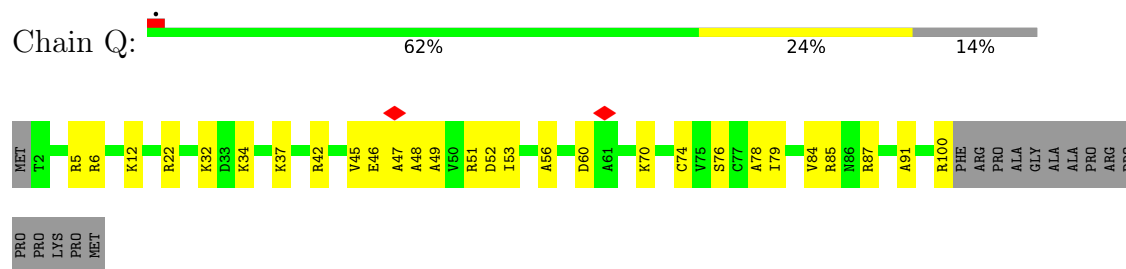
- Molecule 24: 40S ribosomal protein S3a



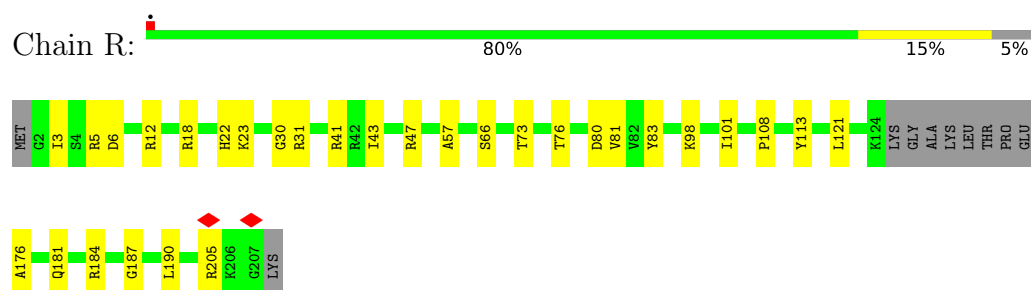
- Molecule 25: 40S ribosomal protein S14



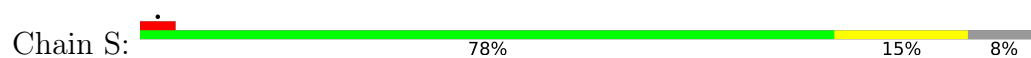
- Molecule 26: 40S ribosomal protein S26

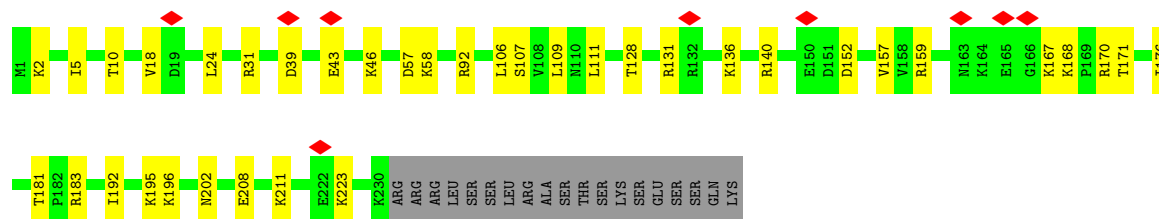


- Molecule 27: 40S ribosomal protein S8

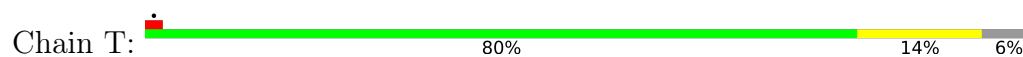


- Molecule 28: 40S ribosomal protein S6

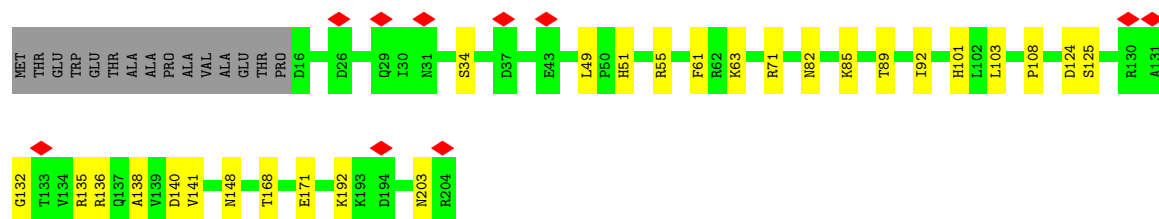
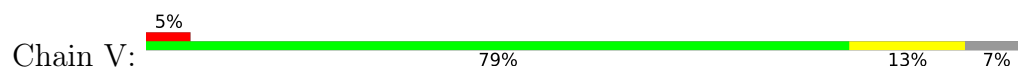




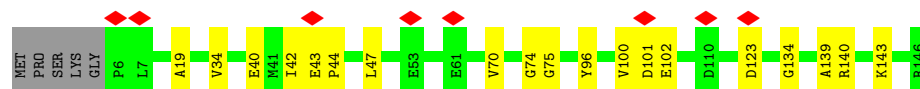
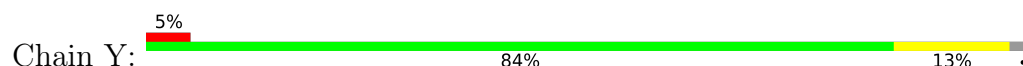
- Molecule 29: 40S ribosomal protein S24



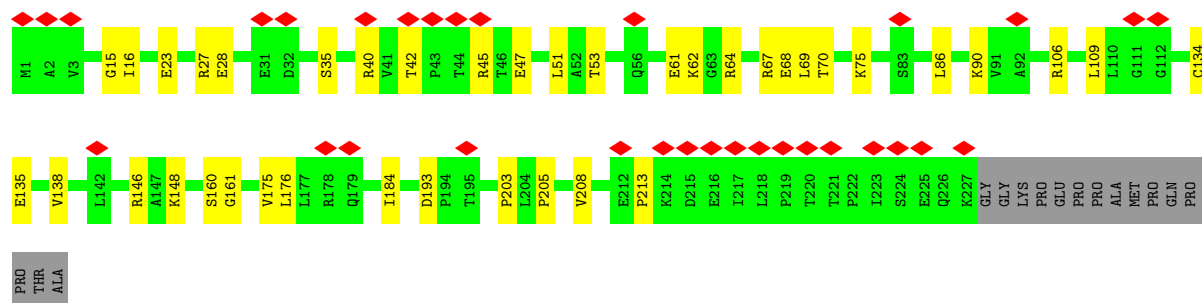
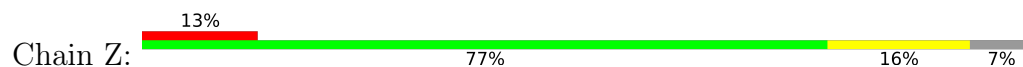
- Molecule 30: 40S ribosomal protein S5



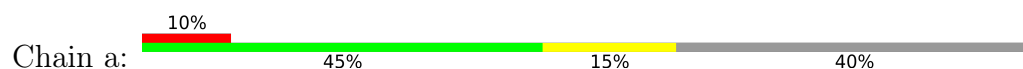
- Molecule 31: 40S ribosomal protein S16

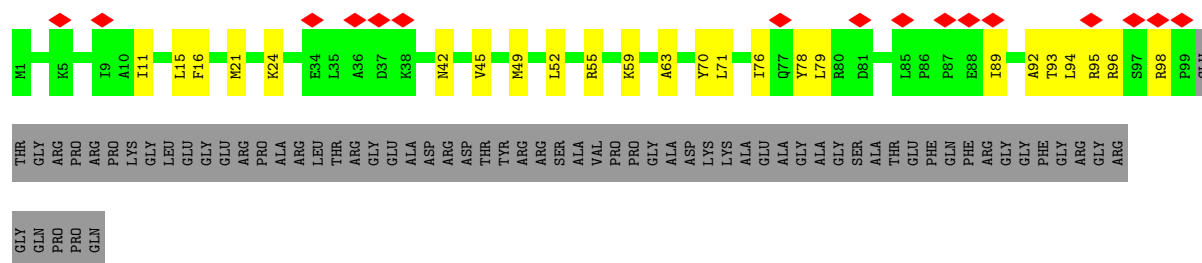


- Molecule 32: 40S ribosomal protein S3

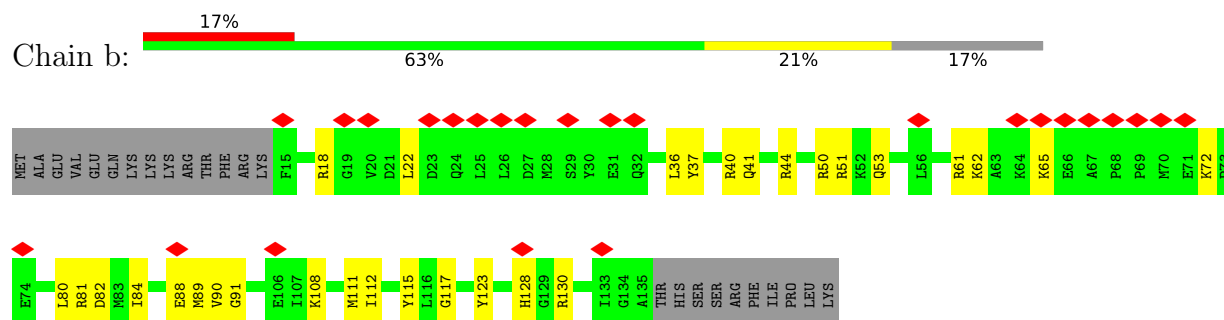


- Molecule 33: 40S ribosomal protein S10

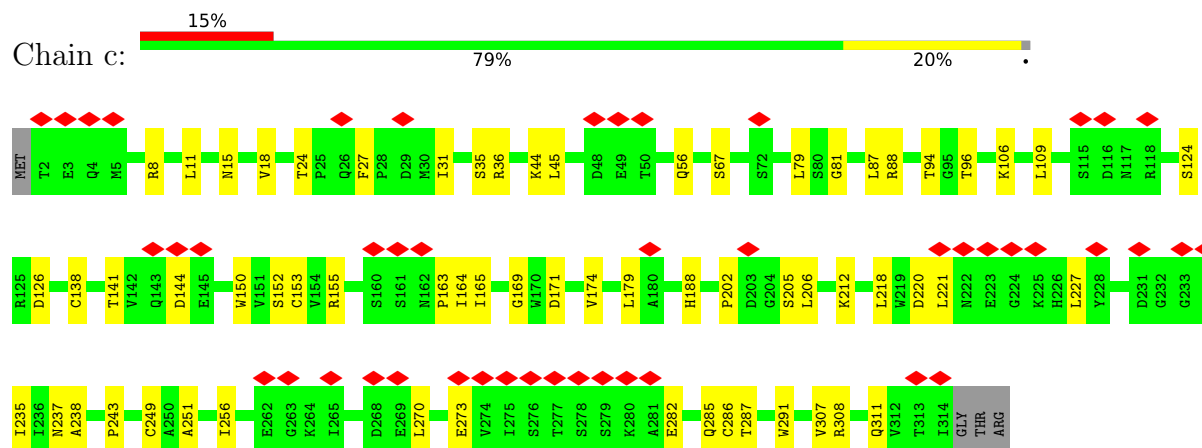




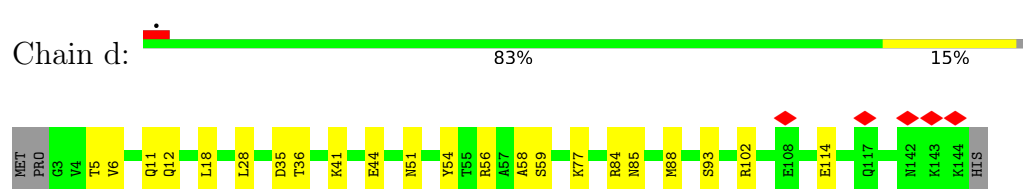
- Molecule 34: 40S ribosomal protein S15



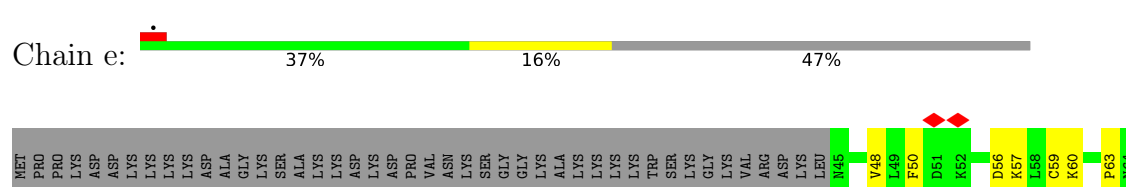
- Molecule 35: Receptor of activated protein C kinase 1

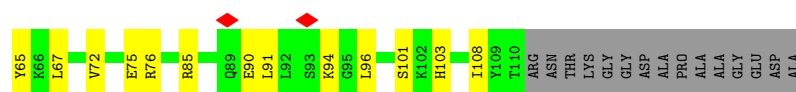


- Molecule 36: 40S ribosomal protein S19

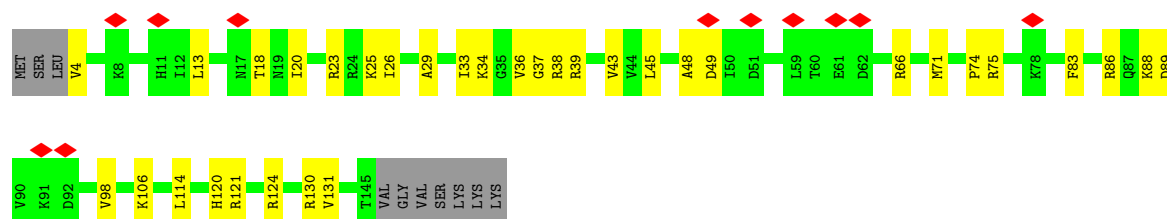


- Molecule 37: 40S ribosomal protein S25

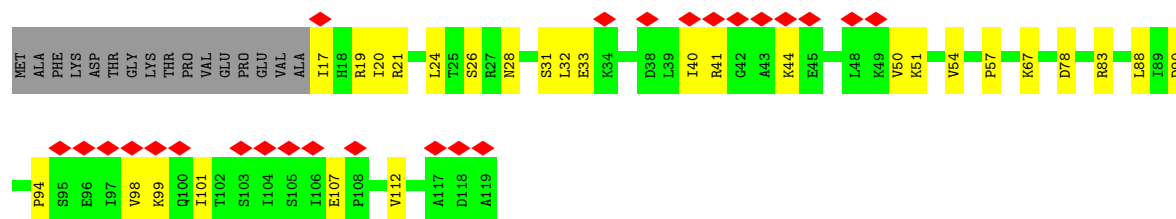




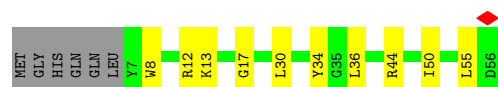
- Molecule 38: 40S ribosomal protein S18



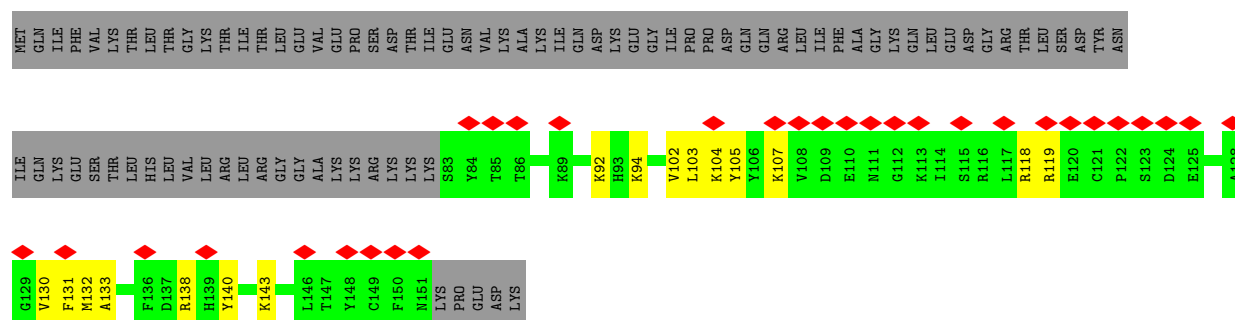
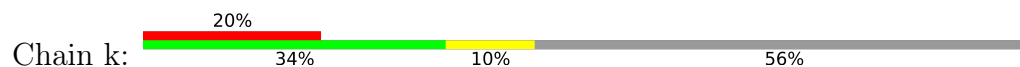
- Molecule 39: 40S ribosomal protein S20



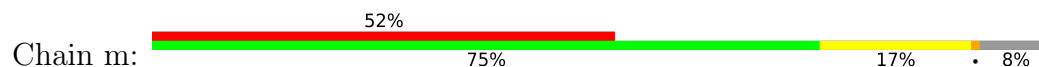
- Molecule 40: 40S ribosomal protein S29

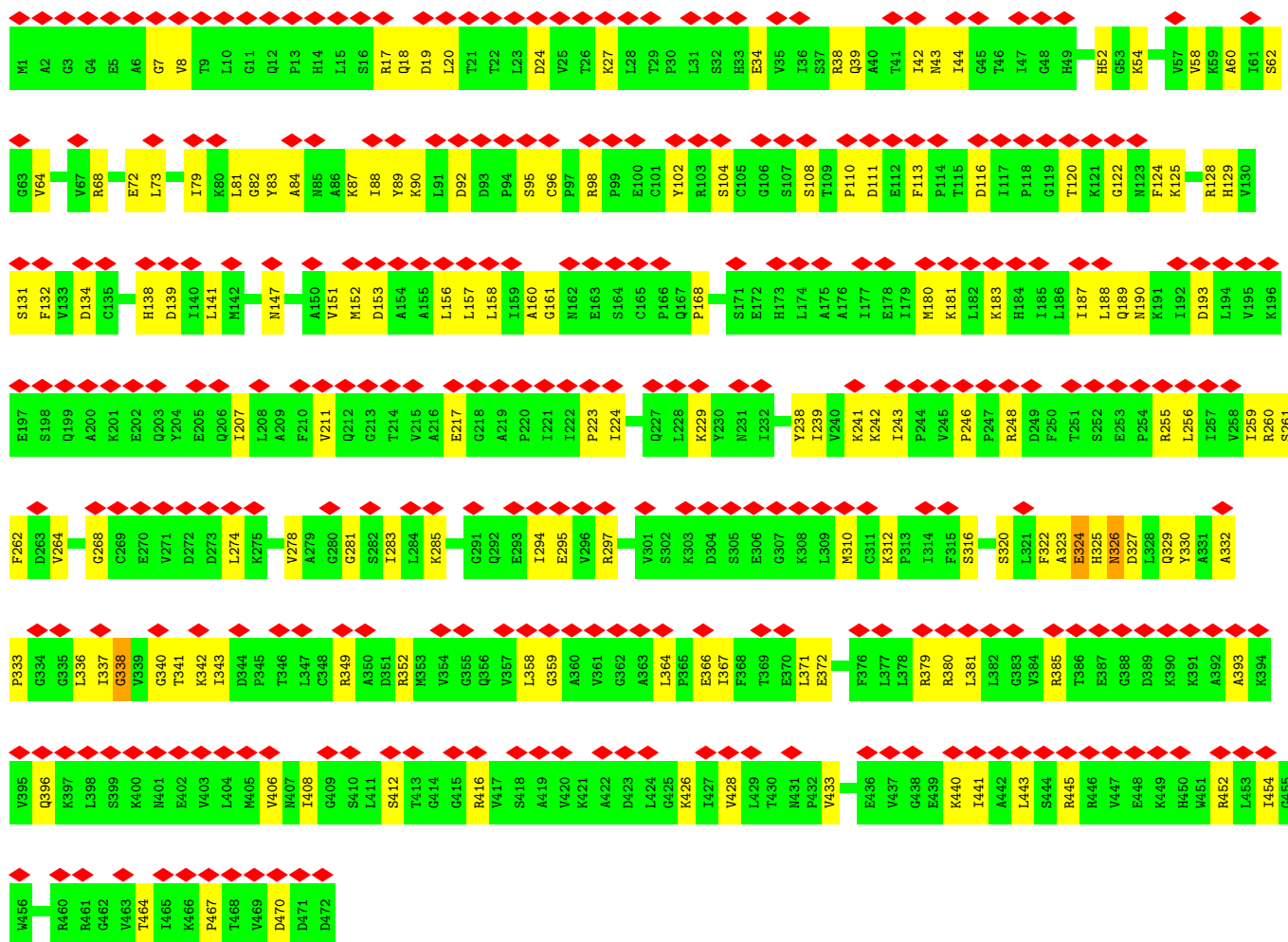


- Molecule 41: Ubiquitin

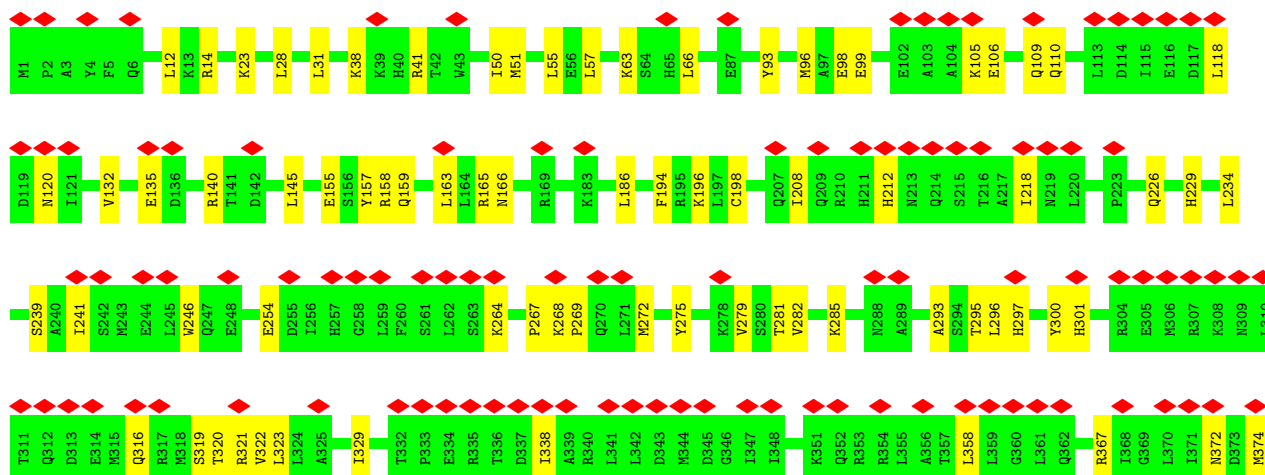


- Molecule 42: 40S ribosomal protein S12

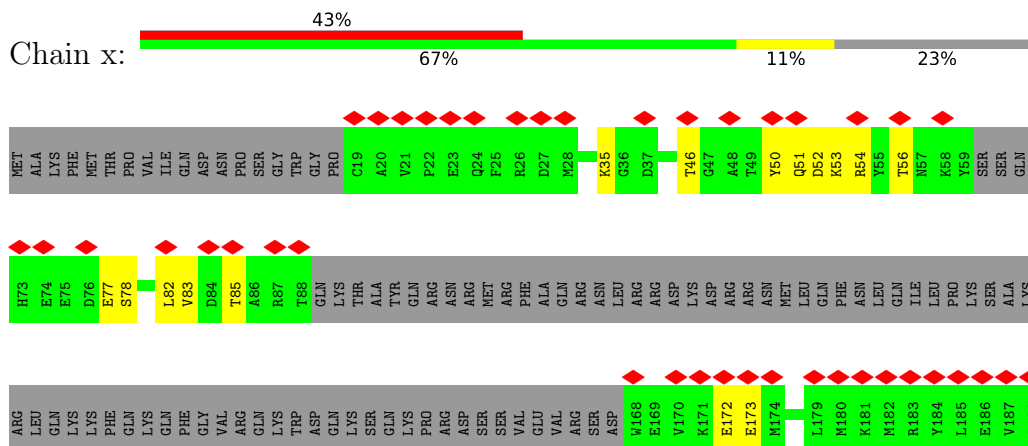




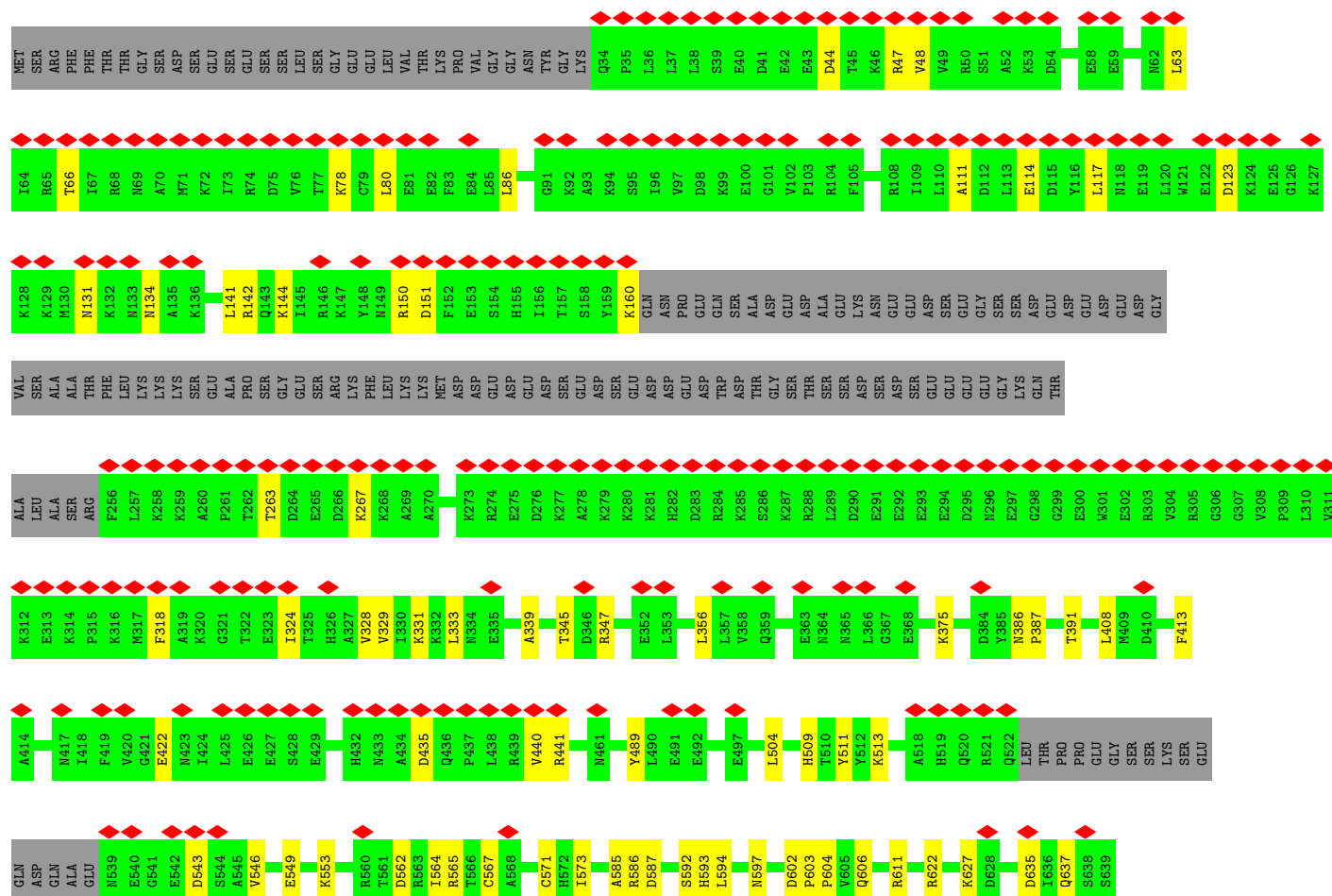
• Molecule 50: Eukaryotic translation initiation factor 3 subunit A

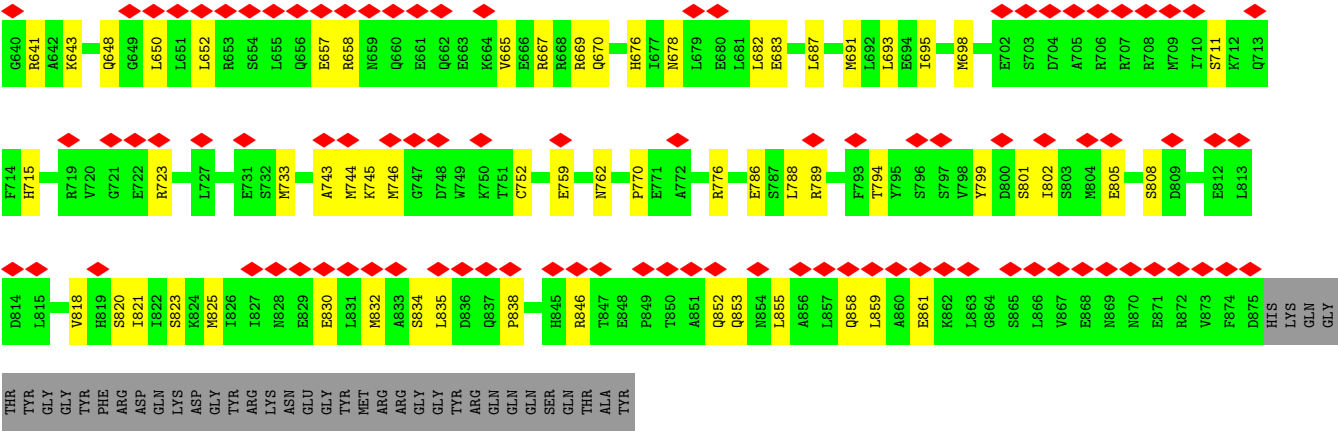






- Molecule 54: Eukaryotic translation initiation factor 3 subunit C





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92749	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	24.146	Depositor
Minimum map value	-8.937	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	417.74402, 417.74402, 417.74402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, OMG, PSU, MG, 5MU, 6MZ, A2M, OMU, 5MC, ZN, MA6, OMC, JMH, UR3, GTP

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	0.18	0/3279	0.45	3/4534 (0.1%)
2	2	0.10	0/1491	0.32	0/2068
3	3	0.10	0/1055	0.30	0/1469
4	4	0.10	0/1269	0.29	0/1762
5	5	0.14	0/4458	0.38	0/6027
6	6	0.15	0/2212	0.42	0/3034
7	7	0.19	0/1126	0.42	0/1750
8	8	0.11	0/1572	0.36	0/2187
9	9	0.21	0/231	0.46	0/294
10	A	0.20	1/41130 (0.0%)	0.33	0/64100
11	B	0.20	0/1186	0.40	0/1585
12	C	0.20	0/2077	0.45	1/2796 (0.0%)
13	D	0.20	0/1502	0.40	0/2008
14	E	0.19	0/1105	0.38	0/1476
15	F	0.15	0/465	0.46	0/612
16	G	0.17	0/1451	0.40	0/1942
17	H	0.19	0/644	0.38	0/864
18	I	0.18	0/1232	0.37	0/1656
19	J	0.24	0/1051	0.46	0/1406
20	K	0.20	0/623	0.46	0/833
21	L	0.22	0/1743	0.48	0/2354
22	M	0.25	0/1078	0.62	0/1447
23	N	0.22	0/1670	0.50	2/2271 (0.1%)
24	O	0.21	0/1742	0.50	0/2330
25	P	0.24	0/1010	0.54	0/1353
26	Q	0.21	0/805	0.40	0/1079
27	R	0.18	0/1654	0.36	0/2203
28	S	0.18	0/1885	0.39	0/2510
29	T	0.17	0/1032	0.38	0/1371
30	V	0.20	0/1516	0.50	0/2037
31	Y	0.21	0/1142	0.50	0/1528
32	Z	0.18	0/1793	0.39	0/2414

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.18	0/859	0.44	0/1159
34	b	0.18	0/1008	0.50	0/1348
35	c	0.16	0/2493	0.43	0/3394
36	d	0.16	0/1123	0.36	0/1504
37	e	0.16	0/529	0.45	0/712
38	f	0.17	0/1194	0.43	0/1599
39	h	0.22	0/827	0.53	0/1110
40	i	0.20	0/429	0.48	0/568
41	k	0.21	0/571	0.60	0/760
42	m	0.16	0/960	0.50	1/1286 (0.1%)
43	n	0.21	0/500	0.53	0/669
44	o	0.19	0/628	0.48	0/846
45	p	0.25	0/843	0.65	0/1134
46	q	0.20	0/764	0.56	0/1020
47	r	0.20	0/2167	0.50	3/2943 (0.1%)
48	s	0.30	0/1295	0.61	0/1739
49	t	0.22	0/3644	0.54	5/4929 (0.1%)
50	u	0.17	0/5475	0.48	1/7432 (0.0%)
51	v	0.17	0/2778	0.47	0/3797
52	w	0.19	0/1795	0.43	0/2798
53	x	0.16	0/2885	0.43	0/3940
54	y	0.18	0/5744	0.46	1/7761 (0.0%)
All	All	0.19	1/124740 (0.0%)	0.41	17/177748 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	668	A2M	O3'-P	5.23	1.61	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	19	MET	CB-CG-SD	-7.77	89.38	112.70
23	N	5	LEU	CA-C-N	6.98	137.81	126.86
23	N	5	LEU	C-N-CA	6.98	137.81	126.86
49	t	338	GLY	CA-C-N	-6.20	115.23	123.17
49	t	338	GLY	C-N-CA	-6.20	115.23	123.17
50	u	571	ARG	CB-CA-C	-5.96	109.71	116.63
49	t	95	SER	CA-C-N	5.89	138.06	120.69
49	t	95	SER	C-N-CA	5.89	138.06	120.69
1	1	287	PHE	N-CA-C	-5.83	104.92	111.28
42	m	35	ILE	N-CA-C	-5.68	107.96	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	284	LYS	N-CA-C	-5.44	105.45	113.72
47	r	236	VAL	N-CA-C	5.40	117.86	108.90
49	t	324	GLU	CB-CA-C	-5.36	110.38	116.54
1	1	288	LYS	N-CA-C	-5.29	107.20	113.97
47	r	231	ALA	CA-C-N	-5.24	114.98	120.38
47	r	231	ALA	C-N-CA	-5.24	114.98	120.38
54	y	48	VAL	N-CA-C	-5.10	105.57	113.16

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	32	0
2	2	1493	0	677	5	0
3	3	1057	0	475	4	0
4	4	1272	0	564	6	0
5	5	4347	0	4294	61	0
6	6	2196	0	1547	21	0
7	7	1003	0	516	22	0
8	8	1574	0	687	5	0
9	9	230	0	276	7	0
10	A	37429	0	18912	377	0
11	B	1166	0	1233	13	0
12	C	2035	0	2138	20	0
13	D	1477	0	1589	25	0
14	E	1087	0	1154	18	0
15	F	459	0	503	8	0
16	G	1430	0	1520	10	0
17	H	631	0	657	11	0
18	I	1208	0	1294	15	0
19	J	1034	0	1080	15	0
20	K	617	0	622	7	0
21	L	1707	0	1794	26	0
22	M	1064	0	1118	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	N	1633	0	1640	27	0
24	O	1715	0	1785	29	0
25	P	997	0	1021	27	0
26	Q	792	0	843	25	0
27	R	1627	0	1706	23	0
28	S	1862	0	2018	30	0
29	T	1015	0	1086	13	0
30	V	1495	0	1549	21	0
31	Y	1124	0	1193	13	0
32	Z	1765	0	1865	30	0
33	a	834	0	861	20	0
34	b	989	0	1033	20	0
35	c	2436	0	2393	36	0
36	d	1105	0	1138	17	0
37	e	523	0	573	14	0
38	f	1176	0	1232	25	0
39	h	817	0	882	20	0
40	i	419	0	415	11	0
41	k	559	0	561	14	0
42	m	950	0	987	15	0
43	n	498	0	525	5	0
44	o	616	0	600	7	0
45	p	830	0	793	18	0
46	q	754	0	773	15	0
47	r	2138	0	1930	36	0
48	s	1275	0	1316	33	0
49	t	3586	0	3735	119	0
50	u	5383	0	5085	98	0
51	v	2740	0	2251	43	0
52	w	1604	0	816	13	0
53	x	2842	0	2209	39	0
54	y	5657	0	5428	85	0
55	A	88	0	0	0	0
55	f	1	0	0	0	0
55	t	1	0	0	0	0
56	Q	1	0	0	0	0
56	k	1	0	0	0	0
56	s	1	0	0	0	0
57	t	32	0	12	0	0
58	w	8	0	8	0	0
All	All	119663	0	94829	1403	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 (1403) 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)
7:7:-8:C:H3'	7:7:-7:A:C2	1.69	1.27
7:7:-8:C:H3'	7:7:-7:A:H2	0.98	1.05
7:7:-8:C:C3'	7:7:-7:A:C2	2.47	0.97
52:w:75:C:H4'	52:w:76:A:C5	2.04	0.92
49:t:323:ALA:HA	49:t:338:GLY:H	1.36	0.91
1:1:286:PRO:HA	1:1:289:ASP:CB	2.09	0.83
7:7:-7:A:C2	7:7:-7:A:OP2	2.32	0.82
7:7:-8:C:C3'	7:7:-7:A:H2	1.85	0.81
7:7:-8:C:H5'	26:Q:42:ARG:HD3	1.66	0.78
10:A:1033:G:H1	10:A:1080:A:HO2'	1.30	0.76
10:A:1652:G:H1	10:A:1672:U:H3	1.30	0.75
47:r:195:ILE:HD11	47:r:237:MET:HE3	1.68	0.74
10:A:1729:U:H3	10:A:1805:G:H1	1.32	0.74
51:v:243:LEU:HA	51:v:247:GLN:HB3	1.68	0.73
48:s:292:GLN:HB2	48:s:308:ARG:HH12	1.53	0.73
49:t:18:GLN:HB2	49:t:38:ARG:HG3	1.70	0.72
54:y:695:ILE:HA	54:y:698:MET:HB2	1.71	0.71
48:s:292:GLN:HB3	48:s:299:PHE:HB2	1.72	0.71
45:p:63:PHE:HB3	45:p:85:LEU:HD21	1.73	0.70
33:a:59:LYS:HB2	33:a:70:TYR:HB2	1.73	0.70
1:1:283:GLU:H	50:u:703:ARG:CB	2.05	0.70
47:r:229:LEU:HA	47:r:235:TYR:HB2	1.75	0.69
49:t:92:ASP:HB2	49:t:122:GLY:HA3	1.75	0.68
7:7:-5:C:H4'	30:V:135:ARG:NH1	2.08	0.68
49:t:349:ARG:HG2	49:t:352:ARG:HH21	1.59	0.68
21:L:108:LYS:HD3	21:L:233:LEU:HD13	1.76	0.67
7:7:-3:A:N3	7:7:-3:A:H3'	2.10	0.67
10:A:1300:U:H1'	34:b:51:ARG:HH21	1.58	0.67
45:p:73:VAL:HG12	45:p:83:ILE:HG12	1.77	0.67
49:t:259:ILE:HG22	49:t:281:GLY:HA2	1.76	0.67
51:v:320:VAL:HG12	51:v:329:LEU:HD11	1.77	0.66
50:u:407:VAL:HG21	50:u:435:THR:HG21	1.77	0.66
16:G:154:ILE:HB	16:G:185:VAL:HG12	1.77	0.66
39:h:67:LYS:HG3	39:h:78:ASP:HB2	1.76	0.66
47:r:229:LEU:HG	47:r:235:TYR:HB2	1.76	0.66
50:u:567:ARG:NH1	50:u:569:LEU:O	2.28	0.65
47:r:24:VAL:HA	47:r:34:VAL:HG12	1.78	0.65
13:D:127:ARG:HD3	15:F:105:ARG:HD3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:92:ALA:HA	33:a:96:ARG:HD2	1.78	0.65
49:t:316:SER:HB2	49:t:342:LYS:HB2	1.78	0.65
7:7:-3:A:H4'	7:7:-3:A:OP1	1.96	0.65
10:A:1854:U:H2'	10:A:1855:G:H8	1.61	0.65
47:r:197:VAL:HG22	47:r:235:TYR:CZ	2.32	0.64
54:y:641:ARG:HA	54:y:652:LEU:HD21	1.79	0.64
10:A:528:A:N1	10:A:557:U:O2'	2.31	0.64
17:H:36:LYS:NZ	53:x:78:SER:OG	2.31	0.64
49:t:259:ILE:HG23	49:t:260:ARG:HG3	1.78	0.64
54:y:573:ILE:HG23	54:y:585:ALA:HB1	1.78	0.64
47:r:46:ILE:HG13	47:r:85:LEU:HB2	1.79	0.64
6:6:317:ARG:HH22	50:u:397:GLU:HB2	1.63	0.64
18:I:5:HIS:HB3	18:I:117:LEU:HD13	1.78	0.64
49:t:323:ALA:HB2	49:t:337:ILE:HA	1.79	0.63
12:C:23:LEU:HD11	13:D:6:SER:HB3	1.79	0.63
27:R:101:ILE:HD12	27:R:190:LEU:HD11	1.79	0.63
47:r:139:ASP:HB2	47:r:145:PRO:HA	1.79	0.63
10:A:851:C:H5''	10:A:852:G:H5'	1.79	0.63
49:t:157:LEU:HD23	49:t:187:ILE:HG12	1.81	0.63
32:Z:138:VAL:HG22	32:Z:184:ILE:HG12	1.80	0.63
10:A:606:G:H5''	15:F:130:ASN:HB3	1.80	0.62
45:p:58:LYS:HA	45:p:61:LYS:HB2	1.80	0.62
5:5:167:ILE:O	5:5:237:LYS:NZ	2.33	0.62
26:Q:87:ARG:NH1	26:Q:91:ALA:O	2.33	0.62
34:b:108:LYS:H	34:b:111:MET:HE3	1.62	0.62
39:h:40:ILE:HG23	39:h:50:VAL:HG11	1.82	0.62
27:R:83:TYR:HA	27:R:205:ARG:HH22	1.63	0.62
49:t:34:GLU:O	49:t:38:ARG:HB2	2.00	0.62
49:t:264:VAL:HA	52:w:76:A:H2	1.65	0.62
49:t:248:ARG:HB3	49:t:333:PRO:HG2	1.82	0.61
51:v:399:SER:HA	51:v:403:GLN:HB3	1.81	0.61
11:B:104:LYS:O	14:E:11:ARG:NH2	2.32	0.61
46:q:46:ARG:HD2	46:q:58:LEU:HD21	1.82	0.61
49:t:128:ARG:NH1	49:t:243:ILE:O	2.33	0.61
51:v:282:GLN:NE2	51:v:286:TYR:O	2.33	0.61
5:5:191:ILE:HG21	5:5:279:ARG:HE	1.65	0.61
10:A:962:A:H5''	25:P:66:ARG:HG2	1.83	0.61
50:u:105:LYS:HD2	50:u:145:LEU:HB3	1.83	0.61
12:C:11:ARG:HA	12:C:28:ALA:HB2	1.81	0.61
32:Z:16:ILE:HD11	40:i:36:LEU:HD23	1.83	0.61
10:A:943:U:H3	25:P:138:ASP:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1288:U:O4	10:A:1311:C:N3	2.33	0.61
47:r:123:LYS:HE2	47:r:126:GLN:HB2	1.83	0.61
51:v:212:THR:O	51:v:216:HIS:ND1	2.33	0.61
16:G:145:ARG:NH1	19:J:51:GLU:OE1	2.34	0.61
7:7:-8:C:C5'	26:Q:42:ARG:HD3	2.30	0.61
10:A:1033:G:N1	10:A:1080:A:O2'	2.27	0.61
10:A:1760:G:H21	10:A:1772:C:H5''	1.66	0.61
29:T:86:GLU:OE2	29:T:90:ARG:NH2	2.33	0.61
38:f:86:ARG:NH2	38:f:89:ASP:OD1	2.33	0.61
6:6:313:ILE:HD11	50:u:446:ILE:HD13	1.83	0.60
10:A:1076:G:H5''	18:I:106:ARG:HH22	1.66	0.60
10:A:1282:A:OP2	42:m:102:LYS:NZ	2.34	0.60
35:c:8:ARG:HE	35:c:311:GLN:HB3	1.64	0.60
49:t:283:ILE:HB	49:t:333:PRO:HA	1.83	0.60
1:1:546:ILE:HB	1:1:557:ASP:HB2	1.82	0.60
10:A:878:G:H1	10:A:908:A:H61	1.49	0.60
10:A:1124:C:H5''	24:O:150:ILE:HG12	1.84	0.60
10:A:1396:A:O2'	10:A:1398:G:N7	2.32	0.60
10:A:1541:G:N3	36:d:12:GLN:NE2	2.49	0.60
50:u:529:VAL:HA	50:u:532:LYS:HB3	1.83	0.60
32:Z:28:GLU:HG2	32:Z:69:LEU:HD21	1.84	0.60
49:t:68:ARG:NH1	52:w:75:C:O2	2.34	0.60
47:r:132:GLN:HA	47:r:136:TRP:HB2	1.82	0.60
49:t:60:ALA:HB1	49:t:229:LYS:HG2	1.83	0.60
34:b:18:ARG:HD2	38:f:88:LYS:HG2	1.83	0.60
10:A:746:C:N4	10:A:797:C:O2	2.35	0.60
10:A:1825:A:N6	46:q:65:LEU:O	2.35	0.59
13:D:91:LYS:HE3	13:D:96:TYR:HD2	1.67	0.59
50:u:452:PHE:HE1	50:u:491:LEU:HD23	1.67	0.59
10:A:350:C:HO2'	10:A:383:G:H1	1.50	0.59
10:A:1488:C:O2'	10:A:1490:G:OP2	2.18	0.59
23:N:77:ILE:HG12	23:N:99:ILE:HB	1.83	0.59
1:1:507:ARG:HD3	1:1:556:VAL:HG11	1.84	0.59
48:s:219:PHE:HB3	48:s:256:LEU:HB3	1.83	0.59
1:1:565:ILE:HD11	1:1:579:VAL:HB	1.85	0.59
35:c:206:LEU:HD12	35:c:218:LEU:HD23	1.84	0.59
10:A:553:U:O4	10:A:555:A:N6	2.36	0.59
10:A:922:A:OP2	19:J:28:ARG:NH1	2.35	0.59
10:A:1597:C:OP2	37:e:85:ARG:NH2	2.36	0.59
10:A:1864:U:OP2	26:Q:5:ARG:NH2	2.36	0.59
17:H:80:ARG:NH2	53:x:77:GLU:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:28:LYS:NZ	25:P:51:GLU:OE1	2.36	0.59
10:A:1228:A:H2'	10:A:1229:G:H8	1.66	0.59
38:f:49:ASP:OD1	38:f:66:ARG:NH1	2.36	0.59
32:Z:15:GLY:HA3	40:i:50:ILE:HG23	1.85	0.59
50:u:411:LEU:HD11	50:u:428:VAL:HG13	1.82	0.59
2:2:125:PHE:HA	2:2:139:TYR:H	1.67	0.59
10:A:874:G:H2'	10:A:875:A:H8	1.66	0.58
50:u:208:ILE:O	50:u:212:HIS:ND1	2.35	0.58
54:y:667:ARG:HH11	54:y:669:ARG:HH12	1.51	0.58
10:A:962:A:N1	10:A:1055:A:O2'	2.35	0.58
45:p:56:LYS:HB2	45:p:59:LEU:HG	1.85	0.58
49:t:320:SER:HB2	49:t:322:PHE:CZ	2.39	0.58
10:A:1237:C:O2'	10:A:1522:A:N6	2.36	0.58
24:O:110:MET:HE1	24:O:140:VAL:HG11	1.84	0.58
30:V:71:ARG:NH2	30:V:148:ASN:OD1	2.37	0.58
45:p:69:CYS:SG	45:p:89:GLN:NE2	2.77	0.58
51:v:262:ILE:HD11	51:v:296:VAL:HG21	1.85	0.58
10:A:617:G:N7	14:E:67:ARG:NH1	2.51	0.58
10:A:1854:U:OP1	25:P:150:ARG:NH1	2.36	0.58
34:b:81:ARG:NH2	34:b:117:GLY:O	2.36	0.58
35:c:202:PRO:HG3	35:c:243:PRO:HA	1.84	0.58
10:A:4:C:H4'	21:L:207:ALA:HB2	1.86	0.58
25:P:121:ARG:NH1	26:Q:52:ASP:OD2	2.37	0.58
47:r:126:GLN:OE1	47:r:133:ARG:NH2	2.36	0.58
51:v:197:ASP:HA	51:v:211:ARG:HH21	1.68	0.58
1:1:505:ARG:NH1	1:1:554:VAL:O	2.36	0.58
1:1:529:LYS:HE2	1:1:565:ILE:HG21	1.85	0.58
49:t:156:LEU:HD21	49:t:239:ILE:HD11	1.85	0.58
13:D:149:VAL:HG11	13:D:157:ILE:HD11	1.86	0.58
21:L:70:VAL:HG21	21:L:93:ILE:HG23	1.86	0.58
10:A:663:C:O2'	21:L:227:ARG:NH2	2.37	0.58
10:A:1166:G:H1	10:A:1193:U:H3	1.50	0.58
23:N:127:PRO:HG2	23:N:152:SER:HB3	1.85	0.58
10:A:1277:C:H2'	10:A:1278:A:H8	1.69	0.57
10:A:1513:C:H2'	10:A:1514:G:H8	1.68	0.57
12:C:45:ILE:HA	12:C:61:VAL:HG11	1.85	0.57
21:L:70:VAL:HG11	21:L:93:ILE:HG12	1.84	0.57
10:A:1291:A:O2'	41:k:140:TYR:OH	2.12	0.57
10:A:1830:UR3:H6	10:A:1831:A:H62	1.68	0.57
23:N:51:LEU:HA	23:N:54:THR:HG22	1.86	0.57
42:m:99:LYS:O	42:m:101:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1156:U:OP1	19:J:71:LYS:NZ	2.37	0.57
25:P:57:THR:H	25:P:60:MET:HG3	1.68	0.57
30:V:168:THR:OG1	30:V:171:GLU:OE1	2.20	0.57
44:o:246:LEU:HD22	44:o:250:THR:HG21	1.87	0.57
53:x:452:VAL:HG22	53:x:465:ILE:HG22	1.86	0.57
17:H:23:ARG:O	19:J:60:LYS:NZ	2.37	0.57
51:v:398:VAL:HA	54:y:846:ARG:HH22	1.69	0.57
4:4:280:GLN:O	50:u:532:LYS:NZ	2.36	0.57
10:A:54:A:OP1	29:T:111:LYS:NZ	2.38	0.57
38:f:48:ALA:HB1	38:f:66:ARG:HH11	1.69	0.57
48:s:200:ARG:O	48:s:272:ARG:NH1	2.37	0.57
50:u:106:GLU:O	50:u:109:GLN:NE2	2.37	0.57
54:y:593:HIS:O	54:y:597:ASN:ND2	2.36	0.57
10:A:1759:G:N2	10:A:1772:C:OP2	2.36	0.57
21:L:213:LEU:HD23	21:L:240:THR:HG23	1.87	0.57
24:O:196:ASP:OD2	50:u:23:LYS:NZ	2.37	0.57
54:y:683:GLU:HG3	54:y:733:MET:HE3	1.86	0.57
49:t:372:GLU:HG2	49:t:426:LYS:HD3	1.86	0.57
10:A:56:G:OP2	29:T:115:LYS:NZ	2.34	0.57
47:r:199:CYS:HA	47:r:267:GLY:HA3	1.87	0.57
49:t:323:ALA:CB	49:t:337:ILE:HA	2.35	0.57
50:u:398:PHE:HB3	50:u:511:LEU:HB3	1.86	0.57
4:4:92:VAL:HA	4:4:129:VAL:H	1.69	0.57
50:u:118:LEU:HD23	50:u:120:ASN:H	1.70	0.57
8:8:69:GLY:HA3	8:8:78:ILE:HA	1.86	0.56
10:A:1086:G:OP2	26:Q:12:LYS:NZ	2.37	0.56
5:5:367:MET:HA	5:5:370:LEU:HB2	1.87	0.56
10:A:1722:G:H1	10:A:1812:U:H3	1.53	0.56
13:D:170:PRO:O	13:D:175:ARG:NH1	2.38	0.56
35:c:124:SER:OG	35:c:126:ASP:OD1	2.21	0.56
48:s:289:THR:HG22	48:s:302:CYS:HA	1.87	0.56
54:y:743:ALA:HA	54:y:746:MET:HG2	1.86	0.56
10:A:1677:U:H2'	10:A:1678:A2M:H8	1.87	0.56
47:r:204:GLY:N	49:t:342:LYS:O	2.36	0.56
49:t:147:ASN:HD21	49:t:412:SER:HG	1.53	0.56
50:u:55:LEU:HD13	50:u:93:TYR:HB2	1.88	0.56
50:u:268:LYS:HD3	50:u:269:PRO:HD2	1.87	0.56
10:A:1244:U:H2'	10:A:1245:G:H8	1.70	0.56
10:A:1854:U:OP2	25:P:147:ARG:NH2	2.38	0.56
19:J:110:ILE:HD12	19:J:126:LEU:HD11	1.87	0.56
49:t:278:VAL:HG22	49:t:340:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:u:503:GLU:HG2	50:u:505:ALA:H	1.71	0.56
54:y:263:THR:O	54:y:267:LYS:N	2.38	0.56
10:A:834:C:O2'	10:A:836:G:N1	2.38	0.56
11:B:21:LYS:NZ	27:R:157:LYS:O	2.39	0.56
49:t:367:ILE:O	49:t:464:THR:OG1	2.22	0.56
10:A:1566:G:OP2	36:d:102:ARG:NH2	2.36	0.56
39:h:31:SER:HB2	39:h:107:GLU:HG2	1.88	0.56
50:u:372:ASN:HA	50:u:375:VAL:HG22	1.87	0.56
5:5:201:ARG:HB3	5:5:426:PRO:HG2	1.88	0.56
10:A:1036:A:N3	10:A:1844:U:O2'	2.38	0.56
30:V:55:ARG:NH2	31:Y:123:ASP:OD1	2.38	0.56
32:Z:40:ARG:NH2	32:Z:47:GLU:OE1	2.39	0.56
49:t:102:TYR:OH	49:t:241:LYS:NZ	2.37	0.56
21:L:64:THR:HG23	21:L:67:GLY:H	1.70	0.56
48:s:302:CYS:SG	48:s:303:GLU:N	2.79	0.56
1:1:520:GLN:NE2	1:1:574:GLY:O	2.39	0.56
10:A:844:U:H2'	10:A:845:G:H8	1.71	0.56
13:D:18:ARG:O	13:D:24:ARG:NH1	2.39	0.56
37:e:90:GLU:HG2	37:e:94:LYS:HE3	1.88	0.56
50:u:447:TYR:HD2	50:u:450:ILE:HG12	1.71	0.56
51:v:218:SER:O	51:v:229:ARG:NH2	2.39	0.56
3:3:87:CYS:HA	5:5:446:VAL:HG21	1.87	0.55
10:A:1445:U:H4'	39:h:57:PRO:HG3	1.87	0.55
13:D:54:ARG:NH2	21:L:200:ARG:O	2.33	0.55
16:G:69:LEU:HD22	16:G:96:ALA:HB2	1.88	0.55
35:c:24:THR:HG23	35:c:27:PHE:H	1.71	0.55
37:e:101:SER:HB3	37:e:108:ILE:HD12	1.88	0.55
5:5:380:MET:HE1	5:5:516:ALA:HB3	1.89	0.55
6:6:243:ILE:O	6:6:340:ARG:NH1	2.39	0.55
10:A:1615:U:O4	34:b:40:ARG:NH2	2.38	0.55
23:N:80:ARG:NH2	23:N:165:ASN:O	2.39	0.55
51:v:298:CYS:SG	51:v:299:LEU:N	2.78	0.55
54:y:44:ASP:OD1	54:y:47:ARG:NH2	2.39	0.55
54:y:667:ARG:O	54:y:670:GLN:NE2	2.39	0.55
2:2:303:GLY:HA2	2:2:309:VAL:HA	1.87	0.55
5:5:394:TYR:HB3	5:5:397:LYS:HB2	1.88	0.55
10:A:322:C:N4	10:A:323:C:O2	2.39	0.55
11:B:59:LYS:HD3	11:B:134:LEU:HB3	1.89	0.55
24:O:29:ASP:OD1	24:O:51:ARG:NH2	2.39	0.55
34:b:44:ARG:NH1	34:b:82:ASP:O	2.40	0.55
47:r:133:ARG:HD2	47:r:168:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:360:ASN:HA	6:6:363:LYS:HE3	1.89	0.55
10:A:303:C:O2	27:R:184:ARG:NH1	2.38	0.55
50:u:489:ARG:NH2	54:y:805:GLU:OE2	2.40	0.55
32:Z:134:CYS:SG	32:Z:135:GLU:N	2.79	0.55
1:1:283:GLU:N	50:u:703:ARG:CB	2.69	0.55
6:6:360:ASN:ND2	8:8:348:GLN:O	2.39	0.55
10:A:868:G:OP2	10:A:868:G:N2	2.34	0.55
10:A:1678:A2M:OP2	30:V:63:LYS:NZ	2.40	0.55
29:T:5:VAL:O	29:T:43:LYS:NZ	2.39	0.55
30:V:34:SER:HA	43:n:55:VAL:HG23	1.88	0.55
50:u:476:ARG:NH1	54:y:794:THR:O	2.40	0.55
7:7:6:A:N6	46:q:64:LYS:O	2.39	0.55
10:A:1589:A:N3	10:A:1653:U:O2'	2.39	0.55
12:C:37:LYS:HB2	12:C:40:GLU:HG2	1.88	0.55
49:t:89:TYR:HB3	49:t:124:PHE:HB3	1.88	0.55
49:t:322:PHE:HD1	49:t:327:ASP:HA	1.70	0.55
50:u:329:ILE:O	50:u:367:ARG:NH1	2.40	0.55
10:A:1209:A:O2'	26:Q:85:ARG:NH1	2.39	0.55
10:A:1550:G:H3'	10:A:1579:A:H61	1.72	0.55
14:E:140:ARG:HE	14:E:141:PRO:HD2	1.71	0.55
52:w:75:C:H5'	52:w:76:A:C2	2.42	0.55
10:A:973:C:N3	25:P:55:ARG:NH2	2.54	0.55
10:A:1232:U:H3	10:A:1526:G:H1	1.54	0.55
49:t:262:PHE:CZ	52:w:76:A:H5'	2.42	0.55
54:y:603:PRO:HA	54:y:606:GLN:HB2	1.89	0.55
7:7:-7:A:OP2	7:7:-7:A:N3	2.40	0.55
10:A:1232:U:H2'	10:A:1233:G:H8	1.72	0.55
49:t:87:LYS:NZ	49:t:111:ASP:OD1	2.40	0.55
52:w:71:C:H2'	52:w:72:U:H4'	1.89	0.55
32:Z:64:ARG:NH1	33:a:93:THR:OG1	2.40	0.54
53:x:448:LYS:HG2	53:x:470:GLN:HG2	1.89	0.54
18:I:136:PRO:HG2	18:I:139:TRP:HB2	1.89	0.54
32:Z:35:SER:HB2	32:Z:51:LEU:HB3	1.88	0.54
10:A:433:A:H5''	27:R:22:HIS:HB3	1.89	0.54
10:A:589:G:N1	15:F:97:GLU:OE2	2.38	0.54
10:A:925:G:H1	10:A:1017:U:H3	1.55	0.54
10:A:1114:U:O2'	10:A:1119:A:N6	2.40	0.54
10:A:1228:A:H2'	10:A:1229:G:C8	2.41	0.54
12:C:124:CYS:HB3	12:C:141:THR:HB	1.90	0.54
22:M:99:ASP:OD2	23:N:42:LYS:NZ	2.39	0.54
10:A:604:A:N3	10:A:639:C:O2'	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1424:G:H2'	10:A:1425:G:H8	1.72	0.54
33:a:96:ARG:O	33:a:98:ARG:NH1	2.41	0.54
54:y:627:LYS:HA	54:y:693:LEU:HD21	1.87	0.54
5:5:183:LEU:HD22	5:5:269:LEU:HD13	1.89	0.54
10:A:823:PSU:N3	13:D:143:ASN:OD1	2.36	0.54
20:K:38:GLU:OE2	20:K:49:GLN:NE2	2.41	0.54
28:S:18:VAL:HG21	28:S:24:LEU:HD21	1.90	0.54
39:h:28:ASN:OD1	39:h:31:SER:OG	2.25	0.54
10:A:570:C:O2'	29:T:34:THR:O	2.22	0.54
10:A:1032:C:H5''	18:I:109:LYS:HD2	1.89	0.54
13:D:110:LEU:HB2	13:D:147:PHE:HB3	1.89	0.54
39:h:24:LEU:HB3	39:h:32:LEU:HD11	1.90	0.54
49:t:8:VAL:H	49:t:19:ASP:HA	1.72	0.54
53:x:317:THR:O	53:x:321:HIS:ND1	2.39	0.54
7:7:-10:A:H2'	7:7:-9:A:C5	2.43	0.54
10:A:28:U:H2'	10:A:29:G:H8	1.73	0.54
10:A:864:A:H2'	10:A:865:A:H8	1.72	0.54
10:A:1622:U:OP1	38:f:120:HIS:ND1	2.40	0.54
17:H:21:LYS:NZ	18:I:13:GLN:OE1	2.38	0.54
49:t:44:ILE:HD13	49:t:239:ILE:HD12	1.90	0.54
10:A:43:U:OP2	10:A:485:A:N6	2.36	0.54
10:A:681:U:H4'	14:E:9:THR:HG22	1.89	0.54
10:A:1541:G:OP1	36:d:56:ARG:NE	2.40	0.54
11:B:38:LYS:NZ	11:B:64:GLY:O	2.41	0.54
20:K:33:GLN:HE22	21:L:261:PHE:HB3	1.73	0.54
54:y:762:ASN:OD1	54:y:776:ARG:NH1	2.41	0.54
5:5:328:ARG:HA	5:5:499:ASN:HD21	1.73	0.54
22:M:54:VAL:HG12	22:M:58:MET:HE2	1.90	0.54
25:P:145:GLY:O	26:Q:22:ARG:NH2	2.36	0.54
48:s:295:THR:O	48:s:296:ARG:C	2.50	0.54
1:1:387:TYR:HA	1:1:408:ASP:HA	1.89	0.53
10:A:507:G:O6	29:T:105:LYS:NZ	2.39	0.53
47:r:26:SER:HB2	47:r:33:TYR:HB2	1.89	0.53
1:1:529:LYS:HE3	1:1:542:THR:HB	1.90	0.53
10:A:546:G:N2	10:A:547:G:O6	2.35	0.53
24:O:175:GLU:O	24:O:179:ASN:ND2	2.41	0.53
10:A:1160:U:O4	14:E:2:GLY:N	2.40	0.53
10:A:1376:A:OP2	22:M:67:ARG:NH1	2.33	0.53
10:A:1433:C:O2	39:h:19:ARG:NH2	2.41	0.53
19:J:44:HIS:NE2	19:J:112:ASP:OD2	2.40	0.53
44:o:243:VAL:HB	44:o:283:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:18:ARG:HG2	9:9:22:GLN:HE22	1.72	0.53
10:A:1101:U:H2'	10:A:1102:G:H8	1.74	0.53
35:c:79:LEU:HD11	35:c:87:LEU:HD23	1.91	0.53
49:t:7:GLY:N	49:t:329:GLN:OE1	2.40	0.53
49:t:264:VAL:HG12	52:w:76:A:N3	2.23	0.53
10:A:643:A:OP1	13:D:38:ARG:NH1	2.41	0.53
45:p:34:ARG:NH1	48:s:317:GLY:O	2.41	0.53
47:r:71:VAL:HG21	47:r:85:LEU:HD13	1.90	0.53
51:v:212:THR:OG1	51:v:247:GLN:OE1	2.21	0.53
10:A:1528:G:O2'	10:A:1666:C:OP1	2.26	0.53
34:b:123:TYR:OH	38:f:124:ARG:NH1	2.40	0.53
35:c:152:SER:H	35:c:169:GLY:HA2	1.72	0.53
49:t:43:ASN:HB2	49:t:153:ASP:H	1.74	0.53
10:A:1862:G:H22	26:Q:76:SER:HB2	1.74	0.53
16:G:142:LYS:HB3	19:J:54:ASP:HB3	1.90	0.53
17:H:21:LYS:HA	17:H:26:GLN:HG2	1.91	0.53
39:h:41:ARG:HH21	39:h:44:LYS:HG3	1.74	0.53
48:s:177:GLU:HA	48:s:180:LEU:HD12	1.91	0.53
10:A:928:G:H2'	10:A:929:G:C8	2.44	0.53
32:Z:193:ASP:OD1	32:Z:193:ASP:N	2.42	0.53
47:r:228:ASN:HA	49:t:268:GLY:HA2	1.91	0.53
49:t:396:GLN:OE1	49:t:445:ARG:NH1	2.41	0.53
10:A:377:G:H5'	27:R:98:LYS:HB3	1.91	0.53
10:A:482:G:N1	10:A:485:A:OP2	2.42	0.53
10:A:1292:C:H42	41:k:138:ARG:HH21	1.57	0.53
49:t:187:ILE:HG21	49:t:207:ILE:HG21	1.90	0.53
49:t:255:ARG:HD2	49:t:285:LYS:HE3	1.91	0.53
50:u:473:ASP:O	50:u:477:HIS:ND1	2.42	0.53
54:y:687:LEU:HD12	54:y:733:MET:HE1	1.90	0.53
35:c:163:PRO:HB2	35:c:179:LEU:HD23	1.90	0.52
36:d:36:THR:O	38:f:39:ARG:NH2	2.39	0.52
49:t:366:GLU:OE1	49:t:464:THR:OG1	2.27	0.52
5:5:178:LEU:HB3	5:5:182:TRP:HD1	1.74	0.52
10:A:453:C:O2'	28:S:92:ARG:O	2.25	0.52
10:A:1648:G:O2'	10:A:1674:G:O6	2.26	0.52
50:u:384:VAL:HB	50:u:387:VAL:HG22	1.91	0.52
16:G:184:ASP:OD1	16:G:184:ASP:N	2.42	0.52
48:s:175:THR:OG1	49:t:98:ARG:NH1	2.43	0.52
14:E:40:PRO:O	14:E:77:ASN:ND2	2.42	0.52
24:O:224:GLU:HG2	24:O:227:LYS:H	1.74	0.52
28:S:10:THR:HB	28:S:128:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:63:ARG:NH1	43:n:64:GLU:O	2.42	0.52
50:u:415:ARG:HD3	50:u:428:VAL:HG11	1.90	0.52
48:s:294:ASP:OD2	48:s:299:PHE:CE1	2.63	0.52
49:t:108:SER:HA	49:t:325:HIS:HE1	1.73	0.52
10:A:383:G:H21	11:B:133:PRO:HG2	1.73	0.52
10:A:844:U:OP1	12:C:240:ARG:NH2	2.43	0.52
42:m:81:ASP:HB3	42:m:84:LYS:HB2	1.92	0.52
54:y:413:PHE:HE1	54:y:489:TYR:HB2	1.73	0.52
26:Q:32:LYS:O	26:Q:37:LYS:NZ	2.39	0.52
35:c:249:CYS:SG	35:c:291:TRP:NE1	2.83	0.52
38:f:36:VAL:HG21	38:f:71:MET:HE2	1.91	0.52
49:t:88:ILE:HG12	49:t:104:SER:HB3	1.91	0.52
5:5:216:ARG:NH2	5:5:429:ASP:OD1	2.42	0.52
10:A:734:C:O2'	10:A:736:C:N4	2.42	0.52
2:2:173:TYR:HA	2:2:180:VAL:HA	1.91	0.52
10:A:521:A:OP1	13:D:45:ARG:NH1	2.36	0.52
10:A:1092:G:OP1	18:I:2:GLY:N	2.43	0.52
22:M:17:ILE:HD11	22:M:54:VAL:HG13	1.92	0.52
37:e:72:VAL:HA	37:e:75:GLU:HG2	1.92	0.52
50:u:563:LYS:O	50:u:572:ARG:NH2	2.43	0.52
41:k:133:ALA:HB3	41:k:140:TYR:HB3	1.92	0.52
47:r:229:LEU:HD22	49:t:274:LEU:HD21	1.92	0.52
10:A:531:A:N1	10:A:552:G:C6	2.78	0.51
14:E:58:GLU:OE2	14:E:58:GLU:N	2.44	0.51
28:S:152:ASP:OD1	28:S:152:ASP:N	2.43	0.51
50:u:300:TYR:HB2	50:u:322:VAL:HG21	1.92	0.51
54:y:386:ASN:ND2	54:y:391:THR:OG1	2.43	0.51
54:y:622:ARG:HH12	54:y:770:PRO:HD2	1.75	0.51
23:N:118:GLU:N	23:N:118:GLU:OE2	2.44	0.51
24:O:107:ARG:NH1	25:P:133:THR:O	2.33	0.51
32:Z:62:LYS:O	32:Z:67:ARG:NH2	2.43	0.51
38:f:20:ILE:HD11	38:f:33:ILE:HD11	1.92	0.51
38:f:98:VAL:HG11	38:f:106:LYS:HG3	1.92	0.51
4:4:350:LEU:HA	5:5:560:MET:HE1	1.92	0.51
6:6:328:THR:HG23	6:6:329:GLN:HG3	1.91	0.51
10:A:21:U:O2'	13:D:17:ARG:O	2.26	0.51
10:A:1452:A:O2'	10:A:1475:G:N2	2.43	0.51
10:A:1543:U:O2'	31:Y:43:GLU:OE2	2.27	0.51
19:J:80:ASP:N	19:J:80:ASP:OD1	2.43	0.51
22:M:108:LEU:HD13	23:N:39:TYR:HE1	1.75	0.51
49:t:42:ILE:HD12	49:t:246:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:x:51:GLN:O	53:x:53:LYS:NZ	2.42	0.51
53:x:304:ASN:OD1	53:x:311:ASN:ND2	2.40	0.51
5:5:388:LEU:HA	5:5:391:ARG:HB2	1.92	0.51
10:A:393:U:H3'	54:y:150:ARG:HH12	1.75	0.51
10:A:1277:C:H2'	10:A:1278:A:C8	2.46	0.51
45:p:56:LYS:HE3	45:p:58:LYS:HG3	1.92	0.51
47:r:133:ARG:NH1	47:r:172:GLU:OE2	2.43	0.51
50:u:96:MET:HA	50:u:99:GLU:HB3	1.91	0.51
9:9:21:ARG:NH1	10:A:1718:G:OP1	2.43	0.51
10:A:1780:G:O6	10:A:1782:G:N2	2.43	0.51
25:P:33:ILE:HD13	25:P:95:ILE:HG23	1.92	0.51
31:Y:19:ALA:HB2	31:Y:75:GLY:HA3	1.93	0.51
36:d:85:ASN:HB2	36:d:88:MET:HB2	1.91	0.51
45:p:27:THR:HG21	45:p:31:ILE:HD11	1.93	0.51
5:5:299:LEU:O	5:5:316:TYR:OH	2.27	0.51
10:A:1190:A:N3	10:A:1714:U:O2'	2.40	0.51
10:A:1829:G:OP1	45:p:86:GLN:NE2	2.43	0.51
12:C:44:LEU:HD13	12:C:72:ILE:HD11	1.93	0.51
16:G:148:LEU:HA	19:J:42:MET:HE2	1.92	0.51
20:K:56:CYS:SG	20:K:57:GLY:N	2.84	0.51
29:T:23:MET:HE1	29:T:44:LEU:HD11	1.93	0.51
34:b:62:LYS:HA	34:b:65:LYS:HE3	1.93	0.51
49:t:157:LEU:O	49:t:188:LEU:N	2.37	0.51
5:5:195:GLN:HG2	5:5:421:LEU:HD21	1.93	0.51
6:6:249:LEU:HD11	6:6:301:LEU:HD23	1.91	0.51
10:A:1656:G:H1	10:A:1668:U:H3	1.59	0.51
22:M:19:LYS:HD3	32:Z:213:PRO:HD3	1.92	0.51
53:x:291:VAL:HG11	53:x:399:TRP:HE1	1.75	0.51
26:Q:51:ARG:HE	43:n:40:ARG:HE	1.56	0.51
32:Z:75:LYS:HZ3	33:a:21:MET:HA	1.76	0.51
35:c:138:CYS:SG	35:c:141:THR:OG1	2.68	0.51
50:u:602:GLN:O	50:u:606:LYS:N	2.43	0.51
1:1:668:THR:O	1:1:682:TRP:N	2.42	0.51
10:A:1285:G:OP2	42:m:61:TYR:OH	2.25	0.51
10:A:1336:C:O3'	40:i:44:ARG:NH2	2.44	0.51
10:A:1398:G:O2'	35:c:88:ARG:NH2	2.41	0.51
35:c:94:THR:HG23	35:c:96:THR:H	1.76	0.51
50:u:155:GLU:OE2	50:u:158:ARG:NH1	2.44	0.51
10:A:663:C:OP2	14:E:3:LYS:NZ	2.35	0.50
10:A:664:A:O2'	10:A:670:A:N1	2.42	0.50
10:A:1130:G:N2	10:A:1130:G:OP2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:M:37:GLU:OE1	35:c:106:LYS:NZ	2.32	0.50
51:v:342:GLU:HG3	51:v:346:ARG:HH22	1.74	0.50
54:y:820:SER:O	54:y:823:SER:OG	2.27	0.50
10:A:885:U:H3	10:A:901:G:H1	1.59	0.50
10:A:1231:C:O2'	10:A:1253:A:N6	2.44	0.50
12:C:54:TYR:O	29:T:15:ASN:ND2	2.44	0.50
31:Y:34:VAL:HG12	31:Y:70:VAL:HB	1.93	0.50
32:Z:106:ARG:HG3	32:Z:175:VAL:HG22	1.93	0.50
35:c:220:ASP:HB2	35:c:227:LEU:HD11	1.93	0.50
1:1:637:PHE:O	1:1:646:MET:N	2.40	0.50
5:5:247:TYR:HD1	5:5:253:PRO:HG3	1.77	0.50
10:A:1262:C:O2	40:i:17:GLY:N	2.40	0.50
20:K:32:ILE:HD12	20:K:34:MET:HB2	1.94	0.50
50:u:31:LEU:HD22	50:u:50:ILE:HG23	1.93	0.50
5:5:501:VAL:N	5:5:512:GLU:O	2.45	0.50
6:6:312:VAL:HG11	6:6:325:ILE:HD13	1.93	0.50
10:A:531:A:N1	10:A:552:G:O6	2.45	0.50
16:G:46:THR:HG23	16:G:65:PRO:HD3	1.93	0.50
33:a:15:LEU:HG	33:a:71:LEU:HD22	1.94	0.50
39:h:98:VAL:HA	39:h:101:ILE:HB	1.93	0.50
48:s:292:GLN:HB2	48:s:308:ARG:NH1	2.25	0.50
1:1:283:GLU:C	1:1:285:GLN:H	2.17	0.50
10:A:659:G:HO2'	10:A:662:G:HO2'	1.59	0.50
10:A:1047:C:H5'	25:P:143:LYS:HB2	1.93	0.50
27:R:176:ALA:H	27:R:187:GLY:HA2	1.76	0.50
50:u:98:GLU:OE1	50:u:157:TYR:OH	2.29	0.50
10:A:1722:G:N2	10:A:1812:U:O2	2.42	0.50
13:D:106:LEU:HD23	13:D:109:ARG:HD2	1.93	0.50
25:P:101:GLY:HA3	25:P:134:PRO:HG2	1.94	0.50
30:V:61:PHE:CE2	43:n:51:ARG:HG3	2.46	0.50
38:f:33:ILE:HD12	38:f:71:MET:HE1	1.94	0.50
41:k:103:LEU:O	41:k:107:LYS:NZ	2.40	0.50
49:t:189:GLN:O	49:t:224:ILE:N	2.44	0.50
10:A:625:G:N1	14:E:64:SER:O	2.39	0.50
21:L:166:ARG:HD3	21:L:181:PRO:HG3	1.93	0.50
25:P:98:ARG:HH21	25:P:134:PRO:HG3	1.77	0.50
49:t:256:LEU:O	49:t:358:LEU:N	2.43	0.50
50:u:517:GLU:HA	50:u:520:ARG:HE	1.75	0.50
10:A:5:U:H2'	10:A:6:G:H8	1.76	0.50
10:A:106:C:H2'	10:A:107:A:H8	1.77	0.50
10:A:350:C:O2'	10:A:383:G:N1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1360:U:O2'	10:A:1379:A:OP2	2.29	0.50
24:O:28:LYS:HD3	24:O:48:LEU:HD13	1.94	0.50
33:a:24:LYS:O	33:a:42:ASN:ND2	2.45	0.50
45:p:36:GLN:HG2	48:s:245:GLY:HA3	1.94	0.50
47:r:126:GLN:OE1	47:r:129:SER:OG	2.29	0.50
48:s:328:LEU:HB2	48:s:331:LYS:HG2	1.94	0.50
49:t:139:ASP:O	49:t:452:ARG:NH1	2.45	0.50
14:E:93:PHE:O	14:E:140:ARG:NH1	2.45	0.50
25:P:126:ILE:N	26:Q:56:ALA:O	2.43	0.50
39:h:20:ILE:HG21	39:h:98:VAL:HG21	1.93	0.50
47:r:36:LEU:HD11	47:r:83:ILE:HG21	1.94	0.50
51:v:252:HIS:CE1	51:v:255:ARG:HH21	2.30	0.50
1:1:575:SER:OG	1:1:594:VAL:O	2.29	0.49
10:A:1143:A:OP2	21:L:187:ARG:NH2	2.44	0.49
10:A:1465:A:OP1	22:M:56:HIS:NE2	2.42	0.49
33:a:16:PHE:HE2	33:a:89:ILE:HG23	1.77	0.49
42:m:15:ASN:HA	42:m:18:LEU:HD12	1.93	0.49
52:w:72:U:H2'	52:w:73:A:C8	2.47	0.49
33:a:15:LEU:HD22	33:a:49:MET:HE3	1.93	0.49
50:u:272:MET:HA	50:u:275:TYR:HB3	1.94	0.49
10:A:71:G:O6	28:S:170:ARG:NH1	2.45	0.49
10:A:696:G:H4'	10:A:697:G:H5'	1.94	0.49
10:A:1310:U:H4'	41:k:143:LYS:HB2	1.95	0.49
22:M:106:LEU:HD23	22:M:109:LEU:HD23	1.94	0.49
41:k:133:ALA:N	41:k:140:TYR:O	2.33	0.49
50:u:384:VAL:HG12	50:u:386:GLU:H	1.77	0.49
51:v:209:GLN:HA	51:v:212:THR:HG22	1.93	0.49
5:5:456:GLN:O	5:5:459:THR:OG1	2.29	0.49
10:A:167:G:O3'	28:S:131:ARG:NH2	2.46	0.49
12:C:102:ILE:HD12	12:C:239:PRO:HD3	1.94	0.49
32:Z:23:GLU:OE2	32:Z:27:ARG:NE	2.41	0.49
35:c:11:LEU:HB2	35:c:307:VAL:HB	1.94	0.49
54:y:592:SER:HB2	54:y:594:LEU:HD23	1.94	0.49
10:A:197:U:OP2	10:A:203:G:N2	2.43	0.49
10:A:562:U:H2'	10:A:563:G:C8	2.48	0.49
10:A:940:U:H3	10:A:1002:U:H3	1.60	0.49
10:A:1093:A:H5''	19:J:28:ARG:HH22	1.76	0.49
13:D:78:LEU:HD23	13:D:97:ILE:HD11	1.94	0.49
19:J:91:ASN:O	21:L:183:LYS:NZ	2.44	0.49
47:r:227:ILE:HA	47:r:237:MET:SD	2.52	0.49
54:y:562:ASP:OD1	54:y:565:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:238:SER:O	5:5:243:GLN:NE2	2.46	0.49
10:A:693:A:H2'	10:A:694:G:C8	2.48	0.49
10:A:1541:G:H5''	36:d:59:SER:HB2	1.93	0.49
18:I:46:THR:HG22	18:I:48:SER:H	1.77	0.49
21:L:168:GLY:N	21:L:179:THR:O	2.37	0.49
27:R:43:ILE:HG12	27:R:57:ALA:HA	1.95	0.49
49:t:8:VAL:HG13	49:t:17:ARG:HD3	1.94	0.49
53:x:318:TYR:O	53:x:322:ASN:ND2	2.45	0.49
8:8:150:LEU:HA	8:8:166:ALA:HA	1.94	0.49
10:A:1562:C:H2'	10:A:1563:G:H8	1.77	0.49
10:A:1605:G:OP1	36:d:84:ARG:NH2	2.45	0.49
28:S:57:ASP:OD1	28:S:58:LYS:N	2.42	0.49
36:d:114:GLU:N	36:d:114:GLU:OE1	2.45	0.49
46:q:34:GLU:OE2	46:q:53:ASP:N	2.42	0.49
10:A:379:C:O2	27:R:5:ARG:NE	2.44	0.49
11:B:135:SER:OG	11:B:136:LYS:N	2.46	0.49
23:N:42:LYS:HZ1	23:N:48:ILE:HD11	1.77	0.49
26:Q:37:LYS:HB3	26:Q:70:LYS:HE2	1.95	0.49
3:3:37:ALA:HA	3:3:41:ALA:HB3	1.94	0.49
5:5:49:PRO:HD2	5:5:52:ILE:HD12	1.93	0.49
5:5:118:ILE:HG23	5:5:121:GLN:HE21	1.77	0.49
5:5:171:ASP:O	5:5:260:TYR:OH	2.30	0.49
10:A:472:C:O2	10:A:475:C:N4	2.46	0.49
10:A:588:G:H4'	10:A:589:G:H5'	1.95	0.49
10:A:1587:G:H21	36:d:77:LYS:HD3	1.78	0.49
19:J:90:GLN:OE1	19:J:117:ARG:NH2	2.45	0.49
22:M:78:ARG:NH2	23:N:85:ARG:HE	2.11	0.49
37:e:65:TYR:OH	37:e:76:ARG:NH1	2.46	0.49
38:f:74:PRO:HG2	38:f:75:ARG:HD3	1.95	0.49
46:q:42:LEU:HD11	46:q:48:GLU:HB2	1.95	0.49
47:r:232:PRO:HD2	47:r:233:PRO:HD2	1.95	0.49
49:t:52:HIS:CE1	49:t:54:LYS:HG3	2.48	0.49
50:u:135:GLU:OE1	50:u:140:ARG:NH1	2.45	0.49
50:u:374:MET:HE1	50:u:380:LEU:HD13	1.95	0.49
51:v:264:ASN:ND2	51:v:266:ASP:OD1	2.45	0.49
54:y:657:GLU:OE1	54:y:658:ARG:NH2	2.45	0.49
10:A:649:U:H2'	10:A:650:A:H8	1.77	0.49
10:A:1523:C:H2'	10:A:1524:G:H8	1.77	0.49
10:A:1560:U:H2'	10:A:1561:A:H8	1.78	0.49
23:N:127:PRO:HD3	23:N:146:ALA:HB1	1.93	0.49
49:t:24:ASP:HB3	49:t:27:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:u:212:HIS:NE2	50:u:218:ILE:O	2.46	0.49
50:u:226:GLN:HG2	50:u:264:LYS:HE3	1.94	0.49
50:u:316:GLN:O	50:u:319:SER:OG	2.29	0.49
50:u:389:ASP:OD1	50:u:389:ASP:N	2.46	0.49
51:v:255:ARG:HH12	51:v:325:LEU:HD21	1.78	0.49
5:5:384:GLU:OE2	5:5:538:ARG:NH1	2.45	0.48
10:A:64:A:N6	10:A:83:A:OP2	2.46	0.48
10:A:956:G:OP2	25:P:63:LYS:NZ	2.46	0.48
34:b:41:GLN:HG3	34:b:84:ILE:HG21	1.95	0.48
54:y:329:VAL:O	54:y:333:LEU:N	2.44	0.48
5:5:248:THR:HG21	5:5:506:ILE:HD13	1.95	0.48
10:A:609:U:H2'	10:A:610:G:H8	1.78	0.48
10:A:1158:G:H5''	19:J:76:SER:HB2	1.95	0.48
26:Q:60:ASP:OD1	26:Q:60:ASP:N	2.45	0.48
42:m:18:LEU:HD21	42:m:77:ILE:HG13	1.95	0.48
48:s:290:ILE:HG13	48:s:301:GLN:HB3	1.95	0.48
53:x:407:VAL:HG12	53:x:423:THR:HG21	1.95	0.48
54:y:63:LEU:HD23	54:y:86:LEU:HG	1.94	0.48
10:A:919:A:H5''	18:I:16:LEU:HD12	1.96	0.48
10:A:1533:A:N6	10:A:1602:U:C2	2.82	0.48
10:A:1729:U:O4	10:A:1805:G:O6	2.32	0.48
24:O:127:VAL:HG11	24:O:173:THR:HA	1.93	0.48
48:s:219:PHE:N	48:s:256:LEU:O	2.43	0.48
49:t:341:THR:HB	49:t:343:ILE:HG23	1.95	0.48
23:N:145:ILE:HG12	23:N:159:ILE:HB	1.96	0.48
24:O:176:VAL:HG13	24:O:184:VAL:HG21	1.95	0.48
34:b:22:LEU:HD11	34:b:90:VAL:HG21	1.96	0.48
51:v:298:CYS:HA	51:v:301:VAL:HG12	1.95	0.48
54:y:318:PHE:H	54:y:356:LEU:HD21	1.78	0.48
54:y:422:GLU:N	54:y:440:VAL:O	2.44	0.48
54:y:858:GLN:HA	54:y:861:GLU:HB2	1.96	0.48
1:1:478:ILE:HG12	1:1:549:MET:HE1	1.94	0.48
1:1:569:ALA:HB3	1:1:578:ALA:HB3	1.94	0.48
10:A:1139:C:H41	10:A:1149:A:H62	1.60	0.48
30:V:82:ASN:HA	30:V:85:LYS:HD2	1.95	0.48
35:c:205:SER:OG	35:c:220:ASP:OD1	2.31	0.48
39:h:54:VAL:HB	39:h:88:LEU:HB2	1.95	0.48
54:y:511:TYR:OH	54:y:611:ARG:NH1	2.46	0.48
10:A:145:G:H2'	10:A:146:G:C8	2.48	0.48
10:A:1618:C:O3'	34:b:50:ARG:NH2	2.46	0.48
21:L:60:TRP:NE1	21:L:90:GLU:OE1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:N:106:GLY:N	23:N:136:GLU:OE2	2.46	0.48
35:c:109:LEU:HD13	35:c:152:SER:HA	1.96	0.48
35:c:237:ASN:ND2	35:c:286:CYS:O	2.47	0.48
49:t:261:SER:OG	49:t:352:ARG:N	2.47	0.48
50:u:468:GLU:HA	50:u:471:ILE:HD12	1.95	0.48
10:A:1010:G:H2'	10:A:1011:A:C8	2.48	0.48
10:A:1438:A:H2'	10:A:1439:A:C8	2.48	0.48
14:E:107:ARG:HD3	14:E:112:VAL:HG22	1.96	0.48
17:H:57:VAL:HG12	17:H:60:SER:HB3	1.95	0.48
21:L:109:ILE:HD11	21:L:151:ILE:HD11	1.95	0.48
21:L:168:GLY:HA3	21:L:181:PRO:HB3	1.96	0.48
33:a:49:MET:HA	33:a:52:LEU:HB2	1.95	0.48
35:c:171:ASP:OD1	35:c:171:ASP:N	2.44	0.48
46:q:37:GLN:O	46:q:50:MET:N	2.44	0.48
54:y:852:GLN:NE2	54:y:853:GLN:OE1	2.47	0.48
10:A:201:C:H5''	10:A:202:G:H21	1.79	0.48
10:A:1010:G:H2'	10:A:1011:A:H8	1.79	0.48
10:A:1308:U:H4'	41:k:118:ARG:HH21	1.79	0.48
16:G:39:GLN:HG3	16:G:75:ILE:HG21	1.96	0.48
21:L:191:VAL:HG11	21:L:236:PHE:HA	1.95	0.48
30:V:140:ASP:OD1	30:V:141:VAL:N	2.47	0.48
49:t:43:ASN:ND2	49:t:151:VAL:O	2.44	0.48
53:x:35:LYS:O	54:y:586:ARG:NH1	2.44	0.48
3:3:198:PRO:HA	5:5:533:THR:HG22	1.95	0.48
5:5:171:ASP:OD1	5:5:171:ASP:N	2.47	0.48
5:5:325:MET:HE1	5:5:413:PHE:HZ	1.79	0.48
10:A:830:A:OP2	10:A:846:G:N2	2.44	0.48
41:k:105:TYR:OH	42:m:35:ILE:O	2.32	0.48
48:s:297:LEU:HD23	49:t:73:LEU:HB3	1.96	0.48
54:y:788:LEU:HD21	54:y:818:VAL:HG23	1.96	0.48
10:A:752:G:N2	10:A:793:G:O2'	2.47	0.48
10:A:1204:A:O2'	10:A:1700:C:OP2	2.25	0.48
4:4:291:GLU:O	6:6:344:LYS:NZ	2.47	0.47
10:A:1358:U:OP2	21:L:123:ARG:NH2	2.47	0.47
50:u:323:LEU:HD13	50:u:380:LEU:HD11	1.95	0.47
54:y:324:ILE:HG22	54:y:328:VAL:HG21	1.96	0.47
5:5:113:PRO:HB2	5:5:118:ILE:HD11	1.96	0.47
5:5:451:VAL:O	5:5:455:ALA:N	2.47	0.47
13:D:83:ARG:HG2	13:D:150:ARG:HD2	1.97	0.47
16:G:33:ASN:OD1	16:G:34:SER:N	2.47	0.47
24:O:71:LEU:HB2	24:O:82:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:41:ARG:HH11	27:R:43:ILE:HD12	1.79	0.47
32:Z:64:ARG:NH2	33:a:71:LEU:O	2.47	0.47
39:h:24:LEU:HG	39:h:112:VAL:HG12	1.97	0.47
5:5:542:PHE:HA	5:5:545:ARG:HB3	1.96	0.47
10:A:1098:C:H2'	10:A:1099:G:C8	2.49	0.47
10:A:1238:U:H5'	34:b:128:HIS:HB2	1.95	0.47
10:A:1249:C:O2'	31:Y:143:LYS:NZ	2.47	0.47
13:D:158:ASP:OD1	13:D:159:PHE:N	2.48	0.47
30:V:125:SER:HA	30:V:138:ALA:HA	1.96	0.47
32:Z:27:ARG:HD2	33:a:63:ALA:HB2	1.96	0.47
35:c:153:CYS:SG	35:c:155:ARG:NH1	2.87	0.47
5:5:494:LYS:HG3	5:5:498:LYS:HE2	1.96	0.47
6:6:286:ALA:HB1	6:6:334:VAL:HG21	1.96	0.47
10:A:692:G:H2'	10:A:693:A:C8	2.49	0.47
10:A:1232:U:H2'	10:A:1233:G:C8	2.49	0.47
10:A:1386:A:OP2	32:Z:160:SER:OG	2.26	0.47
10:A:1447:G:O2'	39:h:33:GLU:OE2	2.27	0.47
31:Y:42:ILE:HG22	31:Y:44:PRO:HD2	1.96	0.47
49:t:39:GLN:NE2	49:t:332:ALA:O	2.43	0.47
50:u:159:GLN:O	50:u:163:LEU:N	2.47	0.47
54:y:543:ASP:HB3	54:y:546:VAL:HG22	1.97	0.47
10:A:799:U:OP1	10:A:867:G:N2	2.45	0.47
10:A:1367:U:HO2'	10:A:1466:G:HO2'	1.62	0.47
12:C:115:THR:HG22	12:C:117:GLU:H	1.78	0.47
30:V:103:LEU:HD21	37:e:67:LEU:HD13	1.95	0.47
42:m:69:CYS:HB2	42:m:74:ILE:HG22	1.96	0.47
49:t:90:LYS:O	49:t:125:LYS:N	2.47	0.47
49:t:320:SER:HB2	49:t:322:PHE:CE2	2.50	0.47
50:u:241:ILE:HG13	50:u:246:TRP:HZ3	1.79	0.47
50:u:486:HIS:HB3	54:y:802:ILE:HA	1.95	0.47
10:A:367:U:H3	54:y:144:LYS:HE3	1.79	0.47
10:A:1539:U:OP1	36:d:44:GLU:N	2.43	0.47
26:Q:74:CYS:O	26:Q:78:ALA:N	2.47	0.47
28:S:159:ARG:NH2	28:S:171:THR:O	2.47	0.47
39:h:26:SER:HB3	39:h:32:LEU:HD22	1.96	0.47
44:o:259:PHE:HE2	44:o:285:ILE:HG13	1.78	0.47
49:t:295:GLU:N	49:t:359:GLY:O	2.46	0.47
50:u:38:LYS:HA	50:u:41:ARG:HD3	1.96	0.47
53:x:412:LYS:HB3	53:x:416:GLN:HB3	1.97	0.47
53:x:426:LYS:O	53:x:426:LYS:NZ	2.47	0.47
4:4:117:ILE:HA	4:4:174:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:600:G:H2'	10:A:601:G:H8	1.78	0.47
10:A:982:G:H21	10:A:1045:U:H1'	1.79	0.47
10:A:1351:G:H1	10:A:1360:U:H3	1.63	0.47
10:A:1513:C:OP1	40:i:12:ARG:NH1	2.39	0.47
10:A:1631:U:O2'	38:f:34:LYS:NZ	2.46	0.47
30:V:132:GLY:HA3	47:r:55:ARG:HD2	1.97	0.47
32:Z:42:THR:HG23	32:Z:45:ARG:H	1.79	0.47
33:a:15:LEU:HD23	33:a:79:LEU:HD11	1.97	0.47
45:p:13:PHE:HZ	49:t:79:ILE:HD12	1.79	0.47
49:t:445:ARG:HB2	49:t:454:ILE:HD13	1.96	0.47
53:x:322:ASN:O	53:x:326:GLN:HB2	2.15	0.47
54:y:123:ASP:N	54:y:123:ASP:OD1	2.47	0.47
54:y:567:CYS:HB3	54:y:571:CYS:HB2	1.60	0.47
54:y:602:ASP:HB2	54:y:604:PRO:HD2	1.97	0.47
54:y:789:ARG:HD2	54:y:821:ILE:HD11	1.96	0.47
5:5:240:ILE:HD11	5:5:267:LYS:HA	1.96	0.47
9:9:2:ARG:NE	10:A:1842:C:OP2	2.37	0.47
10:A:885:U:H2'	10:A:886:A:C8	2.50	0.47
10:A:929:G:N2	10:A:1013:U:O2	2.48	0.47
10:A:1416:C:C4	10:A:1417:C:N4	2.82	0.47
12:C:18:TRP:HH2	12:C:31:PRO:HD3	1.80	0.47
22:M:102:THR:HA	22:M:105:MET:HB3	1.96	0.47
49:t:262:PHE:HZ	52:w:76:A:H5'	1.79	0.47
50:u:447:TYR:CD2	50:u:450:ILE:HG12	2.50	0.47
54:y:151:ASP:OD1	54:y:151:ASP:N	2.47	0.47
10:A:223:C:H2'	10:A:224:A:C8	2.50	0.47
12:C:122:LYS:NZ	12:C:143:ASP:OD2	2.43	0.47
17:H:67:THR:OG1	17:H:70:LYS:O	2.33	0.47
38:f:26:ILE:HG13	38:f:45:LEU:HD21	1.96	0.47
48:s:180:LEU:HD23	49:t:223:PRO:HG3	1.97	0.47
49:t:337:ILE:O	49:t:338:GLY:C	2.58	0.47
54:y:339:ALA:HB1	54:y:345:THR:HG21	1.96	0.47
10:A:483:C:H5''	14:E:48:LYS:HD2	1.97	0.47
10:A:708:C:H2'	10:A:709:G:H8	1.79	0.47
10:A:931:C:H2'	10:A:932:G:C8	2.50	0.47
10:A:1628:C:H2'	10:A:1629:C:C6	2.49	0.47
12:C:44:LEU:HD11	12:C:70:ILE:HG21	1.96	0.47
20:K:3:ASN:HD22	20:K:7:GLU:HB2	1.80	0.47
20:K:73:ALA:HB1	20:K:78:ILE:HB	1.97	0.47
30:V:125:SER:OG	30:V:136:ARG:NH2	2.47	0.47
39:h:21:ARG:HH11	39:h:88:LEU:HD23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:87:LYS:HA	49:t:129:HIS:HA	1.96	0.47
50:u:272:MET:SD	50:u:272:MET:N	2.87	0.47
9:9:11:ARG:NH2	10:A:1844:U:OP1	2.48	0.46
10:A:1357:A:OP1	21:L:125:LYS:NZ	2.48	0.46
10:A:1629:C:H2'	10:A:1630:A:H8	1.81	0.46
5:5:133:LYS:HA	5:5:136:TYR:HB3	1.96	0.46
5:5:286:ASP:HB3	5:5:289:GLN:HB2	1.97	0.46
5:5:457:LEU:HB3	5:5:493:PHE:HD1	1.80	0.46
10:A:1013:U:OP1	10:A:1129:G:O2'	2.34	0.46
10:A:1542:C:H4'	36:d:11:GLN:HB2	1.97	0.46
10:A:1829:G:H5'	45:p:86:GLN:HE22	1.80	0.46
13:D:67:ASP:HB3	13:D:70:ARG:HB3	1.96	0.46
45:p:33:ILE:HG22	45:p:47:VAL:HG22	1.98	0.46
50:u:526:MET:HB2	50:u:530:LEU:HD23	1.98	0.46
51:v:254:LEU:HB2	51:v:286:TYR:HE2	1.79	0.46
53:x:308:SER:OG	53:x:311:ASN:ND2	2.48	0.46
53:x:380:VAL:HG22	53:x:390:PHE:HD1	1.81	0.46
5:5:91:ILE:HA	5:5:94:ILE:HB	1.97	0.46
10:A:1147:C:OP1	26:Q:6:ARG:NH1	2.40	0.46
10:A:1513:C:H2'	10:A:1514:G:C8	2.49	0.46
23:N:53:ARG:HA	23:N:56:GLU:HG2	1.96	0.46
37:e:67:LEU:HD11	37:e:72:VAL:HG11	1.97	0.46
49:t:108:SER:HA	49:t:325:HIS:CE1	2.50	0.46
49:t:281:GLY:O	49:t:336:LEU:HA	2.15	0.46
50:u:484:ILE:HD12	54:y:799:TYR:HE1	1.80	0.46
54:y:835:LEU:HB3	54:y:838:PRO:HD2	1.97	0.46
6:6:258:ASN:OD1	6:6:259:ASN:N	2.49	0.46
6:6:279:LEU:HB3	6:6:320:MET:HE1	1.96	0.46
6:6:297:MET:HG3	6:6:301:LEU:HD12	1.96	0.46
10:A:613:G:N2	10:A:626:G:OP1	2.41	0.46
10:A:712:G:N2	10:A:715:A:OP2	2.49	0.46
10:A:723:C:H3'	10:A:724:A:H8	1.80	0.46
23:N:42:LYS:HD2	23:N:44:ASP:HB3	1.98	0.46
30:V:135:ARG:HD3	47:r:53:ARG:HH12	1.81	0.46
31:Y:40:GLU:N	31:Y:40:GLU:OE2	2.46	0.46
38:f:121:ARG:HG3	38:f:131:VAL:HB	1.96	0.46
50:u:397:GLU:OE1	50:u:399:ASN:ND2	2.46	0.46
51:v:252:HIS:HB2	51:v:286:TYR:CZ	2.51	0.46
54:y:635:ASP:OD1	54:y:635:ASP:N	2.48	0.46
5:5:490:LEU:HA	5:5:493:PHE:HB3	1.98	0.46
10:A:5:U:H2'	10:A:6:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:S:58:LYS:HA	28:S:107:SER:HB2	1.97	0.46
40:i:13:LYS:O	40:i:13:LYS:NZ	2.39	0.46
1:1:568:PHE:HD1	1:1:579:VAL:HG12	1.80	0.46
10:A:84:A:N3	10:A:150:A:O2'	2.45	0.46
10:A:446:G:OP2	27:R:47:ARG:NH2	2.44	0.46
10:A:1113:A:O2'	10:A:1114:U:O4'	2.28	0.46
10:A:1856:C:OP1	25:P:141:ARG:NH2	2.42	0.46
24:O:128:LYS:NZ	24:O:132:GLY:O	2.49	0.46
25:P:34:PHE:HE1	25:P:100:THR:HA	1.81	0.46
30:V:136:ARG:HB2	30:V:203:ASN:HD21	1.80	0.46
49:t:84:ALA:HB3	49:t:132:PHE:HB2	1.96	0.46
49:t:297:ARG:HB2	49:t:364:LEU:HD13	1.97	0.46
49:t:406:VAL:HG23	49:t:443:LEU:HB3	1.98	0.46
51:v:385:ASP:OD1	51:v:385:ASP:N	2.47	0.46
5:5:457:LEU:HD22	5:5:493:PHE:HB2	1.98	0.46
12:C:148:ARG:NH2	28:S:202:ASN:OD1	2.48	0.46
25:P:45:THR:HG23	25:P:52:THR:HA	1.98	0.46
27:R:76:THR:HG22	27:R:108:PRO:HG2	1.97	0.46
41:k:118:ARG:HB2	41:k:131:PHE:HD2	1.80	0.46
50:u:63:LYS:HB3	50:u:66:LEU:HB2	1.98	0.46
50:u:165:ARG:HH11	50:u:166:ASN:HD22	1.63	0.46
51:v:264:ASN:O	51:v:268:ARG:NH2	2.39	0.46
54:y:759:GLU:OE2	54:y:759:GLU:N	2.45	0.46
1:1:548:ARG:NH1	1:1:595:LYS:O	2.44	0.46
5:5:132:TYR:O	5:5:136:TYR:N	2.45	0.46
5:5:138:ARG:NH1	5:5:185:ASP:O	2.49	0.46
10:A:311:C:H5''	10:A:312:G:H5''	1.98	0.46
10:A:544:G:H2'	10:A:545:A:C8	2.50	0.46
10:A:614:C:OP1	46:q:62:ARG:NH2	2.47	0.46
10:A:941:C:H2'	10:A:942:G:H8	1.79	0.46
10:A:1694:U:O2'	10:A:1833:C:O2'	2.31	0.46
10:A:1863:A:H1'	26:Q:79:ILE:HD11	1.98	0.46
17:H:14:GLU:OE2	17:H:14:GLU:N	2.44	0.46
17:H:56:CYS:HB2	17:H:63:LEU:HD11	1.98	0.46
21:L:92:GLU:OE2	21:L:92:GLU:N	2.48	0.46
33:a:71:LEU:HG	33:a:76:ILE:HG13	1.98	0.46
49:t:264:VAL:HA	52:w:76:A:C2	2.48	0.46
50:u:329:ILE:HB	50:u:367:ARG:HH11	1.81	0.46
51:v:401:TYR:HD2	51:v:402:GLN:HG3	1.81	0.46
1:1:306:TYR:HA	1:1:704:TRP:HA	1.98	0.46
10:A:126:G:H5''	28:S:195:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:191:A:H62	10:A:208:G:H21	1.64	0.46
10:A:1545:A:H4'	31:Y:74:GLY:HA2	1.97	0.46
41:k:94:LYS:HB3	41:k:94:LYS:HE3	1.75	0.46
41:k:130:VAL:HG11	41:k:143:LYS:HD3	1.96	0.46
44:o:269:TYR:HB3	44:o:284:PHE:HB2	1.97	0.46
45:p:27:THR:HA	45:p:51:ALA:HB2	1.98	0.46
54:y:63:LEU:HA	54:y:66:THR:HG22	1.97	0.46
7:7:-9:A:H5''	26:Q:100:ARG:NH1	2.31	0.46
10:A:1864:U:O2'	10:A:1866:A:N7	2.49	0.46
28:S:43:GLU:HA	28:S:46:LYS:HE3	1.97	0.46
29:T:57:VAL:HB	29:T:60:PHE:HE1	1.79	0.46
48:s:284:CYS:SG	48:s:304:THR:OG1	2.69	0.46
49:t:294:ILE:HB	49:t:358:LEU:HD11	1.98	0.46
10:A:1265:A:O2'	10:A:1327:G:OP2	2.28	0.45
10:A:1324:G:O2'	10:A:1510:G:O2'	2.34	0.45
10:A:1512:C:H5''	40:i:8:TRP:HZ3	1.81	0.45
10:A:1858:G:OP2	25:P:146:ARG:NH1	2.49	0.45
35:c:174:VAL:HB	35:c:188:HIS:HB2	1.98	0.45
42:m:89:VAL:HG11	42:m:109:VAL:HG11	1.97	0.45
50:u:561:SER:HB3	50:u:564:GLU:HB2	1.99	0.45
51:v:375:ILE:HA	51:v:380:LEU:HD12	1.97	0.45
51:v:414:ARG:HA	51:v:417:MET:HB3	1.98	0.45
1:1:283:GLU:C	1:1:285:GLN:N	2.74	0.45
10:A:70:G:OP2	28:S:167:LYS:NZ	2.50	0.45
10:A:1025:U:O3'	10:A:1089:G:N2	2.49	0.45
10:A:1171:G:O2'	10:A:1187:G:O6	2.33	0.45
24:O:38:MET:HE1	24:O:185:VAL:HG13	1.98	0.45
28:S:181:THR:HG23	28:S:183:ARG:H	1.80	0.45
35:c:35:SER:OG	35:c:36:ARG:N	2.49	0.45
49:t:160:ALA:HA	49:t:190:ASN:HB3	1.97	0.45
14:E:101:LEU:HB3	14:E:124:LYS:HB2	1.99	0.45
34:b:72:LYS:NZ	34:b:91:GLY:O	2.47	0.45
35:c:238:ALA:H	35:c:251:ALA:HB3	1.81	0.45
45:p:30:TYR:HB2	45:p:32:HIS:NE2	2.32	0.45
51:v:255:ARG:NH1	51:v:325:LEU:HD21	2.32	0.45
53:x:46:THR:OG1	54:y:641:ARG:NH2	2.49	0.45
10:A:955:A:N1	10:A:968:U:O2'	2.40	0.45
10:A:1845:A:H2'	10:A:1846:G:C8	2.52	0.45
50:u:421:GLU:HB3	50:u:424:LEU:HG	1.99	0.45
53:x:361:ARG:NH1	53:x:441:LEU:O	2.45	0.45
5:5:94:ILE:O	5:5:99:TRP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:283:LEU:HB3	5:5:421:LEU:HD23	1.98	0.45
10:A:1220:A:N3	10:A:1677:U:O2'	2.43	0.45
10:A:1473:G:OP1	35:c:15:ASN:ND2	2.49	0.45
13:D:136:ARG:HH11	13:D:139:LYS:H	1.63	0.45
25:P:78:ALA:HA	25:P:81:VAL:HG12	1.99	0.45
35:c:273:GLU:OE2	35:c:308:ARG:NH2	2.49	0.45
47:r:190:LYS:HA	47:r:240:THR:HA	1.97	0.45
49:t:82:GLY:HA3	49:t:134:ASP:HB3	1.99	0.45
54:y:587:ASP:OD1	54:y:587:ASP:N	2.48	0.45
10:A:857:U:H2'	10:A:858:A:C8	2.51	0.45
10:A:1217:A:H2'	10:A:1218:C:H6	1.81	0.45
21:L:176:LYS:O	21:L:200:ARG:NH1	2.49	0.45
32:Z:53:THR:O	32:Z:90:LYS:NZ	2.50	0.45
32:Z:70:THR:HA	32:Z:86:LEU:HD13	1.98	0.45
37:e:50:PHE:H	38:f:4:VAL:HG12	1.81	0.45
45:p:56:LYS:HD3	45:p:59:LEU:HG	1.98	0.45
50:u:281:THR:O	50:u:285:LYS:NZ	2.47	0.45
53:x:69:TYR:HD1	54:y:565:ARG:HD3	1.81	0.45
53:x:172:GLU:O	53:x:519:VAL:N	2.48	0.45
5:5:291:ILE:HG23	5:5:508:ALA:HB3	1.99	0.45
10:A:1030:A:H2'	10:A:1031:A2M:H8	1.98	0.45
10:A:1101:U:H2'	10:A:1102:G:C8	2.52	0.45
10:A:1579:A:O2'	10:A:1582:C:N4	2.48	0.45
25:P:117:ARG:NH2	26:Q:48:ALA:O	2.50	0.45
34:b:18:ARG:NH1	34:b:36:LEU:O	2.49	0.45
42:m:91:LEU:HD21	42:m:106:CYS:HB2	1.98	0.45
49:t:18:GLN:HG2	49:t:330:TYR:CE1	2.52	0.45
54:y:549:GLU:O	54:y:553:LYS:HG2	2.16	0.45
1:1:512:VAL:HG13	1:1:530:VAL:HG23	1.99	0.45
7:7:-7:A:H2	7:7:-7:A:OP2	1.86	0.45
10:A:520:A:O2'	10:A:825:A:N3	2.37	0.45
10:A:1037:G:H4'	10:A:1845:A:H4'	1.99	0.45
36:d:28:LEU:HD23	36:d:28:LEU:HA	1.88	0.45
47:r:112:LEU:HA	47:r:115:VAL:HG12	1.99	0.45
52:w:75:C:H4'	52:w:76:A:C4	2.50	0.45
10:A:736:C:H2'	10:A:737:G:C8	2.52	0.45
10:A:1722:G:H2'	10:A:1723:G:C8	2.52	0.45
10:A:1746:U:OP1	28:S:31:ARG:NH2	2.49	0.45
27:R:6:ASP:OD1	27:R:6:ASP:N	2.49	0.45
27:R:80:ASP:OD1	27:R:81:VAL:N	2.50	0.45
30:V:49:LEU:HD13	31:Y:47:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f:13:LEU:HB2	38:f:20:ILE:HB	1.97	0.45
48:s:275:ILE:HG13	48:s:279:VAL:HB	1.98	0.45
49:t:43:ASN:HA	49:t:131:SER:HB3	1.97	0.45
50:u:234:LEU:HD21	50:u:275:TYR:HB2	1.99	0.45
50:u:296:LEU:HD11	50:u:321:ARG:HD3	1.98	0.45
50:u:499:TYR:HB3	50:u:518:GLN:HG2	1.97	0.45
53:x:193:ILE:N	53:x:360:TYR:O	2.44	0.45
54:y:117:LEU:HD12	54:y:142:ARG:HB2	1.97	0.45
54:y:786:GLU:OE1	54:y:789:ARG:NH1	2.45	0.45
10:A:106:C:OP1	10:A:431:G:O2'	2.29	0.45
10:A:300:U:H2'	10:A:301:A:H8	1.81	0.45
10:A:326:C:N4	10:A:327:G:N7	2.65	0.45
28:S:192:ILE:HG22	28:S:196:LYS:HE3	1.99	0.45
30:V:124:ASP:OD1	30:V:125:SER:N	2.50	0.45
32:Z:109:LEU:HD12	32:Z:184:ILE:HD11	1.99	0.45
50:u:226:GLN:HE22	50:u:267:PRO:HB3	1.81	0.45
50:u:432:GLN:HG3	50:u:461:PHE:HE1	1.82	0.45
51:v:234:ASP:HB2	51:v:270:ARG:HE	1.81	0.45
5:5:546:GLN:NE2	51:v:406:GLU:OE2	2.49	0.44
10:A:1757:G:O2'	10:A:1776:G:N1	2.50	0.44
27:R:12:ARG:HB3	27:R:18:ARG:HH21	1.82	0.44
32:Z:64:ARG:O	32:Z:68:GLU:HB2	2.17	0.44
35:c:144:ASP:OD1	35:c:144:ASP:N	2.43	0.44
51:v:44:LEU:H	51:v:217:TRP:HZ2	1.65	0.44
5:5:191:ILE:O	5:5:195:GLN:N	2.46	0.44
10:A:15:U:O2'	10:A:669:A:N6	2.48	0.44
10:A:1206:G:O2'	10:A:1208:A:OP1	2.34	0.44
10:A:1447:G:H2'	10:A:1448:A:C8	2.52	0.44
10:A:1797:U:H2'	10:A:1798:C:C6	2.52	0.44
12:C:66:MET:HE1	12:C:78:THR:HB	2.00	0.44
26:Q:45:VAL:HG11	26:Q:53:ILE:HG13	1.99	0.44
30:V:192:LYS:HD2	30:V:192:LYS:HA	1.83	0.44
33:a:52:LEU:HD23	33:a:52:LEU:HA	1.88	0.44
37:e:57:LYS:HA	37:e:60:LYS:HE2	1.99	0.44
42:m:54:SER:HB2	42:m:80:ASP:HA	1.98	0.44
46:q:104:LYS:HD2	46:q:110:PRO:HG3	1.99	0.44
49:t:381:LEU:HB3	49:t:393:ALA:HA	1.99	0.44
51:v:252:HIS:HE1	51:v:255:ARG:HH21	1.65	0.44
53:x:362:ARG:HB3	53:x:372:ILE:HD13	1.98	0.44
6:6:248:LYS:HZ1	6:6:285:MET:HB3	1.82	0.44
10:A:941:C:H2'	10:A:942:G:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1388:A:H61	32:Z:161:GLY:HA3	1.82	0.44
10:A:1499:U:H4'	32:Z:176:LEU:HD13	1.99	0.44
10:A:1550:G:O2'	10:A:1558:C:O2	2.25	0.44
45:p:109:LYS:O	45:p:111:HIS:N	2.48	0.44
50:u:109:GLN:HE22	50:u:110:GLN:HE21	1.64	0.44
10:A:1144:A:H2'	10:A:1145:A:C8	2.53	0.44
10:A:1545:A:N3	10:A:1671:G:O2'	2.41	0.44
15:F:96:GLN:O	15:F:98:LYS:NZ	2.46	0.44
22:M:37:GLU:HG3	35:c:150:TRP:HE1	1.82	0.44
27:R:113:TYR:OH	27:R:156:ALA:O	2.36	0.44
28:S:223:LYS:HD2	28:S:223:LYS:HA	1.81	0.44
38:f:25:LYS:O	38:f:29:ALA:N	2.49	0.44
47:r:50:GLU:OE1	47:r:89:ARG:NH1	2.51	0.44
47:r:64:ARG:HB3	47:r:67:ARG:HH21	1.83	0.44
50:u:28:LEU:HD12	50:u:57:LEU:HB3	1.98	0.44
50:u:436:ILE:HD11	50:u:459:VAL:HG11	1.99	0.44
5:5:55:PHE:CZ	5:5:94:ILE:HG23	2.52	0.44
10:A:1410:C:H2'	10:A:1411:G:H8	1.83	0.44
10:A:1620:A:OP1	34:b:115:TYR:OH	2.25	0.44
18:I:3:ARG:HA	18:I:3:ARG:HD3	1.81	0.44
31:Y:134:GLY:HA3	31:Y:140:ARG:HA	1.99	0.44
51:v:408:THR:HA	51:v:411:LEU:HG	2.00	0.44
54:y:711:SER:O	54:y:715:HIS:ND1	2.38	0.44
1:1:639:ASP:N	1:1:644:THR:O	2.46	0.44
5:5:278:LEU:HD12	5:5:290:ALA:HB1	2.00	0.44
10:A:300:U:H2'	10:A:301:A:C8	2.53	0.44
10:A:527:C:H2'	10:A:528:A:C8	2.52	0.44
10:A:1593:C:OP1	37:e:103:HIS:NE2	2.40	0.44
11:B:49:GLU:HG3	11:B:116:CYS:HA	2.00	0.44
23:N:76:VAL:HG12	23:N:123:VAL:HB	1.98	0.44
48:s:279:VAL:O	48:s:289:THR:OG1	2.23	0.44
48:s:295:THR:O	48:s:297:LEU:N	2.50	0.44
49:t:256:LEU:HB3	49:t:358:LEU:HB3	1.99	0.44
4:4:118:GLY:O	4:4:173:TYR:N	2.50	0.44
6:6:59:ASP:O	6:6:63:VAL:N	2.47	0.44
10:A:550:C:O2'	10:A:551:U:O4'	2.30	0.44
10:A:602:G:H3'	10:A:603:C:H2'	2.00	0.44
10:A:1120:U:O4	53:x:85:THR:OG1	2.26	0.44
10:A:1337:C:H5'	40:i:44:ARG:NH2	2.33	0.44
10:A:1657:G:H1	10:A:1667:U:H3	1.66	0.44
23:N:184:ARG:HH11	23:N:191:ARG:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:O:123:ALA:HB2	24:O:165:ARG:HG3	2.00	0.44
24:O:136:ARG:HB2	24:O:218:LEU:HD11	2.00	0.44
24:O:217:MET:HB3	24:O:217:MET:HE3	1.72	0.44
29:T:79:LEU:HD11	29:T:96:LEU:HD21	1.99	0.44
36:d:35:ASP:OD1	36:d:35:ASP:N	2.41	0.44
36:d:41:LYS:HE3	36:d:93:SER:HB2	1.99	0.44
54:y:855:LEU:HA	54:y:859:LEU:HD13	1.99	0.44
1:1:528:VAL:HB	1:1:545:GLU:HB2	1.99	0.44
10:A:106:C:H2'	10:A:107:A:C8	2.53	0.44
10:A:441:C:H2'	10:A:442:C:C6	2.53	0.44
10:A:1549:U:OP1	40:i:34:TYR:OH	2.31	0.44
24:O:105:LEU:HD23	24:O:213:ARG:HA	1.99	0.44
27:R:22:HIS:ND1	27:R:23:LYS:O	2.42	0.44
33:a:11:ILE:HD13	33:a:45:VAL:HA	2.00	0.44
38:f:114:LEU:HD11	38:f:121:ARG:HH21	1.82	0.44
44:o:241:ILE:HB	44:o:285:ILE:HB	1.99	0.44
46:q:62:ARG:HB3	46:q:65:LEU:HD23	2.00	0.44
48:s:242:ALA:HA	48:s:316:THR:HG23	2.00	0.44
49:t:83:TYR:OH	52:w:76:A:OP2	2.36	0.44
49:t:312:LYS:HB2	49:t:470:ASP:H	1.83	0.44
50:u:293:ALA:O	50:u:297:HIS:ND1	2.48	0.44
5:5:523:ILE:HG12	5:5:528:ILE:HG23	2.00	0.44
10:A:987:A:C6	24:O:120:MET:HE1	2.53	0.44
10:A:1351:G:O2'	10:A:1378:A:N1	2.41	0.44
10:A:1433:C:H1'	39:h:19:ARG:HH22	1.83	0.44
10:A:1630:A:H5''	38:f:37:GLY:H	1.83	0.44
31:Y:96:TYR:HA	31:Y:100:VAL:HG22	2.00	0.44
5:5:535:VAL:O	5:5:537:ARG:N	2.49	0.43
10:A:846:G:C5	12:C:19:MET:HE2	2.53	0.43
10:A:866:U:H2'	10:A:867:G:C8	2.53	0.43
10:A:1738:C:OP1	28:S:92:ARG:NH1	2.51	0.43
47:r:231:ALA:HB3	47:r:234:ARG:O	2.18	0.43
53:x:506:TYR:HA	53:x:521:SER:HA	1.99	0.43
54:y:643:LYS:HD2	54:y:650:LEU:HB2	1.99	0.43
7:7:-10:A:H2'	7:7:-9:A:C4	2.53	0.43
9:9:11:ARG:NH2	10:A:1184:G:OP1	2.50	0.43
10:A:64:A:O5'	28:S:136:LYS:NZ	2.51	0.43
10:A:476:A:N3	10:A:488:U:O2'	2.36	0.43
10:A:1588:A:H2'	10:A:1589:A:C8	2.53	0.43
47:r:232:PRO:CD	47:r:233:PRO:HD2	2.47	0.43
49:t:161:GLY:N	49:t:190:ASN:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:168:PRO:HG3	49:t:385:ARG:HG2	2.00	0.43
49:t:193:ASP:OD1	49:t:193:ASP:N	2.51	0.43
49:t:359:GLY:HA3	49:t:364:LEU:HD21	2.01	0.43
51:v:244:ASN:HB3	53:x:35:LYS:HD3	2.00	0.43
54:y:78:LYS:HA	54:y:78:LYS:HD3	1.67	0.43
1:1:638:VAL:HA	1:1:645:VAL:HA	1.99	0.43
5:5:461:ARG:HH22	5:5:518:GLU:H	1.66	0.43
10:A:877:C:H2'	10:A:878:G:C8	2.53	0.43
14:E:68:LYS:HB3	14:E:91:LEU:HD22	2.00	0.43
24:O:121:ILE:HD13	24:O:164:ILE:HG21	2.00	0.43
27:R:113:TYR:CG	27:R:121:LEU:HD22	2.54	0.43
35:c:164:ILE:HD11	35:c:221:LEU:HB3	2.00	0.43
49:t:297:ARG:HH12	49:t:467:PRO:HB3	1.83	0.43
50:u:485:ASP:OD1	54:y:801:SER:OG	2.33	0.43
54:y:435:ASP:OD1	54:y:435:ASP:N	2.51	0.43
1:1:493:VAL:HG11	1:1:528:VAL:HG21	2.00	0.43
6:6:249:LEU:HG	6:6:281:THR:HG21	2.00	0.43
10:A:71:G:OP2	28:S:168:LYS:NZ	2.42	0.43
10:A:317:C:OP2	28:S:183:ARG:NH2	2.47	0.43
10:A:1221:G:O2'	10:A:1676:U:O2	2.30	0.43
10:A:1825:A:OP2	46:q:67:LYS:NZ	2.52	0.43
47:r:205:ILE:O	47:r:209:LYS:CB	2.66	0.43
47:r:229:LEU:HA	47:r:235:TYR:CB	2.45	0.43
49:t:180:MET:HA	49:t:440:LYS:HE2	2.00	0.43
51:v:371:ILE:HA	51:v:374:LEU:HG	1.99	0.43
51:v:409:LYS:HA	51:v:412:SER:HB3	2.00	0.43
53:x:197:GLY:HA3	53:x:357:ALA:HA	2.00	0.43
10:A:1650:A:H5''	31:Y:139:ALA:HB2	2.00	0.43
23:N:42:LYS:NZ	23:N:48:ILE:HD11	2.32	0.43
34:b:53:GLN:HG3	34:b:80:LEU:HD13	2.00	0.43
46:q:37:GLN:HB3	46:q:50:MET:HB3	1.99	0.43
48:s:211:ARG:NH2	48:s:213:GLY:O	2.52	0.43
48:s:294:ASP:OD1	48:s:299:PHE:CD1	2.71	0.43
50:u:132:VAL:O	54:y:678:ASN:ND2	2.36	0.43
50:u:226:GLN:HA	50:u:229:HIS:HD2	1.83	0.43
54:y:504:LEU:HD22	54:y:564:ILE:HG12	2.01	0.43
54:y:825:MET:HB3	54:y:830:GLU:HB3	2.01	0.43
2:2:300:TYR:O	2:2:312:HIS:N	2.43	0.43
8:8:236:SER:O	8:8:241:LYS:N	2.51	0.43
10:A:447:A:H4'	12:C:3:ARG:HB2	2.01	0.43
10:A:639:C:H2'	10:A:640:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:838:G:O2'	10:A:840:C:OP2	2.34	0.43
10:A:1244:U:H2'	10:A:1245:G:C8	2.53	0.43
32:Z:146:ARG:O	32:Z:148:LYS:NZ	2.45	0.43
35:c:165:ILE:HD11	35:c:179:LEU:HD13	2.01	0.43
49:t:138:HIS:HB3	49:t:141:LEU:HB2	2.00	0.43
50:u:12:LEU:HD13	50:u:50:ILE:HD13	2.00	0.43
6:6:119:VAL:O	6:6:123:VAL:N	2.45	0.43
10:A:12:U:H2'	10:A:13:C:C6	2.54	0.43
17:H:8:LEU:HD23	17:H:8:LEU:HA	1.85	0.43
30:V:101:HIS:HB2	30:V:108:PRO:HG3	2.00	0.43
35:c:44:LYS:HB2	35:c:56:GLN:HB2	2.00	0.43
39:h:51:LYS:HB2	39:h:90:ASP:HB3	2.00	0.43
49:t:72:GLU:HG2	49:t:79:ILE:H	1.83	0.43
54:y:648:GLN:HE21	54:y:676:HIS:CG	2.37	0.43
10:A:1036:A:H4'	10:A:1855:G:N2	2.34	0.43
10:A:1755:C:O2'	10:A:1778:C:O2	2.37	0.43
13:D:32:ILE:HD11	13:D:40:LYS:HA	2.00	0.43
14:E:100:VAL:HG12	14:E:125:VAL:HG23	1.99	0.43
25:P:106:LYS:HD2	25:P:135:ILE:HG12	2.01	0.43
7:7:-10:A:C8	7:7:-9:A:N6	2.87	0.43
10:A:1283:C:H41	42:m:102:LYS:HE3	1.82	0.43
21:L:178:HIS:ND1	21:L:179:THR:OG1	2.49	0.43
23:N:176:TRP:CZ2	23:N:180:ARG:HD2	2.54	0.43
39:h:99:LYS:HD2	39:h:99:LYS:HA	1.90	0.43
47:r:105:SER:HA	47:r:108:VAL:HG22	2.00	0.43
48:s:240:LEU:HD13	48:s:270:VAL:HG11	2.00	0.43
49:t:310:MET:HE2	49:t:310:MET:HB2	1.91	0.43
50:u:320:THR:HG22	50:u:383:VAL:HB	2.01	0.43
50:u:320:THR:HG21	50:u:384:VAL:HG23	2.00	0.43
5:5:478:PHE:HE1	51:v:369:ARG:HA	1.83	0.43
10:A:17:C:O2'	10:A:1194:A:N1	2.45	0.43
10:A:107:A:H2'	10:A:108:G:C8	2.53	0.43
10:A:929:G:H2'	10:A:930:C:O4'	2.19	0.43
10:A:1005:G:OP2	24:O:162:ARG:NH2	2.51	0.43
10:A:1039:C:O2'	54:y:47:ARG:HG3	2.18	0.43
10:A:1236:G:H21	34:b:130:ARG:HH12	1.65	0.43
23:N:124:VAL:HG21	23:N:134:LEU:HD21	2.01	0.43
48:s:246:THR:OG1	48:s:247:SER:N	2.52	0.43
53:x:267:ILE:O	53:x:508:ILE:N	2.44	0.43
10:A:1083:A:N7	10:A:1841:C:O2'	2.41	0.42
25:P:117:ARG:HE	26:Q:49:ALA:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:149:ARG:HE	25:P:151:LEU:HD11	1.83	0.42
35:c:256:ILE:HB	35:c:270:LEU:HB2	2.00	0.42
46:q:90:ASP:N	46:q:90:ASP:OD1	2.52	0.42
50:u:455:LEU:HG	50:u:467:LEU:HD21	2.00	0.42
50:u:492:SER:OG	50:u:495:SER:OG	2.37	0.42
1:1:391:PHE:HA	1:1:404:ILE:HA	2.02	0.42
10:A:15:U:H2'	10:A:16:G:O4'	2.19	0.42
10:A:116:OMU:H1'	10:A:116:OMU:HM23	1.67	0.42
10:A:1213:C:H2'	10:A:1214:A:C8	2.54	0.42
22:M:98:VAL:HG22	23:N:19:LEU:HD12	2.01	0.42
23:N:176:TRP:NE1	23:N:197:VAL:O	2.51	0.42
38:f:18:THR:HG21	38:f:33:ILE:HA	2.00	0.42
53:x:82:LEU:HD21	54:y:665:VAL:HG21	2.00	0.42
54:y:131:ASN:H	54:y:134:ASN:HB2	1.83	0.42
1:1:569:ALA:N	1:1:578:ALA:O	2.52	0.42
5:5:302:LYS:HD2	5:5:306:SER:HB3	2.00	0.42
6:6:325:ILE:HG22	6:6:332:VAL:HG12	2.00	0.42
10:A:751:G:H22	10:A:789:G:H5''	1.85	0.42
10:A:1391:C:O2'	39:h:83:ARG:NH2	2.53	0.42
10:A:1604:G:OP2	38:f:38:ARG:NH2	2.52	0.42
21:L:87:PRO:HG3	23:N:140:VAL:HA	2.01	0.42
24:O:192:SER:HB2	50:u:23:LYS:HG3	2.00	0.42
29:T:49:LYS:HE2	29:T:49:LYS:HB2	1.89	0.42
49:t:98:ARG:HE	49:t:98:ARG:HB3	1.66	0.42
1:1:473:SER:HB2	1:1:478:ILE:H	1.84	0.42
2:2:286:GLY:HA3	2:2:305:GLU:H	1.84	0.42
8:8:315:ASP:O	8:8:319:ILE:N	2.52	0.42
10:A:604:A:O3'	13:D:22:LYS:NZ	2.53	0.42
22:M:42:PRO:HG3	32:Z:203:PRO:HG2	2.01	0.42
36:d:5:THR:OG1	36:d:6:VAL:N	2.52	0.42
38:f:43:VAL:HG21	38:f:83:PHE:HE2	1.84	0.42
38:f:124:ARG:NE	38:f:130:ARG:O	2.48	0.42
42:m:68:LEU:O	42:m:72:HIS:ND1	2.44	0.42
48:s:207:PRO:HB3	48:s:225:ILE:HD11	2.02	0.42
50:u:51:MET:HE3	50:u:51:MET:HB3	1.74	0.42
51:v:262:ILE:HG23	51:v:335:ASN:HB2	2.02	0.42
53:x:54:ARG:HB3	53:x:56:THR:HG23	2.02	0.42
10:A:555:A:N6	10:A:557:U:O2	2.53	0.42
10:A:693:A:H2'	10:A:694:G:H8	1.85	0.42
17:H:20:LYS:NZ	18:I:13:GLN:O	2.48	0.42
20:K:30:ALA:O	20:K:60:ARG:NH1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:T:104:ARG:HG2	29:T:108:LYS:HD2	2.01	0.42
49:t:20:LEU:HB3	49:t:330:TYR:CD1	2.54	0.42
50:u:301:HIS:HA	50:u:376:ARG:HH21	1.84	0.42
10:A:194:C:H2'	10:A:195:C:C6	2.54	0.42
10:A:640:A:H2'	10:A:641:A:C8	2.54	0.42
24:O:86:LEU:HB3	24:O:98:THR:HB	2.01	0.42
28:S:5:ILE:HD13	28:S:111:LEU:HB2	2.00	0.42
42:m:79:VAL:HG11	42:m:85:LEU:HB2	2.02	0.42
49:t:322:PHE:HA	49:t:326:ASN:O	2.20	0.42
50:u:415:ARG:HD2	50:u:415:ARG:HA	1.71	0.42
53:x:394:LYS:HD3	53:x:435:TRP:CD2	2.55	0.42
5:5:303:SER:OG	5:5:304:MET:N	2.53	0.42
5:5:463:PHE:HA	51:v:376:ARG:HH12	1.85	0.42
5:5:475:LEU:HD12	5:5:528:ILE:HD12	2.01	0.42
7:7:-26:C:OP2	54:y:723:ARG:NH1	2.53	0.42
10:A:647:U:H2'	10:A:648:A:H8	1.85	0.42
10:A:960:U:O2'	10:A:962:A:N7	2.40	0.42
11:B:48:LYS:NZ	11:B:52:GLU:OE2	2.33	0.42
27:R:66:SER:HB2	27:R:73:THR:HG22	2.01	0.42
33:a:16:PHE:HE1	33:a:76:ILE:HG23	1.83	0.42
34:b:89:MET:HE2	34:b:89:MET:HB3	1.87	0.42
48:s:318:PHE:HB2	48:s:321:VAL:HG13	2.01	0.42
50:u:486:HIS:O	50:u:489:ARG:NH1	2.52	0.42
1:1:548:ARG:HD3	1:1:555:PRO:HG2	2.00	0.42
10:A:1447:G:H2'	10:A:1448:A:H8	1.85	0.42
15:F:79:SER:OG	15:F:80:LEU:N	2.50	0.42
21:L:62:PRO:HD3	21:L:71:LYS:HE3	2.02	0.42
36:d:51:ASN:HB3	36:d:54:TYR:HD2	1.84	0.42
37:e:63:PRO:HG2	37:e:96:LEU:HD23	2.01	0.42
45:p:56:LYS:HB3	45:p:59:LEU:H	1.84	0.42
50:u:194:PHE:O	50:u:198:CYS:N	2.51	0.42
54:y:567:CYS:HA	54:y:571:CYS:H	1.84	0.42
10:A:641:A:OP1	13:D:40:LYS:NZ	2.42	0.42
10:A:1854:U:H5''	25:P:150:ARG:HH12	1.85	0.42
10:A:1860:A:N7	26:Q:34:LYS:NZ	2.67	0.42
10:A:1863:A:N3	26:Q:79:ILE:HD11	2.35	0.42
12:C:35:PRO:HG2	12:C:36:HIS:CD2	2.55	0.42
12:C:100:ARG:HB2	12:C:114:ILE:HD13	2.02	0.42
12:C:197:ASN:OD1	12:C:198:ARG:N	2.52	0.42
24:O:145:LYS:HE3	24:O:145:LYS:HB2	1.73	0.42
47:r:16:VAL:HG12	47:r:17:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:294:ILE:HD12	49:t:358:LEU:HD11	2.01	0.42
49:t:327:ASP:OD1	49:t:327:ASP:N	2.52	0.42
49:t:416:ARG:HB3	49:t:428:VAL:HB	2.01	0.42
50:u:254:GLU:HA	50:u:358:LEU:HD11	2.02	0.42
54:y:422:GLU:HG3	54:y:441:ARG:HH21	1.84	0.42
54:y:832:MET:HE1	54:y:834:SER:OG	2.20	0.42
10:A:69:C:H5'	28:S:167:LYS:NZ	2.35	0.42
10:A:305:U:O3'	27:R:41:ARG:NH1	2.41	0.42
10:A:692:G:H2'	10:A:693:A:N9	2.34	0.42
10:A:710:C:H2'	10:A:711:C:C6	2.55	0.42
28:S:157:VAL:HG21	28:S:176:ILE:HD11	2.02	0.42
35:c:31:ILE:HG23	35:c:45:LEU:HD11	2.02	0.42
36:d:18:LEU:HD22	36:d:58:ALA:HA	2.02	0.42
49:t:81:LEU:HD13	49:t:259:ILE:HG13	2.02	0.42
51:v:383:LYS:HB3	51:v:392:VAL:HG23	2.01	0.42
1:1:680:ALA:HA	1:1:695:ASN:HA	2.01	0.41
5:5:115:ALA:HB1	5:5:129:LEU:HD12	2.02	0.41
5:5:475:LEU:HD23	5:5:478:PHE:HD2	1.84	0.41
5:5:495:HIS:HA	5:5:498:LYS:HE3	2.02	0.41
7:7:-10:A:C8	7:7:-9:A:C6	3.08	0.41
7:7:6:A:H5''	7:7:7:A:C8	2.54	0.41
10:A:170:A:OP2	28:S:140:ARG:NH1	2.53	0.41
10:A:1867:U:C4	26:Q:84:VAL:HG12	2.55	0.41
11:B:93:LEU:HD21	14:E:8:ARG:HH21	1.85	0.41
34:b:61:ARG:NH1	34:b:88:GLU:OE2	2.48	0.41
37:e:48:VAL:HG11	38:f:23:ARG:HA	2.02	0.41
41:k:102:VAL:HB	41:k:104:LYS:HE3	2.02	0.41
44:o:302:GLY:HA2	44:o:309:ILE:HG23	2.02	0.41
47:r:77:ASP:HB3	47:r:82:TYR:HB2	2.02	0.41
49:t:7:GLY:HA3	49:t:20:LEU:H	1.85	0.41
49:t:181:LYS:O	49:t:183:LYS:NZ	2.48	0.41
49:t:323:ALA:O	49:t:324:GLU:C	2.63	0.41
53:x:357:ALA:HB3	53:x:377:HIS:HB2	2.01	0.41
10:A:729:C:H2'	10:A:730:C:C6	2.55	0.41
10:A:897:U:N3	10:A:899:U:O4	2.53	0.41
10:A:924:G:H5'	18:I:4:MET:HE3	2.03	0.41
10:A:1413:G:H2'	10:A:1414:A:H8	1.84	0.41
10:A:1574:C:H2'	10:A:1575:G:C8	2.55	0.41
13:D:136:ARG:HD2	13:D:139:LYS:HA	2.02	0.41
14:E:63:ASN:ND2	14:E:114:ASP:OD2	2.46	0.41
16:G:37:LYS:HA	16:G:37:LYS:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:93:LEU:O	25:P:127:GLY:N	2.46	0.41
32:Z:61:GLU:O	33:a:95:ARG:NH2	2.53	0.41
49:t:64:VAL:HG12	49:t:68:ARG:HH21	1.85	0.41
50:u:321:ARG:HG3	50:u:423:GLU:HG3	2.01	0.41
53:x:289:LEU:HD23	53:x:317:THR:HG22	2.01	0.41
54:y:375:LYS:HB3	54:y:408:LEU:HD13	2.01	0.41
10:A:126:G:OP2	28:S:195:LYS:NZ	2.41	0.41
10:A:1372:U:OP1	10:A:1385:G:N2	2.35	0.41
10:A:1844:U:H3	10:A:1855:G:H1	1.67	0.41
11:B:88:ILE:HD11	11:B:109:MET:HE3	2.01	0.41
23:N:79:SER:OG	23:N:130:ASP:OD1	2.35	0.41
24:O:71:LEU:HD21	24:O:189:ILE:HG23	2.01	0.41
26:Q:46:GLU:HG3	26:Q:47:ALA:H	1.86	0.41
35:c:212:LYS:HA	35:c:235:ILE:HG23	2.02	0.41
49:t:158:LEU:HA	49:t:188:LEU:HB2	2.01	0.41
49:t:408:ILE:HA	49:t:441:ILE:HG23	2.01	0.41
50:u:564:GLU:HA	50:u:572:ARG:HH22	1.85	0.41
53:x:52:ASP:CG	53:x:54:ARG:HH12	2.28	0.41
54:y:637:GLN:HE21	54:y:682:LEU:HG	1.85	0.41
9:9:18:ARG:HG2	9:9:22:GLN:NE2	2.35	0.41
10:A:85:A:H2'	10:A:86:C:H6	1.86	0.41
10:A:130:G:O2'	10:A:131:C:O3'	2.37	0.41
10:A:156:G:OP1	28:S:2:LYS:NZ	2.44	0.41
10:A:375:U:H2'	10:A:376:A:C8	2.55	0.41
10:A:839:C:N4	29:T:9:THR:O	2.39	0.41
10:A:1405:A:H2'	10:A:1406:G:O4'	2.20	0.41
10:A:1575:G:H2'	10:A:1576:G:H8	1.85	0.41
15:F:128:GLY:HA2	15:F:129:PRO:HD3	1.94	0.41
43:n:38:THR:HG22	53:x:426:LYS:HZ1	1.85	0.41
46:q:27:VAL:O	46:q:95:TYR:OH	2.31	0.41
49:t:147:ASN:ND2	49:t:412:SER:OG	2.36	0.41
51:v:39:GLN:HA	51:v:251:PRO:HA	2.02	0.41
54:y:80:LEU:HA	54:y:141:LEU:HD13	2.02	0.41
6:6:278:ARG:HB3	6:6:311:PHE:CZ	2.56	0.41
10:A:1410:C:H2'	10:A:1411:G:C8	2.56	0.41
10:A:1705:C:H2'	10:A:1706:G:C8	2.56	0.41
32:Z:64:ARG:HD3	33:a:94:LEU:HD13	2.02	0.41
34:b:37:TYR:HE1	34:b:112:ILE:HG22	1.85	0.41
47:r:155:HIS:O	47:r:158:SER:OG	2.34	0.41
48:s:294:ASP:CG	48:s:295:THR:H	2.28	0.41
49:t:110:PRO:HG2	49:t:113:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:t:152:MET:HE3	49:t:152:MET:HB3	1.86	0.41
49:t:379:ARG:O	49:t:380:ARG:NH1	2.38	0.41
53:x:83:VAL:HG13	53:x:85:THR:HG22	2.02	0.41
1:1:505:ARG:HD2	1:1:505:ARG:HA	1.94	0.41
5:5:184:TRP:HH2	5:5:279:ARG:HH12	1.67	0.41
10:A:1391:C:H4'	40:i:55:LEU:HD21	2.02	0.41
11:B:80:MET:HE3	11:B:80:MET:HB3	1.81	0.41
19:J:3:ARG:NH1	19:J:9:ASP:OD2	2.54	0.41
22:M:41:ILE:HG12	32:Z:208:VAL:HG13	2.02	0.41
22:M:57:LEU:O	22:M:61:ILE:HG12	2.21	0.41
35:c:18:VAL:O	35:c:287:THR:OG1	2.39	0.41
39:h:17:ILE:HD13	39:h:94:PRO:HD3	2.02	0.41
50:u:186:LEU:HD11	50:u:239:SER:HA	2.02	0.41
54:y:111:ALA:HB1	54:y:160:LYS:HE3	2.03	0.41
6:6:294:PHE:HA	6:6:297:MET:HE2	2.03	0.41
10:A:71:G:H2'	10:A:72:C:O4'	2.20	0.41
10:A:545:A:O2'	10:A:546:G:O4'	2.37	0.41
10:A:1017:U:H5'	18:I:55:ARG:HD3	2.03	0.41
27:R:3:ILE:O	27:R:30:GLY:N	2.48	0.41
49:t:238:TYR:O	49:t:242:LYS:HB3	2.21	0.41
49:t:297:ARG:HE	49:t:367:ILE:HG13	1.85	0.41
49:t:371:LEU:HD23	49:t:371:LEU:HA	1.95	0.41
54:y:509:HIS:O	54:y:513:LYS:NZ	2.44	0.41
5:5:502:TRP:HA	5:5:511:GLY:HA2	2.02	0.41
10:A:186:C:H2'	10:A:187:G:H8	1.85	0.41
10:A:1221:G:H2'	10:A:1222:G:C8	2.56	0.41
10:A:1579:A:O2'	10:A:1581:C:OP2	2.29	0.41
24:O:99:ASN:OD1	24:O:100:PHE:N	2.54	0.41
35:c:67:SER:OG	35:c:81:GLY:O	2.36	0.41
41:k:119:ARG:HB2	41:k:132:MET:HB2	2.03	0.41
46:q:22:GLU:HG2	46:q:23:LYS:HD3	2.03	0.41
48:s:292:GLN:CB	48:s:308:ARG:NH1	2.83	0.41
51:v:270:ARG:NH1	51:v:273:VAL:HG23	2.36	0.41
53:x:475:GLU:HG2	53:x:479:GLN:HE21	1.86	0.41
10:A:3:C:O2'	13:D:18:ARG:NH2	2.53	0.41
10:A:186:C:H2'	10:A:187:G:C8	2.56	0.41
10:A:1539:U:H2'	10:A:1540:G:C8	2.55	0.41
10:A:1862:G:H1'	10:A:1863:A:H2'	2.02	0.41
14:E:105:PHE:CD2	14:E:112:VAL:HB	2.56	0.41
18:I:83:ASP:OD1	18:I:83:ASP:N	2.53	0.41
22:M:120:THR:OG1	22:M:121:GLN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:N:190:SER:HB2	23:N:193:HIS:CE1	2.56	0.41
24:O:62:LEU:O	24:O:88:THR:OG1	2.26	0.41
31:Y:101:ASP:OD1	31:Y:102:GLU:N	2.53	0.41
42:m:22:LEU:HD22	42:m:89:VAL:HG12	2.03	0.41
49:t:58:VAL:O	49:t:62:SER:OG	2.35	0.41
49:t:96:CYS:HB2	49:t:120:THR:HG21	2.03	0.41
49:t:381:LEU:H	49:t:393:ALA:HB1	1.85	0.41
49:t:408:ILE:HG21	49:t:433:VAL:HG21	2.03	0.41
50:u:338:ILE:HG23	54:y:745:LYS:HD3	2.02	0.41
50:u:448:GLN:HA	50:u:493:PHE:HB2	2.03	0.41
50:u:539:PRO:HB2	50:u:542:ILE:HB	2.02	0.41
51:v:35:LYS:O	51:v:252:HIS:NE2	2.47	0.41
51:v:290:ASP:HA	51:v:291:PRO:HD3	1.93	0.41
53:x:414:ASP:OD1	53:x:414:ASP:N	2.53	0.41
54:y:691:MET:HE2	54:y:691:MET:HB3	1.91	0.41
54:y:808:SER:HB3	54:y:818:VAL:HG11	2.03	0.41
9:9:12:ARG:NH2	10:A:1847:G:N7	2.69	0.41
10:A:380:G:OP1	27:R:31:ARG:NH1	2.44	0.41
10:A:1256:G:N2	40:i:30:LEU:O	2.52	0.41
10:A:1403:C:OP1	10:A:1433:C:N4	2.54	0.41
10:A:1436:C:O2'	10:A:1438:A:O5'	2.37	0.41
10:A:1674:G:OP1	30:V:51:HIS:NE2	2.49	0.41
13:D:142:VAL:HG12	13:D:144:ILE:H	1.86	0.41
23:N:99:ILE:HD11	23:N:117:ARG:HD2	2.02	0.41
24:O:78:GLU:HB3	50:u:14[A]:ARG:HH22	1.85	0.41
49:t:211:VAL:HB	49:t:217:GLU:HA	2.02	0.41
49:t:256:LEU:N	49:t:358:LEU:O	2.45	0.41
49:t:297:ARG:HH22	49:t:467:PRO:HD3	1.85	0.41
52:w:75:C:H4'	52:w:76:A:C6	2.54	0.41
6:6:116:ASN:O	6:6:120:ARG:N	2.50	0.40
10:A:85:A:H2'	10:A:86:C:C6	2.57	0.40
10:A:379:C:OP2	27:R:181:GLN:NE2	2.54	0.40
10:A:799:U:H2'	10:A:800:U:O4'	2.20	0.40
10:A:982:G:H2'	10:A:983:A:C8	2.56	0.40
10:A:1269:G:H2'	10:A:1270:G:C8	2.56	0.40
18:I:64:ARG:HD3	18:I:70:LYS:HG2	2.03	0.40
24:O:91:VAL:HG12	24:O:96:CYS:HA	2.02	0.40
28:S:208:GLU:HA	28:S:211:LYS:HG2	2.03	0.40
44:o:247:SER:OG	44:o:249:ASP:OD1	2.36	0.40
50:u:279:VAL:HG12	50:u:295:THR:HG21	2.03	0.40
50:u:400:PRO:HA	50:u:403:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:417:MET:HA	51:v:420:MET:HE2	2.03	0.40
54:y:114:GLU:OE2	54:y:160:LYS:NZ	2.41	0.40
3:3:47:ASN:O	3:3:51:LEU:N	2.51	0.40
7:7:-3:A:N3	7:7:-3:A:C3'	2.83	0.40
10:A:640:A:P	15:F:115:ARG:HH22	2.45	0.40
10:A:1092:G:H2'	10:A:1093:A:H8	1.87	0.40
10:A:1408:U:H2'	10:A:1409:A:C8	2.57	0.40
48:s:295:THR:C	48:s:297:LEU:N	2.77	0.40
50:u:196:LYS:HE2	50:u:196:LYS:HB2	1.92	0.40
50:u:279:VAL:HA	50:u:282:VAL:HG12	2.02	0.40
50:u:413:TRP:CD1	50:u:417:GLN:HE22	2.40	0.40
54:y:331:LYS:HD2	54:y:331:LYS:HA	1.81	0.40
5:5:200:TYR:O	5:5:207:LYS:NZ	2.39	0.40
10:A:72:C:O2'	10:A:74:G:N2	2.54	0.40
10:A:198:U:N3	10:A:203:G:O6	2.55	0.40
10:A:603:C:N4	10:A:620:G:O6	2.51	0.40
10:A:796:G:N2	10:A:798:G:OP1	2.55	0.40
10:A:1308:U:H2'	10:A:1309:C:H6	1.86	0.40
10:A:1726:G:H2'	10:A:1727:G:H8	1.86	0.40
13:D:33:GLY:HA3	15:F:112:TYR:CG	2.55	0.40
21:L:68:ARG:NH1	21:L:276:THR:HA	2.36	0.40
28:S:106:LEU:HD13	28:S:109:LEU:HD13	2.02	0.40
33:a:55:ARG:NH1	33:a:78:TYR:OH	2.55	0.40
35:c:282:GLU:HG3	35:c:285:GLN:HE22	1.86	0.40
41:k:92:LYS:HD2	41:k:92:LYS:HA	1.89	0.40
49:t:189:GLN:HB3	49:t:223:PRO:HA	2.03	0.40
53:x:173:GLU:HA	53:x:518:ARG:HA	2.03	0.40
54:y:347:ARG:HH22	54:y:387:PRO:HD3	1.87	0.40
7:7:-7:A:C2	7:7:-7:A:P	3.14	0.40
10:A:109:U:O2	11:B:71:ARG:NH2	2.54	0.40
10:A:1018:U:H2'	10:A:1019:C:H6	1.87	0.40
10:A:1736:G:H2'	10:A:1737:G:H8	1.86	0.40
11:B:49:GLU:HG2	11:B:118:ARG:NH1	2.37	0.40
18:I:45:LEU:HD23	18:I:45:LEU:HA	1.92	0.40
19:J:101:PHE:HA	19:J:113:HIS:CE1	2.56	0.40
21:L:134:ASN:ND2	21:L:134:ASN:O	2.54	0.40
28:S:39:ASP:OD1	28:S:39:ASP:N	2.55	0.40
30:V:89:THR:HA	30:V:92:ILE:HG12	2.04	0.40
37:e:56:ASP:HA	37:e:59:CYS:HB2	2.02	0.40
49:t:116:ASP:OD1	49:t:116:ASP:N	2.51	0.40
49:t:408:ILE:HD13	49:t:433:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:v:311:LYS:HA	51:v:314:GLU:HG2	2.03	0.40
10:A:1648:G:H22	10:A:1675:A:P	2.45	0.40
22:M:42:PRO:HG2	32:Z:205:PRO:HA	2.04	0.40
23:N:66:VAL:HG23	23:N:186:ARG:HG3	2.03	0.40
23:N:147:LEU:HD13	23:N:161:ILE:HB	2.04	0.40
37:e:91:LEU:HD23	37:e:91:LEU:HA	1.96	0.40
46:q:76:ILE:HG22	46:q:95:TYR:HD2	1.86	0.40
48:s:216:LYS:HE2	48:s:216:LYS:HB3	1.93	0.40
50:u:526:MET:HA	50:u:529:VAL:HG12	2.04	0.40
50:u:563:LYS:HA	50:u:567:ARG:HB3	2.03	0.40
53:x:50:TYR:OH	54:y:635:ASP:OD2	2.37	0.40
54:y:744:MET:HB2	54:y:752:CYS:SG	2.62	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%)	541 (93%)	43 (7%)	0	100	100
2	2	300/325 (92%)	296 (99%)	4 (1%)	0	100	100
3	3	209/218 (96%)	197 (94%)	12 (6%)	0	100	100
4	4	251/357 (70%)	240 (96%)	11 (4%)	0	100	100
5	5	518/564 (92%)	508 (98%)	10 (2%)	0	100	100
6	6	360/374 (96%)	347 (96%)	13 (4%)	0	100	100
8	8	313/352 (89%)	293 (94%)	20 (6%)	0	100	100
9	9	22/25 (88%)	22 (100%)	0	0	100	100
11	B	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
12	C	254/263 (97%)	248 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	D	175/194 (90%)	172 (98%)	3 (2%)	0	100	100
14	E	138/143 (96%)	133 (96%)	5 (4%)	0	100	100
15	F	56/59 (95%)	48 (86%)	8 (14%)	0	100	100
16	G	171/194 (88%)	164 (96%)	7 (4%)	0	100	100
17	H	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
18	I	148/151 (98%)	148 (100%)	0	0	100	100
19	J	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
20	K	79/83 (95%)	73 (92%)	6 (8%)	0	100	100
21	L	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
22	M	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
23	N	205/295 (70%)	196 (96%)	9 (4%)	0	100	100
24	O	209/264 (79%)	202 (97%)	7 (3%)	0	100	100
25	P	131/151 (87%)	121 (92%)	10 (8%)	0	100	100
26	Q	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
27	R	194/208 (93%)	189 (97%)	5 (3%)	0	100	100
28	S	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
29	T	123/133 (92%)	123 (100%)	0	0	100	100
30	V	187/204 (92%)	174 (93%)	13 (7%)	0	100	100
31	Y	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
32	Z	225/243 (93%)	219 (97%)	6 (3%)	0	100	100
33	a	97/165 (59%)	90 (93%)	7 (7%)	0	100	100
34	b	119/145 (82%)	117 (98%)	2 (2%)	0	100	100
35	c	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
36	d	140/145 (97%)	138 (99%)	2 (1%)	0	100	100
37	e	64/125 (51%)	63 (98%)	1 (2%)	0	100	100
38	f	140/152 (92%)	134 (96%)	6 (4%)	0	100	100
39	h	101/119 (85%)	97 (96%)	4 (4%)	0	100	100
40	i	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
41	k	67/157 (43%)	55 (82%)	12 (18%)	0	100	100
42	m	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
43	n	61/69 (88%)	55 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	o	75/320 (23%)	70 (93%)	5 (7%)	0	100	100
45	p	108/113 (96%)	96 (89%)	12 (11%)	0	100	100
46	q	91/144 (63%)	87 (96%)	4 (4%)	0	100	100
47	r	294/315 (93%)	276 (94%)	18 (6%)	0	100	100
48	s	157/333 (47%)	138 (88%)	19 (12%)	0	100	100
49	t	470/472 (100%)	431 (92%)	39 (8%)	0	100	100
50	u	705/1382 (51%)	672 (95%)	33 (5%)	0	100	100
51	v	403/445 (91%)	377 (94%)	26 (6%)	0	100	100
53	x	417/548 (76%)	396 (95%)	21 (5%)	0	100	100
54	y	725/913 (79%)	697 (96%)	28 (4%)	0	100	100
All	All	10720/13491 (80%)	10218 (95%)	502 (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
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%)	158 (100%)	0	100	100
14	E	112/115 (97%)	112 (100%)	0	100	100
15	F	47/48 (98%)	47 (100%)	0	100	100
16	G	159/174 (91%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	119 (100%)	0	100	100
23	N	173/243 (71%)	173 (100%)	0	100	100
24	O	192/231 (83%)	192 (100%)	0	100	100
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	159/170 (94%)	159 (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%)	90 (100%)	0	100	100
34	b	107/130 (82%)	107 (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	58/103 (56%)	58 (100%)	0	100	100
38	f	123/132 (93%)	123 (100%)	0	100	100
39	h	94/107 (88%)	94 (100%)	0	100	100
40	i	44/49 (90%)	44 (100%)	0	100	100
41	k	61/140 (44%)	61 (100%)	0	100	100
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	p	79/96 (82%)	79 (100%)	0	100	100
46	q	79/123 (64%)	79 (100%)	0	100	100
47	r	190/280 (68%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	s	142/304 (47%)	142 (100%)	0	100	100
49	t	397/397 (100%)	396 (100%)	1 (0%)	86	84
50	u	528/1259 (42%)	528 (100%)	0	100	100
51	v	206/406 (51%)	206 (100%)	0	100	100
53	x	207/494 (42%)	207 (100%)	0	100	100
54	y	569/811 (70%)	569 (100%)	0	100	100
All	All	7302/10993 (66%)	7301 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	t	326	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	477	ASN
1	1	518	HIS
1	1	522	ASN
5	5	92	GLN
5	5	368	HIS
5	5	407	GLN
5	5	434	ASN
5	5	514	GLN
6	6	273	ASN
12	C	50	ASN
12	C	142	HIS
12	C	188	ASN
13	D	156	HIS
14	E	16	HIS
15	F	77	HIS
15	F	89	GLN
15	F	132	ASN
16	G	162	GLN
16	G	168	HIS
17	H	9	HIS
19	J	98	GLN
21	L	134	ASN
22	M	74	GLN

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Mol	Chain	Res	Type
24	O	124	HIS
24	O	186	ASN
25	P	26	ASN
25	P	113	GLN
28	S	56	ASN
28	S	105	ASN
28	S	110	ASN
29	T	89	HIS
30	V	79	HIS
30	V	179	ASN
33	a	28	HIS
34	b	24	GLN
34	b	35	GLN
34	b	103	ASN
36	d	137	GLN
37	e	45	ASN
38	f	72	GLN
38	f	105	ASN
41	k	93	HIS
41	k	139	HIS
41	k	151	ASN
42	m	15	ASN
45	p	48	GLN
45	p	84	GLN
45	p	86	GLN
45	p	89	GLN
45	p	95	GLN
45	p	111	HIS
47	r	187	GLN
49	t	33	HIS
49	t	169	GLN
49	t	401	ASN
50	u	79	GLN
50	u	110	GLN
50	u	138	GLN
50	u	221	ASN
50	u	226	GLN
50	u	236	GLN
50	u	399	ASN
50	u	445	GLN
50	u	521	ASN
50	u	566	GLN

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Mol	Chain	Res	Type
51	v	335	ASN
51	v	395	ASN
53	x	411	GLN
54	y	326	HIS
54	y	334	ASN
54	y	355	GLN
54	y	364	ASN
54	y	377	ASN
54	y	487	GLN
54	y	615	GLN
54	y	631	ASN
54	y	648	GLN
54	y	662	GLN
54	y	670	GLN
54	y	713	GLN
54	y	716	HIS
54	y	819	HIS
54	y	852	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1746/1869 (93%)	412 (23%)	8 (0%)
52	w	74/75 (98%)	28 (37%)	0
7	7	46/255 (18%)	34 (73%)	4 (8%)
All	All	1866/2199 (84%)	474 (25%)	12 (0%)

All (474) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	7	-27	A
7	7	-26	C
7	7	-23	C
7	7	-22	A
7	7	-21	A
7	7	-20	C
7	7	-16	A
7	7	-15	A
7	7	-13	A
7	7	-12	A
7	7	-10	A

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Mol	Chain	Res	Type
7	7	-9	A
7	7	-8	C
7	7	-7	A
7	7	-6	A
7	7	-5	C
7	7	-4	A
7	7	-3	A
7	7	-2	G
7	7	-1	G
7	7	1	A
7	7	3	C
7	7	4	C
7	7	5	A
7	7	7	A
7	7	9	C
7	7	10	A
7	7	11	G
7	7	12	A
7	7	14	C
7	7	15	A
7	7	16	C
7	7	18	A
7	7	19	U
10	A	2	A
10	A	33	G
10	A	41	G
10	A	42	A
10	A	44	U
10	A	45	A
10	A	46	A
10	A	49	C
10	A	56	G
10	A	58	C
10	A	59	U
10	A	62	G
10	A	64	A
10	A	65	C
10	A	67	C
10	A	68	A
10	A	73	C
10	A	74	G
10	A	78	C

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Mol	Chain	Res	Type
10	A	103	A
10	A	114	G
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	149	A
10	A	155	G
10	A	158	A
10	A	163	U
10	A	171	A
10	A	173	A
10	A	175	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	291	G
10	A	292	A
10	A	295	C
10	A	302	A
10	A	306	C
10	A	307	G
10	A	308	G
10	A	318	A
10	A	319	C
10	A	321	C
10	A	323	C
10	A	324	C
10	A	325	C
10	A	326	C
10	A	327	G

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Mol	Chain	Res	Type
10	A	329	G
10	A	332	G
10	A	335	G
10	A	340	C
10	A	347	G
10	A	351	G
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	428	U
10	A	435	A
10	A	438	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	470	G
10	A	471	G
10	A	472	C
10	A	473	A
10	A	474	G
10	A	476	A
10	A	482	G
10	A	487	U
10	A	492	C
10	A	493	A
10	A	508	A
10	A	509	OMG
10	A	517	OMC
10	A	536	A
10	A	537	C

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Mol	Chain	Res	Type
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	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	587	A
10	A	589	G
10	A	590	A
10	A	591	U
10	A	593	C
10	A	594	A
10	A	603	C
10	A	607	U
10	A	614	C
10	A	617	G
10	A	628	A
10	A	629	A
10	A	631	U
10	A	643	A
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	684	G

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Mol	Chain	Res	Type
10	A	688	U
10	A	689	U
10	A	690	G
10	A	691	G
10	A	692	G
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	710	C
10	A	716	G
10	A	717	G
10	A	720	A
10	A	721	G
10	A	722	C
10	A	728	C
10	A	731	G
10	A	732	U
10	A	733	C
10	A	734	C
10	A	735	C
10	A	737	G
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	790	C
10	A	791	C
10	A	798	G
10	A	799	U
10	A	800	U
10	A	801	U
10	A	810	A
10	A	821	G
10	A	822	PSU
10	A	827	A
10	A	830	A

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Mol	Chain	Res	Type
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	847	A
10	A	870	A
10	A	872	A
10	A	873	G
10	A	880	G
10	A	887	U
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
10	A	899	U
10	A	900	C
10	A	901	G
10	A	903	A
10	A	913	A
10	A	914	U
10	A	920	A
10	A	922	A
10	A	933	G
10	A	934	G
10	A	963	A
10	A	969	U
10	A	972	A
10	A	982	G
10	A	989	C
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	1039	C
10	A	1040	G

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Mol	Chain	Res	Type
10	A	1045	U
10	A	1047	C
10	A	1061	U
10	A	1062	A
10	A	1078	C
10	A	1083	A
10	A	1085	C
10	A	1096	G
10	A	1109	C
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	1133	A
10	A	1138	C
10	A	1149	A
10	A	1150	A
10	A	1153	C
10	A	1154	U
10	A	1155	U
10	A	1170	A
10	A	1195	A
10	A	1207	G
10	A	1208	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	1248	B8N
10	A	1251	A
10	A	1253	A
10	A	1256	G
10	A	1257	G
10	A	1259	A
10	A	1264	C
10	A	1274	G
10	A	1275	G

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Mol	Chain	Res	Type
10	A	1283	C
10	A	1284	A
10	A	1286	G
10	A	1287	A
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	1320	G
10	A	1322	G
10	A	1326	U
10	A	1333	U
10	A	1341	C
10	A	1342	U
10	A	1348	G
10	A	1354	G
10	A	1356	G
10	A	1371	U
10	A	1372	U
10	A	1375	G
10	A	1376	A
10	A	1378	A
10	A	1382	A
10	A	1397	U
10	A	1401	A
10	A	1402	A
10	A	1409	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

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Mol	Chain	Res	Type
10	A	1436	C
10	A	1437	C
10	A	1438	A
10	A	1442	U
10	A	1446	A
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	1494	U
10	A	1497	G
10	A	1498	A
10	A	1507	G
10	A	1508	A
10	A	1521	C
10	A	1522	A
10	A	1533	A
10	A	1534	C
10	A	1536	G
10	A	1544	C
10	A	1552	G
10	A	1553	C
10	A	1556	A
10	A	1560	U
10	A	1570	G
10	A	1578	U
10	A	1579	A
10	A	1580	A
10	A	1585	U
10	A	1587	G
10	A	1588	A
10	A	1600	G
10	A	1601	A
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	1646	C

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Mol	Chain	Res	Type
10	A	1648	G
10	A	1649	U
10	A	1654	G
10	A	1661	A
10	A	1663	A
10	A	1665	G
10	A	1671	G
10	A	1687	C
10	A	1699	A
10	A	1706	G
10	A	1712	A
10	A	1713	C
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
10	A	1755	C
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	1777	G
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

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Mol	Chain	Res	Type
10	A	1821	U
10	A	1822	A
10	A	1824	A
10	A	1825	A
10	A	1826	G
10	A	1829	G
10	A	1831	A
10	A	1835	A
10	A	1838	U
10	A	1849	G
10	A	1851	MA6
10	A	1861	G
10	A	1862	G
10	A	1863	A
10	A	1865	C
52	w	2	G
52	w	4	A
52	w	12	G
52	w	16	C
52	w	18	G
52	w	19	G
52	w	20	A
52	w	21	A
52	w	33	C
52	w	34	C
52	w	35	A
52	w	36	U
52	w	48	C
52	w	53	G
52	w	57	G
52	w	58	A
52	w	59	A
52	w	61	C
52	w	65	C
52	w	68	C
52	w	69	U
52	w	70	G
52	w	71	C
52	w	72	U
52	w	73	A
52	w	74	C
52	w	75	C

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Mol	Chain	Res	Type
52	w	76	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	7	-21	A
7	7	-10	A
7	7	-8	C
7	7	-4	A
10	A	1	U
10	A	291	G
10	A	367	U
10	A	606	G
10	A	688	U
10	A	731	G
10	A	797	C
10	A	1600	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	5MU	A	814	10	19,22,23	0.49	0	28,32,35	1.35	4 (14%)
10	OMG	A	644	10	23,26,27	0.52	0	33,38,41	0.46	0
10	A2M	A	1678	10	22,25,26	3.96	12 (54%)	31,36,39	3.48	14 (45%)
10	OMG	A	683	10	23,26,27	0.53	0	33,38,41	0.56	0
10	OMG	A	509	55,10	23,26,27	0.56	0	33,38,41	0.50	0
10	PSU	A	1243	10	18,21,22	1.10	1 (5%)	22,30,33	1.77	4 (18%)
10	OMU	A	121	10	19,22,23	2.97	6 (31%)	26,31,34	1.67	5 (19%)
10	UR3	A	1830	10	19,22,23	2.79	8 (42%)	26,32,35	1.50	3 (11%)
10	OMC	A	174	55,10	19,22,23	0.56	0	26,31,34	0.70	0
10	OMC	A	517	10	19,22,23	0.56	0	26,31,34	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MA6	A	1850	10	23,26,27	1.57	3 (13%)	34,38,41	3.17	12 (35%)
10	A2M	A	668	55,10	22,25,26	3.92	12 (54%)	31,36,39	3.36	14 (45%)
10	PSU	A	612	10	18,21,22	1.00	1 (5%)	22,30,33	1.73	5 (22%)
10	B8N	A	1248	10	24,29,30	3.11	6 (25%)	29,42,45	1.76	5 (17%)
10	A2M	A	159	10	22,25,26	3.92	10 (45%)	31,36,39	3.35	13 (41%)
10	A2M	A	27	55,10	22,25,26	3.93	12 (54%)	31,36,39	3.36	12 (38%)
10	5MC	A	1374	10	18,22,23	0.59	0	26,32,35	0.70	0
10	6MZ	A	1832	55,10	22,25,26	2.48	5 (22%)	30,36,39	2.53	11 (36%)
10	PSU	A	823	10	18,21,22	1.10	1 (5%)	22,30,33	1.71	4 (18%)
10	A2M	A	166	10	22,25,26	3.97	11 (50%)	31,36,39	3.41	15 (48%)
10	A2M	A	484	10	22,25,26	3.87	11 (50%)	31,36,39	3.32	12 (38%)
10	MA6	A	1851	10	23,26,27	1.57	2 (8%)	34,38,41	3.18	12 (35%)
10	PSU	A	119	10	18,21,22	0.97	1 (5%)	22,30,33	1.60	4 (18%)
10	A2M	A	1031	10	22,25,26	3.93	11 (50%)	31,36,39	3.37	13 (41%)
10	PSU	A	1081	10	18,21,22	1.02	1 (5%)	22,30,33	1.71	5 (22%)
10	JMH	A	1219	55,10	18,22,23	2.88	5 (27%)	21,32,35	1.45	3 (14%)
10	OMC	A	1703	10	19,22,23	0.55	0	26,31,34	0.68	0
10	OMU	A	116	10	19,22,23	2.98	6 (31%)	26,31,34	1.65	5 (19%)
10	PSU	A	822	10	18,21,22	1.05	1 (5%)	22,30,33	1.71	5 (22%)

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	5MU	A	814	10	-	1/7/25/26	0/2/2/2
10	OMG	A	644	10	-	3/9/27/28	0/3/3/3
10	A2M	A	1678	10	-	1/9/27/28	0/3/3/3
10	OMG	A	683	10	-	2/9/27/28	0/3/3/3
10	OMG	A	509	55,10	-	2/9/27/28	0/3/3/3
10	PSU	A	1243	10	-	2/7/25/26	0/2/2/2
10	OMU	A	121	10	-	0/9/27/28	0/2/2/2
10	UR3	A	1830	10	-	2/7/25/26	0/2/2/2
10	OMC	A	174	55,10	-	0/9/27/28	0/2/2/2
10	OMC	A	517	10	-	2/9/27/28	0/2/2/2
10	MA6	A	1850	10	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	A2M	A	668	55,10	-	2/9/27/28	0/3/3/3
10	PSU	A	612	10	-	0/7/25/26	0/2/2/2
10	B8N	A	1248	10	-	9/16/34/35	0/2/2/2
10	A2M	A	159	10	-	2/9/27/28	0/3/3/3
10	A2M	A	27	55,10	-	2/9/27/28	0/3/3/3
10	5MC	A	1374	10	-	0/7/25/26	0/2/2/2
10	6MZ	A	1832	55,10	-	0/9/27/28	0/3/3/3
10	PSU	A	823	10	-	0/7/25/26	0/2/2/2
10	A2M	A	166	10	-	1/9/27/28	0/3/3/3
10	A2M	A	484	10	-	0/9/27/28	0/3/3/3
10	MA6	A	1851	10	-	3/11/29/30	0/3/3/3
10	PSU	A	119	10	-	1/7/25/26	0/2/2/2
10	A2M	A	1031	10	-	1/9/27/28	0/3/3/3
10	PSU	A	1081	10	-	1/7/25/26	0/2/2/2
10	JMH	A	1219	55,10	-	1/7/25/26	0/2/2/2
10	OMC	A	1703	10	-	0/9/27/28	0/2/2/2
10	OMU	A	116	10	-	1/9/27/28	0/2/2/2
10	PSU	A	822	10	-	2/7/25/26	0/2/2/2

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	166	A2M	C3'-C2'	-12.88	1.24	1.52
10	A	1678	A2M	C3'-C2'	-12.82	1.24	1.52
10	A	1031	A2M	C3'-C2'	-12.79	1.24	1.52
10	A	27	A2M	C3'-C2'	-12.70	1.24	1.52
10	A	159	A2M	C3'-C2'	-12.63	1.24	1.52
10	A	484	A2M	C3'-C2'	-12.33	1.25	1.52
10	A	668	A2M	C3'-C2'	-12.28	1.25	1.52
10	A	1832	6MZ	C6-N6	9.98	1.45	1.34
10	A	1248	B8N	C4-N3	-8.33	1.25	1.40
10	A	1219	JMH	C2-N1	8.05	1.50	1.38
10	A	1248	B8N	C6-N1	7.71	1.55	1.36
10	A	1830	UR3	C2-N1	7.45	1.49	1.38
10	A	116	OMU	C2-N3	7.03	1.50	1.38
10	A	668	A2M	O4'-C4'	-7.00	1.29	1.45
10	A	121	OMU	C2-N3	6.92	1.50	1.38
10	A	116	OMU	C2-N1	6.91	1.49	1.38
10	A	121	OMU	C2-N1	6.87	1.49	1.38
10	A	1678	A2M	O4'-C4'	-6.78	1.29	1.45
10	A	159	A2M	O4'-C4'	-6.77	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	484	A2M	O4'-C4'	-6.69	1.30	1.45
10	A	27	A2M	O4'-C4'	-6.60	1.30	1.45
10	A	166	A2M	O4'-C4'	-6.59	1.30	1.45
10	A	1031	A2M	O4'-C4'	-6.51	1.30	1.45
10	A	121	OMU	C6-C5	6.13	1.49	1.35
10	A	1830	UR3	C6-C5	6.07	1.49	1.35
10	A	116	OMU	C6-C5	6.06	1.49	1.35
10	A	1219	JMH	C6-C5	6.01	1.49	1.35
10	A	1248	B8N	C6-C5	5.61	1.42	1.34
10	A	668	A2M	C3'-C4'	5.29	1.66	1.53
10	A	1248	B8N	C2-N1	5.24	1.54	1.39
10	A	1678	A2M	C3'-C4'	5.23	1.66	1.53
10	A	1219	JMH	C2-N3	5.23	1.49	1.39
10	A	484	A2M	C3'-C4'	5.19	1.66	1.53
10	A	27	A2M	C3'-C4'	5.12	1.66	1.53
10	A	1830	UR3	C2-N3	5.08	1.48	1.39
10	A	1851	MA6	C6-N6	5.05	1.51	1.36
10	A	159	A2M	C3'-C4'	5.03	1.65	1.53
10	A	1850	MA6	C6-N6	5.01	1.51	1.36
10	A	1031	A2M	C3'-C4'	4.94	1.65	1.53
10	A	166	A2M	C3'-C4'	4.86	1.65	1.53
10	A	166	A2M	C6-N6	4.55	1.45	1.34
10	A	668	A2M	C1'-N9	-4.54	1.33	1.46
10	A	166	A2M	C1'-N9	-4.52	1.33	1.46
10	A	159	A2M	C6-N6	4.52	1.45	1.34
10	A	484	A2M	C6-N6	4.51	1.45	1.34
10	A	1031	A2M	C6-N6	4.51	1.45	1.34
10	A	1678	A2M	C6-N6	4.50	1.45	1.34
10	A	27	A2M	C6-N6	4.50	1.45	1.34
10	A	668	A2M	C6-N6	4.50	1.45	1.34
10	A	27	A2M	C1'-N9	-4.37	1.33	1.46
10	A	1031	A2M	O4'-C1'	4.34	1.52	1.42
10	A	1678	A2M	C1'-N9	-4.33	1.34	1.46
10	A	166	A2M	O4'-C1'	4.32	1.52	1.42
10	A	159	A2M	C1'-N9	-4.32	1.34	1.46
10	A	1031	A2M	C1'-N9	-4.25	1.34	1.46
10	A	1678	A2M	O4'-C1'	4.22	1.52	1.42
10	A	116	OMU	C4-N3	4.21	1.46	1.38
10	A	159	A2M	O4'-C1'	4.19	1.51	1.42
10	A	484	A2M	C1'-N9	-4.11	1.34	1.46
10	A	27	A2M	O4'-C1'	4.08	1.51	1.42
10	A	121	OMU	C4-N3	4.04	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	484	A2M	O4'-C1'	3.81	1.51	1.42
10	A	1248	B8N	C1'-C5	3.70	1.58	1.50
10	A	1243	PSU	C6-C5	3.63	1.39	1.35
10	A	668	A2M	O4'-C1'	3.57	1.50	1.42
10	A	27	A2M	O2'-C2'	3.45	1.51	1.42
10	A	823	PSU	C6-C5	3.42	1.39	1.35
10	A	159	A2M	O2'-C2'	3.42	1.51	1.42
10	A	1248	B8N	O2-C2	-3.41	1.16	1.22
10	A	166	A2M	O2'-C2'	3.39	1.51	1.42
10	A	822	PSU	C6-C5	3.36	1.39	1.35
10	A	484	A2M	O2'-C2'	3.34	1.51	1.42
10	A	1678	A2M	O2'-C2'	3.33	1.51	1.42
10	A	1031	A2M	O2'-C2'	3.31	1.51	1.42
10	A	668	A2M	O2'-C2'	3.28	1.51	1.42
10	A	119	PSU	C6-C5	3.22	1.39	1.35
10	A	484	A2M	C2'-C1'	3.11	1.61	1.53
10	A	1081	PSU	C6-C5	3.09	1.38	1.35
10	A	668	A2M	C2'-C1'	3.09	1.61	1.53
10	A	668	A2M	C5-C4	-3.05	1.33	1.39
10	A	612	PSU	C6-C5	3.03	1.38	1.35
10	A	1830	UR3	C6-N1	3.03	1.45	1.38
10	A	1851	MA6	C5-C4	-2.98	1.33	1.39
10	A	1832	6MZ	C5-N7	-2.97	1.33	1.39
10	A	1850	MA6	C5-C4	-2.97	1.33	1.39
10	A	166	A2M	C5-C4	-2.95	1.33	1.39
10	A	159	A2M	C2'-C1'	2.95	1.60	1.53
10	A	1031	A2M	C5-C4	-2.93	1.33	1.39
10	A	166	A2M	C2'-C1'	2.91	1.60	1.53
10	A	27	A2M	C5-C4	-2.89	1.33	1.39
10	A	1031	A2M	C2'-C1'	2.89	1.60	1.53
10	A	484	A2M	C5-C4	-2.87	1.33	1.39
10	A	1678	A2M	C5-C4	-2.83	1.33	1.39
10	A	1219	JMH	C6-N1	2.80	1.44	1.38
10	A	159	A2M	C5-C4	-2.78	1.33	1.39
10	A	1678	A2M	C2'-C1'	2.68	1.60	1.53
10	A	484	A2M	C5-N7	-2.67	1.34	1.39
10	A	27	A2M	C2'-C1'	2.67	1.60	1.53
10	A	121	OMU	C6-N1	2.61	1.44	1.38
10	A	1219	JMH	C5-C4	2.60	1.48	1.42
10	A	668	A2M	C5-N7	-2.58	1.34	1.39
10	A	27	A2M	C5-N7	-2.58	1.34	1.39
10	A	159	A2M	C5-N7	-2.58	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1031	A2M	C5-N7	-2.57	1.34	1.39
10	A	116	OMU	C6-N1	2.52	1.44	1.38
10	A	1678	A2M	C5-N7	-2.46	1.34	1.39
10	A	166	A2M	C5-N7	-2.44	1.34	1.39
10	A	1832	6MZ	C6-N1	-2.31	1.31	1.35
10	A	668	A2M	O3'-C3'	2.29	1.48	1.43
10	A	1830	UR3	O4-C4	-2.23	1.18	1.23
10	A	1830	UR3	C5-C4	2.19	1.49	1.43
10	A	668	A2M	C8-N9	-2.18	1.33	1.37
10	A	1830	UR3	C4-N3	2.16	1.45	1.40
10	A	1830	UR3	O2-C2	-2.16	1.18	1.22
10	A	1678	A2M	C8-N9	-2.16	1.33	1.37
10	A	484	A2M	O3'-C3'	2.16	1.48	1.43
10	A	1678	A2M	O3'-C3'	2.13	1.48	1.43
10	A	1832	6MZ	C5-C4	-2.12	1.35	1.39
10	A	121	OMU	C5-C4	2.12	1.48	1.43
10	A	1832	6MZ	C8-N9	-2.10	1.33	1.37
10	A	116	OMU	C5-C4	2.09	1.48	1.43
10	A	1850	MA6	C4-N3	2.09	1.38	1.34
10	A	1031	A2M	O3'-C3'	2.08	1.47	1.43
10	A	27	A2M	O3'-C3'	2.05	1.47	1.43
10	A	27	A2M	C8-N9	-2.04	1.33	1.37
10	A	166	A2M	C8-N9	-2.01	1.33	1.37

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1851	MA6	N1-C6-N6	-12.15	103.80	117.08
10	A	1850	MA6	N1-C6-N6	-12.07	103.89	117.08
10	A	1678	A2M	C1'-N9-C8	-9.56	105.56	127.14
10	A	668	A2M	C1'-N9-C8	-9.24	106.26	127.14
10	A	159	A2M	C1'-N9-C8	-9.20	106.36	127.14
10	A	27	A2M	C1'-N9-C8	-9.00	106.82	127.14
10	A	1031	A2M	C1'-N9-C8	-8.97	106.88	127.14
10	A	484	A2M	C1'-N9-C8	-8.92	107.00	127.14
10	A	166	A2M	C1'-N9-C8	-8.87	107.11	127.14
10	A	1678	A2M	C4-N9-C1'	8.03	145.74	126.59
10	A	159	A2M	C4-N9-C1'	7.87	145.35	126.59
10	A	484	A2M	C4-N9-C1'	7.83	145.24	126.59
10	A	1031	A2M	C4-N9-C1'	7.73	145.01	126.59
10	A	668	A2M	C4-N9-C1'	7.69	144.93	126.59
10	A	27	A2M	C4-N9-C1'	7.65	144.82	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	166	A2M	C4-N9-C1'	7.30	143.99	126.59
10	A	1851	MA6	C5-C6-N6	6.67	136.91	125.30
10	A	1850	MA6	C5-C6-N6	6.55	136.71	125.30
10	A	166	A2M	N3-C2-N1	-5.83	119.49	128.60
10	A	1832	6MZ	N1-C2-N3	-5.82	119.50	128.60
10	A	1832	6MZ	C9-N6-C6	5.75	127.83	122.87
10	A	1678	A2M	N6-C6-N1	-5.67	105.93	118.35
10	A	484	A2M	N6-C6-N1	-5.66	105.96	118.35
10	A	1678	A2M	N3-C2-N1	-5.63	119.80	128.60
10	A	27	A2M	N3-C2-N1	-5.61	119.82	128.60
10	A	1031	A2M	N6-C6-N1	-5.61	106.07	118.35
10	A	166	A2M	N6-C6-N1	-5.58	106.13	118.35
10	A	27	A2M	N6-C6-N1	-5.57	106.15	118.35
10	A	1031	A2M	N3-C2-N1	-5.56	119.90	128.60
10	A	159	A2M	N3-C2-N1	-5.54	119.94	128.60
10	A	1850	MA6	N1-C2-N3	-5.53	119.96	128.60
10	A	668	A2M	N6-C6-N1	-5.52	106.26	118.35
10	A	159	A2M	N6-C6-N1	-5.51	106.28	118.35
10	A	1851	MA6	N1-C2-N3	-5.42	120.13	128.60
10	A	668	A2M	N3-C2-N1	-5.41	120.14	128.60
10	A	484	A2M	N3-C2-N1	-5.40	120.15	128.60
10	A	1248	B8N	C5-C4-N3	5.34	126.07	116.17
10	A	484	A2M	C5-C4-N3	-5.17	120.00	126.75
10	A	1031	A2M	C5-C4-N3	-5.14	120.05	126.75
10	A	1678	A2M	C5-C4-N3	-5.12	120.07	126.75
10	A	27	A2M	C5-C4-N3	-5.04	120.18	126.75
10	A	121	OMU	C4-N3-C2	-5.03	119.94	126.58
10	A	159	A2M	C5-C4-N3	-4.95	120.29	126.75
10	A	116	OMU	C4-N3-C2	-4.94	120.06	126.58
10	A	1832	6MZ	C5-C4-N3	-4.93	120.32	126.75
10	A	166	A2M	N9-C8-N7	-4.88	107.24	113.91
10	A	1850	MA6	N9-C8-N7	-4.87	107.25	113.91
10	A	159	A2M	C5-C6-N6	4.86	134.00	123.43
10	A	484	A2M	C5-C6-N6	4.83	133.93	123.43
10	A	1678	A2M	C5-C6-N6	4.82	133.92	123.43
10	A	27	A2M	C5-C6-N6	4.81	133.90	123.43
10	A	166	A2M	C5-C6-N6	4.81	133.89	123.43
10	A	1031	A2M	C5-C6-N6	4.80	133.88	123.43
10	A	1851	MA6	C5-C4-N3	-4.80	120.49	126.75
10	A	668	A2M	C5-C6-N6	4.78	133.83	123.43
10	A	668	A2M	C5-C4-N3	-4.77	120.53	126.75
10	A	166	A2M	C5-C4-N3	-4.70	120.62	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1850	MA6	C5-C4-N3	-4.69	120.63	126.75
10	A	1851	MA6	N9-C8-N7	-4.67	107.53	113.91
10	A	668	A2M	N9-C8-N7	-4.66	107.54	113.91
10	A	1248	B8N	C4-N3-C2	-4.65	119.58	125.46
10	A	1678	A2M	N9-C8-N7	-4.65	107.56	113.91
10	A	1243	PSU	N1-C2-N3	4.59	120.33	115.13
10	A	27	A2M	N9-C8-N7	-4.49	107.77	113.91
10	A	1830	UR3	C4-N3-C2	-4.45	120.37	124.56
10	A	1243	PSU	C4-N3-C2	-4.44	119.94	126.34
10	A	823	PSU	C4-N3-C2	-4.43	119.95	126.34
10	A	612	PSU	N1-C2-N3	4.43	120.15	115.13
10	A	1081	PSU	C4-N3-C2	-4.42	119.97	126.34
10	A	1031	A2M	N9-C8-N7	-4.40	107.90	113.91
10	A	822	PSU	N1-C2-N3	4.37	120.08	115.13
10	A	159	A2M	N9-C8-N7	-4.37	107.94	113.91
10	A	1832	6MZ	N9-C8-N7	-4.36	107.94	113.91
10	A	823	PSU	N1-C2-N3	4.34	120.05	115.13
10	A	1081	PSU	N1-C2-N3	4.31	120.01	115.13
10	A	612	PSU	C4-N3-C2	-4.28	120.17	126.34
10	A	822	PSU	C4-N3-C2	-4.28	120.18	126.34
10	A	1219	JMH	C1'-N1-C2	4.23	124.13	116.99
10	A	484	A2M	N9-C8-N7	-4.15	108.23	113.91
10	A	119	PSU	N1-C2-N3	4.14	119.82	115.13
10	A	119	PSU	C4-N3-C2	-4.04	120.52	126.34
10	A	1832	6MZ	C5-N7-C8	3.98	109.16	103.51
10	A	27	A2M	O4'-C1'-N9	3.93	115.81	108.06
10	A	1678	A2M	O4'-C1'-N9	3.90	115.74	108.06
10	A	1031	A2M	O4'-C1'-N9	3.89	115.72	108.06
10	A	166	A2M	O4'-C1'-N9	3.83	115.61	108.06
10	A	1850	MA6	C2-N1-C6	3.77	120.67	111.75
10	A	668	A2M	C4'-O4'-C1'	-3.74	101.23	109.47
10	A	1851	MA6	C2-N1-C6	3.68	120.45	111.75
10	A	121	OMU	N3-C2-N1	3.65	119.74	114.89
10	A	1830	UR3	C1'-N1-C2	3.63	123.12	116.99
10	A	116	OMU	N3-C2-N1	3.61	119.69	114.89
10	A	1832	6MZ	C2-N3-C4	3.61	120.28	111.75
10	A	1851	MA6	C4-C5-C6	3.60	119.91	115.88
10	A	1678	A2M	C2-N3-C4	3.59	120.23	111.75
10	A	1031	A2M	C2-N3-C4	3.52	120.07	111.75
10	A	166	A2M	C2-N3-C4	3.50	120.03	111.75
10	A	27	A2M	C2-N3-C4	3.49	119.99	111.75
10	A	484	A2M	C2-N3-C4	3.47	119.95	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1850	MA6	C4-C5-C6	3.46	119.75	115.88
10	A	159	A2M	C2-N3-C4	3.41	119.80	111.75
10	A	166	A2M	C2'-C1'-N9	-3.38	107.84	113.53
10	A	1851	MA6	C2-N3-C4	3.38	119.73	111.75
10	A	814	5MU	C1'-N1-C2	3.37	123.66	117.57
10	A	1850	MA6	C2-N3-C4	3.32	119.59	111.75
10	A	121	OMU	C5-C4-N3	3.31	119.79	114.84
10	A	668	A2M	C2-N3-C4	3.31	119.57	111.75
10	A	1850	MA6	C5-N7-C8	3.30	108.19	103.51
10	A	1832	6MZ	C4-C5-N7	-3.29	106.61	110.62
10	A	1678	A2M	C5-N7-C8	3.27	108.16	103.51
10	A	166	A2M	C5-N7-C8	3.25	108.13	103.51
10	A	814	5MU	O2-C2-N1	3.23	127.08	122.79
10	A	116	OMU	C5-C4-N3	3.21	119.64	114.84
10	A	1678	A2M	N3-C4-N9	3.18	132.32	127.08
10	A	1851	MA6	C5-N7-C8	3.18	108.03	103.51
10	A	1219	JMH	C6-N1-C2	-3.17	118.95	121.79
10	A	27	A2M	C5-N7-C8	3.13	107.96	103.51
10	A	159	A2M	O4'-C1'-N9	3.12	114.21	108.06
10	A	1031	A2M	C5-N7-C8	3.09	107.90	103.51
10	A	159	A2M	N3-C4-N9	3.07	132.14	127.08
10	A	668	A2M	C5-N7-C8	3.07	107.86	103.51
10	A	27	A2M	N3-C4-N9	3.04	132.10	127.08
10	A	1832	6MZ	C4-C5-C6	3.04	119.16	116.81
10	A	1031	A2M	N3-C4-N9	3.04	132.09	127.08
10	A	159	A2M	C5-N7-C8	3.03	107.82	103.51
10	A	484	A2M	N3-C4-N9	3.03	132.07	127.08
10	A	1248	B8N	N3-C2-N1	3.02	121.02	116.76
10	A	484	A2M	C5-N7-C8	3.01	107.78	103.51
10	A	1678	A2M	C4'-O4'-C1'	-2.99	102.86	109.47
10	A	668	A2M	N3-C4-N9	2.99	132.01	127.08
10	A	1850	MA6	C4-N9-C8	2.93	108.90	105.73
10	A	166	A2M	C4-N9-C8	2.93	108.90	105.73
10	A	121	OMU	O4-C4-C5	-2.89	120.08	125.16
10	A	484	A2M	O4'-C1'-N9	2.88	113.74	108.06
10	A	116	OMU	O4-C4-C5	-2.87	120.11	125.16
10	A	166	A2M	N3-C4-N9	2.87	131.81	127.08
10	A	166	A2M	C4'-O4'-C1'	-2.81	103.28	109.47
10	A	1851	MA6	N3-C4-N9	2.81	131.71	127.08
10	A	612	PSU	O2-C2-N1	-2.79	119.72	122.79
10	A	822	PSU	O2-C2-N1	-2.78	119.73	122.79
10	A	1219	JMH	O2-C2-N3	-2.78	117.42	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	668	A2M	C4-N9-C8	2.78	108.74	105.73
10	A	1851	MA6	C4-N9-C8	2.77	108.73	105.73
10	A	1830	UR3	C6-N1-C2	-2.75	119.32	121.79
10	A	1850	MA6	N3-C4-N9	2.75	131.61	127.08
10	A	1678	A2M	C4-N9-C8	2.67	108.62	105.73
10	A	1832	6MZ	C5-C4-N9	2.63	108.84	105.78
10	A	1243	PSU	O2-C2-N1	-2.63	119.90	122.79
10	A	119	PSU	O2-C2-N1	-2.59	119.94	122.79
10	A	1248	B8N	O4-C4-N3	-2.52	115.71	119.98
10	A	823	PSU	O2-C2-N1	-2.50	120.04	122.79
10	A	668	A2M	C2'-C1'-N9	2.50	117.74	113.53
10	A	612	PSU	C6-N1-C2	-2.46	120.16	122.68
10	A	1081	PSU	O2-C2-N1	-2.45	120.09	122.79
10	A	27	A2M	C4-N9-C8	2.42	108.35	105.73
10	A	1243	PSU	C6-N1-C2	-2.41	120.22	122.68
10	A	159	A2M	C4-N9-C8	2.36	108.28	105.73
10	A	823	PSU	C6-N1-C2	-2.35	120.28	122.68
10	A	119	PSU	C6-N1-C2	-2.34	120.29	122.68
10	A	159	A2M	C4'-O4'-C1'	-2.32	104.34	109.47
10	A	121	OMU	O2-C2-N1	-2.32	119.70	122.79
10	A	814	5MU	C1'-N1-C6	-2.32	117.26	121.12
10	A	1031	A2M	C4'-O4'-C1'	-2.29	104.43	109.47
10	A	822	PSU	C6-N1-C2	-2.28	120.35	122.68
10	A	1832	6MZ	C4-N9-C1'	-2.28	121.16	126.59
10	A	1832	6MZ	N3-C4-N9	2.28	130.84	127.08
10	A	1850	MA6	C4-C5-N7	-2.24	107.89	110.62
10	A	1851	MA6	C4-C5-N7	-2.23	107.91	110.62
10	A	612	PSU	O4'-C1'-C2'	2.21	108.26	105.14
10	A	1031	A2M	C4-N9-C8	2.20	108.11	105.73
10	A	814	5MU	C6-N1-C2	-2.19	119.08	121.30
10	A	116	OMU	O2-C2-N1	-2.13	119.95	122.79
10	A	822	PSU	O4'-C1'-C2'	2.13	108.14	105.14
10	A	1678	A2M	C4-C5-N7	-2.11	108.05	110.62
10	A	1081	PSU	C6-N1-C2	-2.10	120.53	122.68
10	A	1248	B8N	C31-N3-C4	2.10	120.40	117.31
10	A	668	A2M	C3'-C2'-C1'	2.07	106.77	102.89
10	A	1081	PSU	O4'-C1'-C2'	2.06	108.04	105.14
10	A	166	A2M	C4-C5-N7	-2.02	108.16	110.62
10	A	484	A2M	C6-C5-C4	2.01	119.89	117.18

There are no chirality outliers.

All (41) 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	668	A2M	O4'-C4'-C5'-O5'
10	A	668	A2M	C3'-C4'-C5'-O5'
10	A	1031	A2M	C1'-C2'-O2'-CM'
10	A	1851	MA6	O4'-C4'-C5'-O5'
10	A	1851	MA6	C3'-C4'-C5'-O5'
10	A	1248	B8N	C2'-C1'-C5-C6
10	A	1248	B8N	C2'-C1'-C5-C4
10	A	1248	B8N	N34-C33-C34-O35
10	A	1830	UR3	O4'-C1'-N1-C2
10	A	517	OMC	C3'-C4'-C5'-O5'
10	A	683	OMG	O4'-C4'-C5'-O5'
10	A	1248	B8N	N34-C33-C34-O36
10	A	1830	UR3	O4'-C1'-N1-C6
10	A	644	OMG	C3'-C4'-C5'-O5'
10	A	683	OMG	C3'-C4'-C5'-O5'
10	A	1243	PSU	C3'-C4'-C5'-O5'
10	A	517	OMC	O4'-C4'-C5'-O5'
10	A	1243	PSU	O4'-C4'-C5'-O5'
10	A	27	A2M	O4'-C4'-C5'-O5'
10	A	822	PSU	C3'-C4'-C5'-O5'
10	A	166	A2M	C1'-C2'-O2'-CM'
10	A	159	A2M	C4'-C5'-O5'-P
10	A	1248	B8N	C32-C33-C34-O36
10	A	644	OMG	O4'-C4'-C5'-O5'
10	A	1248	B8N	C32-C33-C34-O35
10	A	509	OMG	O4'-C4'-C5'-O5'
10	A	822	PSU	O4'-C4'-C5'-O5'
10	A	644	OMG	C4'-C5'-O5'-P
10	A	1851	MA6	C4'-C5'-O5'-P
10	A	1248	B8N	O4'-C1'-C5-C4
10	A	1678	A2M	C1'-C2'-O2'-CM'
10	A	1219	JMH	C2'-C1'-N1-C2
10	A	1081	PSU	C4'-C5'-O5'-P
10	A	1248	B8N	O4'-C1'-C5-C6
10	A	1248	B8N	C31-C32-C33-N34
10	A	814	5MU	C2'-C1'-N1-C2
10	A	119	PSU	O4'-C4'-C5'-O5'
10	A	509	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1678	A2M	2	0
10	A	1830	UR3	1	0
10	A	823	PSU	1	0
10	A	1031	A2M	1	0
10	A	116	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 93 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	MET	w	101	-	6,7,8	0.68	0	2,7,9	0.70	0
57	GTP	t	501	55	30,34,34	0.83	1 (3%)	46,54,54	1.78	11 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MET	w	101	-	-	1/5/6/8	-
57	GTP	t	501	55	-	7/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	t	501	GTP	C2-N3	2.25	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	t	501	GTP	C5-C4-N3	-5.25	119.94	128.46
57	t	501	GTP	C2-N3-C4	4.57	120.44	112.30
57	t	501	GTP	PB-O3B-PG	-3.78	119.84	132.83
57	t	501	GTP	N9-C4-N3	3.40	132.77	125.94
57	t	501	GTP	C2-N1-C6	-2.98	119.67	125.10
57	t	501	GTP	PA-O3A-PB	-2.95	122.69	132.83
57	t	501	GTP	C8-N7-C5	2.54	108.84	104.24
57	t	501	GTP	C5-C6-N1	2.51	119.57	113.19
57	t	501	GTP	N9-C8-N7	-2.47	108.73	113.39
57	t	501	GTP	O6-C6-C5	-2.40	120.24	126.60
57	t	501	GTP	C3'-C2'-C1'	2.22	105.65	101.43

There are no chirality outliers.

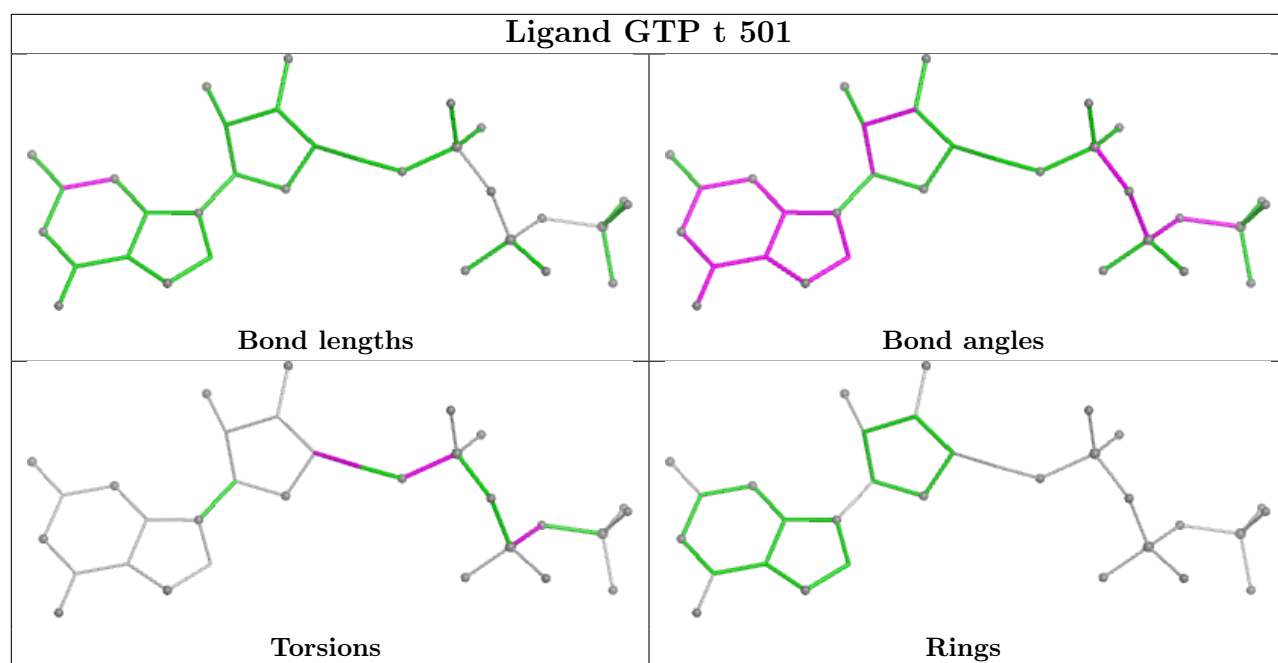
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	t	501	GTP	C5'-O5'-PA-O1A
57	t	501	GTP	C5'-O5'-PA-O2A
58	w	101	MET	O-C-CA-CB
57	t	501	GTP	C3'-C4'-C5'-O5'
57	t	501	GTP	O4'-C4'-C5'-O5'
57	t	501	GTP	C5'-O5'-PA-O3A
57	t	501	GTP	PG-O3B-PB-O2B
57	t	501	GTP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

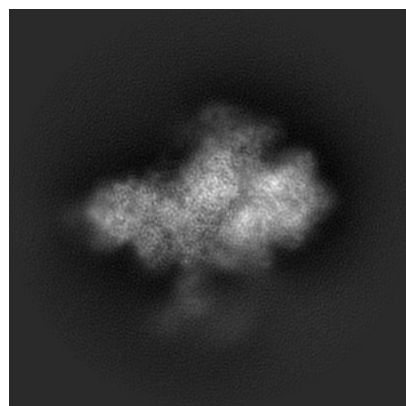
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17696. These allow visual inspection of the internal detail of the map and identification of artifacts.

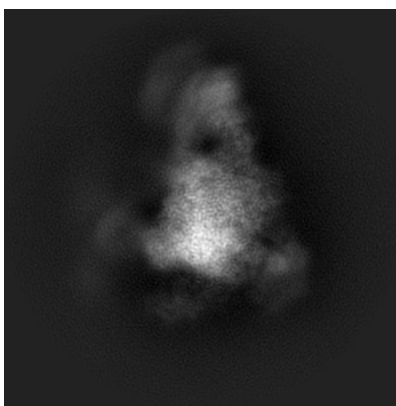
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

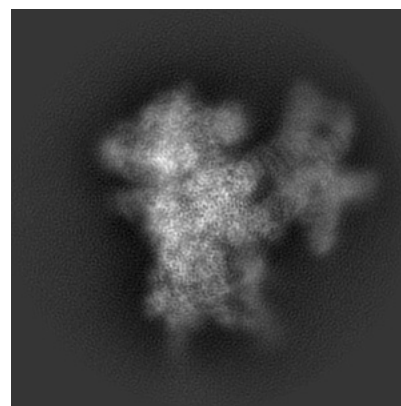
6.1.1 Primary map



X

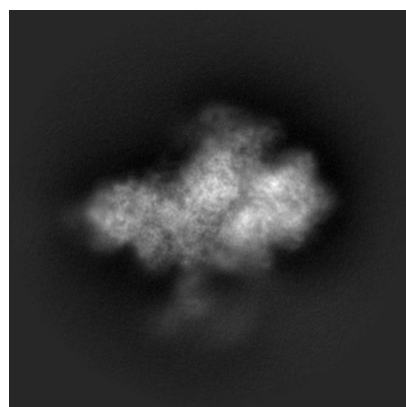


Y

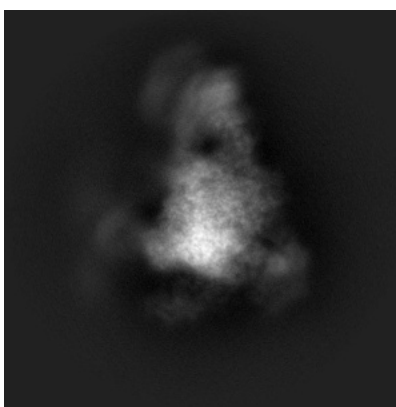


Z

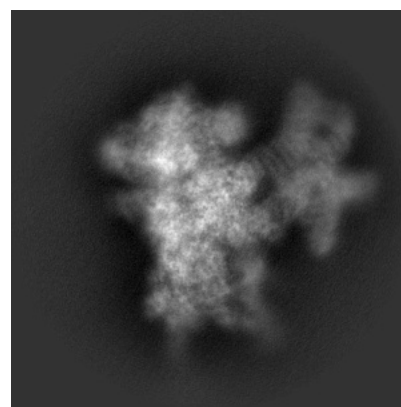
6.1.2 Raw map



X



Y

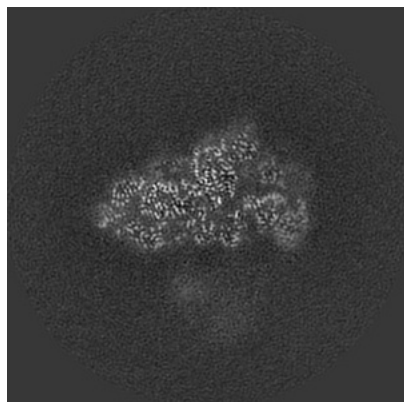


Z

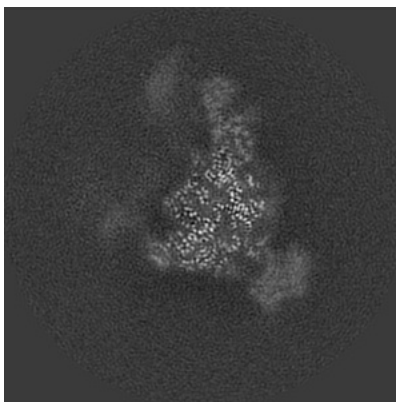
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

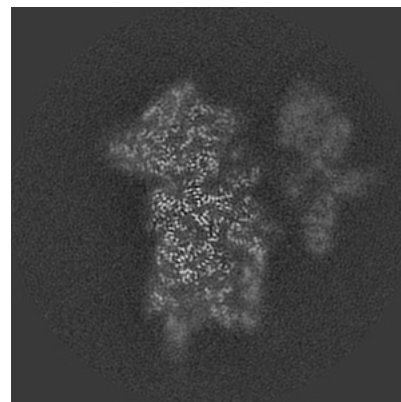
6.2.1 Primary map



X Index: 216

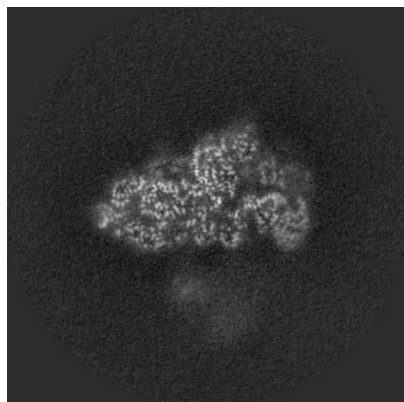


Y Index: 216

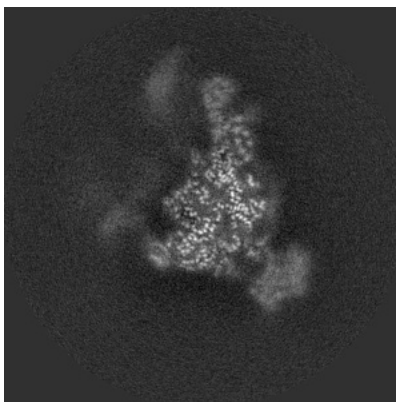


Z Index: 216

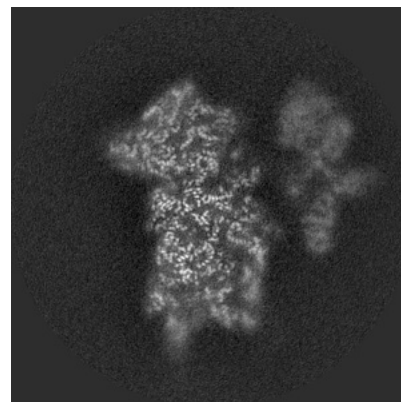
6.2.2 Raw map



X Index: 180



Y Index: 180

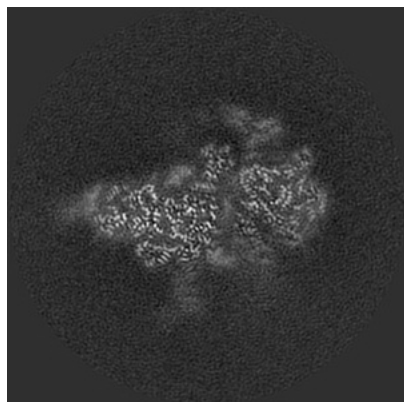


Z Index: 180

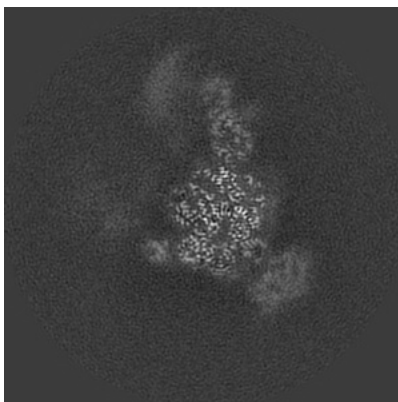
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

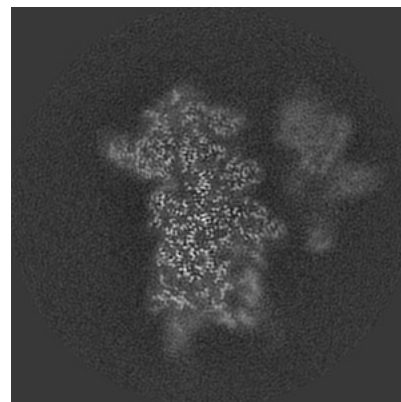
6.3.1 Primary map



X Index: 175

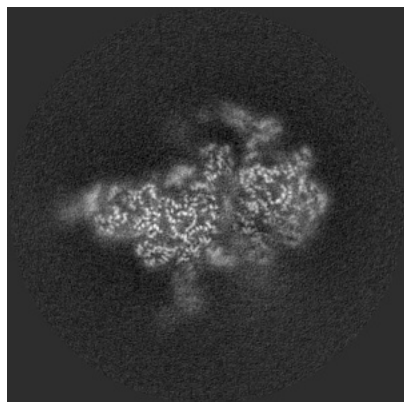


Y Index: 221

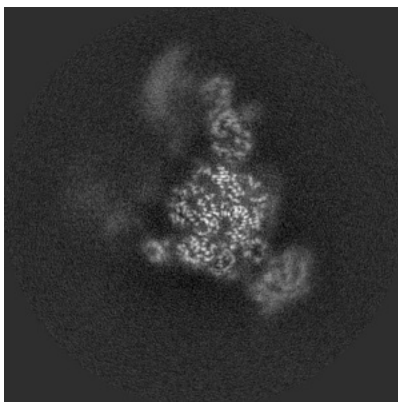


Z Index: 210

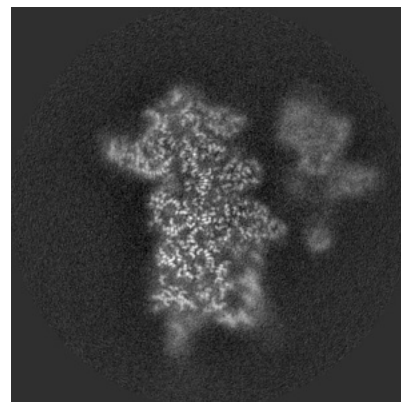
6.3.2 Raw map



X Index: 145



Y Index: 185

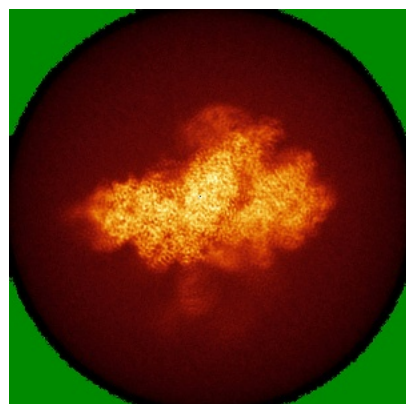


Z Index: 174

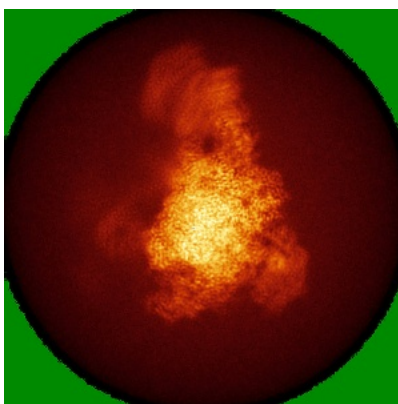
The images above show the largest variance slices of the map in three orthogonal directions.

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

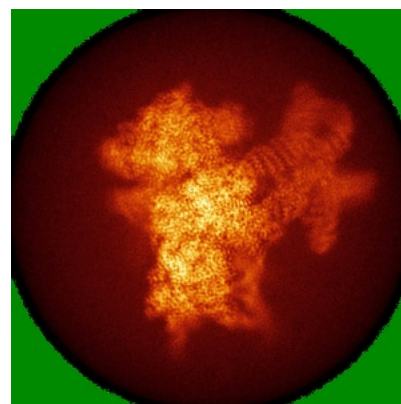
6.4.1 Primary map



X

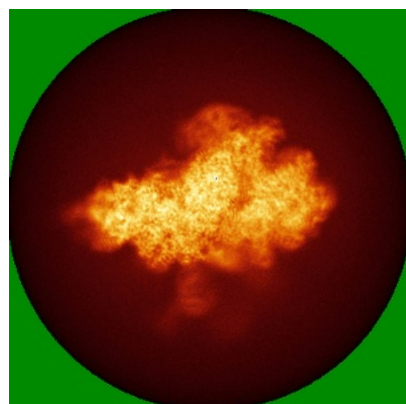


Y

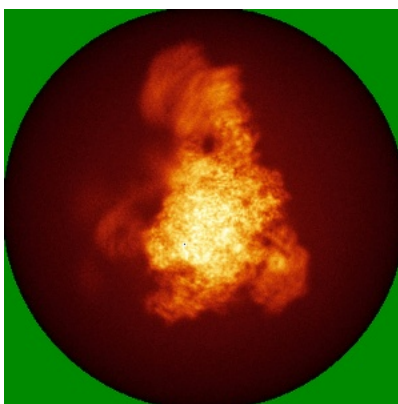


Z

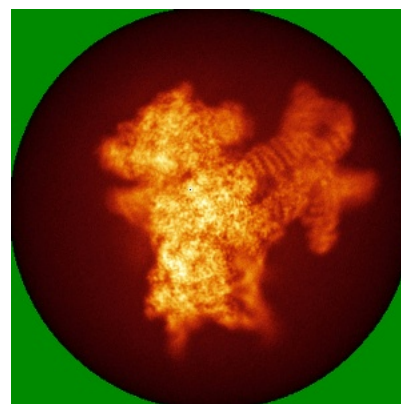
6.4.2 Raw map



X



Y

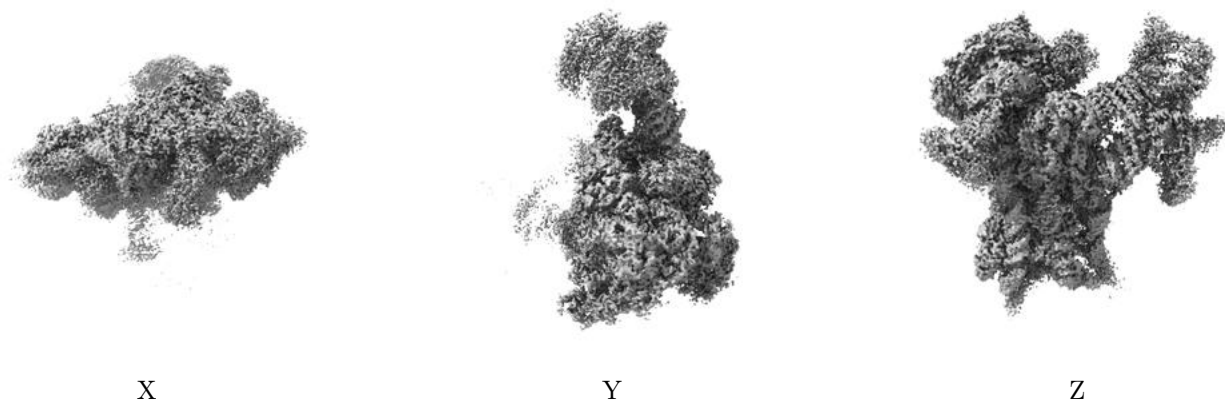


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. 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.

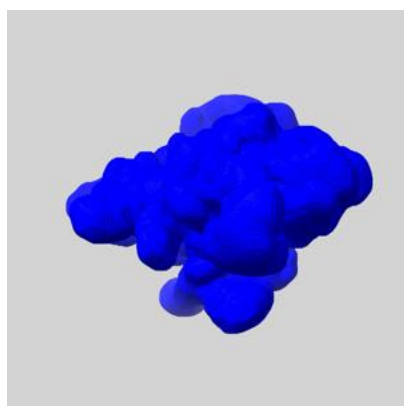
6.6 Mask visualisation [i](#)

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

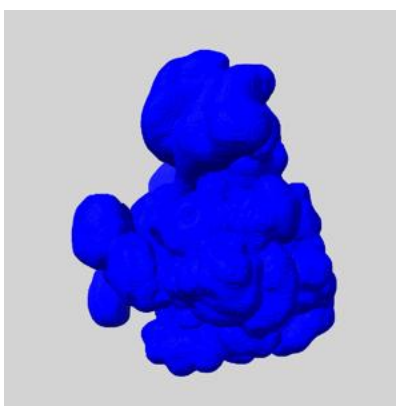
A mask typically either:

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

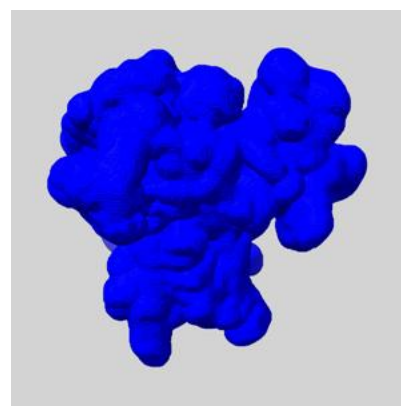
6.6.1 emd_17696_msk_1.map [i](#)



X



Y

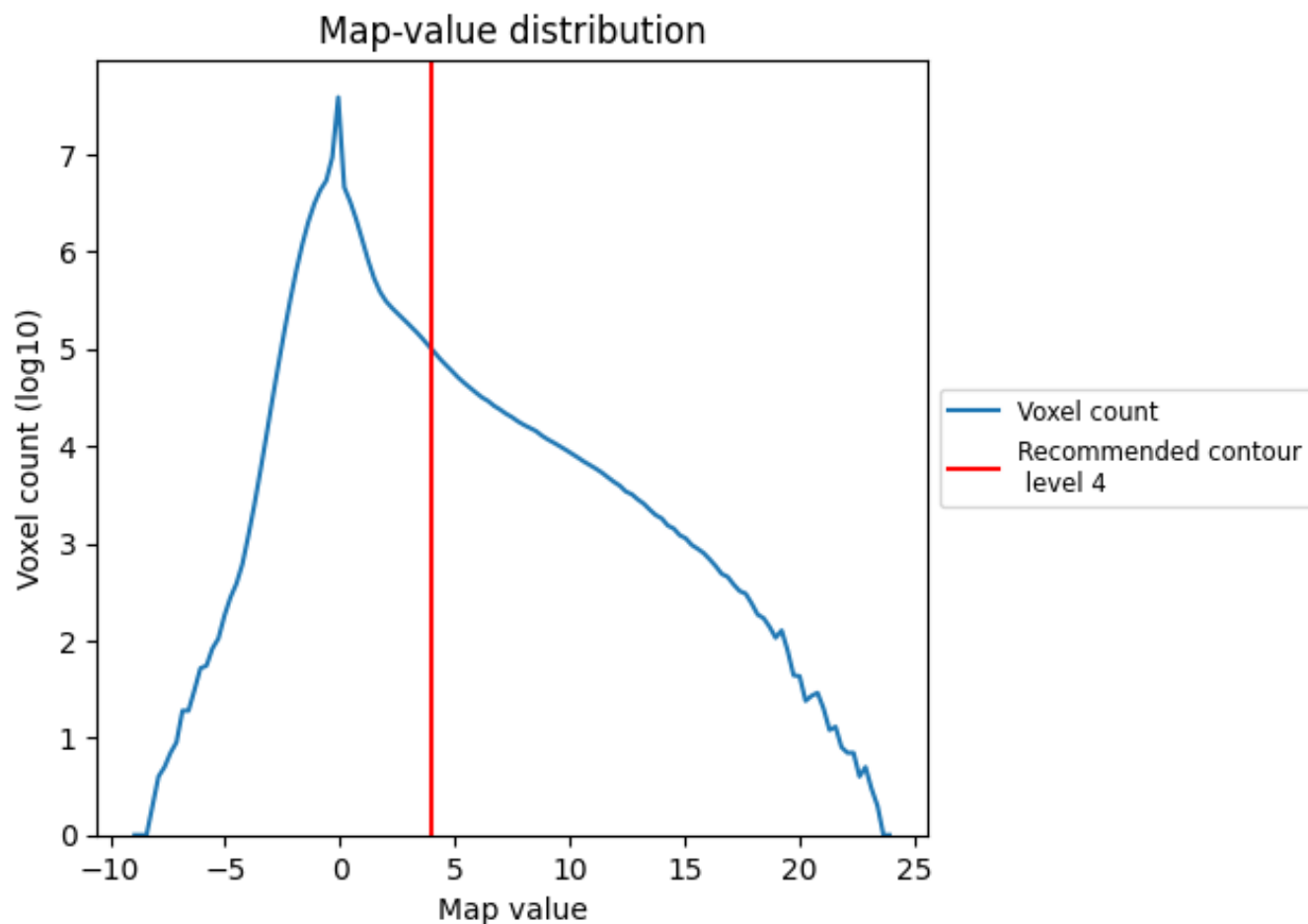


Z

7 Map analysis [i](#)

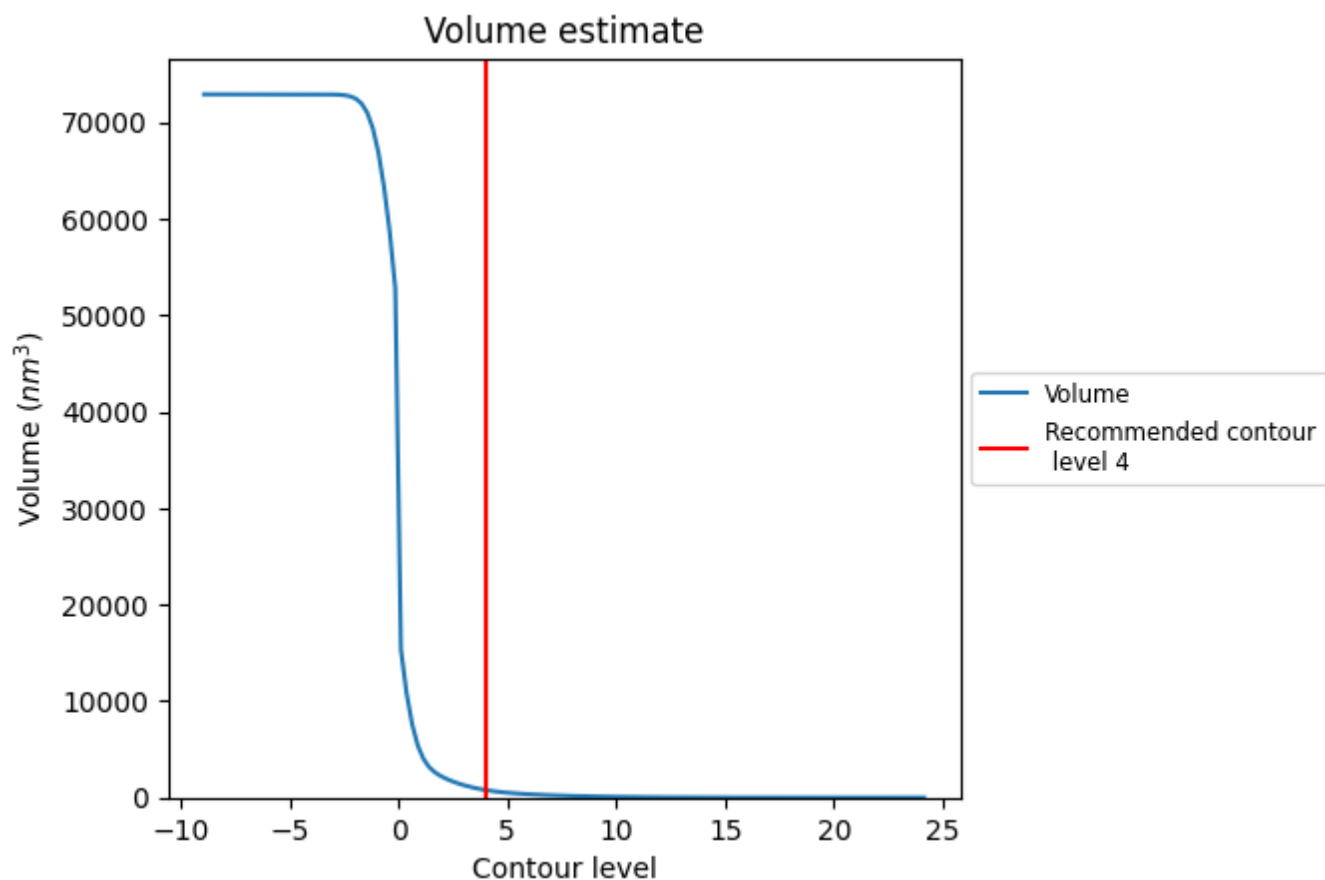
This section contains the results of statistical analysis of the map.

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.

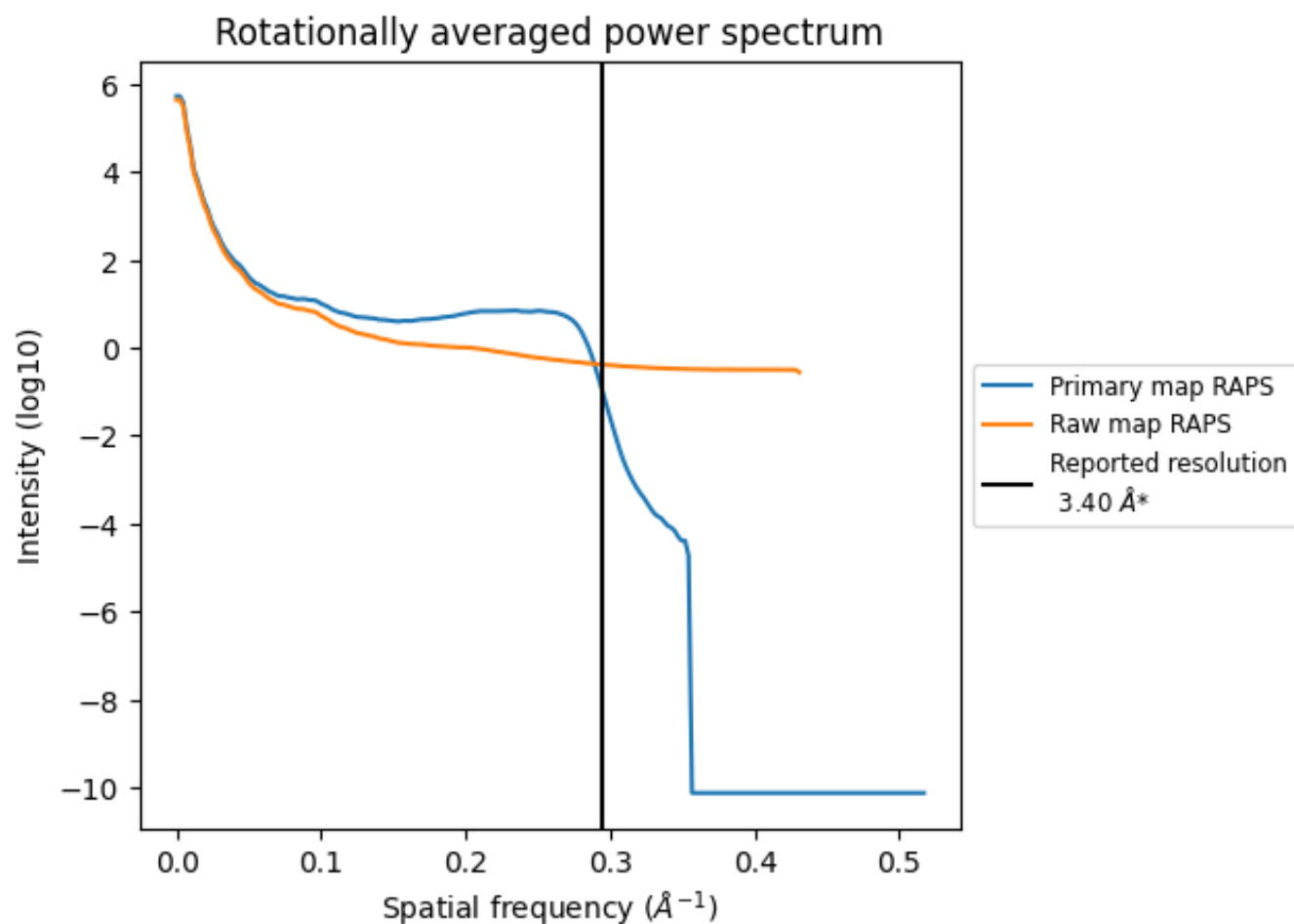
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 777 nm³; this corresponds to an approximate mass of 702 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 ⓘ

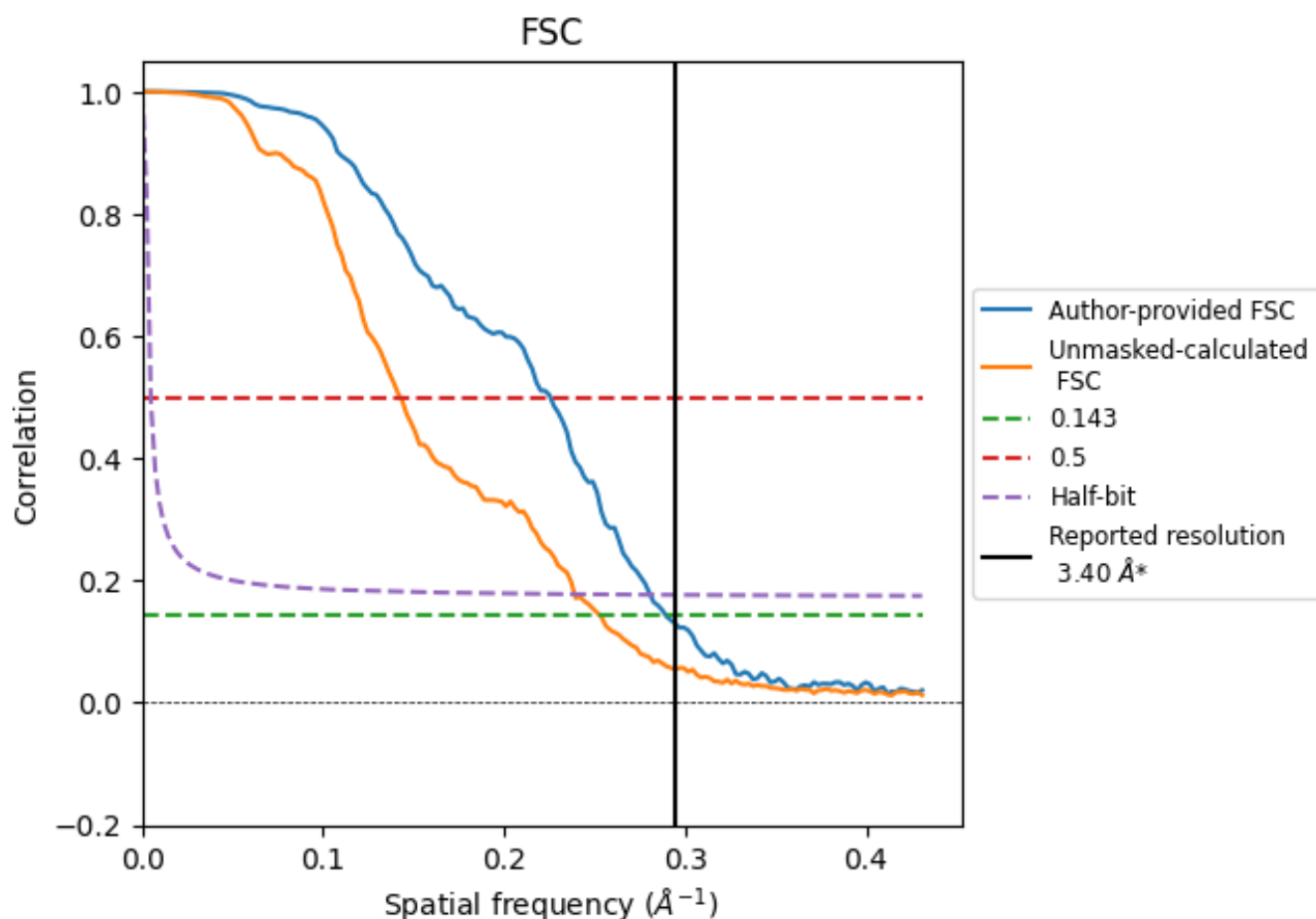


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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](#)

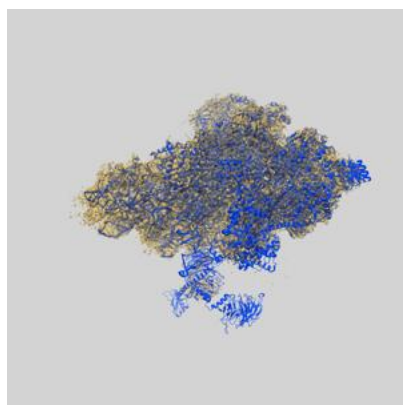
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.46	4.43	3.56
Unmasked-calculated*	3.96	7.02	4.19

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

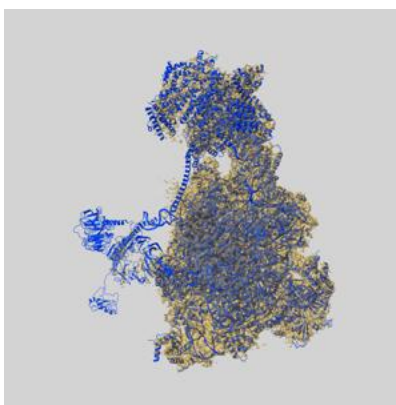
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17696 and PDB model 8PJ1. Per-residue inclusion information can be found in section 3 on page 16.

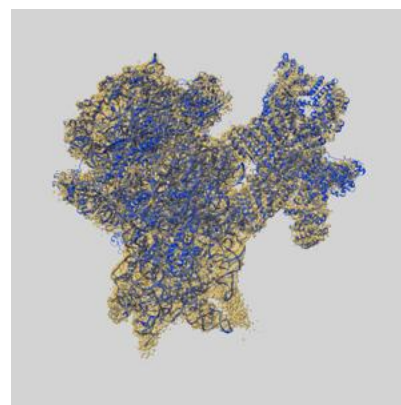
9.1 Map-model overlay [i](#)



X



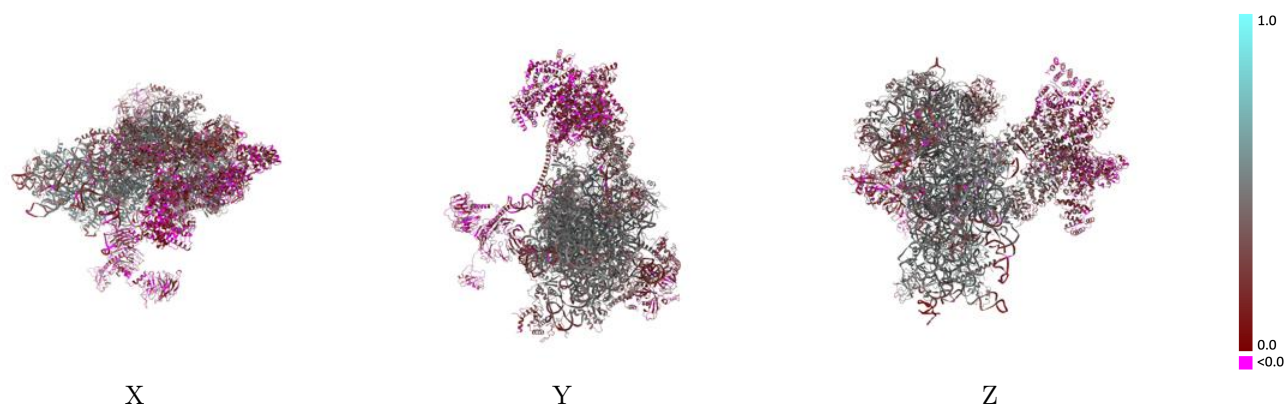
Y



Z

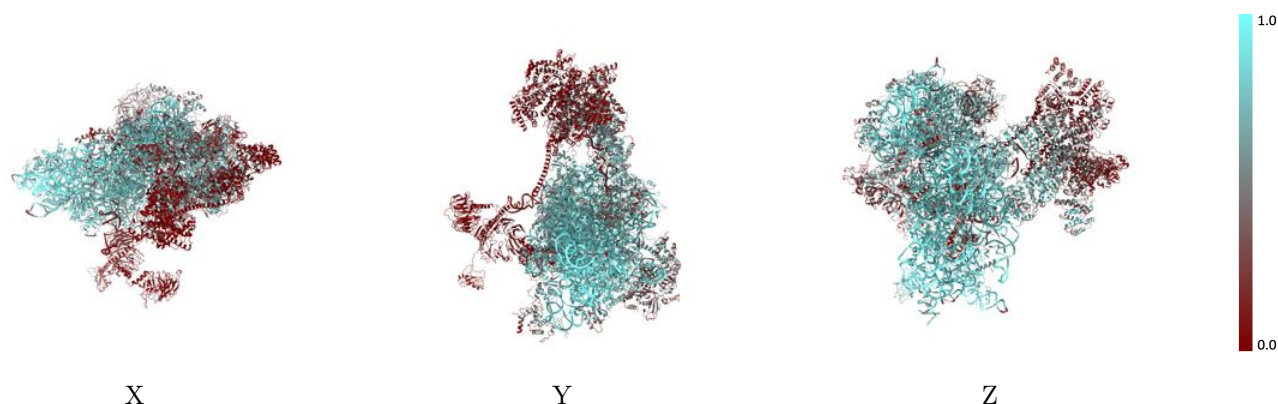
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



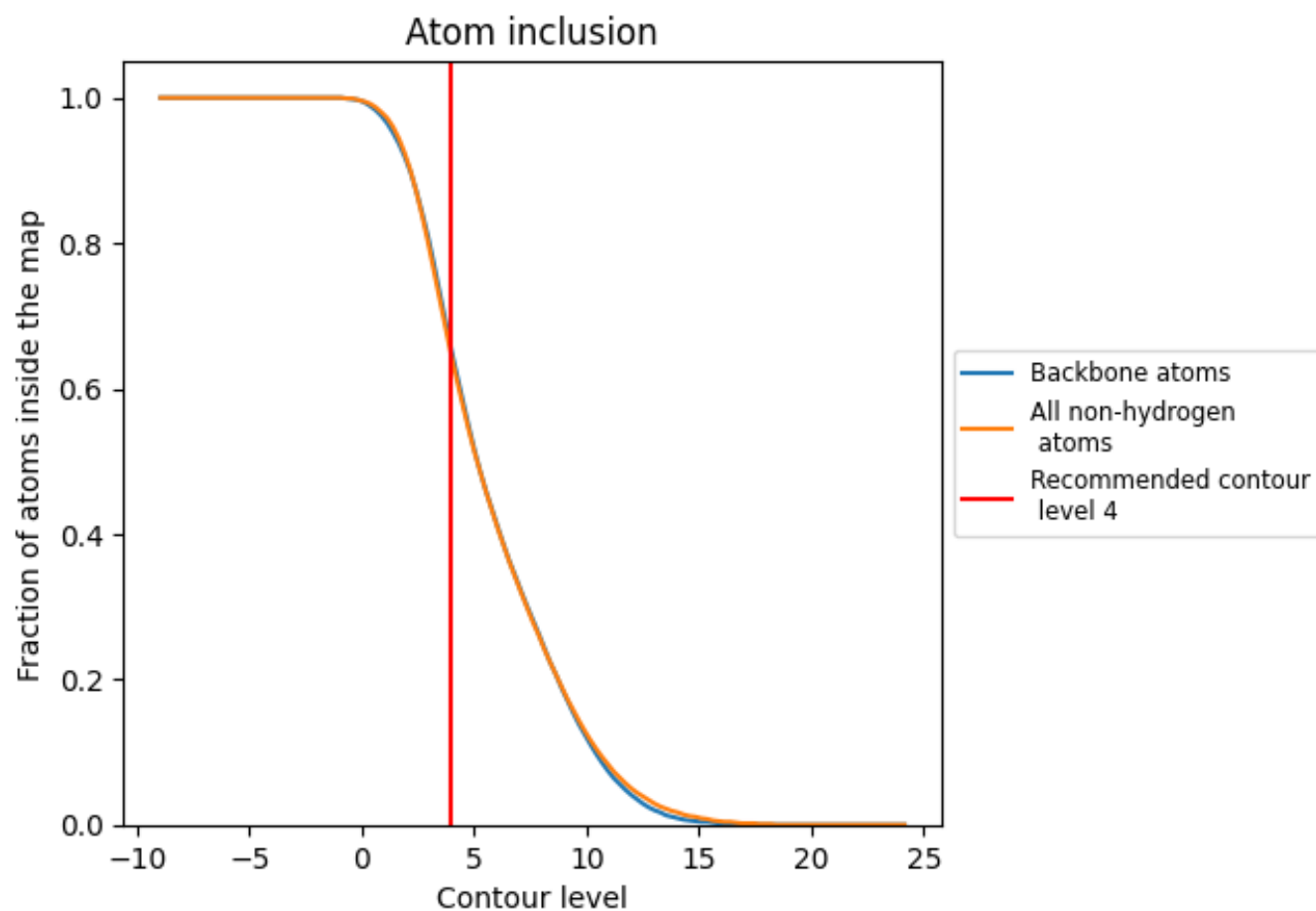
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 64% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6440	 0.3680
1	 0.0360	 0.1280
2	 0.0010	 0.1030
3	 0.0860	 0.0960
4	 0.1970	 0.1250
5	 0.0910	 0.0960
6	 0.2010	 0.1480
7	 0.2940	 0.2100
8	 0.2170	 0.1350
9	 0.6790	 0.4710
A	 0.9040	 0.4360
B	 0.8380	 0.5120
C	 0.8510	 0.5170
D	 0.8220	 0.5000
E	 0.8480	 0.5240
F	 0.7070	 0.4540
G	 0.7250	 0.4520
H	 0.7820	 0.4910
I	 0.8020	 0.4990
J	 0.8410	 0.5180
K	 0.7740	 0.4930
L	 0.7640	 0.4920
M	 0.6780	 0.4520
N	 0.7880	 0.4960
O	 0.7900	 0.4840
P	 0.7840	 0.4810
Q	 0.8440	 0.5230
R	 0.8540	 0.4880
S	 0.8060	 0.4460
T	 0.8690	 0.5030
V	 0.7300	 0.4670
Y	 0.7770	 0.4750
Z	 0.6300	 0.4460
a	 0.6600	 0.4140
b	 0.6490	 0.4180



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Chain	Atom inclusion	Q-score
c	 0.6500	 0.4070
d	 0.7950	 0.4590
e	 0.6990	 0.4350
f	 0.7070	 0.4220
h	 0.6220	 0.4380
i	 0.8530	 0.4940
k	 0.4480	 0.2430
m	 0.3430	 0.2390
n	 0.5900	 0.4560
o	 0.2420	 0.2490
p	 0.5620	 0.4100
q	 0.6710	 0.4500
r	 0.5010	 0.3140
s	 0.4910	 0.3350
t	 0.3330	 0.1900
u	 0.4040	 0.2780
v	 0.3690	 0.1990
w	 0.8210	 0.2820
x	 0.4000	 0.3140
y	 0.4760	 0.3240