Full wwPDB EM Validation Report ⓘ

Jun 4, 2025 – 05:17 PM EDT

PDB ID	:	9OFV / pdb_00009ofv
EMDB ID	:	EMD-70444
Title	:	Consensus reconstruction of the eukaryotic Ribosome-associated Quality Control complex
Authors	:	Li, W.; Cahoon, T.; Shen, P.S.
Deposited on	:	2025-04-30
Resolution	:	3.16 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:

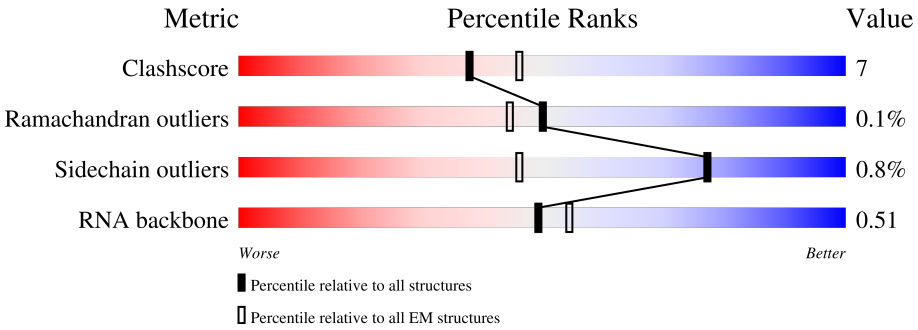
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.16 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	835	65% 57% 9% 34%
1	B	835	78% 67% 11% 22%
1	C	835	59% 48% 11% 41%
1	D	835	59% 50% 8% 41%
1	E	835	59% 49% 9% 41%
1	F	835	64% 53% 10% 36%
2	H	76	100% 83% 17%

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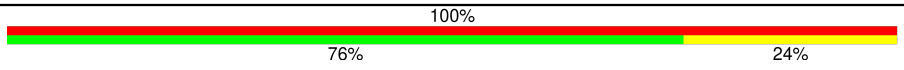
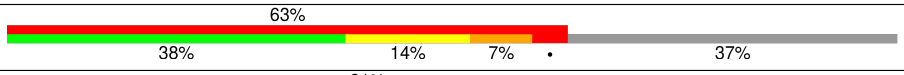
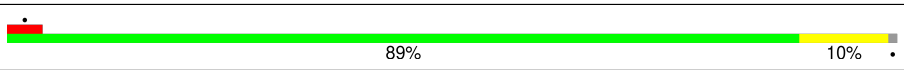
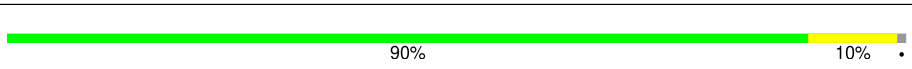
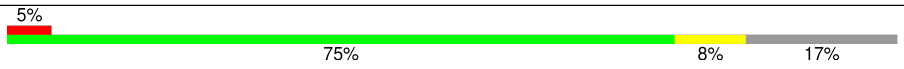
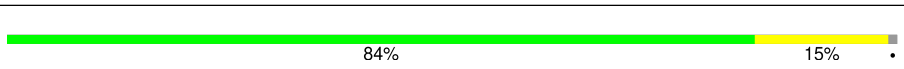
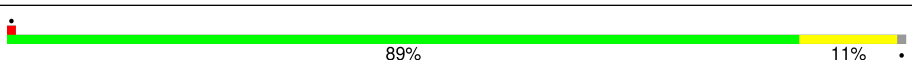
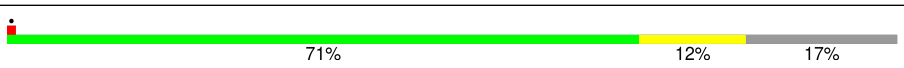
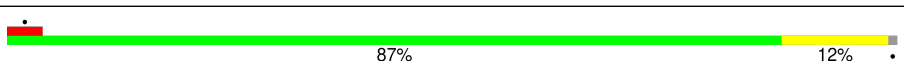
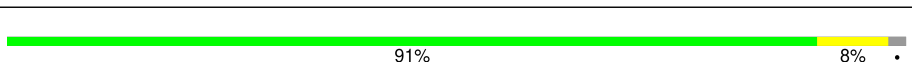
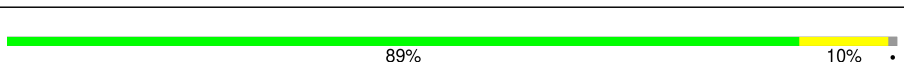
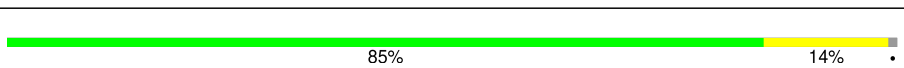
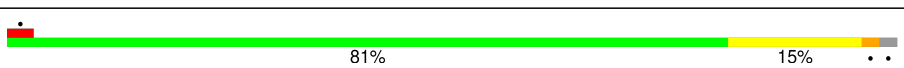
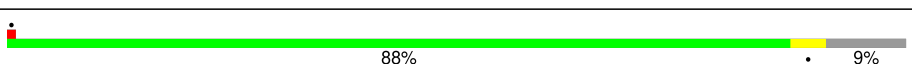
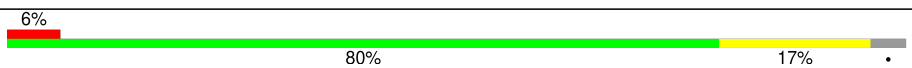
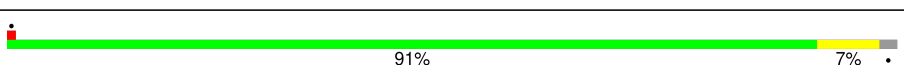
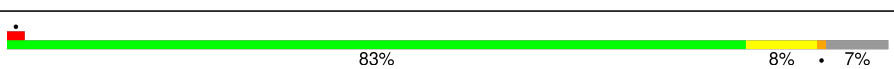
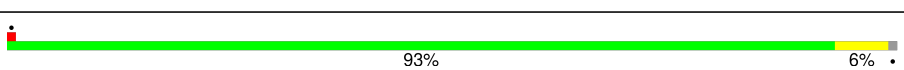
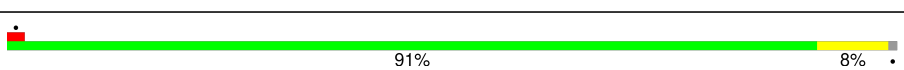
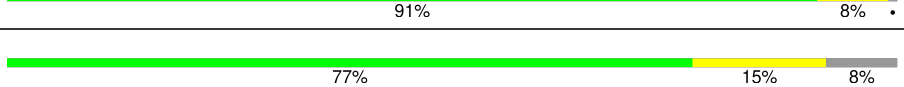
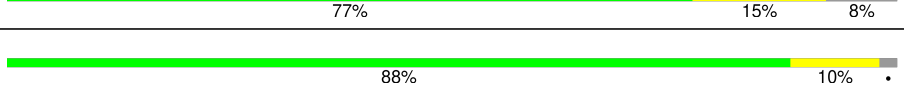
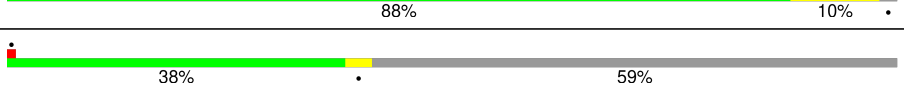
Mol	Chain	Length	Quality of chain
2	J	76	
2	K	76	
3	G	580	
4	3	184	
5	4	186	
6	5	189	
7	6	172	
8	7	160	
9	8	121	
10	I	137	
11	9	155	
12	L	127	
13	M	136	
14	N	149	
15	O	59	
16	P	105	
17	Q	113	
18	R	130	
19	S	107	
20	T	121	
21	U	120	
22	V	100	
23	W	88	
24	Y	51	
25	Z	128	

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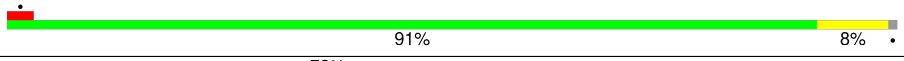
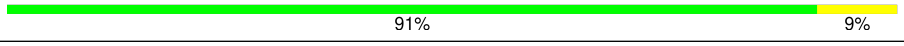
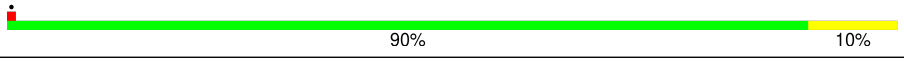
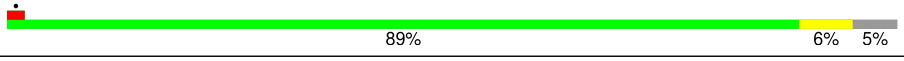
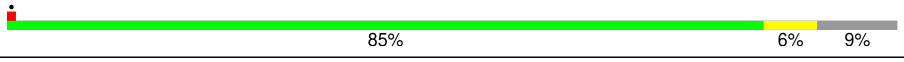
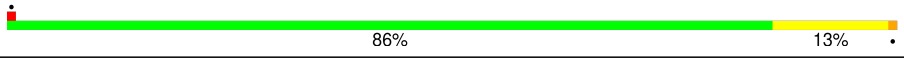
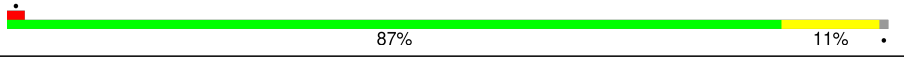
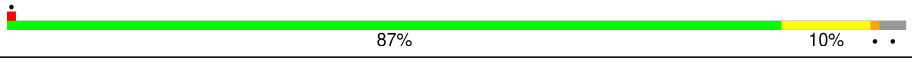
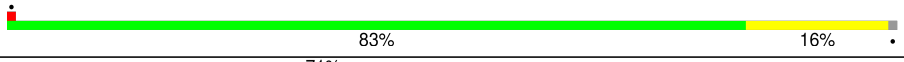
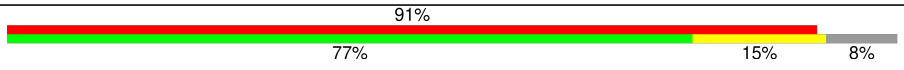
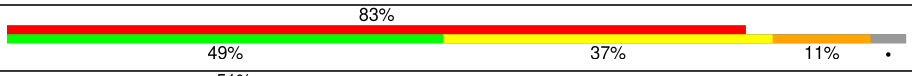
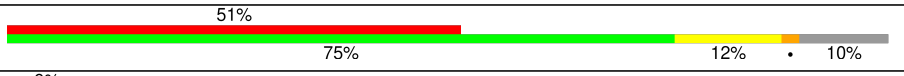
Mol	Chain	Length	Quality of chain
26	b	106	
27	c	92	
28	d	25	
29	f	3395	
30	h	121	
31	i	158	
32	j	254	
33	k	387	
34	l	362	
35	m	297	
36	n	176	
37	o	244	
38	p	256	
39	q	191	
40	r	221	
41	s	174	
42	t	199	
43	u	138	
44	a	1038	
45	e	1562	
46	g	245	
47	x	76	
47	y	76	
48	z	165	
49	0	312	

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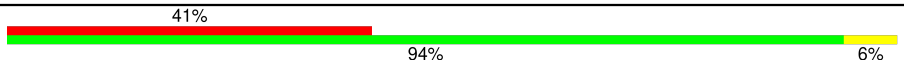
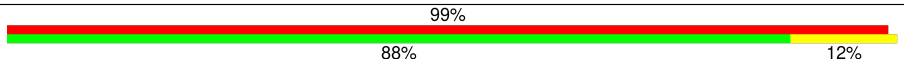
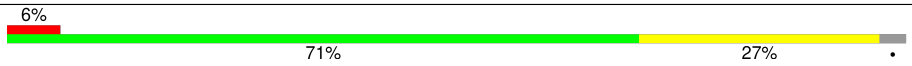
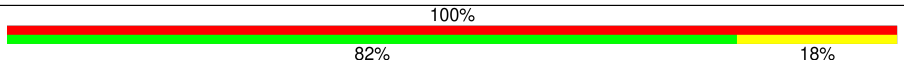
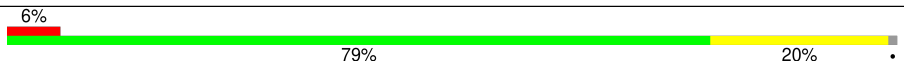
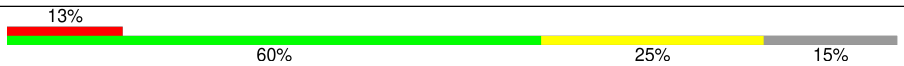
Mol	Chain	Length	Quality of chain
50	1	17	
51	w	217	
52	X	78	
53	v	753	
54	2	76	
55	a0	199	
56	b0	142	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	ATP	A	901	-	-	X	-
57	ATP	C	1001	-	-	X	-
57	ATP	C	1003	-	-	X	-
57	ATP	D	901	-	-	X	-
57	ATP	D	902	-	-	X	-
57	ATP	E	902	-	-	X	-
57	ATP	F	901	-	-	X	-
58	ADP	E	901	-	-	X	-

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 183852 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 Cell division control protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	547	Total 4206	C 2641	N 732	O 814	S 19	0	0
1	B	654	Total 5049	C 3184	N 880	O 964	S 21	0	0
1	C	492	Total 3759	C 2363	N 656	O 723	S 17	0	0
1	D	489	Total 3747	C 2354	N 659	O 717	S 17	0	0
1	E	496	Total 3786	C 2380	N 660	O 729	S 17	0	0
1	F	533	Total 4093	C 2567	N 720	O 787	S 19	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	588	GLN	GLU	conflict	UNP P25694
B	588	GLN	GLU	conflict	UNP P25694
C	588	GLN	GLU	conflict	UNP P25694
D	588	GLN	GLU	conflict	UNP P25694
E	588	GLN	GLU	conflict	UNP P25694
F	588	GLN	GLU	conflict	UNP P25694

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	48	Total 376	C 237	N 63	O 76		0	0
2	H	76	Total 601	C 375	N 105	O 120	S 1	0	0
2	J	76	Total 601	C 375	N 105	O 120	S 1	0	0

- Molecule 3 is a protein called Nuclear protein localization protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	468	Total	C	N	O	S	0	0
			3762	2381	628	732	21		

- Molecule 4 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	183	Total	C	N	O	0	0
			1416	879	284	253		

- Molecule 5 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 6 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 7 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 8 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

- Molecule 9 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 10 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 11 is a protein called Large ribosomal subunit protein eL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	63	Total	C	N	O	S	0	0
			518	333	102	82	1		

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	135	Total	C	N	O	0	0
			1080	701	199	180		

- Molecule 14 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 15 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 17 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 18 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 19 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 21 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 23 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 24 is a protein called 60S ribosomal protein L39.

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

- Molecule 25 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 26 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 27 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 28 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	22	Total	C	N	O	S	0	0
			207	127	56	23	1		

- Molecule 29 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	3216	Total	C	N	O	P	1	0
			68802	30732	12391	22462	3217		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	?	-	G	deletion	GB 1262303
f	1956	U	-	insertion	GB 1262303
f	?	-	A	deletion	GB 1262303
f	2255	U	-	insertion	GB 1262303
f	?	-	G	deletion	GB 1262303

- Molecule 30 is a RNA chain called 5S rRNA.

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

- Molecule 31 is a RNA chain called 5.8S rRNA.

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

- Molecule 32 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 33 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 34 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 36 is a protein called Large ribosomal subunit protein eL6B.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	n	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 37 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 38 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	p	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 39 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 40 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 41 is a protein called Large ribosomal subunit protein uL5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 42 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	t	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 43 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 44 is a protein called Ribosome quality control complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	a	848	Total	C	N	O	S	0	0
			6573	4191	1139	1226	17		

- Molecule 45 is a protein called E3 ubiquitin-protein ligase listerin.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	e	1530	Total	C	N	O	S	0	0
			11556	7383	1946	2189	38		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	g	225	Total	C	N	O	S	0	0
			1651	1030	282	332	7		

- Molecule 47 is a RNA chain called Ala tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	74	Total	C	N	O	P	0	0
			1579	702	278	525	74		
47	y	73	Total	C	N	O	P	0	0
			1556	692	273	518	73		

- Molecule 48 is a protein called Large ribosomal subunit protein uL11A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	z	148	Total	C	N	O	0	0
			728	432	148	148		

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	0	121	Total	C	N	O	S	0	0
			961	618	167	173	3		

- Molecule 50 is a protein called CAT-tailed nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	1	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 51 is a protein called Large ribosomal subunit protein uL1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	216	Total	C	N	O	S	0	0
			1709	1092	298	310	9		

- Molecule 52 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	X	76	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 53 is a protein called Ribosome quality control complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	531	Total	C	N	O	S	0	0
			4376	2824	729	807	16		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	724	THR	-	expression tag	UNP Q05468
v	725	SER	-	expression tag	UNP Q05468
v	726	GLY	-	expression tag	UNP Q05468
v	727	SER	-	expression tag	UNP Q05468
v	728	PRO	-	expression tag	UNP Q05468
v	729	GLY	-	expression tag	UNP Q05468
v	730	ASP	-	expression tag	UNP Q05468
v	731	TYR	-	expression tag	UNP Q05468
v	732	LYS	-	expression tag	UNP Q05468
v	733	ASP	-	expression tag	UNP Q05468
v	734	ASP	-	expression tag	UNP Q05468
v	735	ASP	-	expression tag	UNP Q05468
v	736	ASP	-	expression tag	UNP Q05468
v	737	LYS	-	expression tag	UNP Q05468
v	738	ASP	-	expression tag	UNP Q05468
v	739	TYR	-	expression tag	UNP Q05468
v	740	LYS	-	expression tag	UNP Q05468
v	741	ASP	-	expression tag	UNP Q05468
v	742	ASP	-	expression tag	UNP Q05468
v	743	ASP	-	expression tag	UNP Q05468
v	744	ASP	-	expression tag	UNP Q05468
v	745	LYS	-	expression tag	UNP Q05468
v	746	ASP	-	expression tag	UNP Q05468
v	747	TYR	-	expression tag	UNP Q05468
v	748	LYS	-	expression tag	UNP Q05468

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Chain	Residue	Modelled	Actual	Comment	Reference
v	749	ASP	-	expression tag	UNP Q05468
v	750	ASP	-	expression tag	UNP Q05468
v	751	ASP	-	expression tag	UNP Q05468
v	752	ASP	-	expression tag	UNP Q05468
v	753	LYS	-	expression tag	UNP Q05468

- Molecule 54 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	76	Total	C	N	O	S	0	0
			602	378	105	118	1		

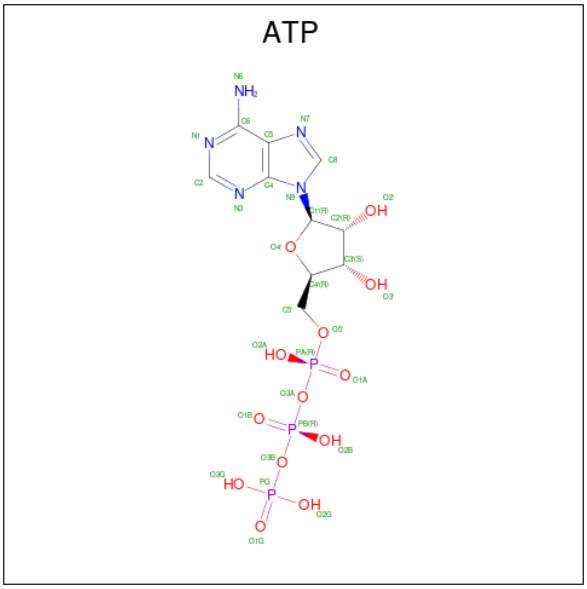
- Molecule 55 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	a0	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 56 is a protein called 60S ribosomal protein L25.

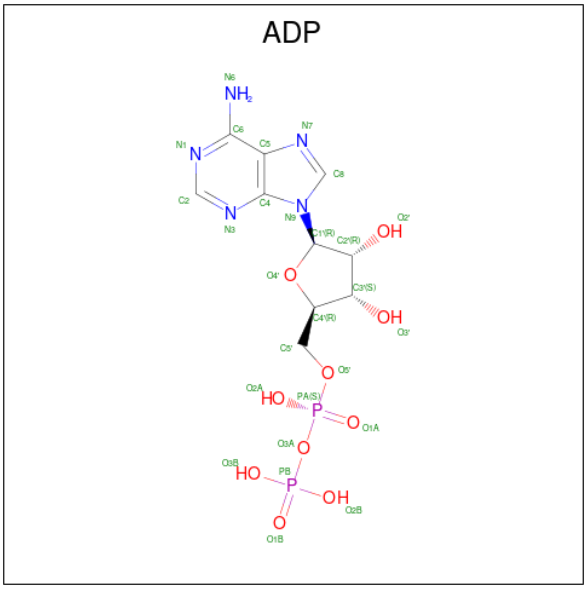
Mol	Chain	Residues	Atoms					AltConf	Trace
56	b0	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 57 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
57	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
57	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
58	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

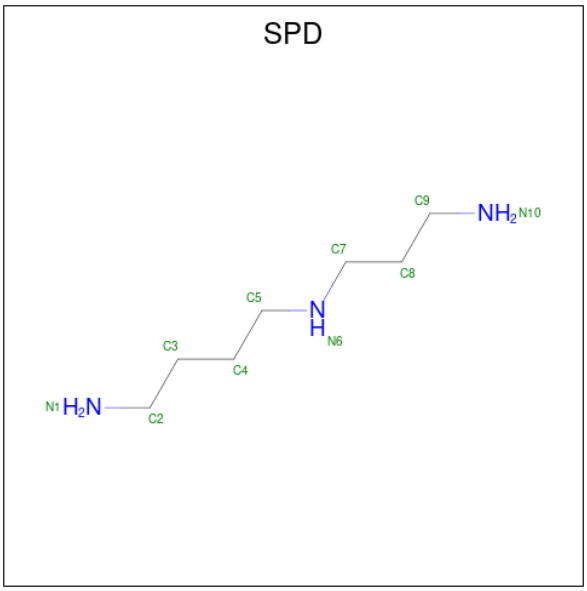
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	G	2	Total Zn 2 2	0
59	T	1	Total Zn 1 1	0
59	W	1	Total Zn 1 1	0
59	Z	1	Total Zn 1 1	0
59	b	1	Total Zn 1 1	0
59	c	1	Total Zn 1 1	0

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
60	3	1	Total Mg 1 1	0
60	5	1	Total Mg 1 1	0
60	I	1	Total Mg 1 1	0
60	R	1	Total Mg 1 1	0
60	T	1	Total Mg 1 1	0
60	f	3	Total Mg 3 3	0
60	h	1	Total Mg 1 1	0
60	j	2	Total Mg 2 2	0
60	k	1	Total Mg 1 1	0

- Molecule 61 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



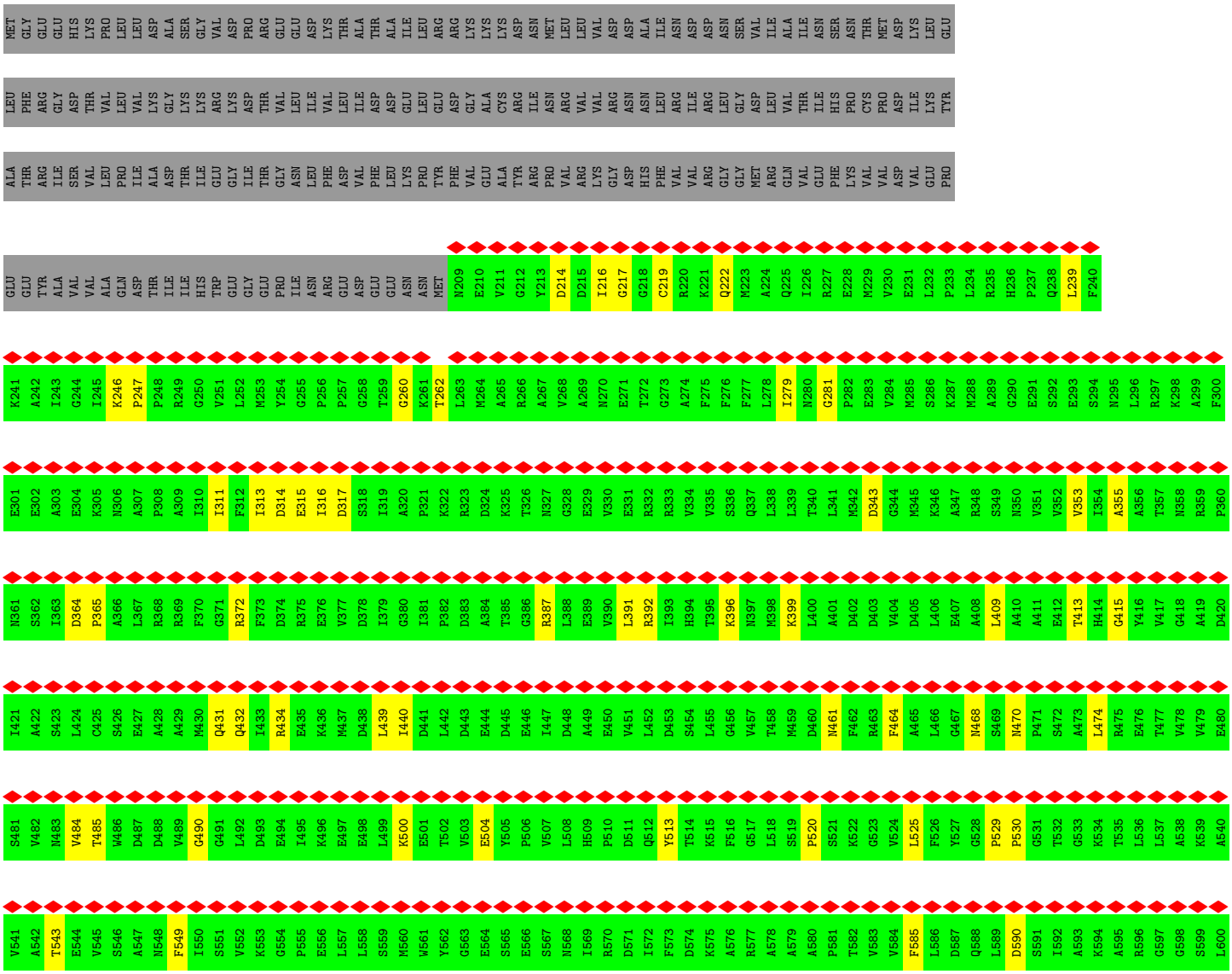
Mol	Chain	Residues	Atoms			AltConf
61	f	1	Total	C	N	0
			10	7	3	

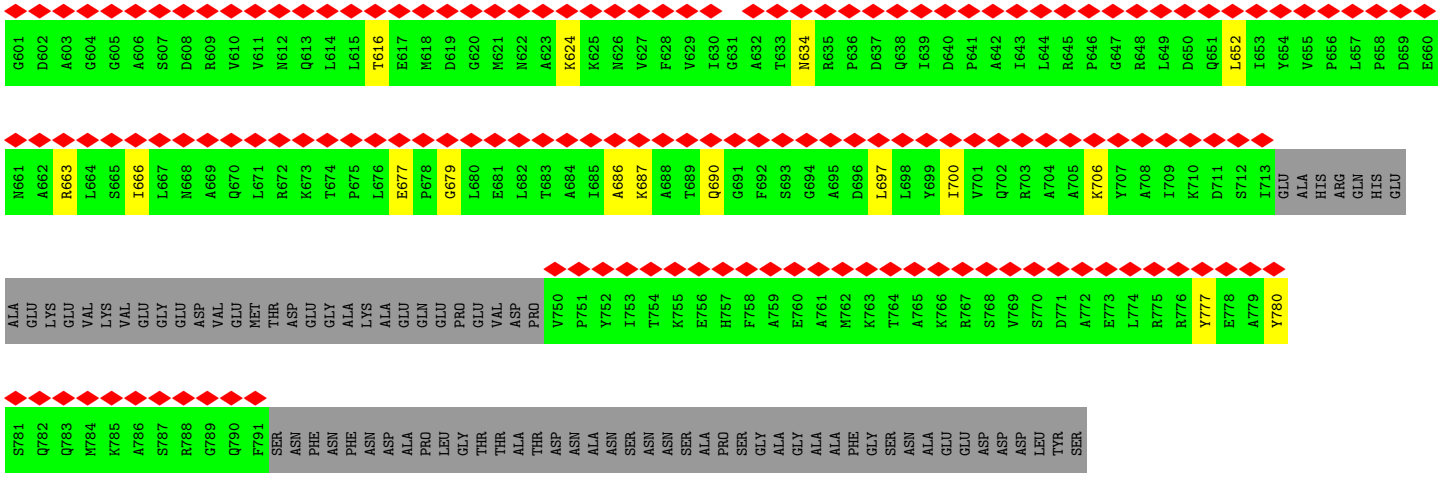
3 Residue-property plots (i)

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

- Molecule 1: Cell division control protein 48

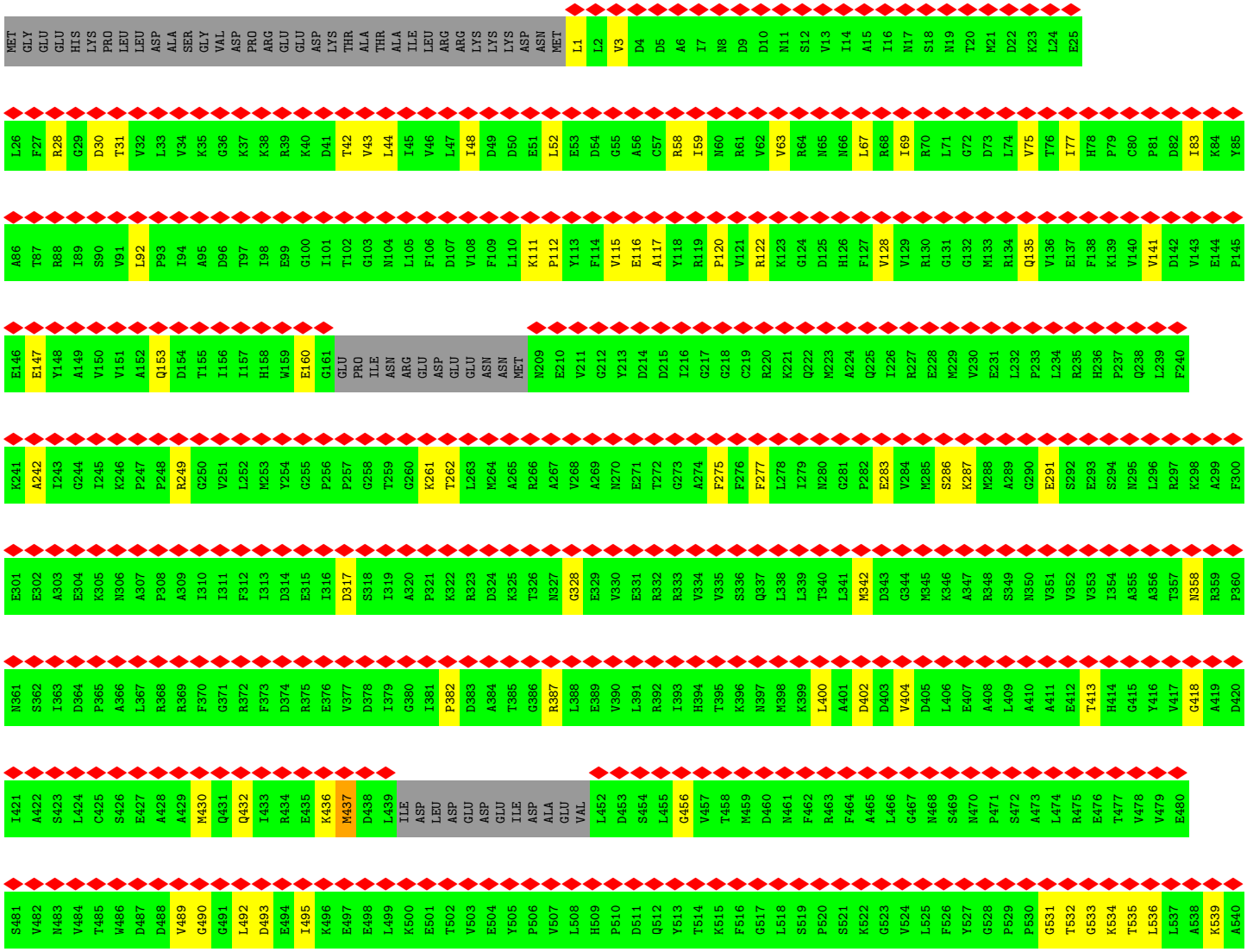
Chain A:

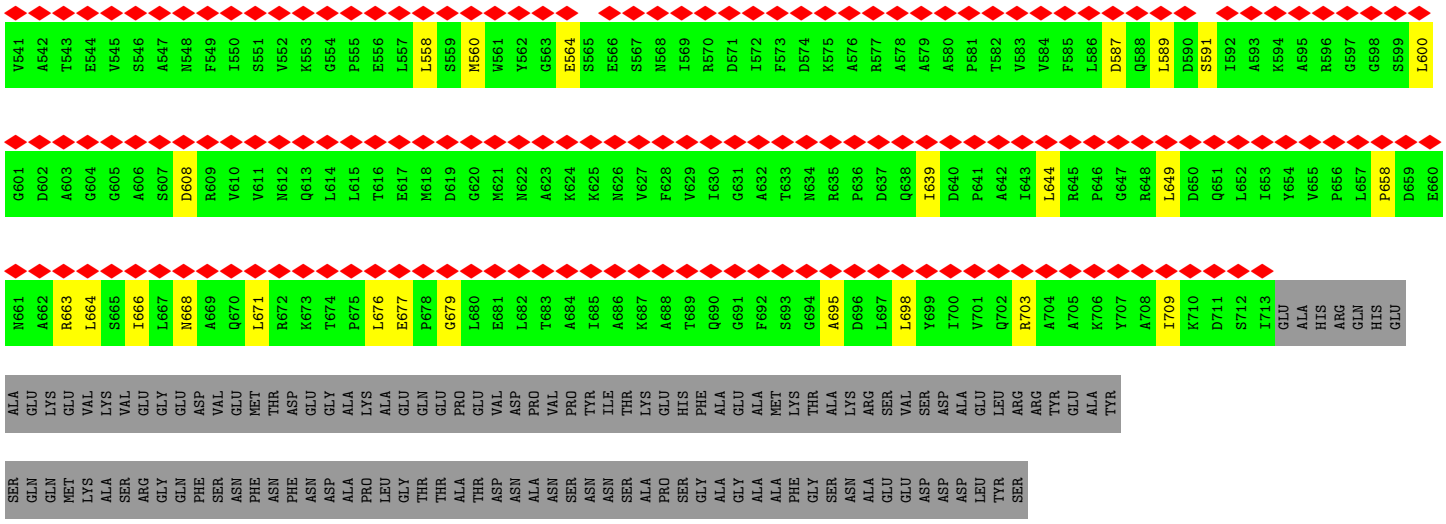




• Molecule 1: Cell division control protein 48

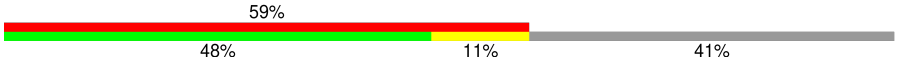
Chain B:

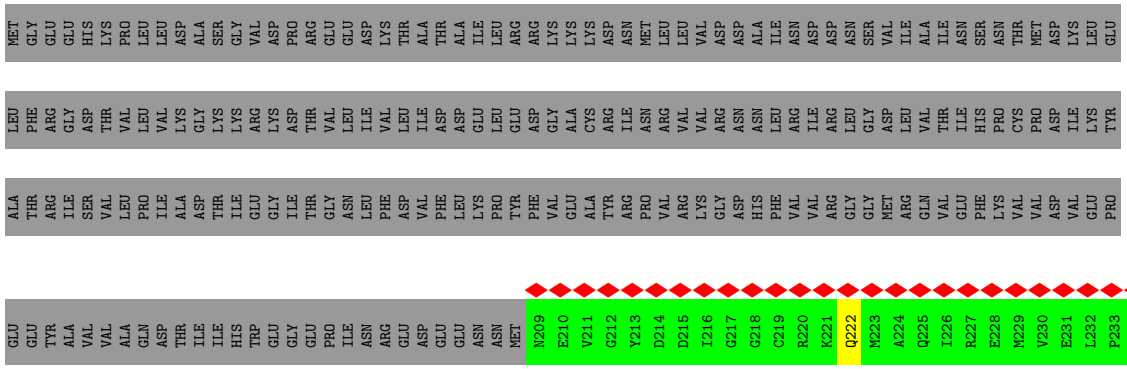


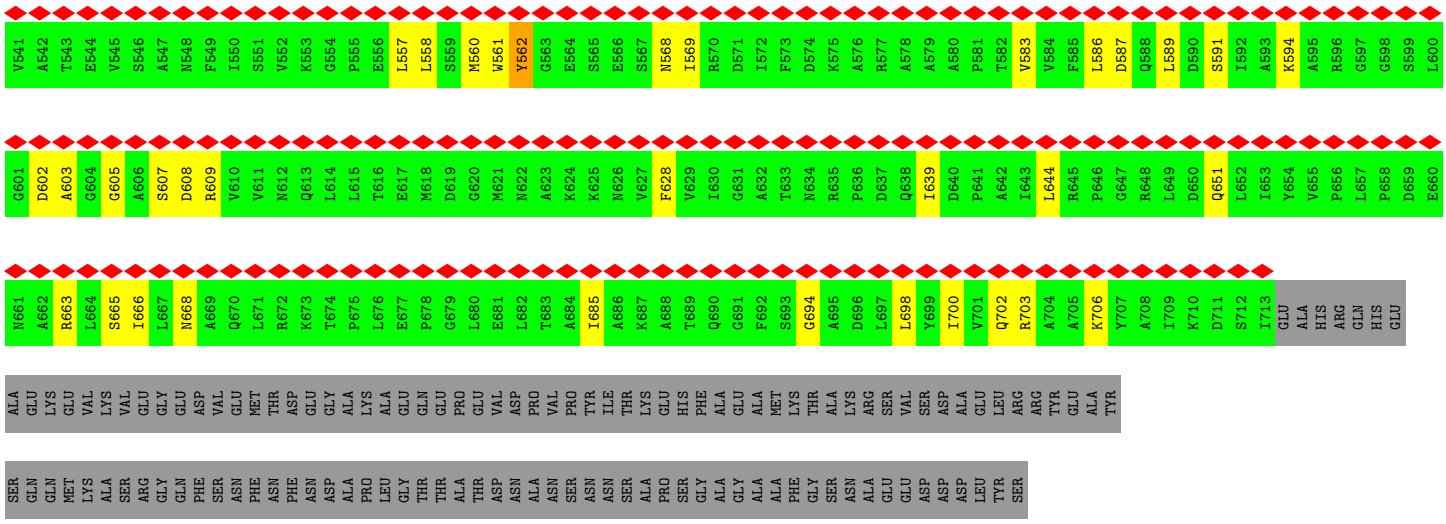


• Molecule 1: Cell division control protein 48

Chain C:

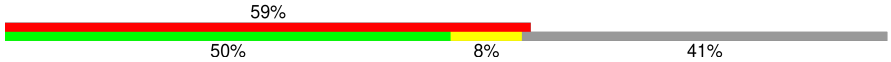


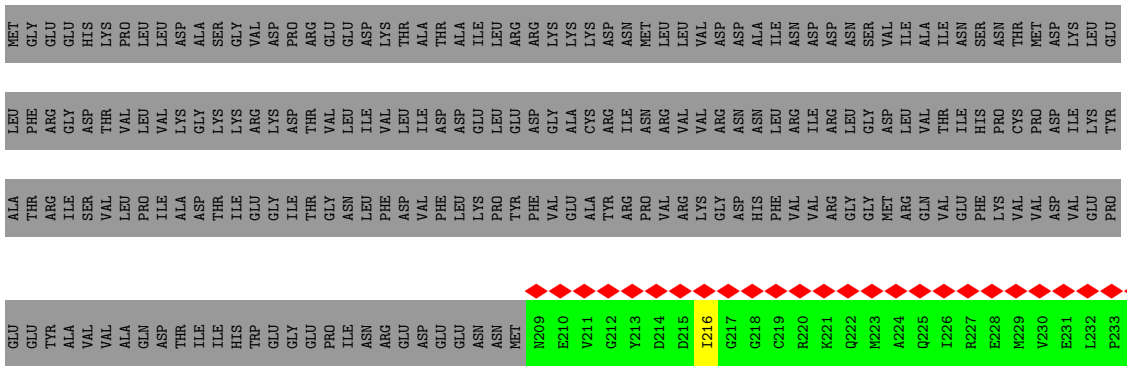


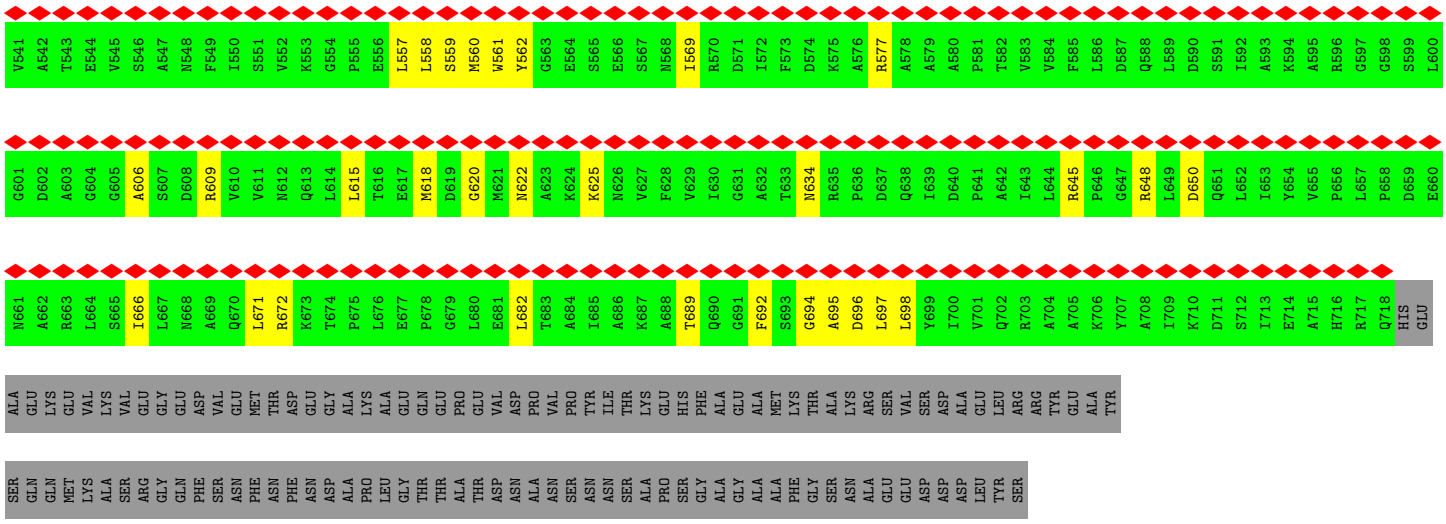


• Molecule 1: Cell division control protein 48

Chain D:

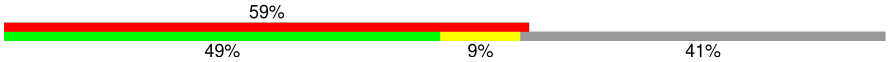


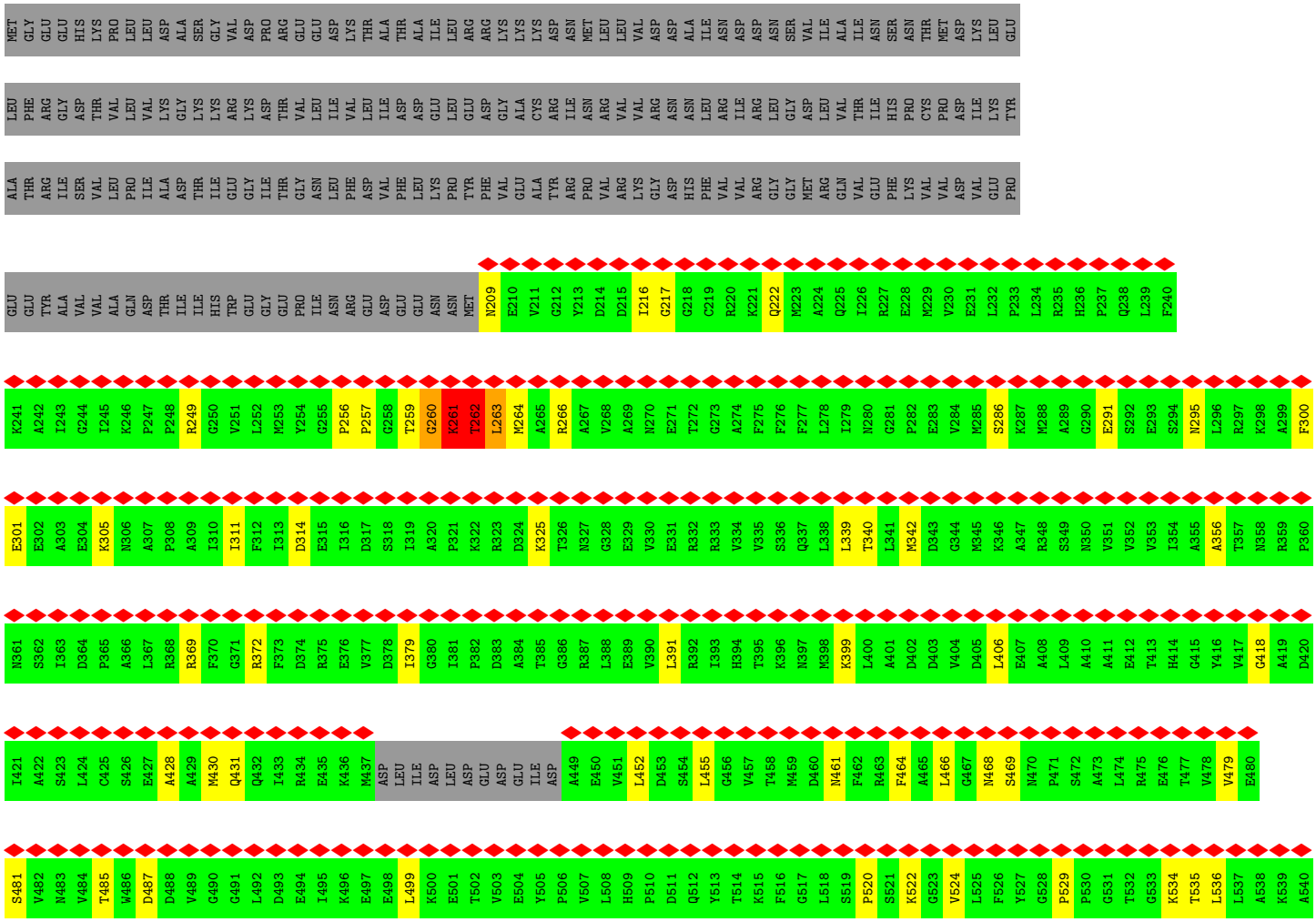


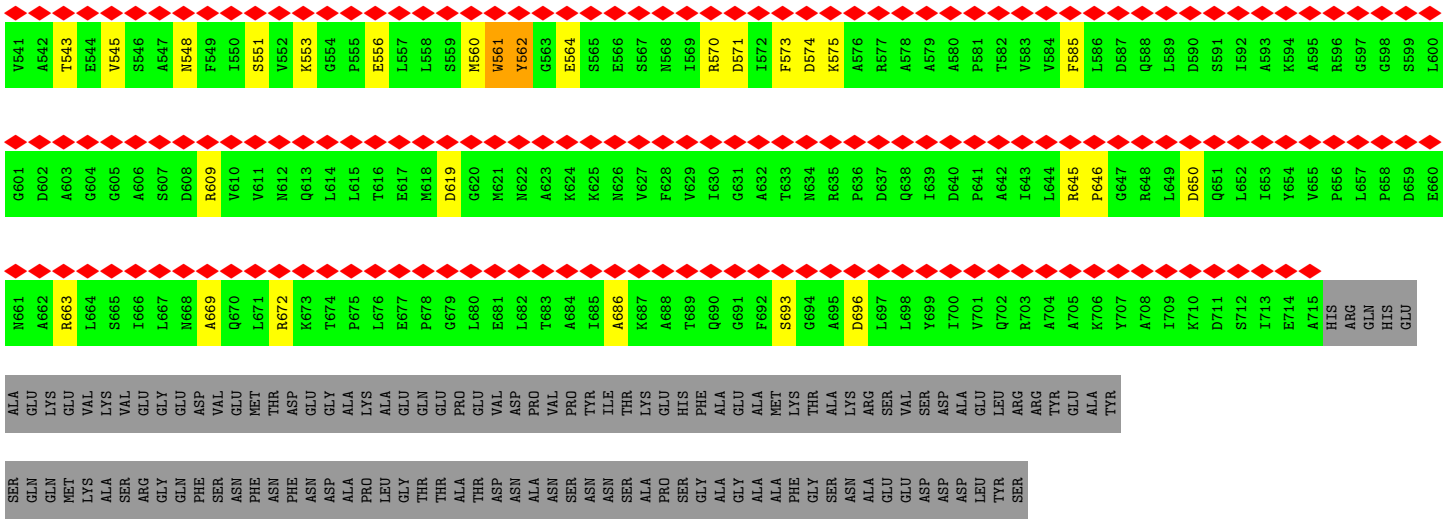


• Molecule 1: Cell division control protein 48

Chain E:

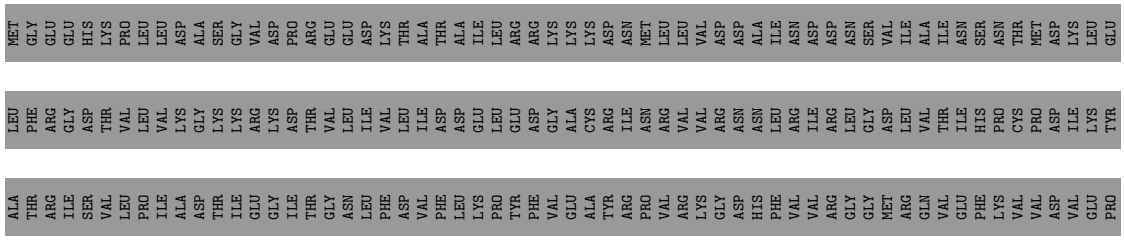


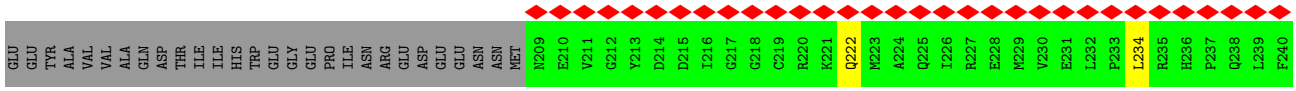


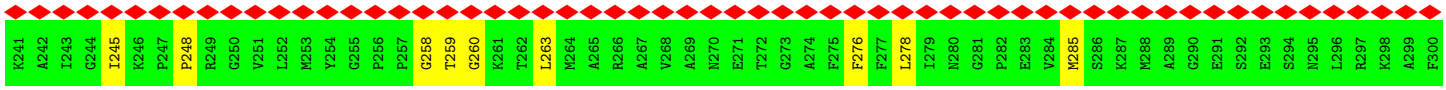


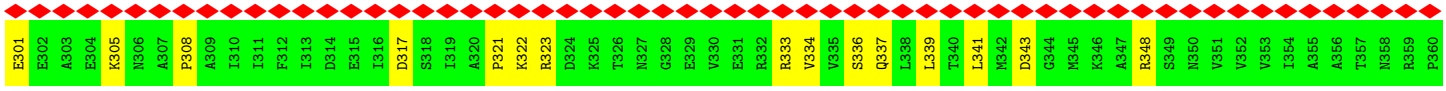
• Molecule 1: Cell division control protein 48

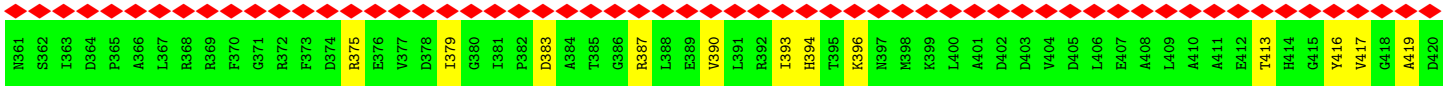
Chain F:

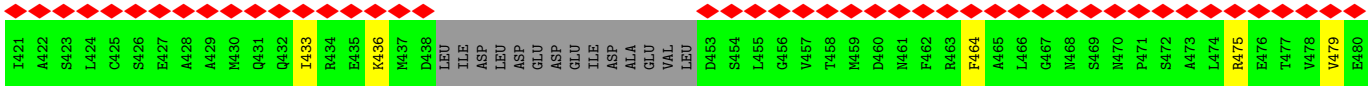


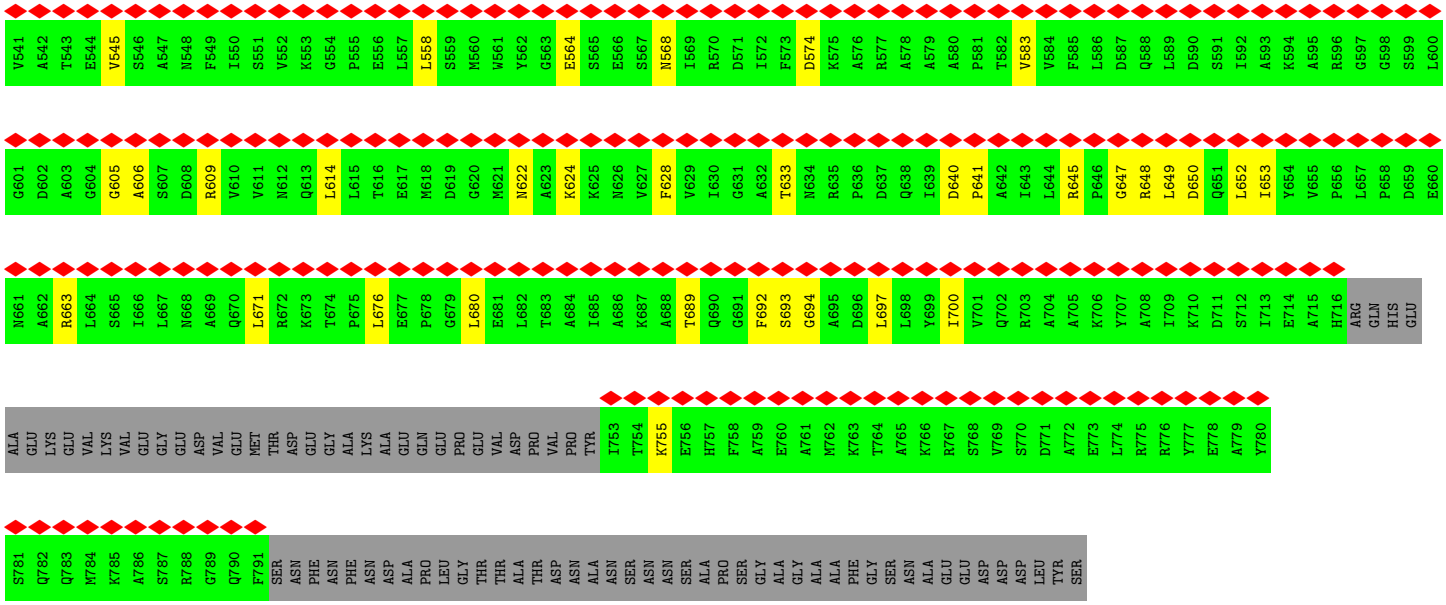






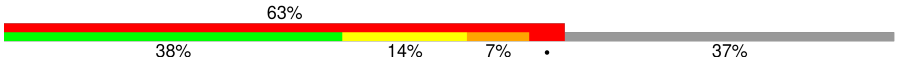


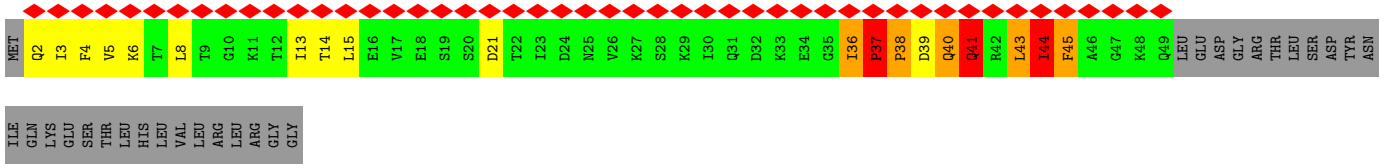




• Molecule 2: Ubiquitin

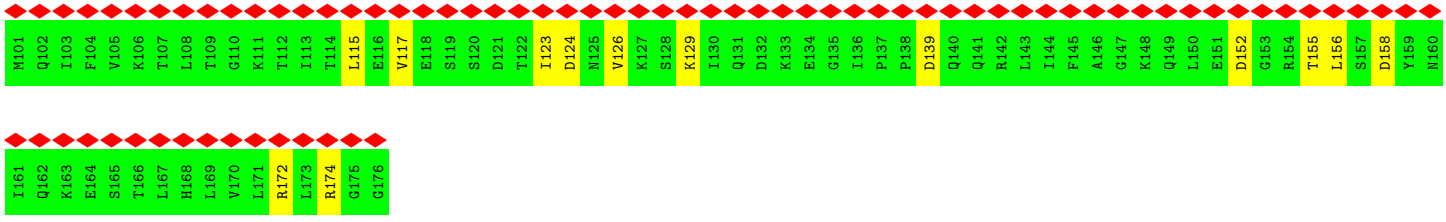
Chain K:





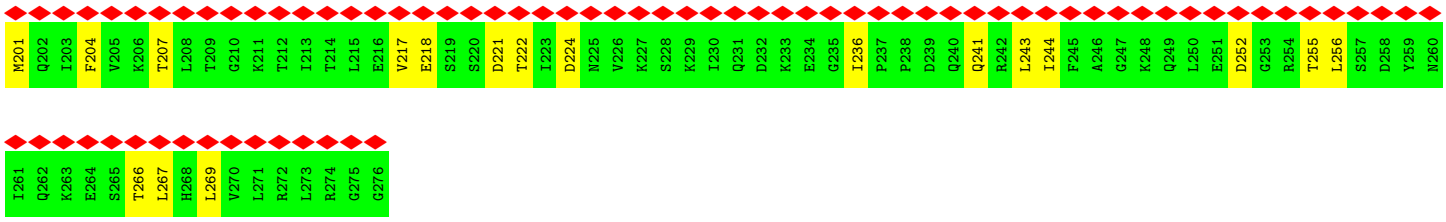
• Molecule 2: Ubiquitin

Chain H:



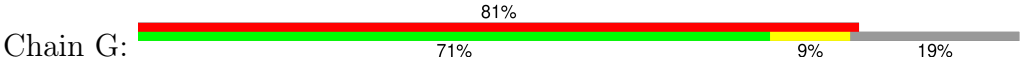
• Molecule 2: Ubiquitin

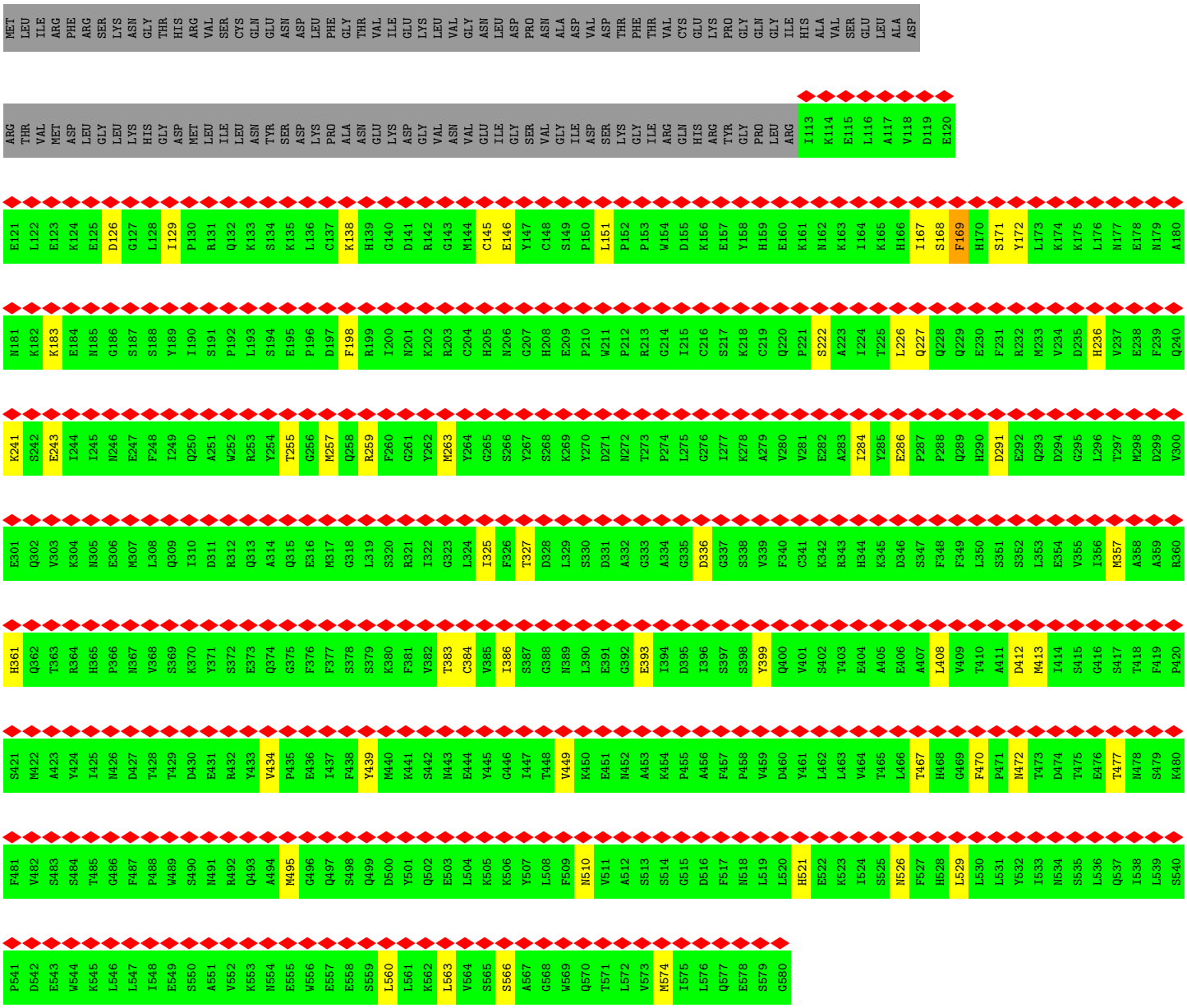
Chain J:



• Molecule 3: Nuclear protein localization protein 4

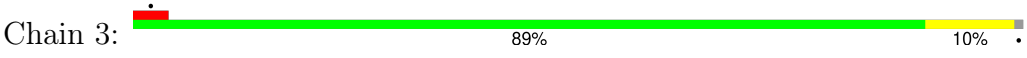
Chain G:

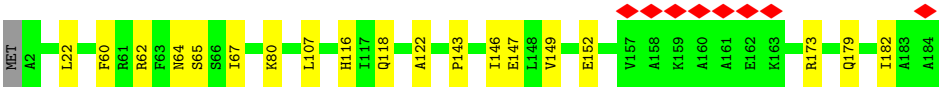




• Molecule 4: 60S ribosomal protein L17-A

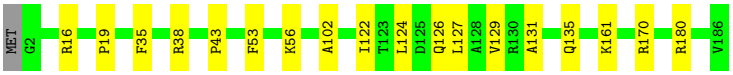
Chain 3:



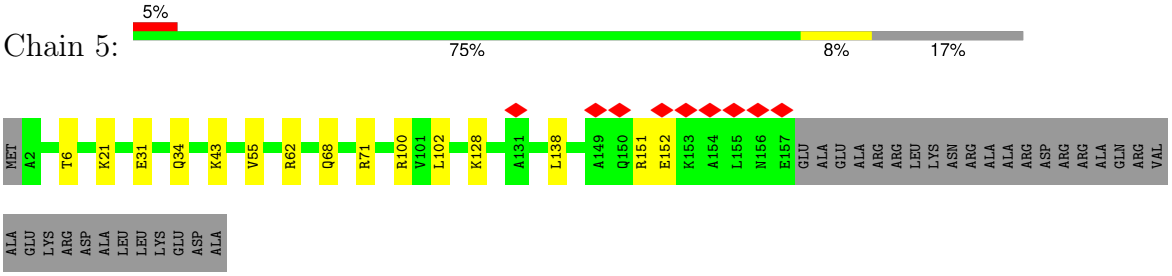


• Molecule 5: 60S ribosomal protein L18-A

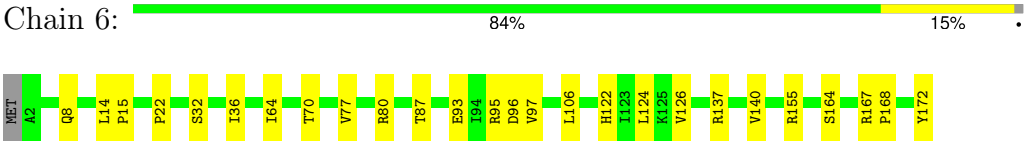
Chain 4:



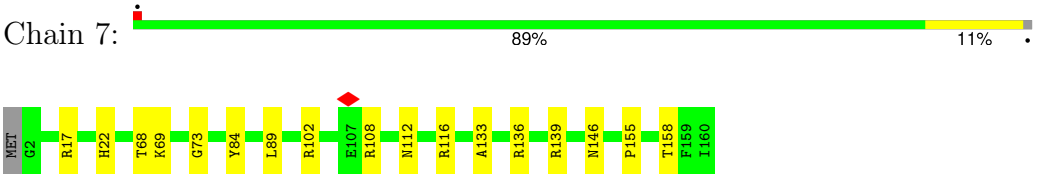
• Molecule 6: 60S ribosomal protein L19-A



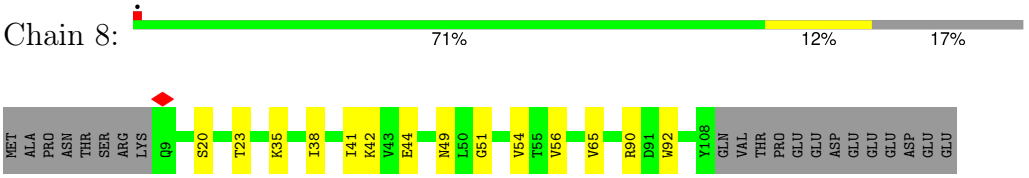
• Molecule 7: 60S ribosomal protein L20-A



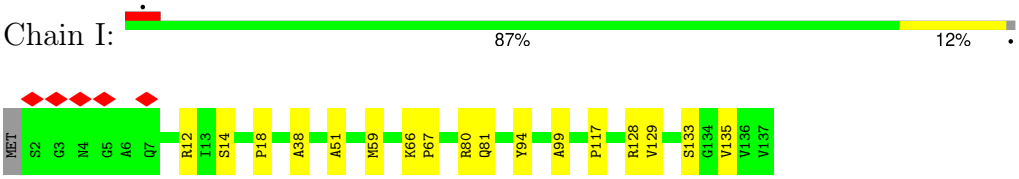
• Molecule 8: 60S ribosomal protein L21-A



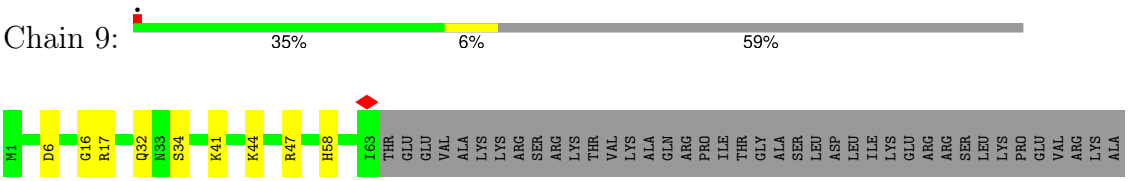
• Molecule 9: 60S ribosomal protein L22-A



• Molecule 10: 60S ribosomal protein L23-A



• Molecule 11: Large ribosomal subunit protein eL24A

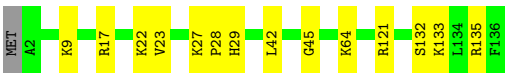


• Molecule 12: 60S ribosomal protein L26-A

Chain L:

• Molecule 13: 60S ribosomal protein L27-A

Chain M:

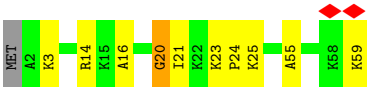


• Molecule 14: 60S ribosomal protein L28

Chain N:

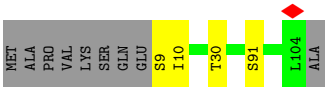
• Molecule 15: Large ribosomal subunit protein eL29

Chain O:



• Molecule 16: 60S ribosomal protein L30

Chain P:

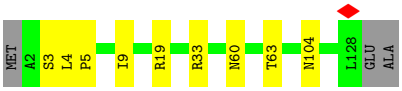


• Molecule 17: 60S ribosomal protein L31-A

Chain Q:

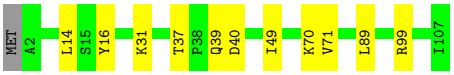
• Molecule 18: Large ribosomal subunit protein eL32

Chain R:



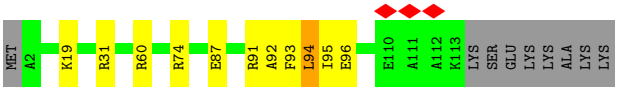
• Molecule 19: 60S ribosomal protein L33-A

Chain S:



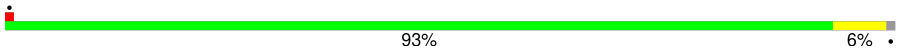
• Molecule 20: 60S ribosomal protein L34-A

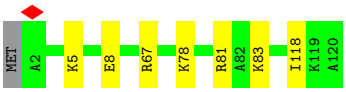
Chain T:



• Molecule 21: 60S ribosomal protein L35-A

Chain U:



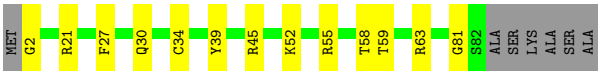


• Molecule 22: 60S ribosomal protein L36-A

Chain V:

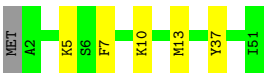
• Molecule 23: 60S ribosomal protein L37-A

Chain W:



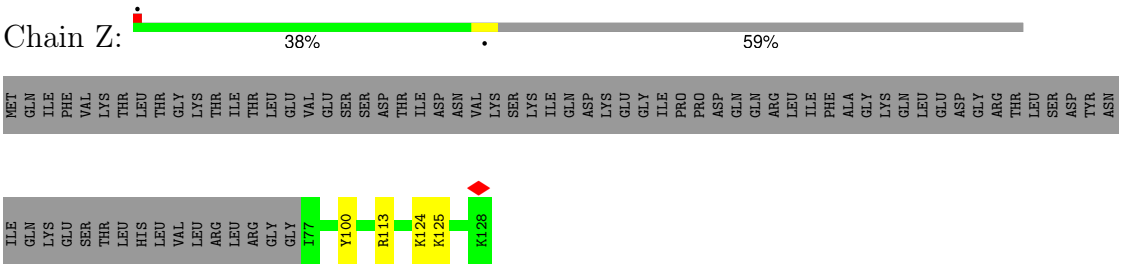
• Molecule 24: 60S ribosomal protein L39

Chain Y:



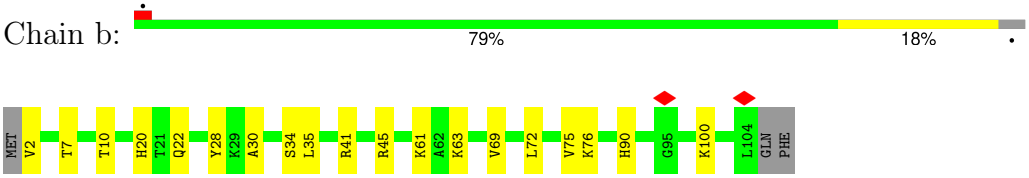
• Molecule 25: Ubiquitin-60S ribosomal protein L40

Chain Z:



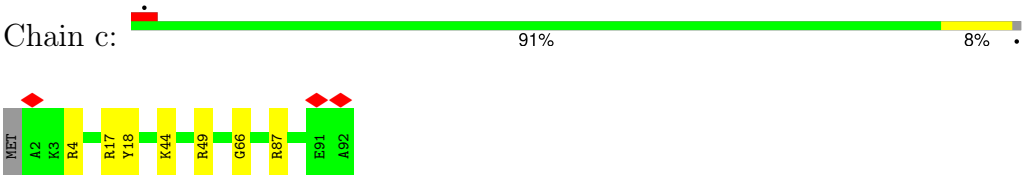
• Molecule 26: 60S ribosomal protein L42-A

Chain b:



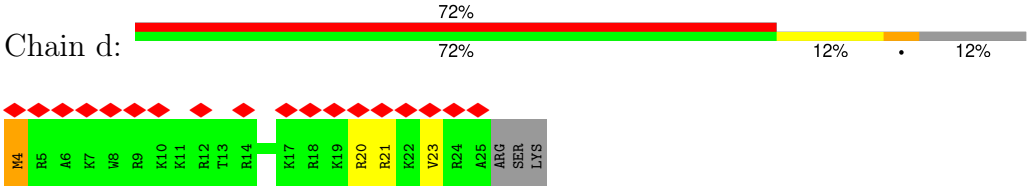
• Molecule 27: 60S ribosomal protein L43-A

Chain c:



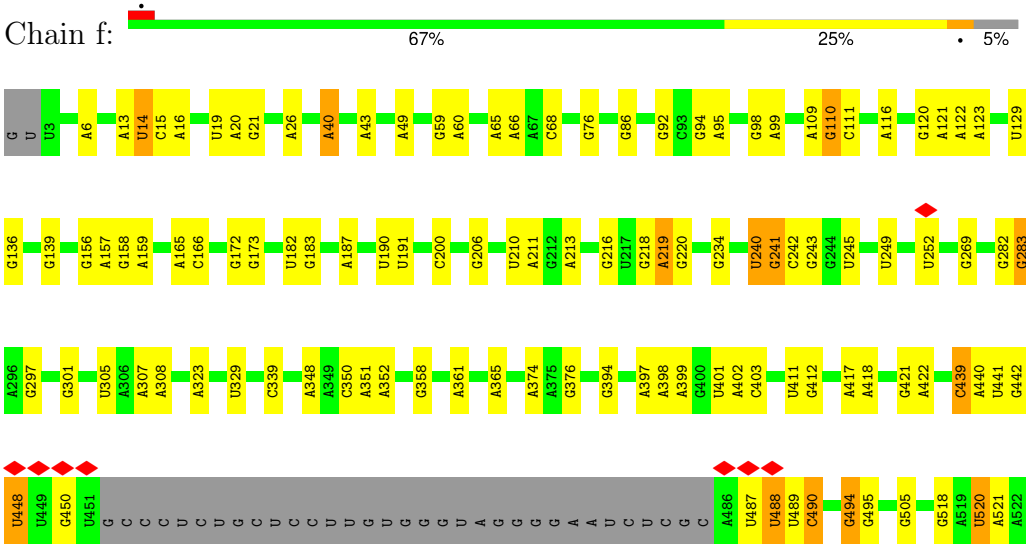
• Molecule 28: 60S ribosomal protein L41-A

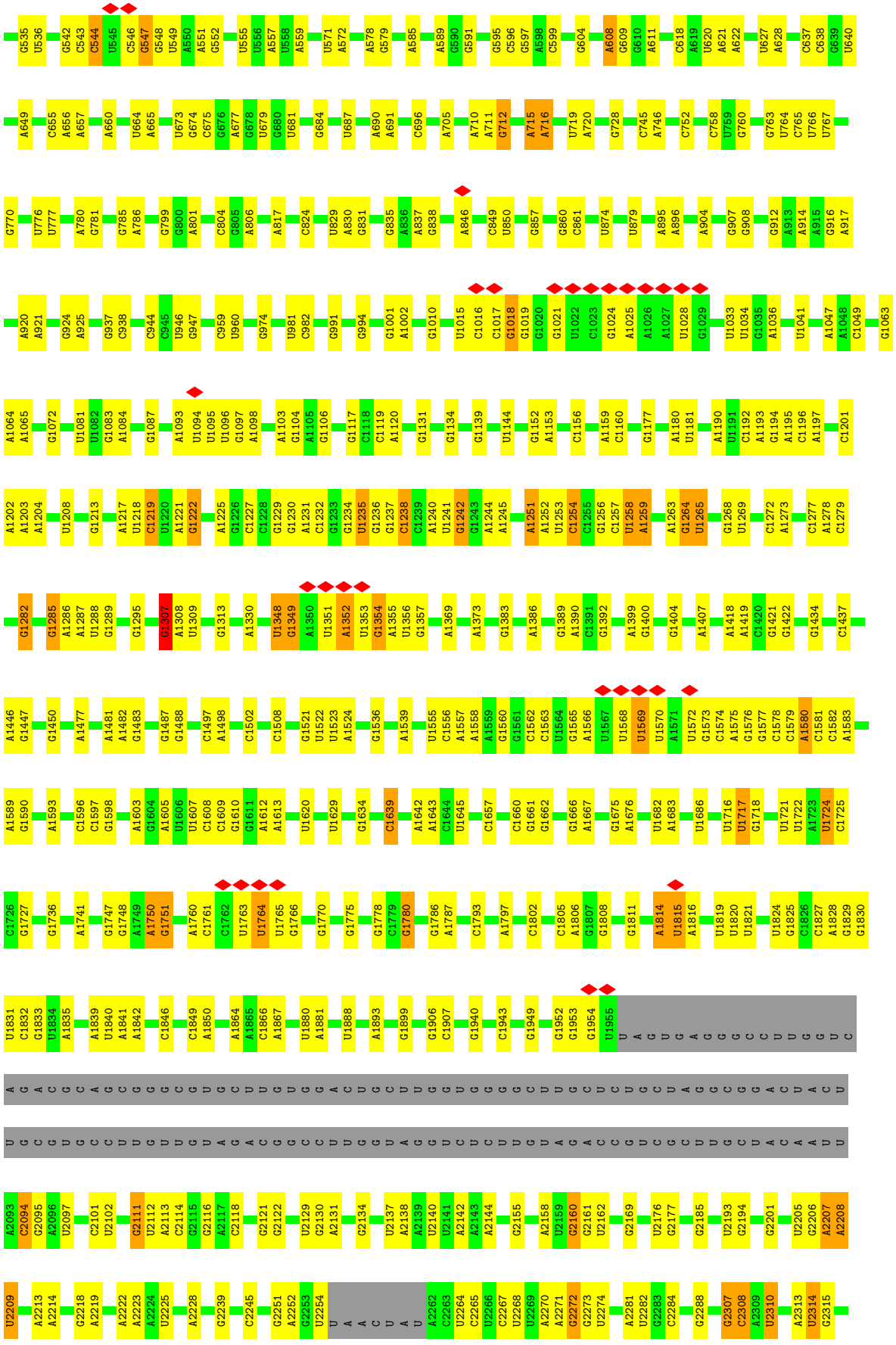
Chain d:

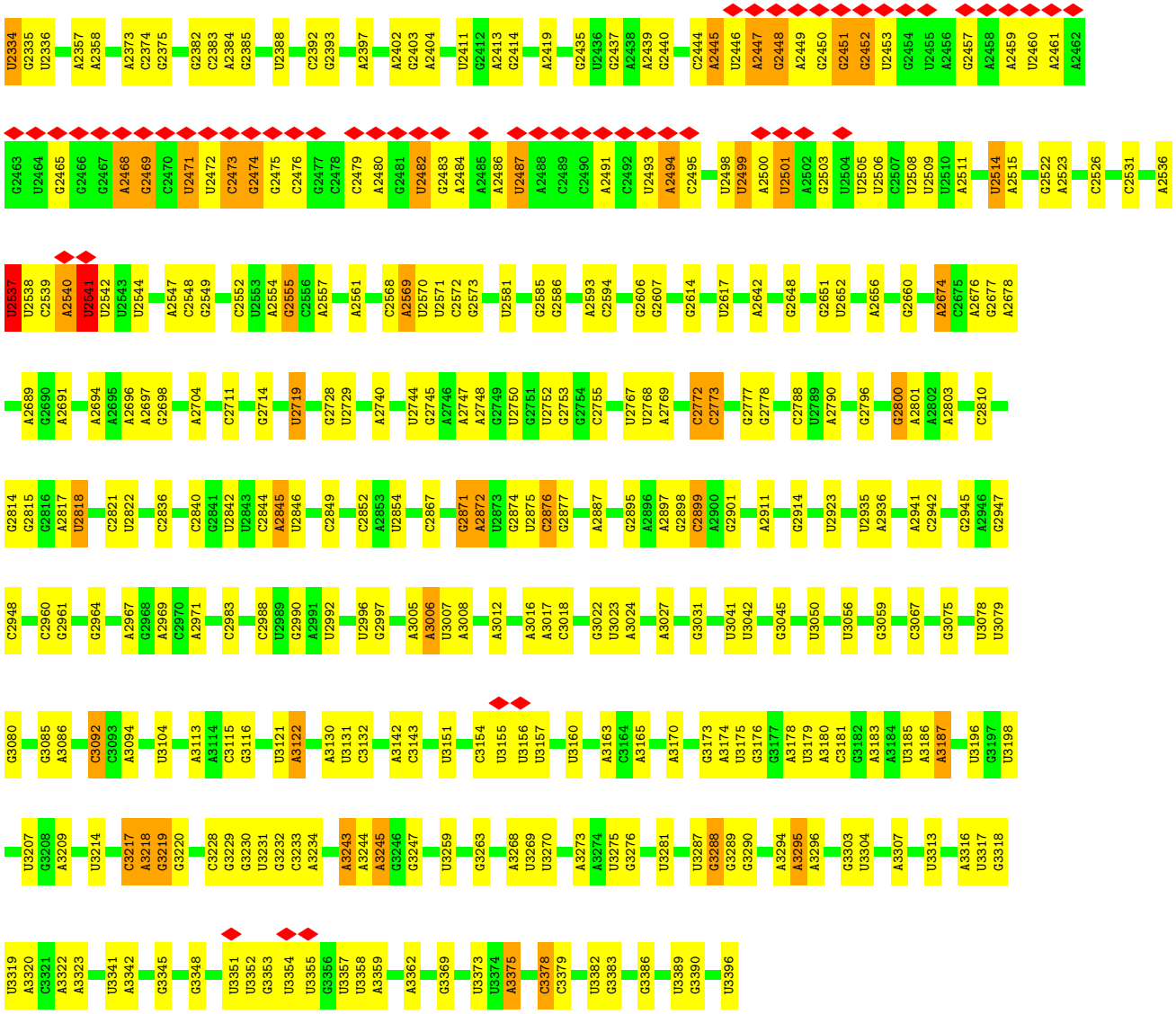


• Molecule 29: 25S rRNA

Chain f:





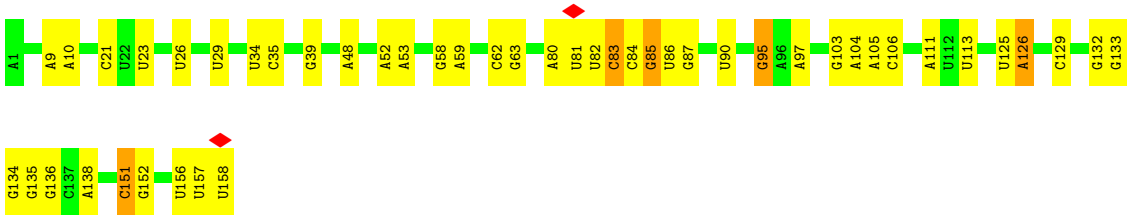


• Molecule 30: 5S rRNA

Chain h:

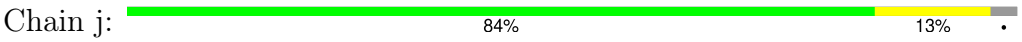
• Molecule 31: 5.8S rRNA

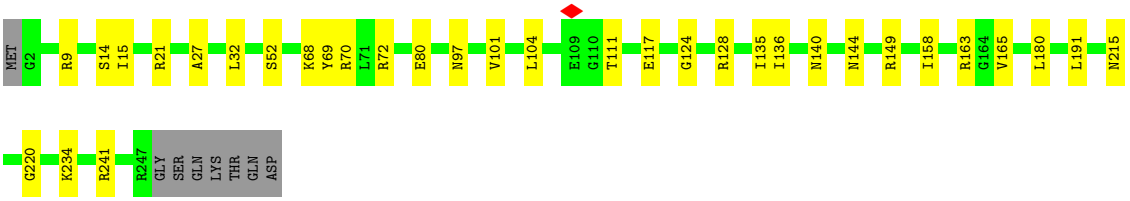
Chain i:



• Molecule 32: 60S ribosomal protein L2-A

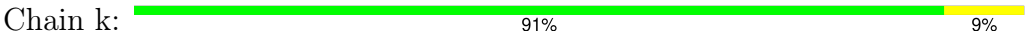
Chain j:

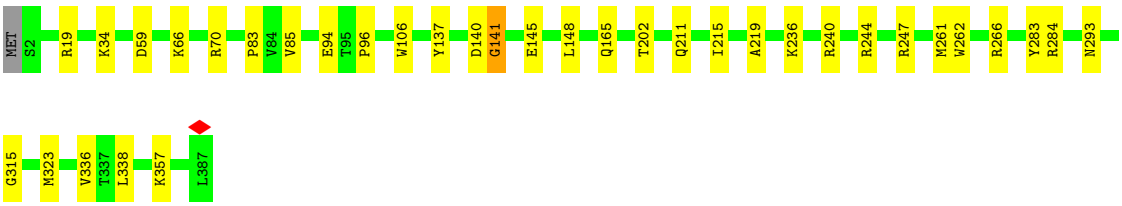




• Molecule 33: Large ribosomal subunit protein uL3

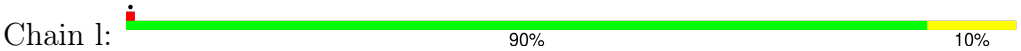
Chain k:

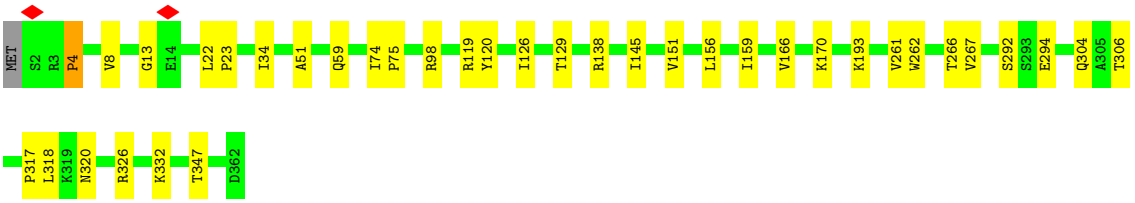




• Molecule 34: Large ribosomal subunit protein uL4A

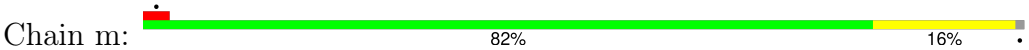
Chain l:

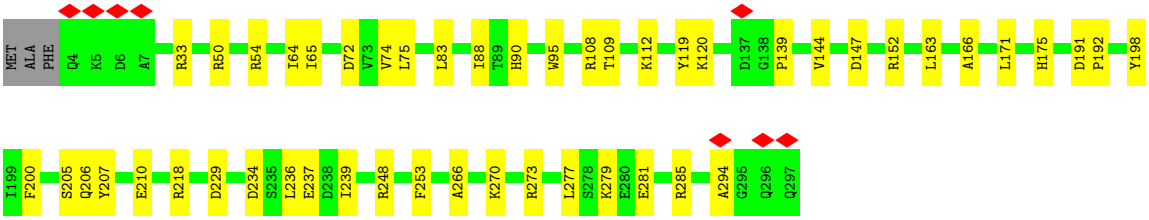




• Molecule 35: Large ribosomal subunit protein uL18

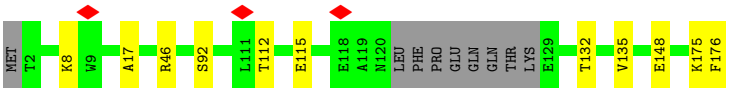
Chain m:





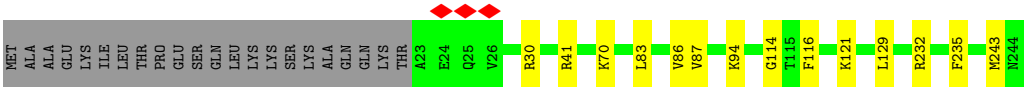
• Molecule 36: Large ribosomal subunit protein eL6B

Chain n:



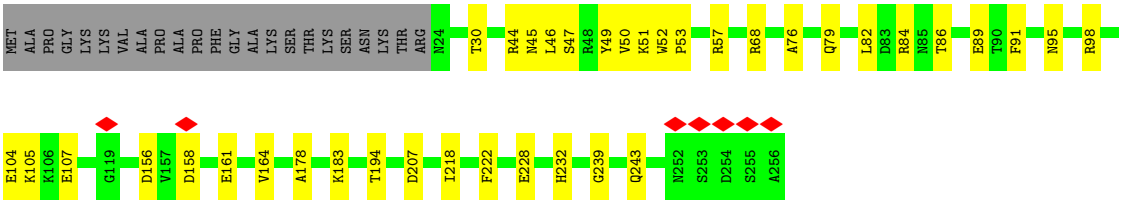
• Molecule 37: 60S ribosomal protein L7-A

Chain o:



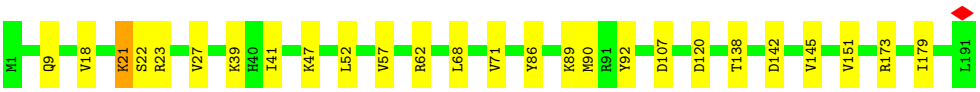
• Molecule 38: 60S ribosomal protein L8-A

Chain p:



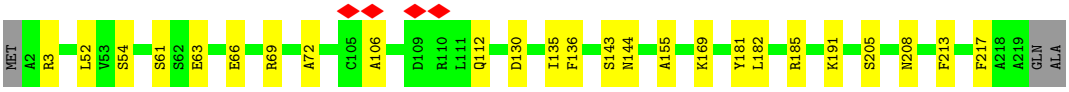
• Molecule 39: 60S ribosomal protein L9-A

Chain q:



• Molecule 40: Large ribosomal subunit protein uL16

Chain r:

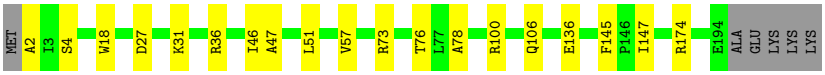


• Molecule 41: Large ribosomal subunit protein uL5A

Chain s:

• Molecule 42: 60S ribosomal protein L13-A

Chain t:

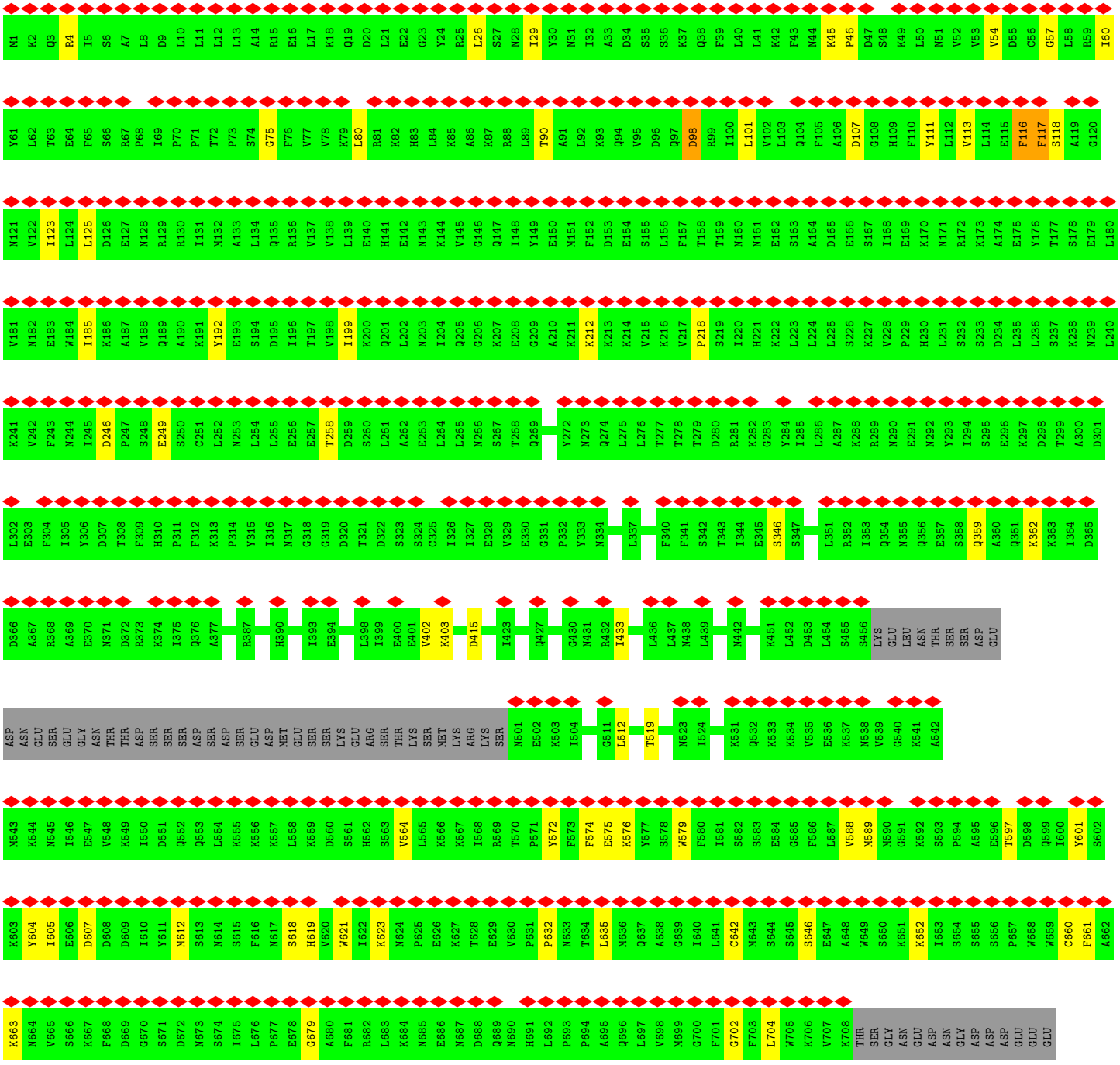


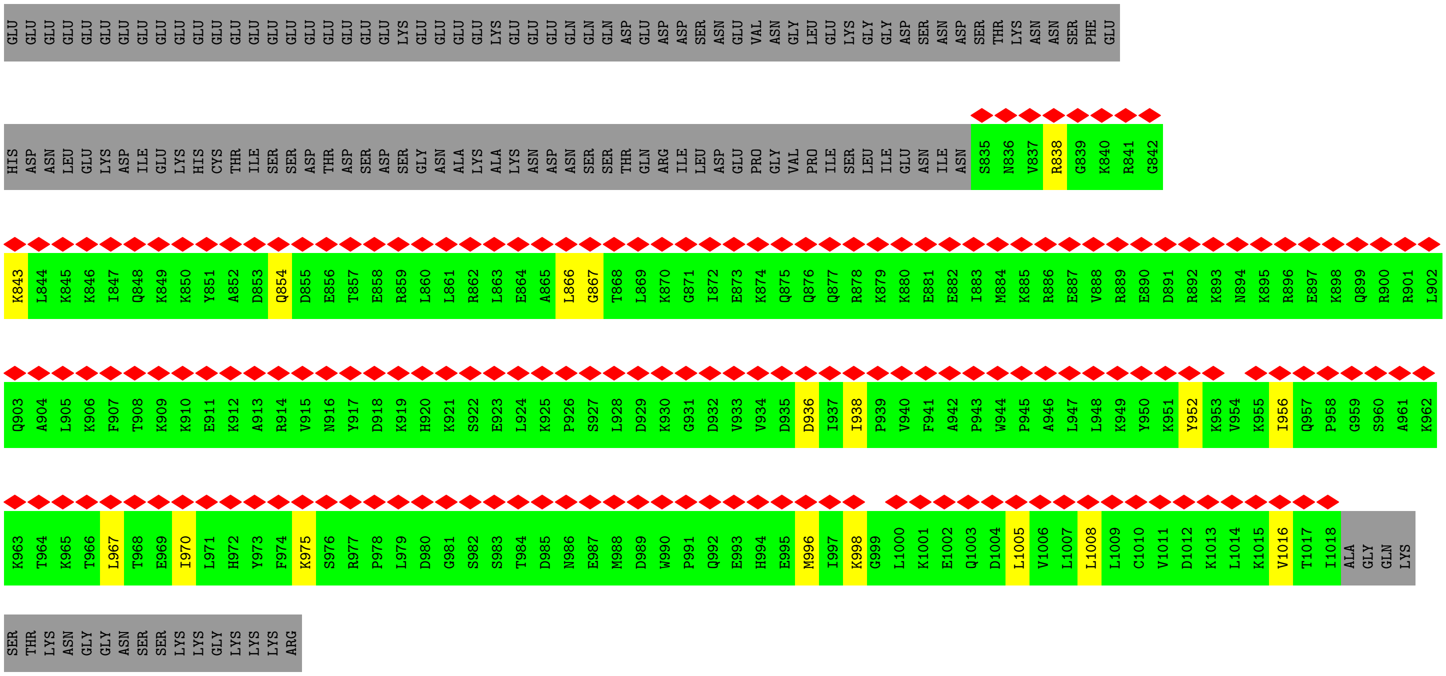
• Molecule 43: 60S ribosomal protein L14-A

Chain u:

• Molecule 44: Ribosome quality control complex subunit 2

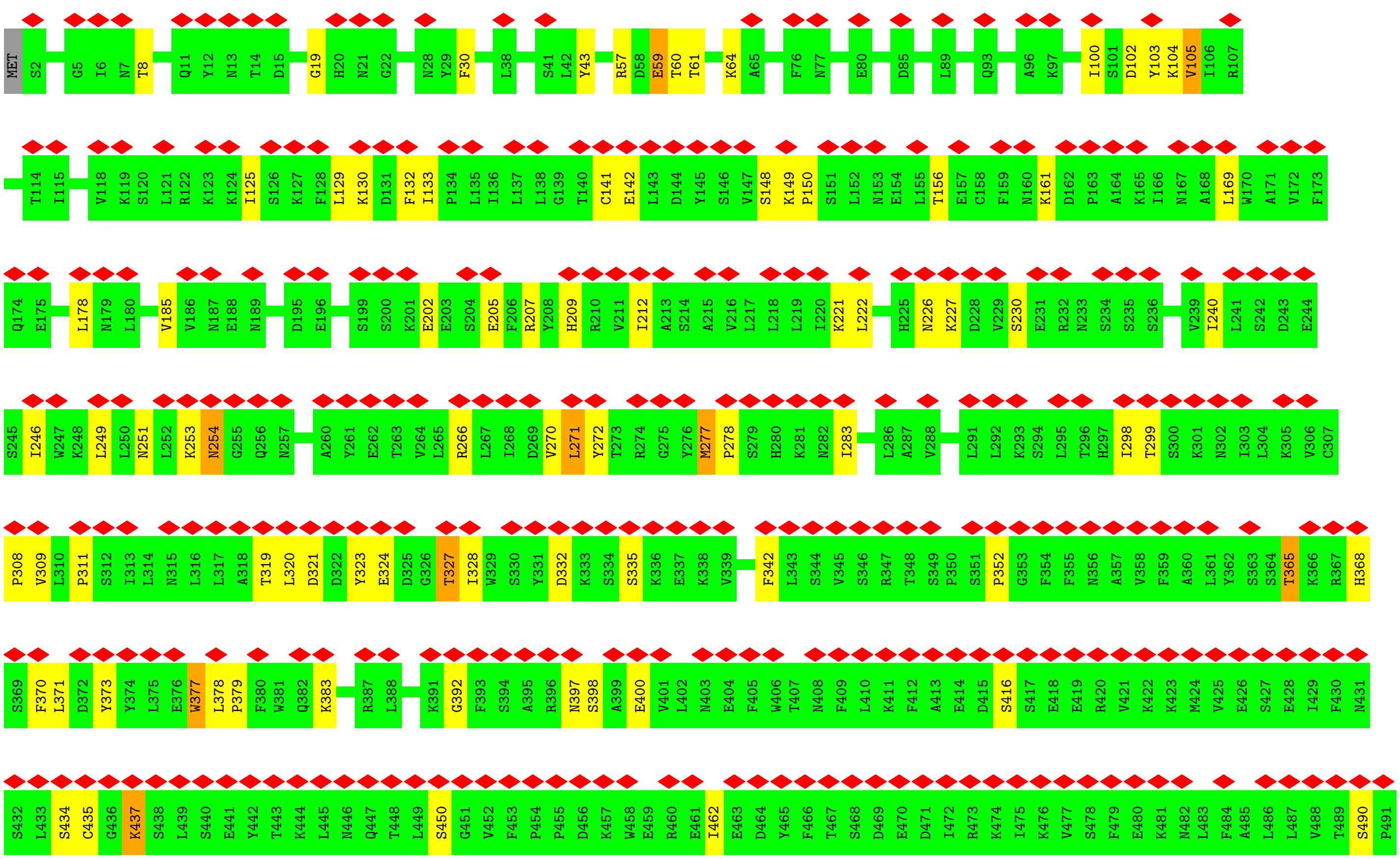
Chain a:

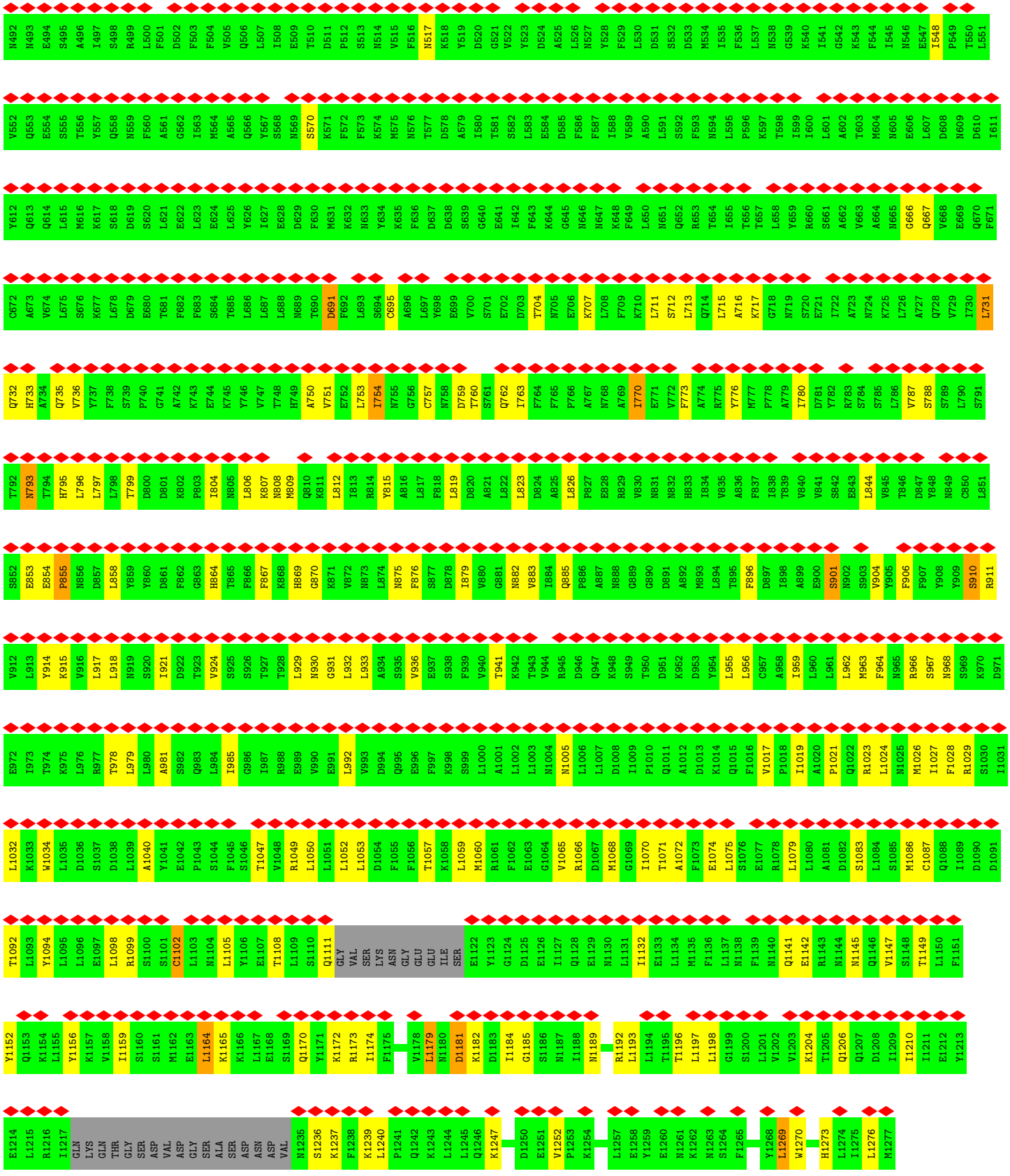


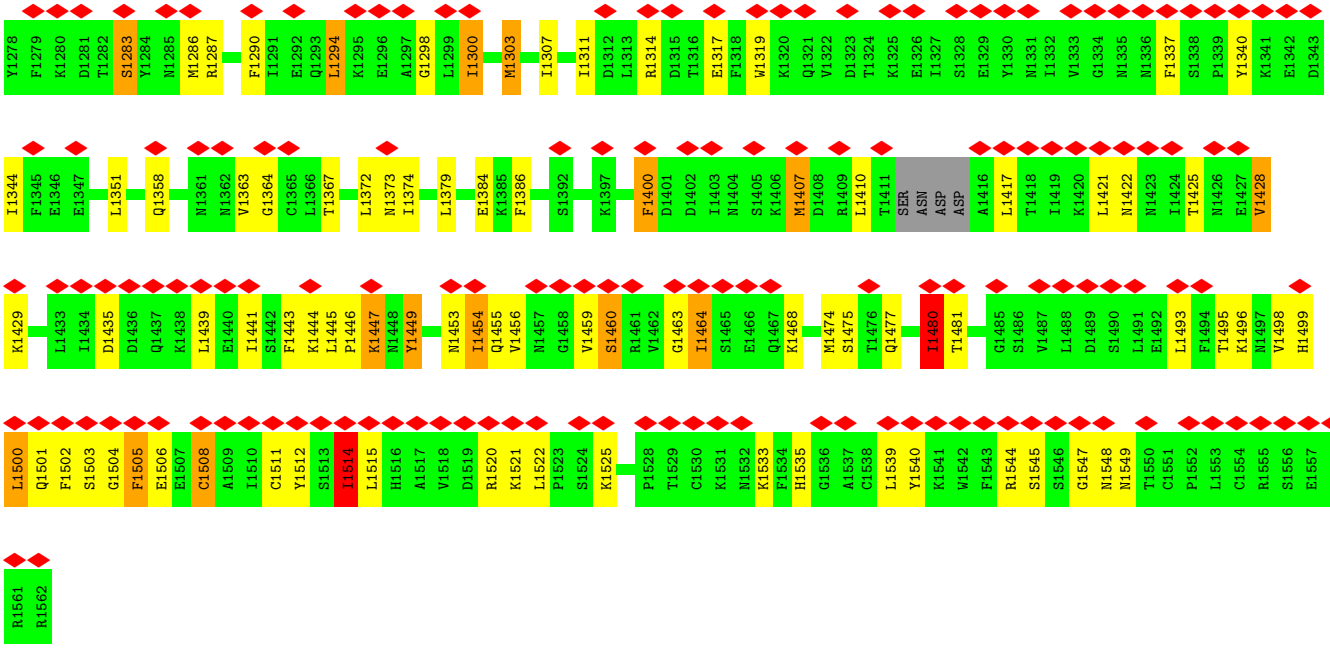


• Molecule 45: E3 ubiquitin-protein ligase listerin

Chain e:

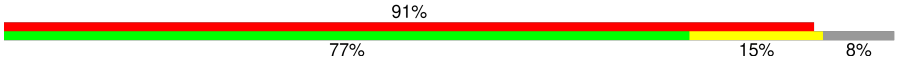


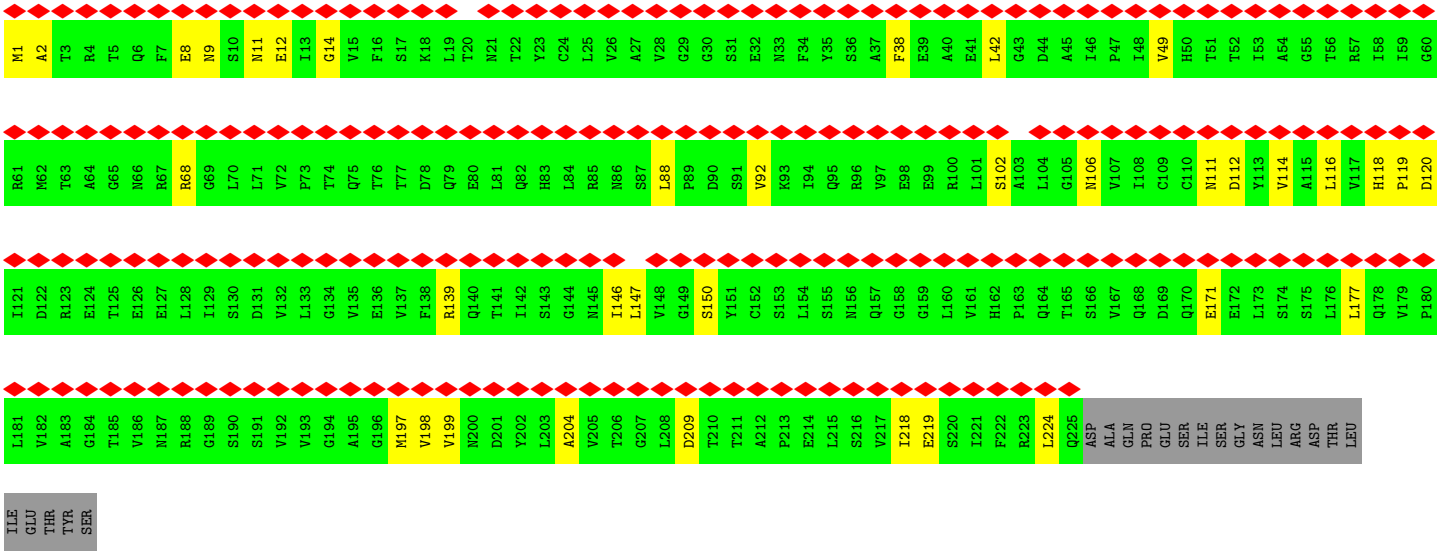

N492 N493 E494 S495 A496 I497 S498 R499 L500 F501 D502 F503 F504 V505 Q506 L507 I508 E509 T510 D511 P512 S513 N514 V515 F516 N517 K518 Y519 D520 G521 V522 Y523 D524 A525 L526 N527 Y528 F529 L530 D531 S532 D533 M534 I535 F536 L537 N538 G539 K540 I541 G542 K543 F544 I545 N546 E547 I548 P549 T550 L551
V552 Q553 E554 S555 T556 Y557 Q558 N559 F560 A561 G562 I563 M564 A565 Q566 Y567 S568 N569 S570 K571 F572 F573 K574 M575 N576 T577 D578 A579 I580 T581 S582 L583 E584 D585 F586 F587 I588 V589 A590 L591 S592 F593 N594 L595 P596 K597 T598 I599 I600 L601 A602 T603 M604 N605 E606 L607 D608 N609 D610 I611
Y612 Q613 Q614 L615 M616 K617 S618 D619 S620 L621 E622 L623 E624 L625 Y626 I627 E628 D629 F630 M631 K632 N633 Y634 K635 F636 D637 D638 S639 G640 E641 I642 F643 K644 G645 N646 N647 K648 F649 L650 N651 Q652 R653 T654 I655 T656 T657 L658 Y659 R660 S661 A662 V663 A664 N665 G666 Q667 V668 E669 Q670 F671
C672 A673 V674 L675 S676 K677 L678 D679 E680 T681 F682 F683 S684 T685 L686 L687 L688 N689 T690 D691 F692 L693 S694 C695 A696 L697 Y698 E699 V700 S701 E702 D703 T704 N705 E706 K707 L708 F709 K710 L711 S712 L713 Q714 L715 A716 K717 G718 N719 S720 E721 I722 A723 N724 K725 L726 A727 Q728 V729 I730 L731
Q732 H733 A734 Q735 V736 Y737 F738 S739 P740 G741 A742 K743 E744 K745 Y746 V747 T748 H749 A750 V751 E752 L753 I754 N755 G756 C757 N758 D759 T760 S761 Q762 I763 F764 F765 P766 A767 N768 A769 I770 E771 V772 F773 A774 R775 Y776 M777 P778 A779 I780 D781 Y782 R783 S784 S785 L786 V787 S788 S789 L790 S791
T792 N793 T794 H795 L796 L797 L798 T799 D800 D801 K802 P803 I804 N805 L806 K807 N808 M809 Q810 K811 L812 I813 R814 Y815 A816 L817 F818 L819 D820 A821 L822 L823 D824 A825 L826 P827 E828 R829 V830 N831 N832 H833 I834 V835 A836 F837 I838 T839 V840 V841 S842 E843 L844 V845 T846 D847 Y848 N849 C850 L851
S852 E853 E854 P855 N856 D857 L858 Y859 Y860 D861 F862 G863 H864 T865 F866 F867 K868 H869 G870 K871 V872 N873 L874 N875 F876 S877 D878 I879 V880 G881 N882 V883 I884 Q885 P886 A887 N888 G889 G890 D891 A892 M893 L894 T895 F896 D897 I898 A899 E900 S901 N902 S903 V904 Y905 F906 F907 Y908 Y909 S910 R911
V912 L913 Y914 K915 V916 L917 L918 N919 S920 I921 D922 T923 V924 S925 S926 T927 T928 L929 N930 G931 L932 L933 A934 S935 V936 E937 S938 F939 V940 T941 K942 T943 V944 R945 D946 Q947 K948 S949 T950 D951 K952 D953 Y954 L955 L956 C957 A958 I959 L960 L961 L962 M963 F964 N965 R966 S967 N968 S969 K970 D971
E972 I973 T974 K975 L976 R977 T978 L979 L980 A981 S982 Q983 L984 I985 G986 I987 R988 E989 V990 E991 L992 V993 D994 Q995 E996 F997 K998 S999 L1000 A1001 L1002 L1003 N1004 N1005 L1006 L1007 D1008 I1009 P1010 Q1011 A1012 D1013 K1014 Q1015 F1016 V1017 P1018 I1019 A1020 P1021 Q1022 R1023 L1024 N1025 M1026 I1027 F1028 R1029 S1030 I1031
L1032 K1033 W1034 L1035 D1036 S1037 D1038 L1039 A1040 Y1041 E1042 P1043 S1044 F1045 S1046 T1047 V1048 R1049 L1050 L1051 L1052 L1053 D1054 F1055 F1056 T1057 K1058 L1059 M1060 R1061 F1062 E1063 G1064 V1065 R1066 D1067 M1068 G1069 I1070 T1071 A1072 F1073 E1074 L1075 S1076 E1077 R1078 L1079 L1080 A1081 D1082 S1083 L1084 S1085 M1086 C1087 Q1088 I1089 D1090 D1091
T1092 L1093 Y1094 L1095 L1096 E1097 L1098 R1099 S1100 S1101 C1102 L1103 N1104 L1105 Y1106 E1107 T1108 L1109 S1110 Q1111 GLY VAL SER LYS ASN GLY GLU GLU ILE SER E1122 Y1123 G1124 D1125 E1126 I1127 Q1128 E1129 N1130 L1131 I1132 E1133 L1134 M1135 F1136 L1137 N1138 F1139 N1140 Q1141 E1142 R1143 N1144 N1145 Q1146 V1147 S1148 T1149 L1150 F1151
Y1152 Q1153 K1154 L1155 Y1156 K1157 V1158 I1159 S1160 S1161 M1162 E1163 L1164 K1165 K1166 L1167 E1168 S1169 Q1170 Y1171 K1172 R1173 I1174 F1175 V1178 L1179 N1180 D1181 K1182 D1183 I1184 G1185 S1186 N1187 I1188 N1189 R1192 L1193 L1194 T1195 T1196 L1197 L1198 G1199 S1200 L1201 V1202 V1203 K1204 T1205 Q1206 Q1207 D1208 I1209 I1210 I1211 E1212 Y1213
E1214 L1215 R1216 I1217 GLN LYS GLN THR GLY SER ASP VAL ASP GLY SER ALA SER ASP ASN ASP VAL N1235 S1236 K1237 F1238 K1239 L1240 P1241 Q1242 K1243 L1244 L1245 Q1246 K1247 D1250 E1251 V1252 P1253 K1254 L1257 E1258 Y1259 E1260 N1261 K1262 N1263 S1264 F1265 Y1268 L1269 W1270 H1273 L1274 I1275 L1276 M1277



• Molecule 46: Eukaryotic translation initiation factor 6

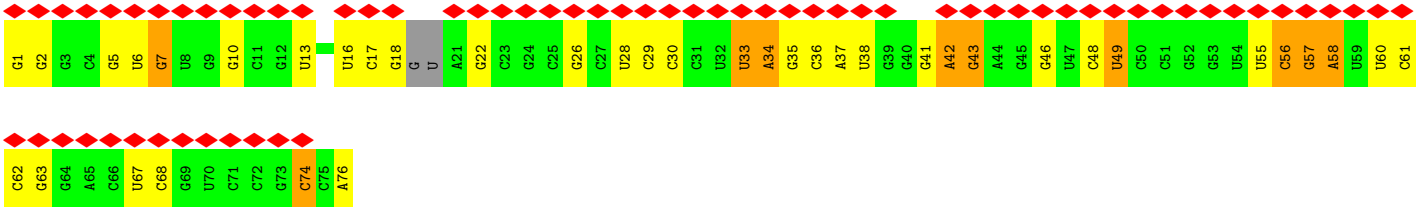
Chain g:





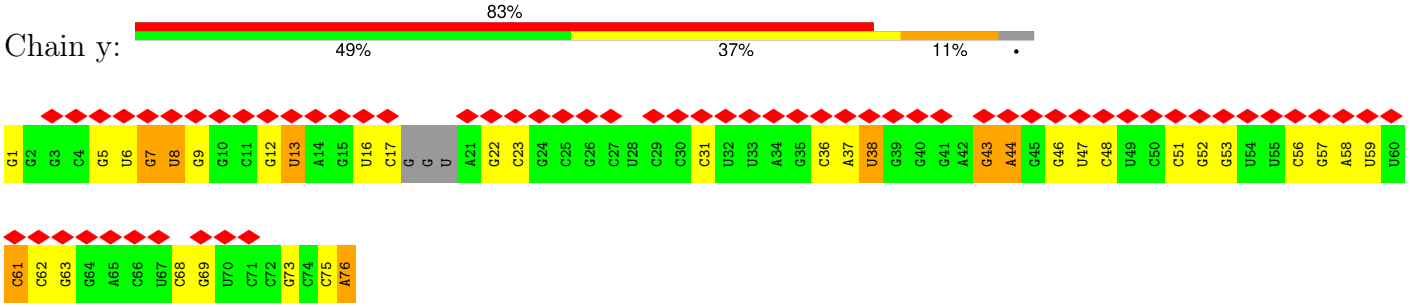
• Molecule 47: Ala tRNA

Chain x:



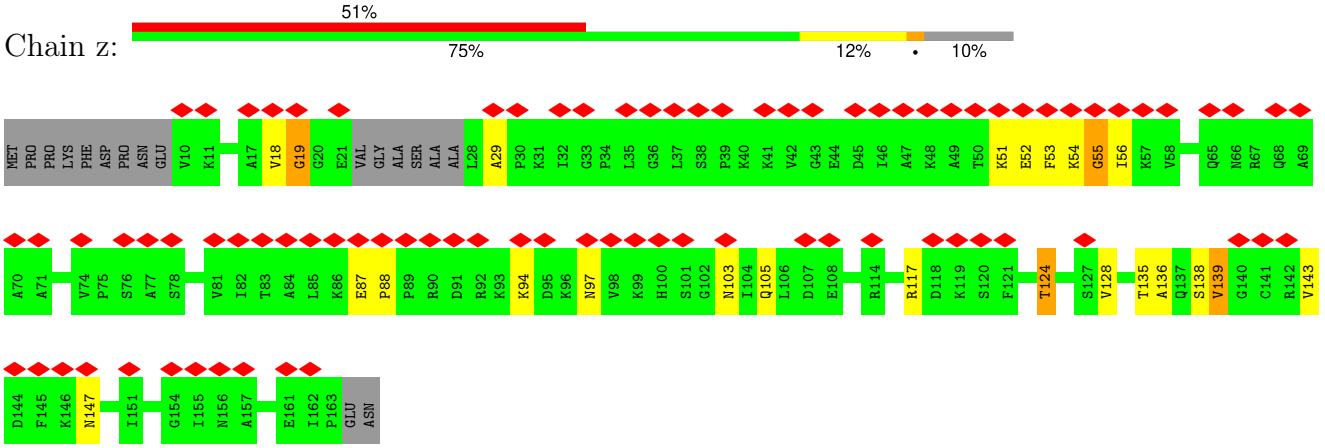
• Molecule 47: Ala tRNA

Chain y:



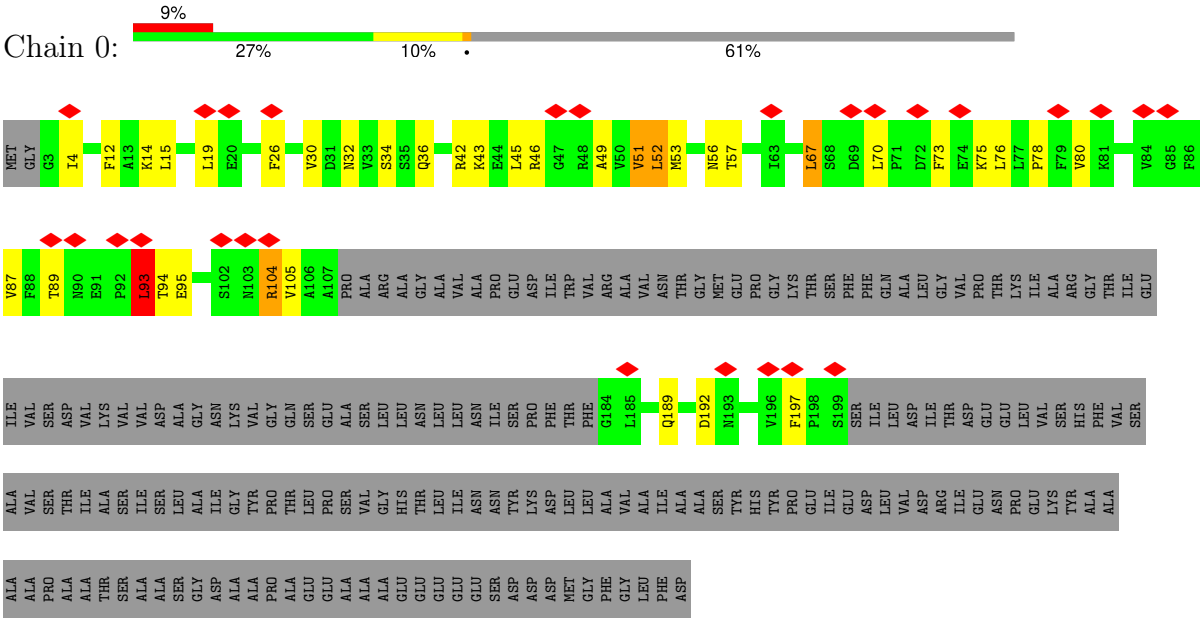
• Molecule 48: Large ribosomal subunit protein uL11A

Chain z:



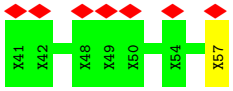
• Molecule 49: 60S acidic ribosomal protein P0

Chain 0:



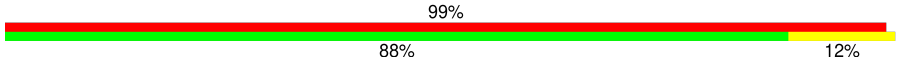
• Molecule 50: CAT-tailed nascent peptide

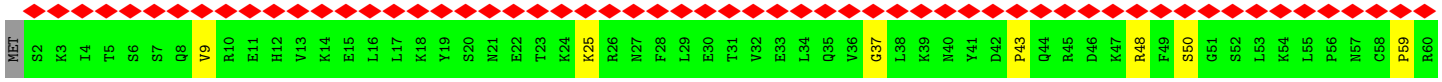
Chain 1:

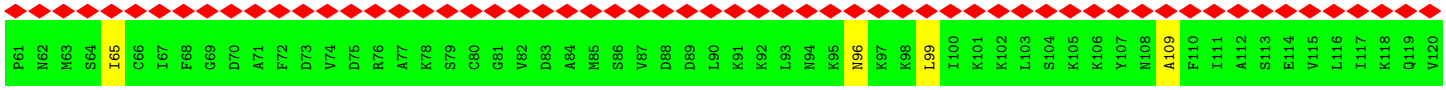


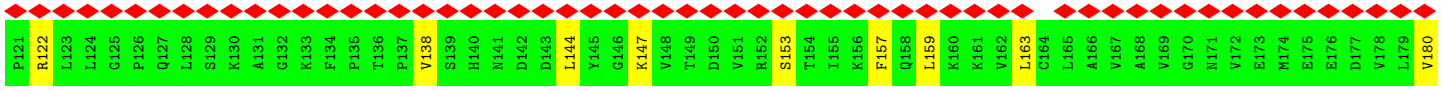
• Molecule 51: Large ribosomal subunit protein uL1A

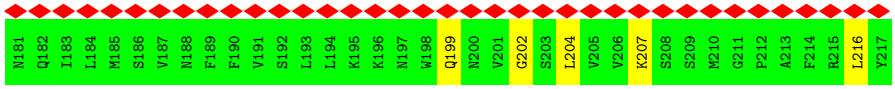
Chain w:





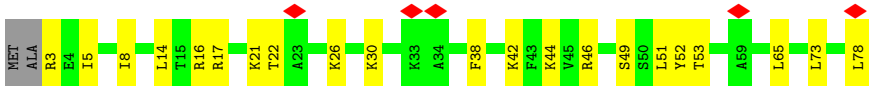






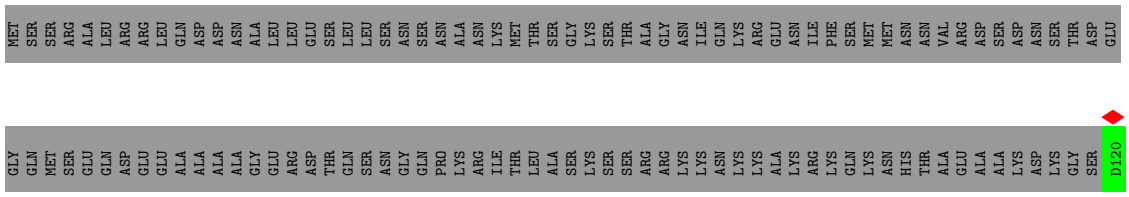
• Molecule 52: Large ribosomal subunit protein eL38

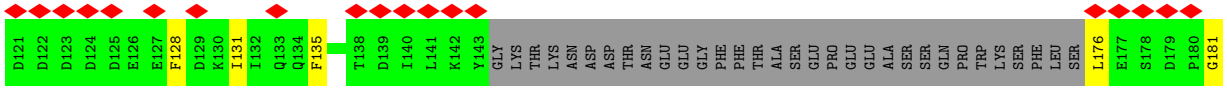
Chain X:

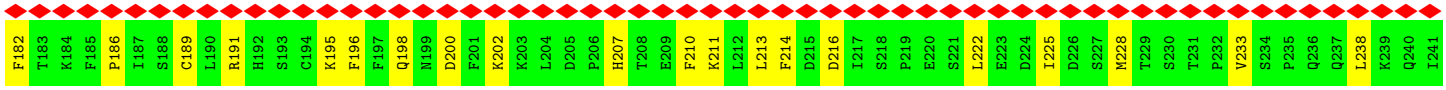


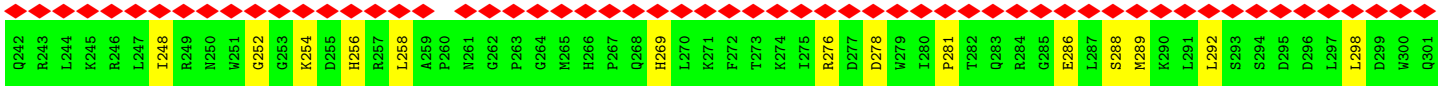
• Molecule 53: Ribosome quality control complex subunit 1

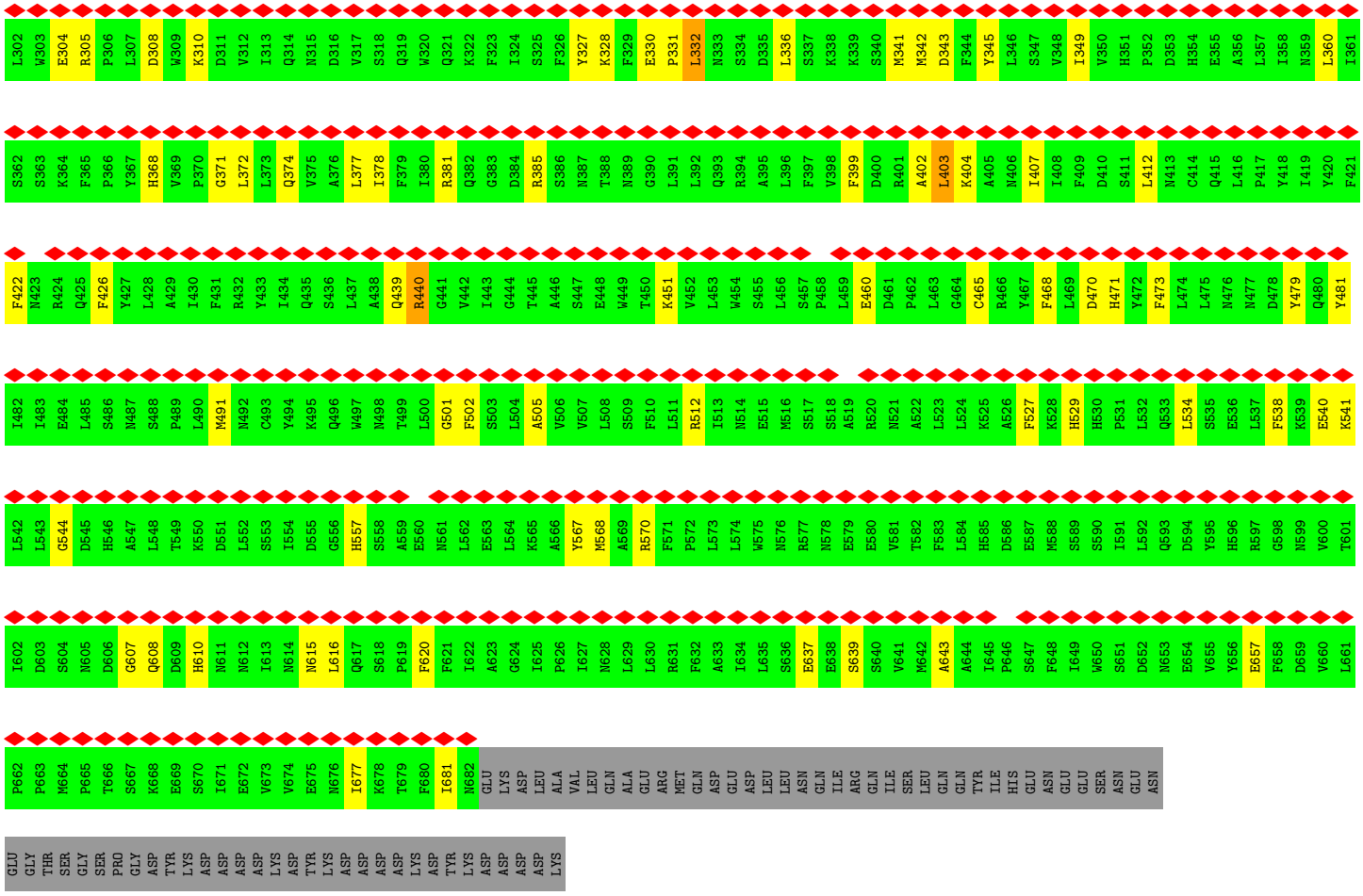
Chain v:





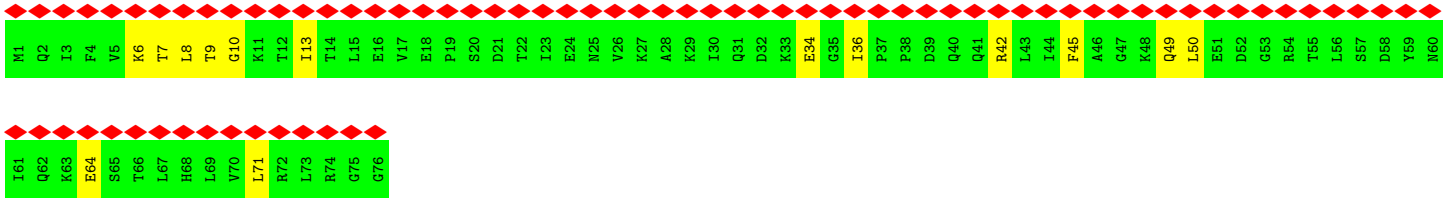






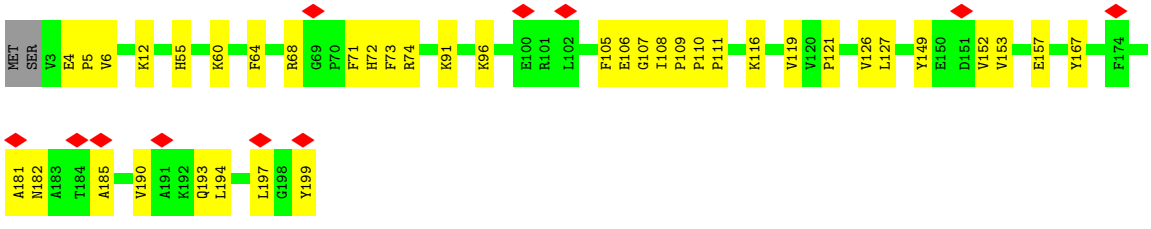
• Molecule 54: Polyubiquitin-C

Chain 2:



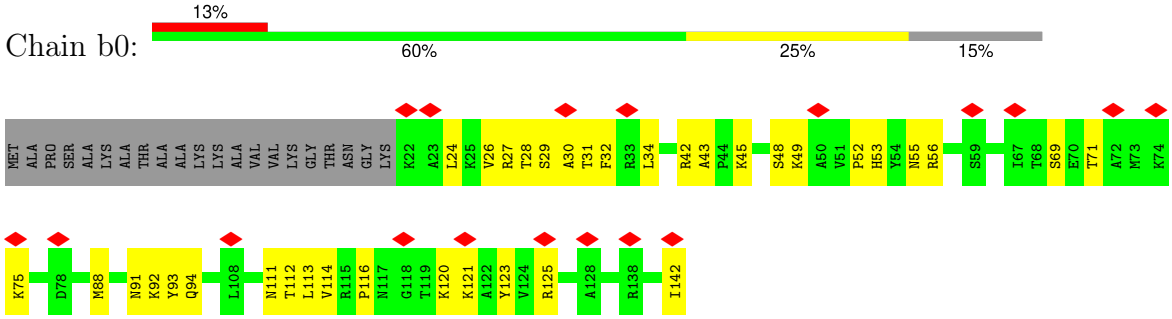
• Molecule 55: 60S ribosomal protein L16-A

Chain a0:



• Molecule 56: 60S ribosomal protein L25

Chain b0:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.553	Depositor
Minimum map value	-0.788	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.187	Depositor
Map size (Å)	677.12, 677.12, 677.12	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ADP, ZN, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.15	0/4273	0.42	0/5775
1	B	0.37	0/5129	0.63	0/6942
1	C	0.18	0/3819	0.46	0/5165
1	D	0.18	0/3808	0.46	0/5148
1	E	0.21	1/3846 (0.0%)	0.45	4/5202 (0.1%)
1	F	0.15	0/4158	0.41	0/5614
2	H	0.17	0/606	0.43	0/812
2	J	0.14	0/606	0.38	0/812
2	K	0.65	0/379	1.15	5/509 (1.0%)
3	G	0.20	0/3851	0.53	2/5201 (0.0%)
4	3	0.30	0/1439	0.61	0/1938
5	4	0.28	0/1465	0.58	0/1965
6	5	0.30	0/1275	0.56	0/1702
7	6	0.31	0/1473	0.56	0/1980
8	7	0.27	0/1296	0.56	0/1739
9	8	0.29	0/812	0.75	2/1099 (0.2%)
10	I	0.27	0/1018	0.50	0/1369
11	9	0.27	0/530	0.52	0/703
12	L	0.27	0/995	0.53	0/1329
13	M	0.27	0/1106	0.56	0/1485
14	N	0.32	0/1200	0.56	1/1607 (0.1%)
15	O	0.26	0/473	0.62	0/629
16	P	0.26	0/745	0.60	0/1001
17	Q	0.31	0/890	0.68	2/1196 (0.2%)
18	R	0.26	0/1034	0.47	0/1385
19	S	0.30	0/868	0.47	0/1168
20	T	0.29	0/890	0.58	2/1189 (0.2%)
21	U	0.27	0/978	0.53	0/1301
22	V	0.28	0/772	0.57	0/1026
23	W	0.32	0/660	0.60	0/875
24	Y	0.29	0/443	0.46	0/588
25	Z	0.28	0/416	0.60	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	b	0.28	0/836	0.53	0/1104
27	c	0.27	0/701	0.56	0/934
28	d	0.22	0/208	0.81	2/267 (0.7%)
29	f	0.31	0/77011	0.40	5/120065 (0.0%)
30	h	0.26	0/2883	0.32	0/4491
31	i	0.30	0/3746	0.36	0/5832
32	j	0.31	0/1908	0.54	0/2564
33	k	0.29	0/3146	0.53	0/4228
34	l	0.29	0/2800	0.57	4/3790 (0.1%)
35	m	0.27	0/2400	0.56	0/3239
36	n	0.28	0/1329	0.60	0/1794
37	o	0.31	0/1821	0.58	0/2451
38	p	0.27	0/1836	0.58	1/2481 (0.0%)
39	q	0.30	0/1529	0.64	2/2060 (0.1%)
40	r	0.25	0/1801	0.49	0/2416
41	s	0.27	0/1367	0.69	4/1834 (0.2%)
42	t	0.29	0/1568	0.62	1/2106 (0.0%)
43	u	0.30	0/1068	0.53	0/1438
44	a	0.26	0/6683	0.55	2/9016 (0.0%)
45	e	0.66	0/11755	0.97	58/15956 (0.4%)
46	g	0.24	0/1672	0.59	1/2281 (0.0%)
47	x	0.35	0/1761	0.61	0/2742
47	y	0.37	0/1735	0.64	0/2701
48	z	0.67	0/726	1.24	13/1006 (1.3%)
49	0	0.49	0/976	0.95	3/1313 (0.2%)
51	w	0.27	0/1736	0.61	0/2332
52	X	0.45	0/614	0.50	0/819
53	v	0.84	3/4492 (0.1%)	1.12	7/6087 (0.1%)
54	2	0.72	0/608	1.02	0/816
55	a0	0.32	0/1585	0.54	0/2128
56	b0	0.31	0/979	0.57	0/1321
All	All	0.35	4/194533 (0.0%)	0.55	121/280619 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1
15	O	0	1
21	U	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	k	0	1
34	l	0	2
38	p	0	3
39	q	0	1
43	u	0	1
45	e	0	1
46	g	0	1
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	v	439	GLN	C-N	21.17	1.61	1.33
53	v	372	LEU	C-N	18.31	1.58	1.33
53	v	286	GLU	C-N	8.53	1.45	1.33
1	E	261	LYS	N-CA	-6.29	1.38	1.46

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	36	ILE	C-N-CD	-13.24	70.72	125.00
45	e	1364	GLY	N-CA-C	12.27	127.34	112.49
53	v	440	ARG	O-C-N	11.96	136.70	122.34
45	e	1514	ILE	CA-C-N	-10.41	106.69	122.09
45	e	1514	ILE	C-N-CA	-10.41	106.69	122.09
45	e	1460	SER	N-CA-C	10.06	122.33	111.36
53	v	372	LEU	O-C-N	8.84	131.49	122.12
45	e	1181	ASP	N-CA-C	8.82	120.89	111.28
45	e	1141	GLN	N-CA-C	8.72	120.79	111.28
2	K	43	LEU	N-CA-C	8.70	129.32	110.80
45	e	793	ASN	N-CA-C	-8.70	102.67	113.28
2	K	37	PRO	C-N-CD	-8.67	89.44	125.00
9	8	51	GLY	CA-C-N	7.90	136.62	121.54
9	8	51	GLY	C-N-CA	7.90	136.62	121.54
44	a	116	PHE	N-CA-C	-7.79	103.84	112.72
45	e	437	LYS	N-CA-C	-7.78	94.24	110.80
45	e	901	SER	N-CA-C	7.62	119.59	111.28
45	e	870	GLY	N-CA-C	-7.58	105.36	115.21
45	e	666	GLY	N-CA-C	-7.46	104.91	115.43
53	v	402	ALA	CA-C-N	7.41	131.23	120.71
53	v	402	ALA	C-N-CA	7.41	131.23	120.71
48	z	87	GLU	CA-C-N	-7.36	112.80	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	z	87	GLU	C-N-CA	-7.36	112.80	120.38
45	e	1447	LYS	N-CA-C	-7.31	100.88	110.53
48	z	138	SER	N-CA-C	-7.27	103.28	111.14
45	e	435	CYS	N-CA-C	-7.24	103.32	111.14
45	e	1298	GLY	N-CA-C	-7.22	105.24	115.43
45	e	1449	TYR	CA-C-N	-7.04	111.23	119.05
45	e	1449	TYR	C-N-CA	-7.04	111.23	119.05
44	a	117	PHE	N-CA-CB	-7.02	100.32	110.36
1	E	261	LYS	N-CA-C	-6.98	101.99	112.04
45	e	434	SER	N-CA-C	6.96	118.65	111.14
45	e	43	TYR	N-CA-C	6.83	118.72	111.28
48	z	94	LYS	N-CA-C	-6.77	103.98	111.36
34	l	4	PRO	CA-C-N	6.76	134.45	121.54
34	l	4	PRO	C-N-CA	6.76	134.45	121.54
45	e	57	ARG	N-CA-C	6.68	118.57	111.28
45	e	1182	LYS	N-CA-C	6.53	118.06	111.07
53	v	402	ALA	O-C-N	-6.47	113.22	122.41
14	N	66	ALA	N-CA-C	-6.42	106.41	114.56
45	e	667	GLN	N-CA-C	-6.35	105.48	112.72
45	e	148	SER	N-CA-C	6.32	117.97	111.14
45	e	132	PHE	N-CA-C	6.29	118.22	111.36
39	q	138	THR	CA-C-N	6.27	133.52	121.54
39	q	138	THR	C-N-CA	6.27	133.52	121.54
45	e	1283	SER	N-CA-C	-6.27	99.95	109.85
45	e	1445	LEU	N-CA-C	-6.21	100.61	109.24
28	d	4	MET	CA-C-N	6.17	133.33	121.54
28	d	4	MET	C-N-CA	6.17	133.33	121.54
45	e	736	VAL	N-CA-C	6.17	116.95	110.72
53	v	440	ARG	CA-C-N	-6.13	109.64	121.78
53	v	440	ARG	C-N-CA	-6.13	109.64	121.78
2	K	41	GLN	O-C-N	5.95	130.51	122.59
45	e	365	THR	N-CA-C	5.95	118.72	111.82
45	e	185	VAL	N-CA-C	5.89	116.07	110.53
45	e	383	LYS	N-CA-C	-5.87	104.88	111.28
48	z	124	THR	N-CA-C	5.87	117.68	111.28
45	e	202	GLU	N-CA-C	-5.84	102.99	110.53
45	e	1317	GLU	N-CA-C	5.80	117.27	111.07
45	e	787	VAL	N-CA-C	5.71	116.49	110.72
1	E	545	VAL	N-CA-C	-5.68	105.86	111.77
29	f	2541	U	P-O3'-C3'	5.67	128.71	120.20
2	K	36	ILE	N-CA-C	5.66	121.10	108.88
46	g	171	GLU	N-CA-CB	5.63	119.01	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	e	462	ILE	N-CA-C	-5.60	104.91	110.62
41	s	114	ILE	CA-C-N	5.59	132.22	121.54
41	s	114	ILE	C-N-CA	5.59	132.22	121.54
45	e	490	SER	N-CA-C	5.53	116.66	109.64
41	s	7	ASN	N-CA-C	5.52	117.53	109.30
45	e	1505	PHE	CA-CB-CG	5.51	119.31	113.80
42	t	136	GLU	CA-CB-CG	5.48	125.07	114.10
45	e	517	ASN	N-CA-C	5.48	117.06	111.14
20	T	94	LEU	CA-C-N	-5.45	112.73	121.35
20	T	94	LEU	C-N-CA	-5.45	112.73	121.35
41	s	108	GLU	CA-CB-CG	5.43	124.95	114.10
45	e	788	SER	N-CA-C	5.43	117.08	110.41
45	e	691	ASP	N-CA-C	-5.39	106.47	113.16
45	e	19	GLY	N-CA-C	5.39	118.86	111.54
48	z	19	GLY	N-CA-C	5.39	119.43	112.54
45	e	896	PHE	N-CA-C	5.38	117.22	111.36
49	0	94	THR	N-CA-C	5.35	117.11	111.28
48	z	29	ALA	N-CA-C	-5.34	105.57	113.16
45	e	1500	LEU	N-CA-C	-5.34	102.55	111.37
17	Q	83	GLU	CA-C-N	5.33	131.72	121.54
17	Q	83	GLU	C-N-CA	5.33	131.72	121.54
29	f	1307	G	P-O3'-C3'	5.32	128.19	120.20
45	e	133	ILE	CA-C-N	-5.32	113.14	119.05
45	e	133	ILE	C-N-CA	-5.32	113.14	119.05
45	e	1480	ILE	N-CA-C	5.32	116.09	110.72
29	f	282	G	C2'-C3'-O3'	5.32	121.68	113.70
29	f	1815	U	P-O3'-C3'	5.32	128.17	120.20
45	e	1314	ARG	N-CA-C	5.29	117.79	111.71
45	e	30	PHE	N-CA-C	5.25	117.01	111.28
45	e	548	ILE	CB-CA-C	-5.24	108.80	114.35
45	e	142	GLU	N-CA-C	-5.22	101.37	109.72
48	z	18	VAL	N-CA-C	-5.21	102.86	109.58
45	e	1459	VAL	CB-CA-C	-5.21	107.28	111.71
48	z	117	ARG	N-CA-C	-5.21	105.60	111.28
38	p	79	GLN	CA-CB-CG	5.20	124.50	114.10
45	e	59	GLU	N-CA-C	5.18	117.01	111.36
49	0	89	THR	N-CA-C	5.17	117.85	109.06
34	l	317	PRO	CA-C-N	5.17	131.42	121.54
34	l	317	PRO	C-N-CA	5.17	131.42	121.54
48	z	139	VAL	N-CA-C	5.16	115.38	110.53
45	e	450	SER	N-CA-C	5.15	116.58	111.07
45	e	1252	VAL	CA-C-N	-5.14	114.10	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	e	1252	VAL	C-N-CA	-5.14	114.10	120.79
45	e	570	SER	N-CA-C	5.13	117.30	110.53
48	z	103	ASN	N-CA-C	5.12	116.98	109.24
45	e	1453	ASN	N-CA-C	5.12	117.72	110.50
3	G	449	VAL	CA-C-N	5.11	129.53	121.56
3	G	449	VAL	C-N-CA	5.11	129.53	121.56
49	0	104	ARG	N-CA-C	5.10	118.48	111.54
48	z	147	ASN	CA-C-N	-5.09	114.33	119.83
48	z	147	ASN	C-N-CA	-5.09	114.33	119.83
1	E	260	GLY	CA-C-N	-5.07	110.85	121.80
1	E	260	GLY	C-N-CA	-5.07	110.85	121.80
45	e	796	LEU	N-CA-C	-5.06	105.77	111.28
45	e	1459	VAL	N-CA-C	5.05	116.23	111.48
45	e	377	TRP	N-CA-C	5.01	116.82	111.36
29	f	2537	U	P-O3'-C3'	5.00	127.70	120.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	510	ASN	Peptide
15	O	20	GLY	Peptide
21	U	83	LYS	Peptide
45	e	392	GLY	Peptide
46	g	8	GLU	Peptide
33	k	141	GLY	Peptide
34	l	13	GLY	Peptide
34	l	318	LEU	Peptide
38	p	158	ASP	Peptide
38	p	30	THR	Peptide
38	p	76	ALA	Peptide
39	q	21	LYS	Peptide
43	u	12	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4206	0	4232	63	0
1	B	5049	0	5118	110	0
1	C	3759	0	3798	86	0
1	D	3747	0	3784	127	0
1	E	3786	0	3827	126	0
1	F	4093	0	4121	70	0
2	H	601	0	622	8	0
2	J	601	0	622	10	0
2	K	376	0	392	64	0
3	G	3762	0	3638	45	0
4	3	1416	0	1433	12	0
5	4	1441	0	1543	14	0
6	5	1258	0	1342	18	0
7	6	1437	0	1475	21	0
8	7	1272	0	1312	12	0
9	8	796	0	812	8	0
10	I	1003	0	1048	11	0
11	9	518	0	542	7	0
12	L	984	0	1075	7	0
13	M	1080	0	1122	10	0
14	N	1169	0	1211	16	0
15	O	462	0	491	8	0
16	P	737	0	792	2	0
17	Q	876	0	912	10	0
18	R	1013	0	1077	6	0
19	S	850	0	880	7	0
20	T	880	0	942	9	0
21	U	969	0	1078	4	0
22	V	766	0	842	6	0
23	W	645	0	645	11	0
24	Y	436	0	475	6	0
25	Z	410	0	442	4	0
26	b	824	0	888	12	0
27	c	694	0	734	8	0
28	d	207	0	250	3	0
29	f	68802	0	34573	604	0
30	h	2579	0	1304	9	0
31	i	3353	0	1695	41	0
32	j	1874	0	1943	24	0
33	k	3075	0	3142	26	0
34	l	2748	0	2859	23	0
35	m	2351	0	2294	31	0
36	n	1307	0	1377	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	o	1784	0	1862	10	0
38	p	1804	0	1877	55	0
39	q	1508	0	1572	17	0
40	r	1764	0	1804	16	0
41	s	1346	0	1370	9	0
42	t	1543	0	1608	15	0
43	u	1053	0	1149	51	0
44	a	6573	0	6471	60	0
45	e	11556	0	10822	475	0
46	g	1651	0	1613	22	0
47	x	1579	0	800	24	0
47	y	1556	0	788	16	0
48	z	728	0	337	20	0
49	0	961	0	979	48	0
50	1	85	0	21	1	0
51	w	1709	0	1797	15	0
52	X	608	0	677	66	0
53	v	4376	0	4289	116	0
54	2	602	0	629	26	0
55	a0	1555	0	1659	133	0
56	b0	964	0	1025	187	0
57	A	31	0	12	23	0
57	B	31	0	12	2	0
57	C	93	0	32	64	0
57	D	62	0	22	49	0
57	E	31	0	10	14	0
57	F	31	0	12	18	0
58	E	27	0	11	23	0
59	G	2	0	0	0	0
59	T	1	0	0	0	0
59	W	1	0	0	0	0
59	Z	1	0	0	0	0
59	b	1	0	0	0	0
59	c	1	0	0	0	0
60	3	1	0	0	0	0
60	5	1	0	0	0	0
60	I	1	0	0	0	0
60	R	1	0	0	0	0
60	T	1	0	0	0	0
60	f	3	0	0	0	0
60	h	1	0	0	0	0
60	j	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	k	1	0	0	0	0
61	f	10	0	19	1	0
All	All	183852	0	145983	2352	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 (2352) 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)
45:e:917:LEU:HD13	45:e:963:MET:SD	1.21	1.74
45:e:272:TYR:HA	45:e:277:MET:SD	1.28	1.66
45:e:277:MET:SD	45:e:278:PRO:HD3	1.34	1.65
1:E:536:LEU:HD22	58:E:901:ADP:C5'	1.23	1.60
1:E:536:LEU:CD2	58:E:901:ADP:H3'	1.14	1.60
45:e:751:VAL:HA	45:e:754:ILE:CD1	1.30	1.58
45:e:272:TYR:HD1	45:e:277:MET:CE	1.13	1.56
1:D:559:SER:CB	1:E:562:TYR:HE1	1.18	1.56
45:e:371:LEU:HD12	45:e:377:TRP:CZ2	1.39	1.55
1:E:536:LEU:CD2	58:E:901:ADP:C3'	1.85	1.55
45:e:272:TYR:CD1	45:e:277:MET:HE1	1.39	1.54
45:e:906:PHE:CE2	45:e:955:LEU:HD23	1.04	1.51
45:e:1053:LEU:CD1	45:e:1105:LEU:HD22	1.38	1.51
1:D:216:ILE:HG22	57:D:902:ATP:N6	1.19	1.50
45:e:906:PHE:CE2	45:e:955:LEU:CD2	1.98	1.46
45:e:371:LEU:HB2	45:e:377:TRP:NE1	1.19	1.46
45:e:918:LEU:CD1	45:e:966:ARG:HH11	1.24	1.45
45:e:1544:ARG:NH2	53:v:276:ARG:HH12	1.00	1.45
1:E:536:LEU:CD2	58:E:901:ADP:H5'2	1.45	1.44
29:f:1259:A:C8	49:0:53:MET:HB2	1.51	1.44
47:y:76:A:O3'	50:1:57:UNK:C	1.64	1.43
29:f:1258:U:H4'	49:0:42:ARG:NH1	1.26	1.43
45:e:277:MET:SD	45:e:278:PRO:CD	2.07	1.42
45:e:917:LEU:CD1	45:e:963:MET:SD	2.08	1.41
45:e:1032:LEU:CD2	45:e:1075:LEU:HD21	1.51	1.40
6:5:34:GLN:CD	53:v:254:LYS:HE2	1.11	1.40
45:e:1501:GLN:O	45:e:1522:LEU:CD1	1.68	1.39
1:D:559:SER:CB	1:E:562:TYR:CE1	2.03	1.38
45:e:918:LEU:HD11	45:e:966:ARG:NH1	1.33	1.38
45:e:1053:LEU:CD1	45:e:1105:LEU:CD2	1.99	1.38
45:e:883:VAL:CB	45:e:956:LEU:HD11	1.52	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:1258:U:C4'	49:0:42:ARG:HH12	1.36	1.38
45:e:751:VAL:CA	45:e:754:ILE:HD11	1.53	1.37
29:f:1748:G:OP1	52:X:44:LYS:CE	1.72	1.37
45:e:1303:MET:HA	45:e:1303:MET:CE	1.48	1.37
45:e:1456:VAL:CG2	45:e:1480:ILE:HD11	1.51	1.37
45:e:323:TYR:CE1	45:e:324:GLU:CG	2.07	1.36
45:e:883:VAL:O	45:e:956:LEU:HD21	1.21	1.36
45:e:918:LEU:CD1	45:e:966:ARG:NH1	1.80	1.35
1:B:489:VAL:HG13	57:C:1001:ATP:N6	1.39	1.35
1:D:562:TYR:CE1	1:D:609:ARG:NH2	1.92	1.35
45:e:323:TYR:CE1	45:e:324:GLU:HG3	1.61	1.34
29:f:1523:U:O4'	56:b0:113:LEU:HD23	1.23	1.33
1:D:561:TRP:CD1	2:K:4:PHE:HB2	1.65	1.31
45:e:272:TYR:CA	45:e:277:MET:SD	2.18	1.31
45:e:751:VAL:O	45:e:754:ILE:HG13	1.29	1.31
57:C:1003:ATP:O1B	1:D:645:ARG:NH1	1.61	1.30
1:D:216:ILE:CG2	57:D:902:ATP:HN61	1.43	1.30
1:E:418:GLY:O	57:E:902:ATP:N3	1.62	1.30
45:e:809:MET:CE	45:e:844:LEU:HD21	1.59	1.30
57:C:1003:ATP:O1B	1:D:645:ARG:CZ	1.78	1.30
45:e:1463:GLY:HA3	45:e:1515:LEU:CD1	1.59	1.29
45:e:1070:ILE:HG22	45:e:1072:ALA:N	1.47	1.29
45:e:1544:ARG:NH2	53:v:276:ARG:NH1	1.81	1.29
38:p:45:ASN:CG	56:b0:26:VAL:HG23	1.58	1.27
1:D:216:ILE:CG2	57:D:902:ATP:N6	1.97	1.26
45:e:906:PHE:CD2	45:e:955:LEU:HD23	1.69	1.26
1:D:559:SER:OG	1:E:562:TYR:CE1	1.86	1.25
2:H:124:ASP:OD1	2:H:152:ASP:HB2	1.27	1.25
47:x:56:C:O2'	47:x:57:G:H5"	1.30	1.25
29:f:1751:G:N1	52:X:78:LEU:CD1	2.00	1.25
29:f:3244:A:N6	55:a0:105:PHE:HD1	1.35	1.25
38:p:46:LEU:N	56:b0:27:ARG:O	1.67	1.25
45:e:371:LEU:HD12	45:e:377:TRP:CE2	1.70	1.25
1:E:536:LEU:CD2	58:E:901:ADP:C5'	1.98	1.24
43:u:120:VAL:CG1	55:a0:197:LEU:HB3	1.68	1.24
45:e:272:TYR:CD1	45:e:277:MET:CE	2.05	1.24
1:D:531:GLY:HA2	57:D:901:ATP:O1B	1.11	1.24
45:e:883:VAL:CG1	45:e:956:LEU:CG	2.14	1.23
29:f:1523:U:C2	56:b0:123:TYR:CE2	2.25	1.23
45:e:371:LEU:CB	45:e:377:TRP:NE1	2.01	1.23
1:C:558:LEU:HD11	1:D:562:TYR:CZ	1.74	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:SER:HB2	1:E:562:TYR:CE1	1.64	1.22
45:e:750:ALA:O	45:e:754:ILE:HG12	1.37	1.21
45:e:1053:LEU:HD12	45:e:1105:LEU:CD2	1.64	1.21
1:E:536:LEU:HD22	58:E:901:ADP:C4'	1.69	1.21
2:K:36:ILE:CG2	2:K:40:GLN:HB3	1.71	1.21
1:D:216:ILE:HG22	57:D:902:ATP:C6	1.74	1.21
29:f:3178:A:O4'	55:a0:4:GLU:OE1	1.59	1.20
29:f:3244:A:C6	55:a0:105:PHE:CE1	2.29	1.20
45:e:1303:MET:HE2	45:e:1303:MET:CA	1.63	1.20
45:e:1463:GLY:CA	45:e:1515:LEU:HD13	1.69	1.20
45:e:906:PHE:CD2	45:e:955:LEU:CD2	2.21	1.20
29:f:1751:G:C2	52:X:78:LEU:HD13	1.74	1.20
1:C:536:LEU:HD11	57:C:1003:ATP:C8	1.78	1.19
45:e:1060:MET:HE1	45:e:1072:ALA:CB	1.72	1.19
29:f:1523:U:C2	56:b0:123:TYR:CD2	2.29	1.19
29:f:3244:A:N1	55:a0:105:PHE:HE1	1.40	1.19
57:D:902:ATP:O1B	1:E:369:ARG:NH1	1.76	1.19
1:B:531:GLY:O	57:C:1001:ATP:O5'	1.58	1.19
29:f:3244:A:N6	55:a0:105:PHE:CD1	2.10	1.18
29:f:1257:C:H5'	48:z:124:THR:CB	1.74	1.18
43:u:120:VAL:HG12	55:a0:197:LEU:CB	1.72	1.18
45:e:932:LEU:C	45:e:933:LEU:N	2.01	1.18
6:5:34:GLN:CD	53:v:254:LYS:CE	2.02	1.17
29:f:1751:G:C6	52:X:78:LEU:CD1	2.27	1.17
45:e:883:VAL:HG12	45:e:956:LEU:CG	1.74	1.17
45:e:1028:PHE:HE2	45:e:1070:ILE:HD13	1.06	1.17
47:x:56:C:O2'	47:x:57:G:C5'	1.93	1.16
1:D:634:ASN:ND2	57:D:901:ATP:O3G	1.78	1.16
45:e:1060:MET:CE	45:e:1072:ALA:HB1	1.75	1.15
1:B:489:VAL:CG1	57:C:1001:ATP:N6	2.09	1.15
1:F:263:LEU:HD22	57:F:901:ATP:C2'	1.77	1.15
43:u:131:VAL:HG11	55:a0:182:ASN:OD1	1.46	1.15
45:e:1070:ILE:O	45:e:1072:ALA:N	1.78	1.15
29:f:1830:G:H5"	56:b0:92:LYS:HB2	1.22	1.14
45:e:917:LEU:HD22	45:e:963:MET:HE1	1.19	1.14
2:K:37:PRO:CB	2:K:38:PRO:HD2	1.76	1.14
29:f:1751:G:N1	52:X:78:LEU:HD11	1.62	1.14
53:v:381:ARG:NH2	53:v:657:GLU:OE1	1.80	1.14
31:i:151:C:C5	56:b0:24:LEU:HD11	1.82	1.14
29:f:1751:G:H5'	52:X:26:LYS:NZ	1.60	1.13
31:i:135:G:H5"	56:b0:49:LYS:HD2	1.26	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:p:45:ASN:CB	56:b0:26:VAL:HG23	1.78	1.13
29:f:1259:A:C8	49:0:53:MET:CB	2.32	1.13
29:f:1523:U:N1	56:b0:123:TYR:CE2	2.14	1.13
45:e:323:TYR:CE1	45:e:324:GLU:HG2	1.77	1.13
45:e:917:LEU:HD22	45:e:963:MET:CE	1.78	1.13
45:e:1501:GLN:O	45:e:1522:LEU:HD11	0.97	1.13
1:B:532:THR:CG2	57:C:1001:ATP:N3	2.12	1.12
1:C:558:LEU:HD11	1:D:562:TYR:OH	1.48	1.12
45:e:1053:LEU:HD11	45:e:1105:LEU:CD2	1.73	1.12
1:E:536:LEU:HD22	58:E:901:ADP:H5'1	1.29	1.12
45:e:809:MET:HE3	45:e:844:LEU:HD21	1.19	1.12
45:e:1456:VAL:HG23	45:e:1480:ILE:CD1	1.79	1.12
45:e:751:VAL:HA	45:e:754:ILE:CG1	1.80	1.12
29:f:1748:G:OP1	52:X:44:LYS:HE2	0.95	1.11
29:f:1608:C:OP1	56:b0:111:ASN:ND2	1.82	1.11
1:F:263:LEU:HD22	57:F:901:ATP:H2'	1.24	1.11
45:e:1050:LEU:HD11	45:e:1098:LEU:HD23	1.31	1.11
29:f:1824:U:OP1	52:X:3:ARG:NH2	1.83	1.11
1:A:216:ILE:HA	57:A:901:ATP:HN61	1.01	1.10
1:D:531:GLY:CA	57:D:901:ATP:O1B	1.98	1.10
29:f:1221:A:C2	49:0:12:PHE:HE2	1.69	1.10
1:C:262:THR:CG2	57:C:1002:ATP:O3G	2.00	1.10
2:K:36:ILE:HG21	2:K:40:GLN:HB3	1.15	1.10
38:p:50:VAL:HG21	56:b0:27:ARG:HD3	1.34	1.10
1:B:532:THR:CG2	57:C:1001:ATP:C2	2.35	1.09
2:K:39:ASP:HB2	3:G:472:ASN:HB2	1.19	1.09
31:i:151:C:C4	56:b0:24:LEU:HD11	1.86	1.09
45:e:921:ILE:HD11	45:e:967:SER:HB3	1.22	1.09
45:e:918:LEU:HD13	45:e:966:ARG:NH1	1.64	1.09
45:e:1477:GLN:NE2	45:e:1481:THR:CG2	2.15	1.09
45:e:882:ASN:O	45:e:885:GLN:O	1.69	1.09
45:e:1477:GLN:NE2	45:e:1481:THR:OG1	1.84	1.09
1:D:562:TYR:CD1	1:D:609:ARG:NH2	2.15	1.08
1:E:536:LEU:CD2	58:E:901:ADP:C4'	2.28	1.08
1:C:262:THR:HG23	57:C:1002:ATP:O3G	1.51	1.08
45:e:371:LEU:CD1	45:e:377:TRP:CZ2	2.34	1.08
45:e:809:MET:CE	45:e:844:LEU:CD2	2.32	1.08
45:e:1032:LEU:HD21	45:e:1075:LEU:HD21	1.30	1.08
45:e:1032:LEU:HD23	45:e:1075:LEU:HD21	1.25	1.08
45:e:1477:GLN:HE22	45:e:1481:THR:CB	1.65	1.08
1:A:216:ILE:CA	57:A:901:ATP:HN61	1.65	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:THR:HG21	57:C:1001:ATP:C2	1.89	1.07
29:f:1523:U:O2	56:b0:123:TYR:CD2	2.06	1.07
29:f:3243:A:O2'	55:a0:110:PRO:HD2	1.53	1.07
29:f:3244:A:O2'	55:a0:111:PRO:HD3	1.55	1.07
1:E:536:LEU:HD21	58:E:901:ADP:C3'	1.66	1.07
6:5:34:GLN:OE1	53:v:254:LYS:HE2	1.52	1.07
45:e:1463:GLY:HA3	45:e:1515:LEU:HD13	1.27	1.07
1:A:217:GLY:H	57:A:901:ATP:N6	1.52	1.06
45:e:1070:ILE:CG2	45:e:1072:ALA:N	2.18	1.06
45:e:1544:ARG:HH21	53:v:276:ARG:NH1	1.41	1.06
6:5:34:GLN:OE1	53:v:254:LYS:CE	1.99	1.06
45:e:1028:PHE:CE2	45:e:1070:ILE:HD13	1.90	1.06
1:D:606:ALA:HB1	1:E:562:TYR:OH	1.56	1.05
53:v:381:ARG:NH2	54:2:6:LYS:HD3	1.69	1.05
43:u:123:LEU:HD12	55:a0:197:LEU:HD12	1.06	1.05
53:v:374:GLN:HE22	54:2:10:GLY:HA3	1.21	1.05
1:E:536:LEU:CB	58:E:901:ADP:H5'2	1.86	1.05
29:f:1751:G:N1	52:X:78:LEU:HD13	1.68	1.05
45:e:713:LEU:O	45:e:717:LYS:HG3	1.55	1.05
1:D:562:TYR:HE1	1:D:609:ARG:CZ	1.70	1.04
1:E:536:LEU:HB2	58:E:901:ADP:H5'2	1.37	1.04
45:e:906:PHE:HE2	45:e:955:LEU:CD2	1.52	1.04
43:u:124:ARG:HA	55:a0:194:LEU:HD11	1.40	1.04
2:K:39:ASP:CB	3:G:472:ASN:HB2	1.87	1.04
29:f:3244:A:C6	55:a0:105:PHE:HE1	1.72	1.04
53:v:374:GLN:NE2	54:2:9:THR:O	1.89	1.03
29:f:1522:U:C4	56:b0:116:PRO:HG3	1.93	1.03
29:f:1825:G:H5'	52:X:17:ARG:NH2	1.71	1.03
1:C:558:LEU:CD1	1:D:562:TYR:OH	2.06	1.03
1:D:561:TRP:HD1	2:K:4:PHE:CB	1.70	1.03
1:E:560:MET:HE3	1:E:561:TRP:HE1	1.22	1.02
7:6:168:PRO:HG3	55:a0:127:LEU:HD11	1.38	1.02
45:e:883:VAL:O	45:e:956:LEU:CD2	2.06	1.02
45:e:1050:LEU:CD1	45:e:1098:LEU:HD23	1.89	1.02
45:e:1456:VAL:CG2	45:e:1480:ILE:CD1	2.34	1.02
45:e:731:LEU:HD12	45:e:732:GLN:N	1.73	1.02
29:f:1523:U:C4'	56:b0:113:LEU:HD23	1.88	1.01
45:e:323:TYR:CZ	45:e:324:GLU:CG	2.44	1.01
45:e:1060:MET:HE1	45:e:1072:ALA:HB1	1.02	1.01
1:C:694:GLY:HA3	57:C:1003:ATP:H2	1.23	1.00
45:e:1071:THR:O	45:e:1074:GLU:CD	2.04	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:37:PRO:CB	2:K:38:PRO:CD	2.40	1.00
45:e:371:LEU:CB	45:e:377:TRP:HE1	1.64	0.99
1:E:536:LEU:HB2	58:E:901:ADP:C5'	1.91	0.99
29:f:1522:U:OP2	56:b0:121:LYS:NZ	1.94	0.99
29:f:1523:U:H4'	56:b0:113:LEU:HB3	1.42	0.99
45:e:1053:LEU:HD11	45:e:1105:LEU:HD23	1.44	0.99
45:e:809:MET:HE2	45:e:844:LEU:HD21	1.42	0.99
29:f:1259:A:N7	49:0:53:MET:CB	2.25	0.99
45:e:1050:LEU:CD2	45:e:1098:LEU:HA	1.93	0.98
1:D:562:TYR:HE1	1:D:609:ARG:NH2	1.41	0.98
1:E:536:LEU:HD23	58:E:901:ADP:C3'	1.89	0.98
45:e:1050:LEU:HD21	45:e:1098:LEU:HA	1.45	0.98
1:E:560:MET:HE3	1:E:561:TRP:NE1	1.78	0.98
31:i:133:G:H4'	56:b0:55:ASN:CG	1.89	0.98
2:K:36:ILE:CG2	2:K:40:GLN:CB	2.41	0.98
31:i:133:G:H5"	56:b0:55:ASN:OD1	1.63	0.98
1:D:262:THR:CG2	57:D:902:ATP:O3G	2.11	0.98
45:e:1053:LEU:CD1	45:e:1105:LEU:HD23	1.91	0.98
45:e:323:TYR:CD1	45:e:324:GLU:HG2	1.98	0.98
29:f:3244:A:N1	55:a0:105:PHE:CE1	2.31	0.97
29:f:3244:A:O2'	55:a0:111:PRO:CD	2.12	0.97
29:f:2473:C:C2	29:f:2475:G:H1'	1.98	0.97
45:e:371:LEU:CD1	45:e:377:TRP:CE2	2.46	0.97
53:v:374:GLN:HE21	54:2:9:THR:C	1.72	0.97
29:f:1523:U:H5'	56:b0:113:LEU:HB3	1.47	0.96
29:f:1751:G:C6	52:X:78:LEU:HD13	1.97	0.96
1:B:532:THR:HG23	57:C:1001:ATP:N3	1.79	0.96
1:D:606:ALA:HB3	1:E:562:TYR:CZ	2.00	0.96
1:A:217:GLY:H	57:A:901:ATP:HN62	1.09	0.96
53:v:639:SER:HB3	54:2:64:GLU:O	1.63	0.96
1:D:606:ALA:CB	1:E:562:TYR:CZ	2.48	0.96
29:f:1830:G:O3'	56:b0:91:ASN:HB2	1.65	0.96
29:f:3178:A:C4'	55:a0:4:GLU:OE1	2.14	0.95
2:K:37:PRO:HB3	2:K:38:PRO:HD2	1.48	0.95
1:E:261:LYS:O	1:E:263:LEU:N	1.99	0.95
29:f:1751:G:C2	52:X:78:LEU:CD1	2.42	0.95
1:E:536:LEU:CG	58:E:901:ADP:H5'2	1.96	0.95
43:u:123:LEU:HD12	55:a0:197:LEU:CD1	1.94	0.95
45:e:731:LEU:HD12	45:e:731:LEU:C	1.90	0.95
29:f:1259:A:H8	49:0:53:MET:HB2	1.29	0.95
45:e:929:LEU:HD23	45:e:967:SER:O	1.64	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:1463:GLY:HA3	45:e:1515:LEU:HD11	1.47	0.94
53:v:374:GLN:NE2	54:2:9:THR:C	2.25	0.94
45:e:1456:VAL:HG23	45:e:1480:ILE:HD11	0.96	0.94
45:e:751:VAL:C	45:e:754:ILE:HG13	1.93	0.94
29:f:3180:A:H4'	55:a0:116:LYS:HD3	1.49	0.94
29:f:1609:C:OP1	56:b0:125:ARG:HD2	1.68	0.94
45:e:323:TYR:CZ	45:e:324:GLU:HG2	2.02	0.94
45:e:1544:ARG:HH22	53:v:276:ARG:HH12	1.00	0.94
45:e:883:VAL:CG1	45:e:956:LEU:HD12	1.45	0.94
45:e:1050:LEU:CG	45:e:1098:LEU:HD23	1.97	0.94
43:u:124:ARG:HG3	55:a0:194:LEU:HD22	1.50	0.94
29:f:3244:A:C6	55:a0:105:PHE:CD1	2.54	0.94
1:D:559:SER:HB2	1:E:562:TYR:HE1	0.77	0.93
31:i:133:G:H4'	56:b0:55:ASN:ND2	1.82	0.93
45:e:1463:GLY:H	45:e:1520:ARG:NH1	1.66	0.93
1:D:606:ALA:CB	1:E:562:TYR:OH	2.16	0.93
45:e:1032:LEU:CD2	45:e:1075:LEU:CD2	2.45	0.93
45:e:751:VAL:CA	45:e:754:ILE:CG1	2.46	0.93
29:f:1751:G:H5'	52:X:26:LYS:HZ2	1.30	0.93
45:e:1463:GLY:H	45:e:1520:ARG:HH11	0.96	0.93
45:e:1463:GLY:HA2	45:e:1515:LEU:HD13	1.47	0.93
45:e:1477:GLN:NE2	45:e:1481:THR:HG21	1.80	0.92
29:f:1258:U:P	49:0:46:ARG:HH22	1.89	0.92
29:f:3243:A:N1	55:a0:108:ILE:N	2.17	0.92
29:f:1257:C:O3'	49:0:46:ARG:NH2	2.02	0.92
43:u:123:LEU:HD13	55:a0:193:GLN:HB3	1.48	0.92
15:O:16:ALA:O	15:O:20:GLY:HA3	1.69	0.92
2:K:44:ILE:HD13	3:G:393:GLU:OE1	1.70	0.92
31:i:134:G:H4'	56:b0:53:HIS:O	1.70	0.92
1:C:694:GLY:HA3	57:C:1003:ATP:C2	2.05	0.91
45:e:883:VAL:CG1	45:e:956:LEU:CD1	0.92	0.91
1:E:261:LYS:H	1:E:261:LYS:HD3	1.34	0.91
1:B:489:VAL:HA	57:C:1001:ATP:HN61	1.33	0.91
45:e:917:LEU:CG	45:e:963:MET:SD	2.58	0.91
45:e:1477:GLN:HE22	45:e:1481:THR:CG2	1.77	0.91
38:p:45:ASN:HB2	56:b0:26:VAL:HG23	1.50	0.91
45:e:1463:GLY:CA	45:e:1515:LEU:CD1	2.35	0.91
1:D:262:THR:HG22	57:D:902:ATP:O3G	1.70	0.91
29:f:1523:U:C4'	56:b0:113:LEU:HB3	2.00	0.91
29:f:1523:U:C5'	56:b0:113:LEU:HB3	1.99	0.91
29:f:1523:U:C5'	56:b0:113:LEU:CD2	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:39:ASP:HB3	3:G:472:ASN:CG	1.96	0.90
1:A:216:ILE:HA	57:A:901:ATP:N6	1.86	0.90
1:D:666:ILE:HD13	57:D:901:ATP:C6	2.05	0.90
1:B:532:THR:HG23	57:C:1001:ATP:C2	2.05	0.90
45:e:918:LEU:HD11	45:e:966:ARG:HH11	0.75	0.90
29:f:3007:U:OP1	55:a0:74:ARG:N	2.04	0.90
43:u:123:LEU:CD1	55:a0:197:LEU:HD12	2.00	0.90
1:A:216:ILE:CA	57:A:901:ATP:N6	2.35	0.89
47:y:8:U:O2	47:y:8:U:H2'	1.71	0.89
1:D:562:TYR:HE1	1:D:609:ARG:NH1	1.69	0.89
1:D:262:THR:HG23	57:D:902:ATP:O3B	1.72	0.89
1:E:562:TYR:CZ	1:E:609:ARG:NH1	2.40	0.89
29:f:1258:U:O5'	49:0:42:ARG:NH1	2.04	0.89
1:A:260:GLY:CA	57:A:901:ATP:H5'2	2.01	0.89
1:D:561:TRP:HD1	2:K:4:PHE:HB2	0.78	0.89
29:f:3243:A:O2'	55:a0:110:PRO:CD	2.21	0.89
1:E:262:THR:HG22	57:E:902:ATP:O2A	1.73	0.88
45:e:277:MET:SD	45:e:278:PRO:HD2	2.12	0.88
29:f:1258:U:C5'	49:0:42:ARG:HH12	1.86	0.88
1:A:217:GLY:N	57:A:901:ATP:N6	2.21	0.88
1:B:532:THR:O	57:C:1001:ATP:O2B	1.91	0.88
29:f:1523:U:H5'	56:b0:113:LEU:CB	2.01	0.88
45:e:883:VAL:C	45:e:956:LEU:HD21	1.99	0.88
57:D:902:ATP:PB	1:E:369:ARG:HH12	1.97	0.88
45:e:1032:LEU:HD21	45:e:1075:LEU:CD2	2.03	0.88
53:v:381:ARG:HH21	54:2:6:LYS:HD3	1.32	0.88
29:f:1522:U:C5	56:b0:116:PRO:HG3	2.09	0.88
29:f:2383:C:N4	55:a0:91:LYS:HG2	1.89	0.87
45:e:929:LEU:HD11	45:e:967:SER:OG	1.71	0.87
43:u:135:LEU:HD22	55:a0:181:ALA:CB	2.04	0.87
45:e:1066:ARG:NH1	45:e:1111:GLN:HE22	1.72	0.87
2:K:37:PRO:HB2	2:K:38:PRO:HD2	1.55	0.87
29:f:1222:G:OP2	49:0:57:THR:OG1	1.90	0.87
45:e:883:VAL:HG13	45:e:956:LEU:CG	1.94	0.87
29:f:2382:G:N7	55:a0:91:LYS:NZ	2.23	0.87
1:A:260:GLY:HA2	57:A:901:ATP:H5'2	1.55	0.87
2:K:39:ASP:OD2	3:G:472:ASN:ND2	2.07	0.87
38:p:45:ASN:OD1	56:b0:27:ARG:N	2.06	0.87
43:u:124:ARG:HG3	55:a0:194:LEU:CD2	2.04	0.87
43:u:120:VAL:HG12	55:a0:197:LEU:HB3	0.90	0.86
29:f:1221:A:C2	49:0:12:PHE:CE2	2.62	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:932:LEU:HB3	45:e:964:PHE:HZ	1.38	0.86
29:f:1751:G:H5'	52:X:26:LYS:HZ1	1.35	0.86
29:f:1751:G:C4	52:X:78:LEU:HD13	2.09	0.86
1:C:536:LEU:CD1	57:C:1003:ATP:C8	2.57	0.86
45:e:751:VAL:O	45:e:754:ILE:CG1	2.19	0.86
1:C:698:LEU:HD13	57:C:1003:ATP:O2'	1.75	0.86
2:K:44:ILE:O	2:K:45:PHE:HB2	1.75	0.86
29:f:1824:U:O2'	52:X:17:ARG:NH2	2.08	0.86
1:E:536:LEU:HD23	58:E:901:ADP:H5'2	1.52	0.85
45:e:277:MET:CE	45:e:278:PRO:HD3	2.06	0.85
1:D:216:ILE:HG22	57:D:902:ATP:C5	2.09	0.85
29:f:1521:G:OP1	56:b0:69:SER:OG	1.95	0.85
45:e:324:GLU:O	45:e:327:THR:OG1	1.93	0.85
29:f:1831:U:OP1	56:b0:91:ASN:HA	1.75	0.85
45:e:809:MET:HE3	45:e:844:LEU:CD2	1.99	0.85
45:e:883:VAL:HG11	45:e:956:LEU:HD12	0.95	0.85
29:f:1258:U:C4'	49:0:42:ARG:NH1	2.13	0.85
29:f:1523:U:C5'	56:b0:113:LEU:HD22	2.07	0.85
29:f:1831:U:H5'	56:b0:91:ASN:HB3	1.57	0.85
1:E:562:TYR:OH	1:E:609:ARG:NH2	2.10	0.84
1:D:216:ILE:CB	57:D:902:ATP:HN61	1.90	0.84
45:e:323:TYR:CD1	45:e:324:GLU:CG	2.59	0.84
1:B:532:THR:HA	57:C:1001:ATP:H5'2	1.57	0.84
1:D:561:TRP:HE1	2:K:5:VAL:H	1.24	0.84
29:f:1259:A:N7	49:0:53:MET:HG3	1.92	0.84
45:e:883:VAL:HG13	45:e:956:LEU:CD1	0.68	0.84
45:e:1502:PHE:HD1	45:e:1522:LEU:HD21	1.42	0.84
45:e:1505:PHE:HB2	45:e:1514:ILE:HG12	1.60	0.84
1:B:532:THR:CG2	57:C:1001:ATP:C4	2.60	0.84
1:E:261:LYS:O	1:E:262:THR:C	2.20	0.84
29:f:1824:U:OP1	52:X:3:ARG:NH1	2.11	0.84
29:f:3007:U:H5'	55:a0:73:PHE:CD2	2.12	0.83
38:p:45:ASN:CG	56:b0:26:VAL:CG2	2.49	0.83
45:e:1053:LEU:HD21	45:e:1102:CYS:HA	1.60	0.83
45:e:809:MET:HE2	45:e:844:LEU:CD2	2.00	0.83
53:v:643:ALA:CB	54:2:64:GLU:HG2	2.08	0.83
45:e:931:GLY:O	45:e:933:LEU:N	2.11	0.83
45:e:1049:ARG:HD2	45:e:1086:MET:HE1	1.61	0.83
29:f:1751:G:C5	52:X:78:LEU:HD13	2.13	0.83
29:f:3243:A:HO2'	55:a0:110:PRO:HD2	1.40	0.83
1:B:489:VAL:CG1	57:C:1001:ATP:HN62	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:1825:G:H5'	52:X:17:ARG:HH21	1.40	0.83
45:e:371:LEU:HB2	45:e:377:TRP:CD1	2.12	0.82
45:e:804:ILE:HD12	45:e:809:MET:SD	2.17	0.82
45:e:906:PHE:CD2	45:e:955:LEU:HD22	2.13	0.82
1:A:216:ILE:HB	57:A:901:ATP:N6	1.94	0.82
29:f:1229:G:H4'	49:0:32:ASN:OD1	1.79	0.82
29:f:1824:U:OP1	52:X:3:ARG:CZ	2.27	0.82
1:B:418:GLY:HA3	57:B:901:ATP:C2	2.15	0.82
2:K:37:PRO:HG2	2:K:40:GLN:OE1	1.79	0.82
45:e:1463:GLY:HA2	45:e:1520:ARG:HD3	1.59	0.82
1:D:418:GLY:HA3	57:D:902:ATP:C2	2.14	0.82
45:e:1028:PHE:HE2	45:e:1070:ILE:CD1	1.89	0.82
45:e:914:TYR:HE1	45:e:962:LEU:HD13	1.44	0.82
1:E:263:LEU:O	1:E:266:ARG:N	2.12	0.81
29:f:1830:G:H5"	56:b0:92:LYS:CB	2.08	0.81
45:e:917:LEU:HB3	45:e:963:MET:SD	2.19	0.81
1:D:561:TRP:NE1	2:K:5:VAL:H	1.79	0.81
29:f:1222:G:N7	49:0:57:THR:HB	1.96	0.81
43:u:131:VAL:CG1	55:a0:182:ASN:OD1	2.27	0.81
1:B:558:LEU:CD1	1:C:562:TYR:OH	2.27	0.81
2:K:39:ASP:CB	3:G:472:ASN:CB	2.59	0.81
45:e:931:GLY:C	45:e:933:LEU:N	2.38	0.81
45:e:1499:HIS:O	45:e:1503:SER:N	2.13	0.81
1:A:262:THR:CG2	57:A:901:ATP:O3G	2.29	0.81
45:e:1050:LEU:HD21	45:e:1098:LEU:HD23	1.61	0.81
1:E:536:LEU:HD22	58:E:901:ADP:C3'	1.79	0.81
45:e:751:VAL:C	45:e:754:ILE:CG1	2.53	0.81
45:e:1049:ARG:NH1	45:e:1086:MET:SD	2.52	0.81
45:e:1070:ILE:C	45:e:1072:ALA:N	2.38	0.81
29:f:1523:U:C1'	56:b0:123:TYR:CE2	2.63	0.81
45:e:222:LEU:HD12	45:e:226:ASN:ND2	1.94	0.81
45:e:272:TYR:CD1	45:e:277:MET:HE3	2.16	0.81
45:e:1444:LYS:HD2	45:e:1455:GLN:HE21	1.45	0.81
53:v:328:LYS:HE2	53:v:330:GLU:HG2	1.62	0.81
29:f:1258:U:H4'	49:0:42:ARG:HH12	0.66	0.80
45:e:910:SER:HB2	45:e:955:LEU:HD21	1.63	0.80
1:E:260:GLY:HA2	57:E:902:ATP:O2A	1.81	0.80
29:f:1750:A:OP2	52:X:42:LYS:NZ	2.11	0.80
29:f:2383:C:C2	55:a0:91:LYS:HE2	2.15	0.80
45:e:371:LEU:CB	45:e:377:TRP:CD1	2.65	0.80
45:e:921:ILE:HD11	45:e:967:SER:CB	2.09	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:1050:LEU:HD21	45:e:1098:LEU:CD2	2.11	0.80
53:v:381:ARG:NH1	54:2:7:THR:O	2.14	0.80
1:D:606:ALA:HB3	1:E:562:TYR:CE2	2.16	0.80
1:A:260:GLY:HA2	57:A:901:ATP:C5'	2.12	0.80
1:D:216:ILE:CB	57:D:902:ATP:N6	2.45	0.80
1:D:559:SER:OG	1:E:562:TYR:CD1	2.32	0.80
29:f:1558:A:N3	56:b0:34:LEU:HD12	1.97	0.80
47:x:58:A:H8	47:x:58:A:OP2	1.63	0.80
2:K:36:ILE:HG22	2:K:40:GLN:CB	2.11	0.79
29:f:1523:U:H5'	56:b0:113:LEU:CD2	2.12	0.79
1:B:489:VAL:HG13	57:C:1001:ATP:C6	2.16	0.79
45:e:1057:THR:OG1	45:e:1105:LEU:HD13	1.82	0.79
45:e:932:LEU:CB	45:e:964:PHE:HZ	1.95	0.79
45:e:1032:LEU:HD23	45:e:1075:LEU:CD2	2.11	0.79
1:B:558:LEU:HD22	1:C:562:TYR:CZ	2.17	0.79
2:K:40:GLN:HA	3:G:470:PHE:O	1.83	0.79
45:e:751:VAL:CA	45:e:754:ILE:CD1	2.27	0.79
45:e:914:TYR:CE1	45:e:962:LEU:HD13	2.17	0.79
45:e:1050:LEU:CD2	45:e:1098:LEU:HD23	2.11	0.79
31:i:134:G:OP1	56:b0:56:ARG:HD3	1.83	0.79
1:D:666:ILE:CD1	57:D:901:ATP:C6	2.66	0.79
38:p:53:PRO:HD3	56:b0:32:PHE:CD2	2.17	0.79
45:e:918:LEU:CD1	45:e:966:ARG:HH12	1.93	0.79
45:e:1502:PHE:CD1	45:e:1522:LEU:HD21	2.18	0.79
29:f:1523:U:O4'	56:b0:113:LEU:CD2	2.19	0.78
45:e:917:LEU:HD22	45:e:963:MET:SD	2.23	0.78
29:f:1523:U:H5'	56:b0:113:LEU:HD22	1.65	0.78
29:f:2523:A:OP1	56:b0:31:THR:HG22	1.83	0.78
38:p:45:ASN:HB2	56:b0:26:VAL:CG2	2.13	0.78
1:F:263:LEU:CD2	57:F:901:ATP:O2'	2.32	0.78
1:D:560:MET:HG3	1:D:561:TRP:CE3	2.19	0.78
29:f:1259:A:N7	49:0:53:MET:CG	2.47	0.78
29:f:1825:G:OP2	52:X:49:SER:OG	2.01	0.78
45:e:222:LEU:CD1	45:e:226:ASN:ND2	2.47	0.78
1:F:263:LEU:CD2	57:F:901:ATP:C2'	2.60	0.77
29:f:1833:G:OP2	56:b0:114:VAL:CG2	2.31	0.77
2:J:224:ASP:OD1	2:J:252:ASP:O	2.02	0.77
38:p:45:ASN:CB	56:b0:26:VAL:CG2	2.62	0.77
43:u:124:ARG:N	55:a0:194:LEU:HD21	1.99	0.77
1:D:606:ALA:HB1	1:E:562:TYR:HH	1.50	0.77
29:f:2988:C:OP1	55:a0:68:ARG:NH1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:i:133:G:C5'	56:b0:55:ASN:OD1	2.33	0.77
45:e:141:CYS:SG	45:e:221:LYS:HD2	2.24	0.77
29:f:3007:U:OP1	55:a0:73:PHE:HA	1.85	0.77
45:e:1050:LEU:HD11	45:e:1098:LEU:CD2	2.13	0.77
45:e:1050:LEU:HD21	45:e:1098:LEU:CA	2.14	0.77
29:f:1523:U:O2	56:b0:123:TYR:CG	2.37	0.77
31:i:134:G:H5"	56:b0:53:HIS:O	1.83	0.77
45:e:1057:THR:HG23	45:e:1108:THR:OG1	1.83	0.77
47:x:26:G:O6	47:x:43:G:O6	2.01	0.77
2:K:36:ILE:HG22	2:K:40:GLN:HB2	1.67	0.76
45:e:883:VAL:HG12	45:e:956:LEU:HD11	0.82	0.76
45:e:1463:GLY:N	45:e:1520:ARG:HH11	1.78	0.76
45:e:1477:GLN:CD	45:e:1481:THR:OG1	2.28	0.76
29:f:2383:C:C4	55:a0:91:LYS:HG2	2.20	0.76
29:f:1523:U:C6	56:b0:123:TYR:CE2	2.74	0.76
29:f:3006:A:HO2'	55:a0:73:PHE:HE2	1.33	0.76
33:k:262:TRP:N	55:a0:64:PHE:O	2.18	0.76
29:f:1612:A:P	52:X:46:ARG:NH1	2.59	0.76
29:f:3006:A:O2'	55:a0:73:PHE:HE2	1.67	0.76
45:e:1070:ILE:CB	45:e:1072:ALA:N	2.49	0.76
45:e:906:PHE:HD2	45:e:955:LEU:CD2	1.96	0.76
29:f:2444:C:H2'	29:f:2445:A:H8	1.51	0.75
45:e:883:VAL:HG11	45:e:956:LEU:CD1	1.24	0.75
45:e:1456:VAL:HG21	45:e:1480:ILE:HD11	1.64	0.75
29:f:1830:G:O2'	56:b0:91:ASN:CB	2.35	0.75
1:D:216:ILE:CG2	57:D:902:ATP:C6	2.58	0.75
2:K:36:ILE:CG2	2:K:37:PRO:HD2	2.16	0.75
29:f:1258:U:C5'	49:0:42:ARG:NH1	2.46	0.75
1:C:536:LEU:CD1	57:C:1003:ATP:N7	2.50	0.75
29:f:1524:A:OP1	56:b0:112:THR:N	2.20	0.75
43:u:127:LYS:CD	55:a0:194:LEU:HD12	2.17	0.75
1:D:216:ILE:HG22	57:D:902:ATP:HN61	0.76	0.74
31:i:134:G:C5'	56:b0:53:HIS:O	2.35	0.74
45:e:272:TYR:CB	45:e:277:MET:SD	2.76	0.74
1:F:258:GLY:O	57:F:901:ATP:H2	1.70	0.74
31:i:135:G:OP1	56:b0:49:LYS:NZ	2.14	0.74
53:v:288:SER:HB3	53:v:332:LEU:HD12	1.70	0.74
45:e:1547:GLY:O	53:v:440:ARG:HG2	1.88	0.74
1:B:128:VAL:HG11	1:B:135:GLN:NE2	2.03	0.74
38:p:46:LEU:HD12	56:b0:28:THR:O	1.88	0.74
45:e:1501:GLN:O	45:e:1522:LEU:HD13	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:ASN:HD21	57:D:901:ATP:PG	2.10	0.74
2:K:40:GLN:O	2:K:41:GLN:O	2.05	0.74
43:u:135:LEU:HD22	55:a0:181:ALA:HB1	1.67	0.74
45:e:323:TYR:HE1	45:e:324:GLU:HG3	1.44	0.74
45:e:1435:ASP:CG	45:e:1514:ILE:H	1.95	0.74
1:F:258:GLY:N	57:F:901:ATP:O1B	2.20	0.74
29:f:3180:A:H4'	55:a0:116:LYS:CD	2.18	0.73
45:e:272:TYR:HD1	45:e:277:MET:HE1	0.57	0.73
47:x:56:C:HO2'	47:x:57:G:C5'	1.92	0.73
43:u:123:LEU:CD1	55:a0:193:GLN:HB3	2.17	0.73
1:C:561:TRP:CD2	2:K:8:LEU:HD11	2.24	0.73
29:f:1523:U:C2	56:b0:123:TYR:CZ	2.76	0.73
43:u:135:LEU:CD2	55:a0:181:ALA:HB3	2.17	0.73
45:e:266:ARG:O	45:e:270:VAL:HG23	1.88	0.73
43:u:135:LEU:HD21	55:a0:181:ALA:HB3	1.71	0.73
31:i:134:G:C4'	56:b0:53:HIS:O	2.37	0.73
43:u:135:LEU:CD2	55:a0:181:ALA:CB	2.66	0.73
1:A:216:ILE:CB	57:A:901:ATP:N6	2.51	0.73
1:B:558:LEU:HD13	1:C:562:TYR:OH	1.89	0.73
45:e:149:LYS:HB3	45:e:150:PRO:HD3	1.69	0.73
29:f:1610:G:P	56:b0:125:ARG:NH2	2.62	0.73
45:e:1499:HIS:HA	45:e:1503:SER:H	1.53	0.73
53:v:211:LYS:HE2	53:v:222:LEU:HD11	1.71	0.73
29:f:1610:G:OP2	56:b0:125:ARG:NH1	2.22	0.72
29:f:1751:G:C5'	52:X:26:LYS:NZ	2.47	0.72
45:e:731:LEU:C	45:e:731:LEU:CD1	2.62	0.72
1:D:262:THR:CG2	57:D:902:ATP:PG	2.77	0.72
45:e:691:ASP:O	45:e:695:CYS:N	2.21	0.72
1:D:562:TYR:HE1	1:D:609:ARG:HH12	1.36	0.72
29:f:1612:A:H5"	52:X:51:LEU:HD22	1.70	0.72
45:e:272:TYR:CE1	45:e:277:MET:HE1	2.18	0.72
15:O:16:ALA:O	15:O:20:GLY:CA	2.36	0.72
31:i:133:G:O3'	56:b0:55:ASN:HA	1.89	0.72
31:i:134:G:O2'	56:b0:52:PRO:HB3	1.90	0.72
45:e:906:PHE:HD2	45:e:955:LEU:HD22	1.52	0.72
45:e:932:LEU:HB3	45:e:964:PHE:CZ	2.23	0.72
48:z:105:GLN:HA	48:z:143:VAL:HA	1.71	0.72
53:v:374:GLN:HE22	54:2:10:GLY:CA	2.02	0.72
1:B:489:VAL:CA	57:C:1001:ATP:HN61	2.03	0.72
29:f:1751:G:N3	52:X:78:LEU:HD13	2.04	0.72
45:e:883:VAL:HG12	45:e:956:LEU:CD1	1.34	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:917:LEU:CB	45:e:963:MET:SD	2.77	0.72
43:u:124:ARG:HD2	55:a0:199:TYR:CG	2.24	0.72
6:5:34:GLN:OE1	53:v:254:LYS:NZ	2.22	0.72
45:e:1145:ASN:HB2	45:e:1147:VAL:HG22	1.72	0.72
47:x:58:A:OP2	47:x:58:A:C8	2.43	0.72
1:D:561:TRP:CD1	2:K:4:PHE:CB	2.55	0.71
45:e:1477:GLN:HE21	45:e:1481:THR:HG21	1.53	0.71
45:e:323:TYR:CZ	45:e:324:GLU:HG3	2.16	0.71
1:C:698:LEU:HD22	57:C:1003:ATP:O2'	1.89	0.71
1:B:532:THR:HG22	57:C:1001:ATP:C4	2.26	0.71
45:e:105:VAL:HG22	46:g:1:MET:HE1	1.72	0.71
45:e:932:LEU:C	45:e:964:PHE:CZ	2.69	0.71
47:x:56:C:O2'	47:x:57:G:O5'	2.05	0.71
48:z:19:GLY:HA3	48:z:55:GLY:HA2	1.72	0.71
38:p:44:ARG:O	56:b0:28:THR:HA	1.91	0.71
45:e:917:LEU:CD2	45:e:963:MET:SD	2.79	0.71
1:E:262:THR:CG2	57:E:902:ATP:O2A	2.39	0.71
2:K:39:ASP:CB	3:G:472:ASN:CG	2.63	0.71
29:f:1524:A:OP2	56:b0:112:THR:O	2.09	0.71
45:e:1514:ILE:HG23	45:e:1522:LEU:HD23	1.73	0.71
45:e:1540:TYR:CE1	53:v:210:PHE:CD2	2.78	0.71
52:X:8:ILE:HD11	52:X:65:LEU:HD13	1.72	0.71
45:e:978:THR:HG23	45:e:1023:ARG:NH1	2.06	0.71
49:0:26:PHE:HB2	49:0:87:VAL:HB	1.74	0.70
29:f:2473:C:N3	29:f:2475:G:H1'	2.04	0.70
29:f:1018:G:H1	29:f:1034:U:H3	1.38	0.70
29:f:1763:U:H3	53:v:202:LYS:HZ3	1.39	0.70
45:e:365:THR:HB	45:e:370:PHE:HB3	1.72	0.70
45:e:921:ILE:CD1	45:e:967:SER:HB3	2.12	0.70
29:f:2473:C:N4	29:f:2475:G:N3	2.40	0.70
45:e:918:LEU:CD2	45:e:966:ARG:HH12	2.04	0.70
45:e:929:LEU:CD2	45:e:967:SER:O	2.37	0.70
29:f:1523:U:H1'	56:b0:123:TYR:CD2	2.26	0.70
1:B:531:GLY:O	57:C:1001:ATP:PA	2.49	0.70
45:e:1049:ARG:HD2	45:e:1086:MET:CE	2.21	0.70
1:E:561:TRP:CD1	1:E:561:TRP:H	2.08	0.70
29:f:1259:A:N7	49:0:53:MET:HB2	1.92	0.70
29:f:1523:U:C4'	56:b0:113:LEU:CD2	2.65	0.70
45:e:930:ASN:O	45:e:933:LEU:CB	2.40	0.70
1:A:217:GLY:N	57:A:901:ATP:HN62	1.82	0.69
29:f:2254:U:H5"	44:a:75:GLY:HA3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:168:PRO:CG	55:a0:127:LEU:HD11	2.18	0.69
29:f:1219:C:OP1	49:0:4:ILE:HG21	1.92	0.69
29:f:1522:U:O4	56:b0:116:PRO:HG3	1.92	0.69
52:X:8:ILE:HD12	53:v:128:PHE:HE1	1.57	0.69
1:D:262:THR:CG2	57:D:902:ATP:O3B	2.39	0.69
38:p:46:LEU:CA	56:b0:27:ARG:O	2.40	0.69
45:e:1053:LEU:HD12	45:e:1105:LEU:HD22	0.73	0.69
1:D:606:ALA:CB	1:E:562:TYR:HH	2.00	0.69
1:E:262:THR:CG2	57:E:902:ATP:PA	2.80	0.69
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.57	0.69
29:f:3183:A:OP1	55:a0:12:LYS:HE3	1.92	0.69
38:p:49:TYR:O	56:b0:30:ALA:HB1	1.93	0.69
1:B:532:THR:HA	57:C:1001:ATP:C5'	2.23	0.69
38:p:52:TRP:HH2	56:b0:27:ARG:CZ	2.05	0.69
45:e:272:TYR:HA	45:e:277:MET:CG	2.23	0.69
1:D:216:ILE:CG2	57:D:902:ATP:C5	2.75	0.69
1:E:536:LEU:HD23	58:E:901:ADP:C2'	2.22	0.69
29:f:1833:G:P	56:b0:114:VAL:HB	2.33	0.69
29:f:3244:A:C8	55:a0:109:PRO:HB3	2.27	0.69
29:f:3244:A:HO2'	55:a0:111:PRO:HD3	1.55	0.69
45:e:104:LYS:H	46:g:1:MET:HE3	1.58	0.69
45:e:1050:LEU:HD22	45:e:1098:LEU:HA	1.74	0.69
47:x:1:G:H2'	47:x:2:G:C8	2.27	0.69
1:E:536:LEU:HD21	58:E:901:ADP:H3'	0.69	0.69
31:i:135:G:OP1	56:b0:53:HIS:HB2	1.93	0.69
45:e:932:LEU:CB	45:e:964:PHE:CZ	2.76	0.69
45:e:1066:ARG:NH1	45:e:1111:GLN:NE2	2.41	0.69
1:D:694:GLY:HA3	57:D:901:ATP:C2	2.28	0.68
53:v:211:LYS:HE2	53:v:222:LEU:CD1	2.22	0.68
29:f:1833:G:OP1	56:b0:114:VAL:HG11	1.92	0.68
45:e:222:LEU:HD12	45:e:226:ASN:HD21	1.57	0.68
29:f:3178:A:C6	55:a0:6:VAL:HB	2.29	0.68
45:e:1545:SER:HB3	53:v:228:MET:HE1	1.75	0.68
1:B:536:LEU:CD1	57:C:1001:ATP:C8	2.77	0.68
29:f:1523:U:C5'	56:b0:113:LEU:HD23	2.20	0.68
38:p:45:ASN:OD1	56:b0:26:VAL:HG23	1.93	0.68
45:e:272:TYR:CD1	45:e:277:MET:SD	2.86	0.68
45:e:1499:HIS:O	45:e:1502:PHE:N	2.26	0.68
51:w:138:VAL:HG23	51:w:147:LYS:HD2	1.75	0.68
29:f:14:U:O2'	56:b0:42:ARG:HG3	1.94	0.68
29:f:1830:G:O2'	56:b0:91:ASN:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:ASN:ND2	57:D:901:ATP:PG	2.67	0.68
29:f:1524:A:P	56:b0:112:THR:O	2.52	0.68
44:a:90:THR:HG21	44:a:107:ASP:OD1	1.94	0.68
39:q:92:TYR:HB2	39:q:142:ASP:HB3	1.73	0.67
45:e:751:VAL:HA	45:e:754:ILE:HD11	0.68	0.67
1:B:558:LEU:CD2	1:C:562:TYR:OH	2.42	0.67
29:f:1523:U:O4	56:b0:75:LYS:HE3	1.94	0.67
1:E:261:LYS:HD3	1:E:261:LYS:N	2.08	0.67
29:f:2969:A:N7	32:j:215:ASN:ND2	2.42	0.67
43:u:127:LYS:CB	55:a0:194:LEU:HD12	2.24	0.67
1:B:30:ASP:OD1	45:e:1023:ARG:NH2	2.27	0.67
2:K:37:PRO:HB2	2:K:38:PRO:CD	2.19	0.67
29:f:2193:U:H5'	29:f:2194:G:H5'	1.75	0.67
45:e:222:LEU:CD1	45:e:226:ASN:HD21	2.08	0.67
45:e:371:LEU:HD12	45:e:377:TRP:HZ2	1.49	0.67
29:f:1610:G:OP1	56:b0:125:ARG:NH2	2.28	0.67
29:f:3005:A:H5"	55:a0:149:TYR:OH	1.95	0.67
29:f:1751:G:N2	52:X:78:LEU:HD22	2.09	0.67
1:B:92:LEU:HD21	1:B:160:GLU:HB2	1.76	0.67
29:f:3180:A:C4'	55:a0:116:LYS:HD3	2.23	0.66
1:E:536:LEU:CD2	58:E:901:ADP:C2'	2.72	0.66
29:f:1222:G:C8	49:0:57:THR:HB	2.29	0.66
29:f:1254:C:O2	48:z:135:THR:CB	2.43	0.66
29:f:2473:C:N4	29:f:2475:G:C2	2.62	0.66
45:e:1021:PRO:HB3	45:e:1068:MET:HE3	1.77	0.66
29:f:1222:G:C8	49:0:57:THR:CB	2.79	0.66
57:D:902:ATP:O1B	1:E:369:ARG:CZ	2.44	0.66
29:f:2472:U:H2'	29:f:2474:G:H22	1.59	0.66
53:v:471:HIS:HB2	53:v:570:ARG:HH11	1.61	0.66
1:D:561:TRP:NE1	2:K:5:VAL:O	2.29	0.66
45:e:883:VAL:CB	45:e:956:LEU:CD1	2.37	0.66
45:e:929:LEU:CD1	45:e:967:SER:OG	2.22	0.66
45:e:1540:TYR:CD2	53:v:225:ILE:HD13	2.31	0.66
53:v:643:ALA:HB2	54:2:64:GLU:HG2	1.78	0.66
29:f:1940:G:H21	29:f:3362:A:H8	1.44	0.66
53:v:374:GLN:NE2	54:2:10:GLY:HA3	2.04	0.66
53:v:381:ARG:NH2	53:v:657:GLU:CD	2.51	0.66
1:B:489:VAL:HG12	57:C:1001:ATP:HN62	1.60	0.66
1:D:666:ILE:HD11	57:D:901:ATP:N6	2.11	0.66
29:f:2988:C:P	55:a0:68:ARG:NH1	2.68	0.66
31:i:134:G:OP1	56:b0:56:ARG:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:2473:C:C5	29:f:2474:G:N2	2.63	0.66
45:e:253:LYS:C	45:e:254:ASN:OD1	2.39	0.66
29:f:1751:G:H1	52:X:78:LEU:HD11	1.56	0.65
45:e:320:LEU:HB3	45:e:328:ILE:HG21	1.79	0.65
29:f:1222:G:C8	49:0:57:THR:HG21	2.31	0.65
44:a:403:LYS:NZ	44:a:512:LEU:O	2.28	0.65
1:D:418:GLY:HA3	57:D:902:ATP:H2	1.59	0.65
29:f:1240:A:OP1	48:z:97:ASN:O	2.14	0.65
1:F:394:HIS:HE1	57:F:901:ATP:H1'	1.60	0.65
45:e:936:VAL:HG21	45:e:964:PHE:CE1	2.31	0.65
1:D:535:THR:OG1	57:D:901:ATP:O2A	2.07	0.65
1:D:562:TYR:CE1	1:D:609:ARG:NH1	2.56	0.65
57:F:901:ATP:O2A	57:F:901:ATP:H3'	1.97	0.65
8:7:84:TYR:HB2	15:O:24:PRO:HD3	1.78	0.65
7:6:164:SER:HB2	55:a0:121:PRO:HG3	1.78	0.65
29:f:3244:A:H61	55:a0:105:PHE:HD1	1.37	0.65
53:v:343:ASP:HB3	53:v:360:LEU:HD12	1.78	0.65
23:W:2:GLY:N	29:f:2138:A:HO2'	1.95	0.65
29:f:1238:C:H4'	48:z:139:VAL:CB	2.27	0.65
45:e:985:ILE:HD11	45:e:1023:ARG:HG3	1.78	0.65
53:v:381:ARG:CZ	54:2:6:LYS:HD3	2.26	0.65
29:f:3018:C:OP1	46:g:9:ASN:ND2	2.29	0.65
2:K:39:ASP:HB3	3:G:472:ASN:CB	2.26	0.65
29:f:687:U:OP2	42:t:36:ARG:NH2	2.30	0.65
29:f:1523:U:C2	56:b0:123:TYR:CG	2.84	0.65
29:f:2836:C:H5	29:f:2852:C:H42	1.44	0.65
29:f:3180:A:C5'	55:a0:116:LYS:HD3	2.27	0.65
53:v:233:VAL:HG21	53:v:278:ASP:HB2	1.78	0.65
45:e:883:VAL:HG12	45:e:956:LEU:CD2	2.26	0.64
45:e:1477:GLN:NE2	45:e:1481:THR:HG23	2.12	0.64
29:f:1221:A:N3	49:0:12:PHE:HE2	1.93	0.64
38:p:45:ASN:OD1	56:b0:26:VAL:HA	1.97	0.64
53:v:328:LYS:HE2	53:v:330:GLU:CG	2.26	0.64
57:C:1003:ATP:O1B	1:D:645:ARG:NH2	2.28	0.64
29:f:2474:G:H1'	29:f:2475:G:C8	2.32	0.64
1:D:562:TYR:HD1	1:D:609:ARG:NH2	1.87	0.64
29:f:1825:G:H5'	52:X:17:ARG:HH22	1.58	0.64
29:f:1610:G:P	56:b0:125:ARG:HH22	2.21	0.64
45:e:1086:MET:HB2	45:e:1092:THR:HG21	1.80	0.64
45:e:1475:SER:OG	45:e:1493:LEU:HD21	1.96	0.64
45:e:1540:TYR:HE1	53:v:210:PHE:CD2	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:43:LEU:H	2:K:43:LEU:HD22	1.62	0.64
43:u:127:LYS:HD2	55:a0:194:LEU:HD12	1.80	0.64
29:f:1523:U:C1'	56:b0:123:TYR:CD2	2.81	0.64
29:f:1523:U:O5'	56:b0:113:LEU:HD22	1.98	0.64
29:f:3243:A:C6	55:a0:108:ILE:O	2.51	0.64
45:e:1050:LEU:HD21	45:e:1098:LEU:CB	2.28	0.64
1:D:560:MET:HG3	1:D:561:TRP:CZ3	2.33	0.63
29:f:1232:C:O2'	49:0:36:GLN:NE2	2.31	0.63
1:E:314:ASP:OD2	57:E:902:ATP:O3G	2.17	0.63
10:I:12:ARG:NH1	29:f:3041:U:OP1	2.32	0.63
45:e:883:VAL:CG1	45:e:956:LEU:HD11	0.20	0.63
45:e:60:THR:O	45:e:64:LYS:HG3	1.98	0.63
45:e:371:LEU:HB3	45:e:377:TRP:CD1	2.32	0.63
45:e:1236:SER:HA	45:e:1239:LYS:HE3	1.80	0.63
47:y:62:C:H2'	47:y:63:G:C8	2.34	0.63
38:p:52:TRP:HH2	56:b0:27:ARG:NH1	1.96	0.63
45:e:1192:ARG:HG2	45:e:1270:TRP:CH2	2.34	0.63
45:e:1506:GLU:HB2	45:e:1533:LYS:HD2	1.79	0.63
48:z:54:LYS:C	48:z:56:ILE:H	2.07	0.63
1:C:262:THR:HG21	57:C:1002:ATP:O3G	1.95	0.63
29:f:2523:A:H3'	56:b0:30:ALA:CB	2.29	0.63
53:v:305:ARG:HD2	53:v:308:ASP:OD2	1.99	0.63
1:E:418:GLY:O	57:E:902:ATP:C2	2.47	0.63
2:K:44:ILE:O	2:K:45:PHE:CB	2.45	0.63
2:J:218:GLU:HB2	2:J:221:ASP:HB2	1.81	0.63
29:f:1610:G:OP2	56:b0:125:ARG:NH2	2.31	0.63
29:f:1751:G:C6	52:X:78:LEU:HD12	2.33	0.63
29:f:3185:U:C5	55:a0:126:VAL:HG11	2.33	0.63
38:p:52:TRP:CH2	56:b0:27:ARG:CZ	2.82	0.63
45:e:59:GLU:HG2	45:e:103:TYR:CD1	2.33	0.63
45:e:807:LYS:CE	45:e:808:ASN:OD1	2.47	0.63
45:e:932:LEU:C	45:e:933:LEU:CA	2.71	0.63
28:d:4:MET:N	29:f:1802:C:OP1	2.32	0.62
1:B:116:GLU:HG2	1:B:153:GLN:HE21	1.63	0.62
29:f:1825:G:P	52:X:49:SER:OG	2.57	0.62
43:u:124:ARG:HA	55:a0:194:LEU:CD1	2.23	0.62
45:e:102:ASP:OD1	45:e:207:ARG:HD2	1.99	0.62
45:e:930:ASN:O	45:e:933:LEU:HB2	1.98	0.62
45:e:1050:LEU:CG	45:e:1098:LEU:CD2	2.74	0.62
45:e:1477:GLN:OE1	45:e:1481:THR:OG1	2.18	0.62
1:F:394:HIS:CE1	57:F:901:ATP:H1'	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:2472:U:H2'	29:f:2474:G:N2	2.13	0.62
1:B:532:THR:HG21	57:C:1001:ATP:N1	2.15	0.62
1:C:531:GLY:N	57:C:1003:ATP:O2B	2.32	0.62
13:M:27:LYS:HB3	13:M:42:LEU:HB2	1.81	0.62
29:f:1523:U:C4	56:b0:123:TYR:CZ	2.88	0.62
45:e:1024:LEU:HD11	45:e:1059:LEU:HD21	1.82	0.62
52:X:8:ILE:CD1	53:v:128:PHE:CE1	2.83	0.62
1:B:489:VAL:HG13	57:C:1001:ATP:HN61	1.56	0.62
24:Y:10:LYS:NZ	56:b0:114:VAL:O	2.31	0.62
29:f:1235:U:O4	48:z:136:ALA:HA	2.00	0.62
45:e:1319:TRP:CD1	45:e:1386:PHE:HE1	2.17	0.62
1:C:698:LEU:CD1	57:C:1003:ATP:O2'	2.47	0.62
27:c:87:ARG:NH1	32:j:97:ASN:OD1	2.32	0.62
31:i:133:G:C4'	56:b0:55:ASN:ND2	2.62	0.62
31:i:151:C:C4	56:b0:24:LEU:CD1	2.75	0.62
29:f:1221:A:N3	49:0:12:PHE:CE2	2.67	0.61
29:f:1751:G:N2	52:X:78:LEU:CD2	2.62	0.61
46:g:111:ASN:ND2	46:g:114:VAL:O	2.32	0.61
48:z:51:LYS:O	48:z:52:GLU:C	2.43	0.61
1:B:52:LEU:HD21	1:B:58:ARG:HG3	1.81	0.61
1:B:536:LEU:HD11	57:C:1001:ATP:N7	2.15	0.61
1:E:216:ILE:HG13	57:E:902:ATP:N7	2.14	0.61
10:I:14:SER:O	10:I:81:GLN:NE2	2.33	0.61
29:f:1610:G:OP2	56:b0:125:ARG:CZ	2.48	0.61
29:f:3348:G:H1	29:f:3357:U:H3	1.47	0.61
1:B:122:ARG:NH1	1:B:147:GLU:HB3	2.15	0.61
1:F:583:VAL:HG23	1:F:628:PHE:HB3	1.83	0.61
29:f:2383:C:N4	55:a0:91:LYS:CG	2.61	0.61
43:u:123:LEU:HD13	55:a0:193:GLN:CB	2.27	0.61
1:B:28:ARG:NE	1:B:48:ILE:HD12	2.15	0.61
29:f:1258:U:P	49:0:46:ARG:NH2	2.64	0.61
29:f:1523:U:O4	56:b0:75:LYS:CE	2.49	0.61
29:f:1750:A:H4'	52:X:26:LYS:NZ	2.15	0.61
1:D:618:MET:HB3	1:D:648:ARG:HH21	1.66	0.61
23:W:21:ARG:HG2	31:i:103:G:H4'	1.82	0.61
29:f:1348:U:O2	29:f:1349:G:N2	2.34	0.61
29:f:1751:G:C5	52:X:78:LEU:CD1	2.79	0.61
45:e:1032:LEU:HG	45:e:1075:LEU:HD11	1.83	0.61
31:i:132:G:H5"	56:b0:94:GLN:CG	2.30	0.61
45:e:883:VAL:CG1	45:e:956:LEU:CD2	2.78	0.61
45:e:1057:THR:OG1	45:e:1105:LEU:CD1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:1439:LEU:HA	45:e:1460:SER:HB2	1.83	0.61
47:y:1:G:C6	47:y:73:G:C2	2.88	0.61
29:f:1612:A:O5'	52:X:46:ARG:NH1	2.34	0.61
42:t:27:ASP:O	42:t:31:LYS:HB2	2.01	0.61
45:e:1060:MET:HE1	45:e:1072:ALA:HB3	1.79	0.61
52:X:8:ILE:HD12	53:v:128:PHE:CE1	2.36	0.61
53:v:527:PHE:HA	53:v:534:LEU:HD12	1.83	0.61
1:C:524:VAL:HG23	1:C:651:GLN:HB2	1.83	0.60
29:f:2254:U:C5'	44:a:75:GLY:HA3	2.31	0.60
45:e:807:LYS:NZ	45:e:808:ASN:OD1	2.35	0.60
45:e:917:LEU:CD2	45:e:963:MET:CE	2.68	0.60
45:e:1340:TYR:O	45:e:1344:ILE:HG12	2.01	0.60
2:K:36:ILE:HG22	2:K:36:ILE:O	2.01	0.60
23:W:55:ARG:NH2	34:l:59:GLN:OE1	2.34	0.60
29:f:1751:G:C6	52:X:78:LEU:HD11	2.16	0.60
29:f:1751:G:OP1	52:X:26:LYS:NZ	2.31	0.60
6:5:43:LYS:NZ	29:f:1764:U:OP1	2.31	0.60
7:6:80:ARG:HH21	7:6:87:THR:HG21	1.66	0.60
29:f:15:C:H5"	56:b0:42:ARG:CG	2.31	0.60
29:f:1253:U:H5"	29:f:1254:C:H5'	1.83	0.60
35:m:277:LEU:HG	35:m:281:GLU:HG3	1.82	0.60
44:a:4:ARG:NH1	44:a:57:GLY:O	2.35	0.60
45:e:917:LEU:CD2	45:e:963:MET:HE1	2.13	0.60
1:D:561:TRP:HE1	2:K:5:VAL:N	1.96	0.60
5:4:38:ARG:NH2	29:f:1348:U:OP2	2.34	0.60
29:f:439:C:O2'	29:f:494:G:N2	2.34	0.60
29:f:1523:U:N3	56:b0:123:TYR:CZ	2.70	0.60
1:B:536:LEU:HD11	57:C:1001:ATP:C8	2.35	0.60
22:V:66:GLU:OE2	51:w:199:GLN:NE2	2.35	0.60
31:i:151:C:C5	56:b0:24:LEU:CD1	2.74	0.60
29:f:1833:G:OP1	56:b0:114:VAL:CG1	2.49	0.60
45:e:751:VAL:CB	45:e:754:ILE:HD11	2.29	0.60
45:e:883:VAL:HG12	45:e:956:LEU:HG	1.79	0.60
29:f:1603:A:N6	56:b0:71:THR:OG1	2.34	0.60
35:m:50:ARG:NH1	35:m:147:ASP:OD2	2.34	0.60
37:o:87:VAL:HG11	37:o:243:MET:HE1	1.83	0.60
1:C:694:GLY:CA	57:C:1003:ATP:C2	2.83	0.60
29:f:804:C:OP1	34:l:98:ARG:NH2	2.35	0.60
38:p:47:SER:HA	56:b0:27:ARG:HB2	1.84	0.60
1:C:222:GLN:HE22	1:C:380:GLY:H	1.50	0.59
29:f:2383:C:H42	55:a0:91:LYS:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:149:LYS:HB3	45:e:150:PRO:CD	2.31	0.59
45:e:883:VAL:HG13	45:e:956:LEU:HD13	0.60	0.59
45:e:1477:GLN:CD	45:e:1481:THR:HG1	2.09	0.59
51:w:65:ILE:HG12	51:w:109:ALA:HB3	1.84	0.59
29:f:14:U:O3'	56:b0:42:ARG:NE	2.34	0.59
29:f:3243:A:HO2'	55:a0:110:PRO:CD	2.10	0.59
45:e:1525:LYS:HE3	53:v:214:PHE:HA	1.84	0.59
45:e:1303:MET:HA	45:e:1303:MET:HE2	0.69	0.59
1:B:536:LEU:CD1	57:C:1001:ATP:N7	2.65	0.59
43:u:127:LYS:HB2	55:a0:194:LEU:HD12	1.84	0.59
45:e:712:SER:O	45:e:716:ALA:N	2.27	0.59
45:e:1040:ALA:O	45:e:1049:ARG:NH2	2.34	0.59
2:K:43:LEU:HD22	2:K:43:LEU:N	2.18	0.59
6:5:34:GLN:OE1	53:v:254:LYS:CD	2.50	0.59
6:5:128:LYS:NZ	29:f:1724:U:OP2	2.31	0.59
29:f:1763:U:H3	53:v:202:LYS:NZ	1.99	0.59
29:f:1829:G:H5'	56:b0:93:TYR:CE1	2.38	0.59
35:m:294:ALA:HB1	40:r:217:PHE:HB3	1.83	0.59
1:D:666:ILE:CD1	57:D:901:ATP:N6	2.66	0.59
4:3:173:ARG:NH2	29:f:618:C:OP1	2.35	0.59
20:T:74:ARG:NH2	29:f:1639:C:OP2	2.31	0.59
44:a:619:HIS:NE2	44:a:679:GLY:O	2.36	0.59
29:f:1522:U:H3'	56:b0:113:LEU:HD22	1.85	0.59
25:Z:125:LYS:O	39:q:173:ARG:NH1	2.35	0.59
29:f:1268:G:O2'	29:f:1273:A:N6	2.36	0.59
29:f:1830:G:C5'	56:b0:92:LYS:HB2	2.14	0.59
29:f:3245:A:O2'	55:a0:110:PRO:HB3	2.03	0.59
44:a:359:GLN:HA	44:a:362:LYS:HD2	1.85	0.59
53:v:403:LEU:HD23	53:v:407:ILE:HB	1.85	0.59
1:E:553:LYS:HB3	1:E:556:GLU:HB2	1.84	0.58
7:6:8:GLN:HB3	7:6:64:ILE:HD11	1.85	0.58
43:u:131:VAL:HG22	55:a0:185:ALA:HB3	1.85	0.58
45:e:731:LEU:HD12	45:e:732:GLN:CA	2.32	0.58
49:0:192:ASP:HB2	49:0:197:PHE:HE2	1.67	0.58
29:f:3243:A:N1	55:a0:107:GLY:HA3	2.18	0.58
45:e:1071:THR:O	45:e:1074:GLU:CG	2.51	0.58
29:f:2254:U:H5"	44:a:75:GLY:CA	2.32	0.58
29:f:3244:A:C2	55:a0:105:PHE:HE1	2.17	0.58
14:N:42:ARG:NH2	29:f:2800:G:O6	2.37	0.58
29:f:3008:A:OP1	55:a0:72:HIS:N	2.23	0.58
38:p:45:ASN:OD1	56:b0:26:VAL:CG2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:917:LEU:HB3	45:e:963:MET:CE	2.33	0.58
14:N:21:ARG:NH2	29:f:640:U:OP1	2.32	0.58
21:U:5:LYS:HB2	21:U:8:GLU:HG2	1.84	0.58
29:f:3007:U:H5'	55:a0:73:PHE:CE2	2.37	0.58
30:h:31:U:O2'	35:m:218:ARG:NH1	2.35	0.58
31:i:21:C:OP1	34:l:193:LYS:NZ	2.36	0.58
54:2:42:ARG:HE	54:2:49:GLN:CD	2.10	0.58
29:f:2384:A:N1	55:a0:96:LYS:CE	2.66	0.58
45:e:1499:HIS:O	45:e:1502:PHE:C	2.46	0.58
6:5:100:ARG:NH1	29:f:1722:U:OP1	2.36	0.58
39:q:89:LYS:HG2	39:q:145:VAL:HG22	1.84	0.58
45:e:1303:MET:CE	45:e:1303:MET:CA	2.30	0.58
32:j:27:ALA:O	32:j:128:ARG:NH2	2.36	0.58
53:v:471:HIS:HB2	53:v:570:ARG:NH1	2.18	0.58
14:N:21:ARG:NH1	29:f:1369:A:OP1	2.36	0.58
27:c:17:ARG:NH1	29:f:860:G:OP1	2.36	0.58
29:f:1354:G:N3	36:n:8:LYS:NZ	2.51	0.58
35:m:166:ALA:HB1	35:m:171:LEU:HD12	1.85	0.58
44:a:975:LYS:HE2	44:a:998:LYS:HA	1.84	0.58
45:e:776:TYR:HB2	45:e:812:LEU:HG	1.85	0.58
45:e:1068:MET:HE2	45:e:1070:ILE:HD11	1.85	0.58
7:6:77:VAL:HG22	7:6:126:VAL:HG23	1.85	0.58
29:f:2471:U:O2	29:f:2474:G:C2	2.56	0.58
45:e:1276:LEU:HD13	45:e:1358:GLN:HG2	1.86	0.57
45:e:1435:ASP:OD2	45:e:1514:ILE:N	2.36	0.57
17:Q:55:LEU:HB2	17:Q:95:PRO:HD3	1.86	0.57
29:f:1257:C:C5'	48:z:124:THR:CB	2.68	0.57
29:f:3187:A:OP1	39:q:23:ARG:NH1	2.37	0.57
31:i:135:G:P	56:b0:53:HIS:H	2.27	0.57
45:e:277:MET:CG	45:e:278:PRO:HD3	2.31	0.57
45:e:1053:LEU:HD11	45:e:1105:LEU:CB	2.35	0.57
29:f:1833:G:OP2	56:b0:114:VAL:HG23	2.03	0.57
40:r:205:SER:OG	40:r:208:ASN:OD1	2.21	0.57
29:f:1231:A:H5"	29:f:1232:C:H5'	1.86	0.57
29:f:1522:U:C4	56:b0:116:PRO:CG	2.80	0.57
45:e:100:ILE:HG22	45:e:207:ARG:HH21	1.69	0.57
47:y:8:U:O2	47:y:8:U:C2'	2.46	0.57
1:C:347:ALA:HB1	1:C:350:ASN:HD22	1.69	0.57
24:Y:5:LYS:HE2	24:Y:13:MET:HE1	1.87	0.57
27:c:49:ARG:NH2	29:f:1793:C:OP2	2.38	0.57
1:A:663:ARG:HG3	1:A:666:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:4:ARG:NH1	29:f:837:A:OP2	2.37	0.57
1:C:557:LEU:O	1:C:568:ASN:ND2	2.38	0.57
1:C:561:TRP:CZ3	2:K:8:LEU:HD12	2.40	0.57
31:i:134:G:OP1	56:b0:56:ARG:CD	2.52	0.57
45:e:793:ASN:ND2	45:e:1005:ASN:HD21	2.02	0.57
29:f:15:C:H5"	56:b0:42:ARG:HG2	1.86	0.57
45:e:156:THR:HG22	45:e:161:LYS:HA	1.86	0.57
45:e:1057:THR:HG22	45:e:1108:THR:HG21	1.87	0.57
45:e:1544:ARG:NH1	53:v:207:HIS:CE1	2.73	0.57
47:y:62:C:H2'	47:y:63:G:H8	1.68	0.57
53:v:211:LYS:CE	53:v:222:LEU:CD1	2.82	0.57
17:Q:4:LEU:O	17:Q:79:ARG:NH2	2.38	0.57
22:V:68:ARG:NH2	29:f:2219:A:OP2	2.38	0.57
29:f:1830:G:O3'	56:b0:91:ASN:CB	2.47	0.57
1:E:561:TRP:CD1	1:E:561:TRP:N	2.72	0.57
45:e:906:PHE:HE2	45:e:955:LEU:CG	2.15	0.56
46:g:118:HIS:HD1	46:g:120:ASP:H	1.52	0.56
1:B:534:LYS:HG2	1:B:535:THR:HG23	1.87	0.56
29:f:1830:G:O2'	56:b0:91:ASN:ND2	2.37	0.56
29:f:2523:A:H3'	56:b0:30:ALA:HB3	1.87	0.56
30:h:52:G:H21	41:s:9:MET:HE1	1.68	0.56
33:k:140:ASP:OD1	33:k:141:GLY:N	2.36	0.56
43:u:124:ARG:HG3	55:a0:194:LEU:HD21	1.86	0.56
45:e:795:HIS:CD2	45:e:1047:THR:HG23	2.39	0.56
1:B:28:ARG:HE	1:B:48:ILE:HD12	1.70	0.56
1:B:532:THR:C	57:C:1001:ATP:O2A	2.48	0.56
1:D:216:ILE:CG2	57:D:902:ATP:N7	2.68	0.56
5:4:43:PRO:HB2	29:f:728:G:H5"	1.86	0.56
27:c:4:ARG:NH2	29:f:838:G:O6	2.38	0.56
29:f:3180:A:N6	55:a0:167:TYR:CE1	2.73	0.56
36:n:132:THR:HA	36:n:135:VAL:HG12	1.87	0.56
45:e:1152:TYR:HD1	45:e:1193:LEU:HD12	1.68	0.56
53:v:378:ILE:HG12	54:2:8:LEU:O	2.05	0.56
1:A:315:GLU:OE2	57:A:901:ATP:PG	2.64	0.56
31:i:133:G:C4'	56:b0:55:ASN:CG	2.71	0.56
1:F:419:ALA:HB2	57:F:901:ATP:H5'2	1.88	0.56
1:F:285:MET:HE1	1:F:334:VAL:HG21	1.87	0.56
29:f:1390:A:N6	29:f:1418:A:O2'	2.38	0.56
44:a:90:THR:HG21	44:a:107:ASP:H	1.70	0.56
44:a:936:ASP:HA	44:a:996:MET:HE1	1.86	0.56
29:f:2162:U:OP1	32:j:234:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:0:43:LYS:HA	49:0:46:ARG:HG2	1.86	0.56
53:v:378:ILE:CG1	54:2:8:LEU:O	2.54	0.56
1:E:562:TYR:OH	1:E:609:ARG:CZ	2.53	0.56
17:Q:9:THR:HG23	17:Q:109:VAL:HG23	1.88	0.56
29:f:2472:U:C2'	29:f:2474:G:N2	2.68	0.56
33:k:59:ASP:HB2	33:k:357:LYS:HE3	1.87	0.56
38:p:49:TYR:O	56:b0:30:ALA:CB	2.53	0.56
1:E:261:LYS:O	1:E:264:MET:N	2.38	0.56
9:8:56:VAL:HG12	9:8:65:VAL:HG22	1.88	0.56
39:q:23:ARG:HE	39:q:39:LYS:HA	1.71	0.56
39:q:57:VAL:HG12	39:q:68:LEU:HD22	1.88	0.56
1:B:532:THR:HG21	57:C:1001:ATP:C4	2.40	0.56
1:B:589:LEU:HB3	1:B:639:ILE:HD13	1.88	0.56
1:C:558:LEU:HD11	1:D:562:TYR:CE1	2.38	0.56
13:M:17:ARG:NH1	29:f:1634:G:N7	2.53	0.56
47:x:55:U:H2'	47:x:56:C:H2'	1.88	0.56
1:D:280:ASN:HB3	1:D:283:GLU:HB2	1.88	0.55
45:e:323:TYR:CG	45:e:324:GLU:HG2	2.40	0.55
45:e:1070:ILE:HB	45:e:1072:ALA:CB	2.35	0.55
45:e:1477:GLN:NE2	45:e:1481:THR:CB	2.43	0.55
52:X:16:ARG:HD2	53:v:135:PHE:CE1	2.41	0.55
2:K:43:LEU:N	2:K:43:LEU:CD2	2.69	0.55
29:f:2447:A:H2'	29:f:2448:G:O4'	2.06	0.55
35:m:64:ILE:HG13	35:m:109:THR:HG21	1.87	0.55
38:p:47:SER:CA	56:b0:27:ARG:HB2	2.37	0.55
40:r:143:SER:C	40:r:144:ASN:HD22	2.14	0.55
1:B:558:LEU:HD11	1:C:562:TYR:OH	2.05	0.55
1:E:431:GLN:HB3	1:E:461:ASN:HD21	1.70	0.55
29:f:1612:A:P	52:X:46:ARG:HH11	2.29	0.55
29:f:2674:A:H5"	41:s:105:GLY:HA3	1.89	0.55
45:e:932:LEU:C	45:e:964:PHE:HZ	2.12	0.55
20:T:87:GLU:OE1	20:T:91:ARG:NH1	2.39	0.55
29:f:2473:C:H5	29:f:2474:G:N2	2.05	0.55
1:E:428:ALA:O	1:E:461:ASN:ND2	2.39	0.55
1:F:337:GLN:HE21	1:F:341:LEU:HD23	1.71	0.55
25:Z:100:TYR:O	29:f:2895:G:O2'	2.24	0.55
29:f:1523:U:N1	56:b0:123:TYR:HE2	1.93	0.55
32:j:111:THR:HB	32:j:136:ILE:HD13	1.87	0.55
45:e:750:ALA:C	45:e:754:ILE:HG12	2.24	0.55
49:0:42:ARG:HG2	49:0:51:VAL:HG11	1.88	0.55
29:f:2482:U:H2'	29:f:2483:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:a:604:TYR:O	44:a:623:LYS:NZ	2.39	0.55
45:e:365:THR:HB	45:e:370:PHE:CB	2.37	0.55
1:B:262:THR:OG1	57:B:901:ATP:O1A	2.25	0.55
32:j:70:ARG:HD2	32:j:72:ARG:HE	1.72	0.55
33:k:66:LYS:O	33:k:70:ARG:NH2	2.39	0.55
45:e:1505:PHE:HB2	45:e:1514:ILE:CG1	2.35	0.55
1:E:562:TYR:CD1	1:E:562:TYR:C	2.85	0.55
10:I:94:TYR:OH	11:9:41:LYS:NZ	2.39	0.55
29:f:1352:A:H4'	29:f:1353:U:H5'	1.88	0.55
29:f:2491:A:H1'	51:w:207:LYS:HE2	1.88	0.55
29:f:3008:A:OP1	55:a0:72:HIS:ND1	2.40	0.55
29:f:3045:G:OP1	33:k:19:ARG:NH2	2.39	0.55
1:A:697:LEU:HD23	1:A:700:ILE:HD13	1.88	0.55
29:f:542:G:H1	29:f:549:U:H3	1.52	0.55
29:f:1259:A:N7	49:0:53:MET:HB3	2.15	0.55
29:f:2473:C:H2'	29:f:2474:G:H4'	1.89	0.55
29:f:2557:A:OP1	32:j:69:TYR:OH	2.24	0.55
45:e:1307:ILE:O	45:e:1311:ILE:HG12	2.06	0.55
7:6:96:ASP:OD1	7:6:97:VAL:N	2.38	0.55
9:8:90:ARG:NH1	29:f:1682:U:O4	2.40	0.55
14:N:44:ASN:ND2	42:t:4:SER:O	2.40	0.55
29:f:1832:C:OP1	56:b0:120:LYS:CE	2.55	0.55
29:f:3180:A:C5	55:a0:167:TYR:CZ	2.95	0.55
45:e:906:PHE:HE2	45:e:955:LEU:HD23	0.74	0.55
45:e:1156:TYR:HB2	45:e:1193:LEU:HD21	1.89	0.55
47:x:1:G:H2'	47:x:2:G:H8	1.72	0.55
1:D:484:VAL:HG13	1:D:488:ASP:HB2	1.88	0.54
29:f:1833:G:OP1	56:b0:114:VAL:HB	2.07	0.54
29:f:2383:C:N3	55:a0:91:LYS:HE2	2.22	0.54
43:u:124:ARG:HD2	55:a0:199:TYR:CD2	2.41	0.54
2:K:40:GLN:C	2:K:41:GLN:O	2.49	0.54
29:f:1221:A:C4	49:0:12:PHE:CZ	2.95	0.54
40:r:61:SER:OG	40:r:63:GLU:OE1	2.25	0.54
45:e:1435:ASP:CG	45:e:1514:ILE:N	2.63	0.54
2:K:40:GLN:O	2:K:41:GLN:C	2.51	0.54
29:f:1256:G:O2'	48:z:124:THR:CB	2.55	0.54
29:f:1522:U:P	56:b0:121:LYS:NZ	2.81	0.54
29:f:1558:A:O2'	56:b0:34:LEU:HD13	2.07	0.54
45:e:917:LEU:HB3	45:e:963:MET:HE3	1.89	0.54
45:e:1070:ILE:HB	45:e:1072:ALA:N	2.22	0.54
1:B:400:LEU:HD12	1:B:404:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:GLY:H	57:C:1001:ATP:N6	2.06	0.54
1:B:535:THR:HB	1:B:539:LYS:HE2	1.90	0.54
1:E:430:MET:HE1	1:F:248:PRO:HG3	1.89	0.54
38:p:45:ASN:OD1	56:b0:26:VAL:CA	2.56	0.54
45:e:272:TYR:CA	45:e:277:MET:CG	2.85	0.54
53:v:195:LYS:HE3	53:v:196:PHE:CZ	2.43	0.54
1:E:562:TYR:CE2	1:E:609:ARG:NH1	2.75	0.54
14:N:95:SER:OG	14:N:98:THR:OG1	2.25	0.54
29:f:3115:C:OP1	39:q:62:ARG:NH2	2.41	0.54
29:f:3214:U:OP2	43:u:128:ARG:NH1	2.34	0.54
45:e:104:LYS:N	46:g:1:MET:HE3	2.22	0.54
1:D:561:TRP:CD1	2:K:5:VAL:H	2.26	0.54
2:K:39:ASP:HB2	3:G:472:ASN:CB	2.10	0.54
29:f:1242:G:H1	44:a:519:THR:HG22	1.73	0.54
29:f:1524:A:C5'	56:b0:111:ASN:CG	2.81	0.54
29:f:2383:C:C4	55:a0:91:LYS:CG	2.90	0.54
53:v:176:LEU:HD11	53:v:182:PHE:CE1	2.43	0.54
18:R:19:ARG:HD3	18:R:33:ARG:HB2	1.89	0.54
29:f:394:G:N1	29:f:397:A:OP2	2.39	0.54
29:f:1222:G:C8	49:0:57:THR:CG2	2.90	0.54
29:f:3178:A:C8	55:a0:5:PRO:HD2	2.42	0.54
45:e:1499:HIS:O	45:e:1500:LEU:C	2.50	0.54
1:C:639:ILE:HD12	1:C:644:LEU:HD21	1.89	0.54
1:D:561:TRP:CG	2:K:6:LYS:HD3	2.43	0.54
1:E:262:THR:HG22	57:E:902:ATP:PA	2.48	0.54
1:F:245:ILE:O	1:F:348:ARG:NH2	2.41	0.54
29:f:1751:G:P	52:X:26:LYS:HZ1	2.30	0.54
29:f:2384:A:N1	55:a0:96:LYS:HE3	2.23	0.54
35:m:236:LEU:HA	35:m:239:ILE:HG12	1.90	0.54
1:A:513:TYR:HE2	1:A:520:PRO:HA	1.73	0.54
1:C:262:THR:HG23	57:C:1002:ATP:PG	2.48	0.54
1:E:536:LEU:HD23	58:E:901:ADP:C4'	2.21	0.54
2:J:204:PHE:HB2	2:J:266:THR:HA	1.90	0.54
8:7:17:ARG:HG2	8:7:22:HIS:HA	1.90	0.54
29:f:1221:A:C4	49:0:12:PHE:CE2	2.96	0.54
29:f:1523:U:C1'	56:b0:123:TYR:HE2	2.14	0.54
29:f:1524:A:H5'	56:b0:111:ASN:CG	2.33	0.54
29:f:3231:U:H2'	29:f:3232:G:H8	1.73	0.54
44:a:607:ASP:HB3	44:a:663:LYS:HB3	1.90	0.54
1:E:340:THR:HG23	3:G:138:LYS:HB3	1.90	0.53
3:G:226:LEU:HD12	3:G:439:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:9:6:ASP:OD1	11:9:32:GLN:N	2.40	0.53
51:w:48:ARG:HG2	51:w:159:LEU:HD23	1.89	0.53
1:A:281:GLY:HA3	1:A:315:GLU:HB2	1.90	0.53
1:F:525:LEU:HD11	1:F:649:LEU:HD23	1.91	0.53
29:f:3042:U:OP2	29:f:3092:C:N4	2.38	0.53
44:a:1005:LEU:HA	44:a:1008:LEU:HD12	1.89	0.53
45:e:332:ASP:HB3	45:e:335:SER:HB3	1.89	0.53
45:e:809:MET:CE	45:e:844:LEU:HD23	2.30	0.53
1:E:286:SER:HB2	1:F:333:ARG:HD2	1.90	0.53
29:f:1751:G:C2	52:X:78:LEU:HD22	2.43	0.53
45:e:1132:ILE:HG21	45:e:1170:GLN:HG3	1.89	0.53
53:v:381:ARG:CZ	54:2:6:LYS:HB3	2.37	0.53
29:f:68:C:OP2	29:f:301:G:N2	2.40	0.53
35:m:120:LYS:O	35:m:248:ARG:NH2	2.42	0.53
45:e:1028:PHE:CD2	45:e:1070:ILE:HG21	2.43	0.53
52:X:21:LYS:HG3	52:X:22:THR:HG23	1.89	0.53
1:B:283:GLU:O	1:B:287:LYS:NZ	2.41	0.53
29:f:1833:G:OP1	56:b0:114:VAL:CB	2.56	0.53
35:m:75:LEU:O	35:m:112:LYS:NZ	2.40	0.53
53:v:198:GLN:HE22	53:v:200:ASP:C	2.16	0.53
1:D:531:GLY:H	57:D:901:ATP:PB	2.31	0.53
1:E:479:VAL:HB	1:E:548:ASN:HD21	1.73	0.53
9:8:44:GLU:OE2	9:8:49:ASN:ND2	2.41	0.53
11:9:44:LYS:HD2	29:f:2111:G:H1'	1.90	0.53
29:f:1256:G:H4'	48:z:128:VAL:CB	2.39	0.53
29:f:2245:C:O2'	32:j:220:GLY:O	2.26	0.53
29:f:2473:C:H5	29:f:2474:G:C2	2.27	0.53
45:e:1560:PHE:CZ	53:v:210:PHE:HE1	2.27	0.53
1:B:536:LEU:HD11	57:C:1001:ATP:C5	2.44	0.53
57:D:902:ATP:PB	1:E:369:ARG:NH1	2.70	0.53
20:T:31:ARG:NH2	29:f:1598:G:OP2	2.42	0.53
29:f:1833:G:OP2	56:b0:114:VAL:HB	2.09	0.53
29:f:3007:U:OP1	55:a0:73:PHE:CA	2.54	0.53
29:f:110:G:OP2	42:t:73:ARG:NH2	2.42	0.53
29:f:1613:A:OP1	52:X:51:LEU:HB3	2.08	0.53
29:f:1747:G:O3'	52:X:53:THR:HG21	2.09	0.53
33:k:284:ARG:NH1	33:k:293:ASN:O	2.42	0.53
35:m:270:LYS:HG2	35:m:273:ARG:HE	1.73	0.53
38:p:51:LYS:N	56:b0:30:ALA:O	2.35	0.53
38:p:51:LYS:O	56:b0:32:PHE:HB3	2.09	0.53
45:e:209:HIS:HA	45:e:212:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:1540:TYR:CE1	53:v:210:PHE:CG	2.96	0.53
53:v:289:MET:O	53:v:404:LYS:HE3	2.09	0.53
1:E:464:PHE:O	1:E:468:ASN:ND2	2.42	0.53
29:f:1558:A:O3'	56:b0:34:LEU:HB2	2.09	0.53
31:i:133:G:C5'	56:b0:55:ASN:CG	2.82	0.53
44:a:111:TYR:HB2	44:a:125:LEU:HB2	1.91	0.53
45:e:323:TYR:CE2	45:e:324:GLU:HG2	2.42	0.53
8:7:158:THR:OG1	40:r:169:LYS:NZ	2.42	0.53
17:Q:102:LYS:NZ	29:f:3373:U:OP2	2.38	0.53
29:f:1156:C:OP2	37:o:94:LYS:NZ	2.40	0.53
1:B:128:VAL:HG11	1:B:135:GLN:HE21	1.73	0.52
1:D:262:THR:HG23	57:D:902:ATP:PG	2.46	0.52
4:3:118:GLN:NE2	4:3:147:GLU:OE2	2.39	0.52
26:b:2:VAL:N	26:b:90:HIS:O	2.42	0.52
35:m:54:ARG:NH1	35:m:147:ASP:O	2.42	0.52
43:u:120:VAL:HG12	55:a0:197:LEU:CG	2.39	0.52
45:e:1070:ILE:HB	45:e:1072:ALA:HB2	1.91	0.52
47:x:7:G:C6	47:x:49:U:C4	2.97	0.52
1:E:291:GLU:O	1:E:295:ASN:ND2	2.43	0.52
5:4:180:ARG:NH2	29:f:2790:A:OP1	2.42	0.52
11:9:47:ARG:HH21	11:9:58:HIS:HB2	1.73	0.52
45:e:918:LEU:HD21	45:e:966:ARG:HH12	1.75	0.52
45:e:1422:ASN:HB2	45:e:1425:THR:HG22	1.90	0.52
53:v:378:ILE:HG23	54:2:8:LEU:HD22	1.91	0.52
6:5:128:LYS:NZ	29:f:1721:U:O4	2.39	0.52
7:6:80:ARG:HB2	7:6:122:HIS:HB2	1.91	0.52
29:f:3268:A:OP1	36:n:46:ARG:NH2	2.35	0.52
1:C:698:LEU:CD2	57:C:1003:ATP:O2'	2.57	0.52
1:E:663:ARG:NH2	1:E:693:SER:O	2.41	0.52
11:9:16:GLY:O	29:f:3050:U:O2'	2.28	0.52
29:f:1899:G:O2'	29:f:2334:U:O4	2.25	0.52
29:f:3180:A:H5"	55:a0:116:LYS:HD3	1.91	0.52
44:a:612:MET:HE1	44:a:642:CYS:HB2	1.92	0.52
45:e:932:LEU:O	45:e:936:VAL:HG23	2.09	0.52
1:B:600:LEU:HD12	1:C:602:ASP:HB2	1.91	0.52
1:E:479:VAL:O	1:E:548:ASN:ND2	2.43	0.52
4:3:107:LEU:HD12	4:3:152:GLU:HG3	1.92	0.52
8:7:136:ARG:HD2	8:7:139:ARG:HH12	1.74	0.52
29:f:1830:G:O2'	56:b0:91:ASN:CG	2.52	0.52
34:l:266:THR:HG23	34:l:267:VAL:HG13	1.92	0.52
41:s:32:ARG:HD2	41:s:120:ILE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:u:127:LYS:CB	55:a0:194:LEU:CD1	2.88	0.52
47:y:6:U:H2'	47:y:7:G:C8	2.44	0.52
1:D:577:ARG:HD2	1:D:625:LYS:HD3	1.90	0.52
1:E:261:LYS:H	1:E:261:LYS:CD	2.13	0.52
7:6:77:VAL:HG11	7:6:106:LEU:HD22	1.92	0.52
29:f:1523:U:H1'	56:b0:123:TYR:HD2	1.71	0.52
29:f:2473:C:C5	29:f:2474:G:N3	2.78	0.52
45:e:271:LEU:C	45:e:277:MET:HG3	2.34	0.52
53:v:607:GLY:O	53:v:610:HIS:CD2	2.63	0.52
3:G:145:CYS:SG	3:G:146:GLU:N	2.79	0.52
19:S:70:LYS:HD2	29:f:585:A:H5"	1.92	0.52
41:s:49:LYS:HG3	41:s:64:LYS:HD3	1.92	0.52
45:e:1515:LEU:HD22	45:e:1520:ARG:O	2.10	0.52
1:A:439:LEU:HD23	1:A:440:ILE:HG12	1.92	0.52
1:B:43:VAL:HG23	1:B:120:PRO:HB2	1.92	0.52
1:D:341:LEU:HD23	3:G:183:LYS:HG2	1.91	0.52
29:f:831:G:O2'	29:f:1864:A:N3	2.39	0.52
29:f:3008:A:OP2	55:a0:74:ARG:NH1	2.43	0.52
32:j:241:ARG:HD3	44:a:866:LEU:HD21	1.92	0.52
45:e:981:ALA:HB1	45:e:1027:ILE:HD11	1.91	0.52
53:v:181:GLY:HA3	53:v:305:ARG:HD3	1.91	0.52
1:C:703:ARG:HD2	1:C:706:LYS:HE2	1.92	0.52
1:E:399:LYS:HE2	1:E:452:LEU:HD13	1.92	0.52
2:J:201:MET:N	2:J:217:VAL:O	2.42	0.52
29:f:3243:A:N6	55:a0:157:GLU:OE2	2.38	0.52
35:m:50:ARG:NH2	35:m:72:ASP:OD2	2.43	0.52
44:a:704:LEU:HB3	44:a:938:ILE:HG13	1.91	0.52
45:e:222:LEU:HD11	45:e:226:ASN:ND2	2.22	0.52
45:e:1050:LEU:CD2	45:e:1098:LEU:CD2	2.78	0.52
45:e:1066:ARG:CZ	45:e:1111:GLN:HE22	2.21	0.52
45:e:1495:THR:O	45:e:1499:HIS:CD2	2.63	0.52
53:v:341:MET:HE3	53:v:677:ILE:HG13	1.92	0.52
1:A:216:ILE:C	57:A:901:ATP:N6	2.68	0.51
1:C:605:GLY:HA2	1:C:609:ARG:HH22	1.74	0.51
29:f:2177:G:OP2	32:j:128:ARG:NH1	2.43	0.51
29:f:3230:G:H4'	43:u:132:LYS:HD3	1.92	0.51
45:e:1477:GLN:NE2	45:e:1481:THR:HG1	2.00	0.51
1:A:525:LEU:HD21	1:A:652:LEU:HD13	1.91	0.51
14:N:100:PRO:HG2	14:N:123:VAL:HG23	1.92	0.51
26:b:75:VAL:HG23	26:b:76:LYS:HD2	1.93	0.51
29:f:2307:G:O2'	29:f:2310:U:OP2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:2493:U:H2'	29:f:2494:A:C8	2.44	0.51
53:v:465:CYS:HA	53:v:468:PHE:CE2	2.45	0.51
1:B:261:LYS:NZ	1:B:358:ASN:OD1	2.44	0.51
1:E:562:TYR:HB3	2:K:2:GLN:HA	1.92	0.51
3:G:412:ASP:OD1	3:G:412:ASP:N	2.43	0.51
45:e:272:TYR:HB2	45:e:277:MET:HE3	1.92	0.51
1:B:493:ASP:N	1:B:493:ASP:OD1	2.41	0.51
1:C:557:LEU:HD21	1:C:569:ILE:HG12	1.92	0.51
2:J:236:ILE:O	2:J:241:GLN:NE2	2.42	0.51
29:f:1256:G:O3'	48:z:124:THR:CB	2.59	0.51
29:f:1751:G:C5'	52:X:26:LYS:HZ1	2.13	0.51
38:p:46:LEU:CD1	56:b0:28:THR:O	2.57	0.51
43:u:127:LYS:HB3	55:a0:194:LEU:CD1	2.40	0.51
45:e:277:MET:SD	45:e:278:PRO:CG	2.94	0.51
53:v:298:LEU:HD21	53:v:310:LYS:HE3	1.92	0.51
1:C:665:SER:HA	1:C:668:ASN:HB2	1.91	0.51
1:E:216:ILE:C	57:E:902:ATP:N6	2.62	0.51
1:E:261:LYS:N	1:E:261:LYS:CD	2.70	0.51
1:F:301:GLU:O	1:F:305:LYS:NZ	2.43	0.51
1:F:558:LEU:HG	1:F:606:ALA:HB1	1.91	0.51
3:G:357:MET:O	3:G:361:HIS:ND1	2.44	0.51
21:U:67:ARG:NH2	31:i:97:A:OP1	2.44	0.51
29:f:2540:A:N3	29:f:2541:U:N3	2.59	0.51
38:p:52:TRP:O	38:p:57:ARG:NH1	2.44	0.51
45:e:1499:HIS:C	45:e:1502:PHE:H	2.17	0.51
51:w:50:SER:HA	51:w:157:PHE:O	2.11	0.51
1:B:31:THR:HG21	1:B:83:ILE:HD13	1.93	0.51
1:B:558:LEU:CD2	1:C:562:TYR:CZ	2.92	0.51
38:p:207:ASP:OD1	38:p:207:ASP:N	2.44	0.51
53:v:248:ILE:HD12	53:v:281:PRO:HB2	1.92	0.51
1:A:260:GLY:HA2	57:A:901:ATP:O2A	2.11	0.51
1:B:591:SER:HB2	1:C:609:ARG:HG3	1.91	0.51
1:C:405:ASP:N	1:C:405:ASP:OD1	2.44	0.51
1:C:561:TRP:CE3	2:K:8:LEU:HD12	2.45	0.51
28:d:20:ARG:HA	28:d:23:VAL:HG12	1.92	0.51
29:f:16:A:H5"	56:b0:43:ALA:O	2.11	0.51
29:f:1234:G:N2	48:z:135:THR:CB	2.73	0.51
29:f:1778:G:O2'	29:f:1780:G:OP2	2.28	0.51
29:f:2568:C:O2'	29:f:2569:A:O4'	2.27	0.51
31:i:29:U:H5"	42:t:27:ASP:HB3	1.92	0.51
38:p:50:VAL:HA	56:b0:30:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:751:VAL:CA	45:e:754:ILE:HG12	2.38	0.51
45:e:804:ILE:CD1	45:e:809:MET:SD	2.96	0.51
45:e:910:SER:CB	45:e:955:LEU:HD21	2.38	0.51
46:g:68:ARG:NH2	46:g:112:ASP:O	2.44	0.51
2:K:39:ASP:CG	3:G:472:ASN:ND2	2.67	0.51
20:T:96:GLU:OE2	29:f:2555:G:N1	2.42	0.51
21:U:118:ILE:HD11	42:t:145:PHE:HE2	1.76	0.51
29:f:655:C:H2'	29:f:656:A:H8	1.76	0.51
29:f:1288:U:H2'	29:f:1289:G:H8	1.74	0.51
29:f:1833:G:P	56:b0:114:VAL:HG21	2.51	0.51
29:f:2901:G:O2'	29:f:3024:A:N1	2.44	0.51
35:m:206:GLN:NE2	35:m:210:GLU:OE2	2.44	0.51
45:e:1444:LYS:HD2	45:e:1455:GLN:NE2	2.22	0.51
1:A:464:PHE:O	1:A:468:ASN:ND2	2.44	0.51
1:B:42:THR:HG22	1:B:67:LEU:HD21	1.93	0.51
1:B:534:LYS:HB2	57:C:1001:ATP:O3B	2.11	0.51
1:C:251:VAL:HB	1:C:354:ILE:HG22	1.92	0.51
29:f:76:G:O2'	42:t:100:ARG:NH1	2.37	0.51
29:f:544:C:H2'	29:f:547:G:H1	1.76	0.51
29:f:1661:G:H2'	29:f:1662:G:C8	2.46	0.51
29:f:1833:G:P	56:b0:114:VAL:CB	2.99	0.51
44:a:192:TYR:HE1	44:a:218:PRO:HD2	1.76	0.51
45:e:751:VAL:CA	45:e:754:ILE:HG13	2.31	0.51
45:e:1057:THR:OG1	45:e:1105:LEU:HA	2.11	0.51
29:f:1830:G:C3'	56:b0:91:ASN:HB2	2.39	0.51
29:f:2471:U:H2'	29:f:2474:G:N2	2.26	0.51
34:l:156:LEU:HD12	34:l:159:ILE:HD12	1.93	0.51
45:e:1505:PHE:CD2	45:e:1514:ILE:HG12	2.46	0.51
1:B:489:VAL:CA	57:C:1001:ATP:N6	2.74	0.50
1:F:663:ARG:NH2	1:F:689:THR:OG1	2.44	0.50
29:f:1751:G:C2	52:X:78:LEU:CD2	2.94	0.50
29:f:3198:U:O2	39:q:21:LYS:N	2.44	0.50
45:e:711:LEU:O	45:e:715:LEU:HG	2.10	0.50
45:e:1548:ASN:OD1	53:v:385:ARG:HD2	2.10	0.50
1:A:485:THR:HA	1:A:543:THR:HG21	1.93	0.50
1:B:92:LEU:HD12	1:B:141:VAL:HG21	1.91	0.50
1:B:558:LEU:HD22	1:C:562:TYR:OH	2.05	0.50
1:E:261:LYS:C	1:E:263:LEU:N	2.65	0.50
45:e:1287:ARG:HA	45:e:1290:PHE:HD2	1.76	0.50
1:C:374:ASP:OD1	1:C:374:ASP:N	2.44	0.50
1:C:432:GLN:HG3	1:C:455:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:3160:U:H3	29:f:3290:G:H1	1.58	0.50
39:q:18:VAL:HG12	39:q:27:VAL:HG22	1.94	0.50
1:B:3:VAL:HG21	1:B:69:ILE:HD12	1.94	0.50
27:c:18:TYR:HB3	32:j:180:LEU:HD22	1.93	0.50
29:f:2137:U:OP2	29:f:2142:A:N6	2.40	0.50
29:f:3132:C:O2'	55:a0:55:HIS:CE1	2.65	0.50
30:h:44:C:H4'	35:m:152:ARG:HG3	1.93	0.50
33:k:261:MET:HA	55:a0:64:PHE:HB2	1.93	0.50
39:q:22:SER:OG	39:q:39:LYS:NZ	2.44	0.50
1:B:317:ASP:OD1	1:B:317:ASP:N	2.45	0.50
1:C:470:ASN:ND2	1:C:471:PRO:O	2.44	0.50
1:D:558:LEU:HD12	1:D:560:MET:H	1.77	0.50
1:E:561:TRP:H	1:E:561:TRP:HD1	1.58	0.50
1:F:258:GLY:O	57:F:901:ATP:C2	2.61	0.50
29:f:1019:G:H1	29:f:1033:U:H3	1.59	0.50
31:i:132:G:H5"	56:b0:94:GLN:HG3	1.93	0.50
45:e:1499:HIS:HB3	45:e:1503:SER:OG	2.12	0.50
1:B:698:LEU:HD12	57:C:1001:ATP:O2'	2.12	0.50
1:D:502:THR:HG23	1:D:503:VAL:HG13	1.93	0.50
4:3:60:PHE:HB3	4:3:64:ASN:HB3	1.93	0.50
4:3:62:ARG:NH1	29:f:412:G:OP1	2.45	0.50
45:e:1159:ILE:HG21	45:e:1197:LEU:HD11	1.93	0.50
51:w:138:VAL:HG21	51:w:144:LEU:HD23	1.94	0.50
1:C:561:TRP:CE3	2:K:8:LEU:CD1	2.95	0.50
1:E:669:ALA:O	1:E:672:ARG:NH1	2.45	0.50
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50
34:l:126:ILE:O	34:l:129:THR:OG1	2.30	0.50
1:C:431:GLN:OE1	1:C:434:ARG:NH2	2.44	0.50
1:E:536:LEU:HD23	58:E:901:ADP:H8	1.77	0.50
14:N:26:ARG:NH1	29:f:938:C:OP2	2.44	0.50
29:f:3027:A:O2'	44:a:415:ASP:OD1	2.29	0.50
1:E:696:ASP:OD1	1:F:645:ARG:NH1	2.45	0.50
1:F:263:LEU:HD22	57:F:901:ATP:O2'	1.97	0.50
7:6:22:PRO:O	8:7:146:ASN:ND2	2.38	0.50
17:Q:77:ARG:HD2	17:Q:89:LEU:HD13	1.94	0.50
18:R:104:ASN:ND2	29:f:1389:G:OP1	2.42	0.50
29:f:505:G:OP1	34:l:320:ASN:ND2	2.43	0.50
29:f:3243:A:C2	55:a0:107:GLY:HA3	2.47	0.50
35:m:90:HIS:NE2	35:m:229:ASP:OD2	2.41	0.50
41:s:90:GLN:NE2	41:s:170:ASP:OD1	2.45	0.50
51:w:59:PRO:HD2	51:w:153:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:THR:OG1	1:F:475:ARG:NH2	2.44	0.49
6:5:68:GLN:OE1	6:5:71:ARG:NH2	2.43	0.49
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	0.49
36:n:92:SER:OG	36:n:148:GLU:OE1	2.30	0.49
38:p:161:GLU:HA	38:p:164:VAL:HG22	1.93	0.49
45:e:1071:THR:O	45:e:1074:GLU:OE1	2.29	0.49
45:e:1443:PHE:HB3	45:e:1454:ILE:HD11	1.94	0.49
45:e:1514:ILE:HG23	45:e:1522:LEU:CD2	2.40	0.49
53:v:460:GLU:HG3	53:v:620:PHE:CE1	2.47	0.49
1:D:281:GLY:HA2	1:D:319:ILE:HD11	1.93	0.49
1:D:671:LEU:HD21	1:D:682:LEU:HD11	1.93	0.49
1:F:336:SER:HA	1:F:339:LEU:HD12	1.95	0.49
1:F:522:LYS:HD2	1:F:648:ARG:HG3	1.93	0.49
3:G:167:ILE:O	3:G:171:SER:OG	2.30	0.49
17:Q:80:ASN:OD1	17:Q:81:GLU:N	2.45	0.49
29:f:664:U:H2'	29:f:665:A:C8	2.47	0.49
29:f:1613:A:OP1	52:X:51:LEU:CB	2.60	0.49
44:a:579:TRP:HA	44:a:588:VAL:O	2.11	0.49
1:E:249:ARG:HB2	1:E:342:MET:HE1	1.94	0.49
1:E:663:ARG:HD3	1:E:686:ALA:HB1	1.94	0.49
1:F:393:ILE:HA	1:F:396:LYS:HE3	1.94	0.49
3:G:521:HIS:HD2	3:G:560:LEU:HD13	1.77	0.49
26:b:45:ARG:NH1	29:f:283:G:OP1	2.46	0.49
29:f:1832:C:OP1	56:b0:120:LYS:NZ	2.45	0.49
29:f:2897:A:H2'	29:f:2899:C:H5"	1.93	0.49
38:p:91:PHE:O	38:p:95:ASN:ND2	2.46	0.49
45:e:1539:LEU:HD23	53:v:214:PHE:HE1	1.77	0.49
1:B:664:LEU:O	1:B:668:ASN:ND2	2.45	0.49
1:F:525:LEU:HB2	1:F:652:LEU:HA	1.94	0.49
29:f:3178:A:N1	55:a0:6:VAL:HB	2.28	0.49
44:a:29:ILE:HD12	44:a:80:LEU:HB3	1.94	0.49
45:e:352:PRO:HG3	45:e:397:ASN:ND2	2.26	0.49
1:A:549:PHE:HE1	1:A:585:PHE:HB3	1.77	0.49
1:F:493:ASP:HA	1:F:496:LYS:HE2	1.94	0.49
3:G:259:ARG:NH2	3:G:286:GLU:OE1	2.46	0.49
5:4:56:LYS:NZ	29:f:674:G:O6	2.46	0.49
29:f:3180:A:C5	55:a0:167:TYR:CE2	3.00	0.49
44:a:970:ILE:HD11	44:a:1016:VAL:HG11	1.94	0.49
45:e:753:LEU:HG	45:e:760:THR:HG21	1.94	0.49
48:z:54:LYS:C	48:z:56:ILE:N	2.71	0.49
54:2:13:ILE:HD13	54:2:34:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:155:ARG:HB2	7:6:172:TYR:HD1	1.77	0.49
15:O:25:LYS:NZ	29:f:1106:G:O3'	2.44	0.49
29:f:1824:U:O2'	52:X:17:ARG:CZ	2.61	0.49
33:k:85:VAL:HG22	33:k:202:THR:HG22	1.95	0.49
45:e:751:VAL:CG2	45:e:754:ILE:HD11	2.42	0.49
45:e:1179:LEU:HD22	45:e:1247:LYS:HZ3	1.77	0.49
1:D:216:ILE:CA	57:D:902:ATP:HN61	2.25	0.49
8:7:108:ARG:O	8:7:112:ASN:HB2	2.12	0.49
45:e:1049:ARG:HD2	45:e:1086:MET:SD	2.52	0.49
45:e:1549:ASN:HB3	53:v:440:ARG:O	2.13	0.49
47:x:62:C:H2'	47:x:63:G:C8	2.48	0.49
1:B:532:THR:CA	57:C:1001:ATP:H5'2	2.37	0.49
1:D:254:TYR:HE2	1:D:376:GLU:HB2	1.78	0.49
1:D:562:TYR:CE1	1:D:609:ARG:CZ	2.59	0.49
7:6:93:GLU:HG3	7:6:140:VAL:HG11	1.95	0.49
45:e:272:TYR:CG	45:e:277:MET:CE	2.86	0.49
45:e:1240:LEU:HG	45:e:1290:PHE:HD1	1.78	0.49
1:A:216:ILE:HB	57:A:901:ATP:HN62	1.74	0.49
1:B:658:PRO:O	1:B:663:ARG:NH1	2.46	0.49
1:D:216:ILE:HB	57:D:902:ATP:N6	2.25	0.49
2:K:13:ILE:HG22	2:K:14:THR:HG22	1.93	0.49
29:f:348:A:N3	29:f:352:A:O2'	2.46	0.49
29:f:2815:G:N2	29:f:2818:U:O2	2.45	0.49
29:f:2948:C:OP1	33:k:244:ARG:NH2	2.36	0.49
31:i:156:U:OP2	38:p:84:ARG:NH2	2.45	0.49
44:a:402:VAL:HG22	44:a:433:ILE:HG23	1.95	0.49
1:E:300:PHE:HE1	1:E:311:ILE:HG21	1.77	0.49
2:K:40:GLN:CA	3:G:470:PHE:O	2.57	0.49
29:f:2155:G:OP1	32:j:241:ARG:NH1	2.46	0.49
45:e:793:ASN:CG	45:e:1005:ASN:HD21	2.20	0.49
45:e:1498:VAL:O	45:e:1501:GLN:HB3	2.13	0.49
1:F:234:LEU:HD22	1:F:308:PRO:HB3	1.95	0.48
1:F:693:SER:OG	1:F:694:GLY:N	2.45	0.48
2:J:244:ILE:HD13	3:G:574:MET:HG3	1.94	0.48
5:4:16:ARG:HB2	29:f:974:G:H5'	1.95	0.48
6:5:151:ARG:NH2	6:5:152:GLU:OE2	2.44	0.48
29:f:123:A:OP1	38:p:105:LYS:NZ	2.37	0.48
29:f:1264:G:N2	29:f:1265:U:O4	2.40	0.48
45:e:941:THR:HA	45:e:979:LEU:HD21	1.94	0.48
1:A:500:LYS:HD2	1:A:504:GLU:HG2	1.95	0.48
1:B:534:LYS:HB2	57:C:1001:ATP:O3G	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:LEU:HD13	1:C:589:LEU:HD13	1.94	0.48
1:D:280:ASN:ND2	1:D:283:GLU:OE1	2.45	0.48
1:E:536:LEU:HD23	58:E:901:ADP:C8	2.48	0.48
1:F:564:GLU:OE1	1:F:568:ASN:ND2	2.42	0.48
29:f:1569:U:H5'	29:f:1570:U:H5"	1.94	0.48
29:f:2854:U:OP2	40:r:3:ARG:NH2	2.47	0.48
29:f:2964:G:N2	29:f:2967:A:OP2	2.41	0.48
4:3:65:SER:OG	29:f:1447:G:OP1	2.28	0.48
12:L:16:ARG:NH1	29:f:216:G:OP1	2.45	0.48
16:P:30:THR:HG23	16:P:91:SER:HB2	1.95	0.48
33:k:211:GLN:NE2	33:k:283:TYR:O	2.45	0.48
38:p:46:LEU:HD12	56:b0:29:SER:HA	1.95	0.48
39:q:120:ASP:OD1	39:q:120:ASP:N	2.44	0.48
45:e:1504:GLY:O	45:e:1506:GLU:N	2.40	0.48
1:B:382:PRO:O	1:B:387:ARG:NH1	2.45	0.48
1:B:532:THR:C	57:C:1001:ATP:O2B	2.56	0.48
3:G:168:SER:OG	3:G:171:SER:OG	2.30	0.48
6:5:62:ARG:HH22	29:f:3067:C:H3'	1.77	0.48
29:f:1523:U:C5	56:b0:123:TYR:CZ	3.02	0.48
29:f:3178:A:C5'	55:a0:4:GLU:OE1	2.61	0.48
45:e:882:ASN:C	45:e:885:GLN:O	2.53	0.48
45:e:1050:LEU:HG	45:e:1098:LEU:CD2	2.42	0.48
48:z:52:GLU:O	48:z:53:PHE:C	2.55	0.48
1:A:392:ARG:O	1:A:396:LYS:NZ	2.47	0.48
1:D:531:GLY:HA2	57:D:901:ATP:PB	2.40	0.48
5:4:131:ALA:HB1	5:4:135:GLN:H	1.78	0.48
29:f:591:G:O2'	36:n:17:ALA:O	2.28	0.48
29:f:655:C:H2'	29:f:656:A:C8	2.49	0.48
33:k:145:GLU:HA	33:k:148:LEU:HB2	1.95	0.48
45:e:1477:GLN:HE21	45:e:1481:THR:CG2	2.12	0.48
46:g:146:ILE:HG13	46:g:147:LEU:HD12	1.96	0.48
23:W:52:LYS:NZ	34:l:59:GLN:O	2.39	0.48
29:f:2209:U:C4	44:a:838:ARG:HD2	2.49	0.48
39:q:47:LYS:H	43:u:7:VAL:HG21	1.78	0.48
45:e:212:ILE:HG23	45:e:249:LEU:HD21	1.95	0.48
45:e:807:LYS:HE3	45:e:808:ASN:OD1	2.13	0.48
45:e:930:ASN:O	45:e:933:LEU:N	2.46	0.48
46:g:116:LEU:HG	46:g:177:LEU:HD21	1.94	0.48
53:v:557:HIS:CE1	53:v:608:GLN:HE21	2.31	0.48
3:G:383:THR:OG1	3:G:399:TYR:O	2.32	0.48
5:4:19:PRO:HB3	5:4:53:PHE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:10:LYS:NZ	56:b0:114:VAL:HG12	2.28	0.48
29:f:712:G:OP1	42:t:174:ARG:NH1	2.47	0.48
29:f:1524:A:OP1	56:b0:111:ASN:HA	2.13	0.48
29:f:3180:A:N6	55:a0:167:TYR:CD1	2.82	0.48
34:l:292:SER:OG	34:l:294:GLU:OE1	2.31	0.48
45:e:757:CYS:HB2	45:e:760:THR:HG23	1.95	0.48
45:e:1477:GLN:OE1	45:e:1477:GLN:C	2.56	0.48
46:g:197:MET:HE3	46:g:218:ILE:HD12	1.96	0.48
52:X:5:ILE:HD11	52:X:52:TYR:HB3	1.94	0.48
1:B:560:MET:HB3	1:B:564:GLU:HB2	1.95	0.48
1:D:287:LYS:HD3	1:D:291:GLU:HB2	1.96	0.48
2:H:158:ASP:N	2:H:158:ASP:OD1	2.46	0.48
29:f:3243:A:H2	55:a0:106:GLU:O	1.97	0.48
41:s:38:GLU:HB2	41:s:45:PRO:HD3	1.95	0.48
45:e:793:ASN:HD21	45:e:1005:ASN:ND2	2.11	0.48
45:e:1373:ASN:O	45:e:1374:ILE:C	2.55	0.48
46:g:88:LEU:HD12	46:g:92:VAL:HG21	1.96	0.48
53:v:377:LEU:HD22	53:v:657:GLU:HB3	1.96	0.48
1:D:531:GLY:CA	57:D:901:ATP:PB	3.02	0.48
2:H:117:VAL:HG11	2:H:126:VAL:HG22	1.96	0.48
29:f:1230:G:H4'	49:0:34:SER:HA	1.96	0.48
29:f:1383:G:O3'	34:l:138:ARG:NH2	2.47	0.48
29:f:1833:G:OP2	56:b0:114:VAL:CB	2.62	0.48
45:e:864:HIS:HA	45:e:869:HIS:HB3	1.96	0.48
45:e:1206:GLN:O	45:e:1210:ILE:HG13	2.13	0.48
1:B:671:LEU:HD23	1:B:676:LEU:HD22	1.96	0.48
1:C:238:GLN:HA	1:C:241:LYS:HE2	1.95	0.48
1:E:222:GLN:HE21	1:E:379:ILE:HG22	1.78	0.48
5:4:102:ALA:HA	5:4:122:ILE:O	2.14	0.48
29:f:1523:U:C6	56:b0:123:TYR:CZ	3.01	0.48
31:i:9:A:H2'	31:i:10:A:C8	2.49	0.48
32:j:117:GLU:HG2	32:j:124:GLY:H	1.79	0.48
38:p:44:ARG:O	56:b0:28:THR:CA	2.62	0.48
43:u:127:LYS:HD3	55:a0:194:LEU:CD1	2.43	0.48
45:e:1463:GLY:CA	45:e:1520:ARG:HD3	2.37	0.48
45:e:1504:GLY:C	45:e:1506:GLU:H	2.20	0.48
53:v:377:LEU:CD2	53:v:657:GLU:CB	2.92	0.48
1:D:262:THR:HG21	57:D:902:ATP:PG	2.54	0.47
1:E:339:LEU:HD22	1:E:372:ARG:HD3	1.96	0.47
14:N:94:ALA:HA	14:N:121:VAL:HG23	1.95	0.47
45:e:1174:ILE:HG22	45:e:1198:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:1499:HIS:C	45:e:1501:GLN:N	2.68	0.47
1:E:369:ARG:HB2	1:E:372:ARG:HD2	1.96	0.47
15:O:3:LYS:HD3	29:f:2617:U:H3'	1.95	0.47
44:a:572:TYR:HB2	44:a:575:GLU:HG3	1.96	0.47
45:e:1083:SER:HA	45:e:1086:MET:HE2	1.96	0.47
45:e:1508:CYS:HA	45:e:1533:LYS:O	2.14	0.47
47:y:8:U:O2	47:y:13:U:O4	2.31	0.47
1:C:493:ASP:OD1	1:C:493:ASP:N	2.47	0.47
1:D:241:LYS:HG3	1:D:348:ARG:HH12	1.79	0.47
1:D:314:ASP:OD1	1:D:314:ASP:N	2.47	0.47
1:E:263:LEU:HD12	1:E:266:ARG:HB3	1.95	0.47
29:f:520:U:OP2	37:o:70:LYS:NZ	2.45	0.47
29:f:1814:A:H4'	29:f:1815:U:H5'	1.95	0.47
1:F:263:LEU:HD13	57:F:901:ATP:O2A	2.13	0.47
3:G:126:ASP:OD1	3:G:126:ASP:N	2.46	0.47
29:f:411:U:H2'	29:f:412:G:H8	1.79	0.47
29:f:1523:U:O5'	56:b0:113:LEU:CD2	2.61	0.47
32:j:32:LEU:HD13	32:j:163:ARG:HD3	1.96	0.47
34:l:304:GLN:NE2	34:l:306:THR:O	2.42	0.47
38:p:156:ASP:N	38:p:156:ASP:OD1	2.47	0.47
45:e:1525:LYS:CE	53:v:214:PHE:HA	2.44	0.47
45:e:1560:PHE:CD1	53:v:213:LEU:HD13	2.49	0.47
53:v:176:LEU:HD11	53:v:182:PHE:CD1	2.49	0.47
1:B:249:ARG:NH1	1:B:342:MET:O	2.48	0.47
1:D:403:ASP:OD2	1:D:459:MET:N	2.47	0.47
1:D:560:MET:CG	1:D:561:TRP:CZ3	2.97	0.47
3:G:336:ASP:OD1	3:G:336:ASP:N	2.45	0.47
29:f:2185:G:O2'	29:f:2314:U:OP2	2.28	0.47
29:f:3006:A:O2'	55:a0:73:PHE:CE2	2.48	0.47
31:i:126:A:O2'	31:i:129:C:N4	2.48	0.47
45:e:882:ASN:O	45:e:885:GLN:C	2.50	0.47
1:E:261:LYS:NZ	57:E:902:ATP:O1G	2.48	0.47
1:F:614:LEU:O	1:F:648:ARG:NH2	2.47	0.47
5:4:170:ARG:HD2	14:N:57:GLY:HA3	1.97	0.47
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.96	0.47
29:f:2473:C:C5	29:f:2474:G:C2	3.03	0.47
35:m:119:TYR:OH	35:m:139:PRO:O	2.33	0.47
45:e:1435:ASP:OD2	45:e:1514:ILE:HB	2.15	0.47
1:A:246:LYS:HD3	1:A:247:PRO:HD2	1.97	0.47
1:C:603:ALA:HB2	2:K:3:ILE:HB	1.96	0.47
1:D:216:ILE:HA	57:D:902:ATP:HN61	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:THR:HG23	1:E:261:LYS:HD2	1.97	0.47
1:E:574:ASP:OD1	1:E:574:ASP:N	2.47	0.47
14:N:115:LYS:HA	29:f:715:A:H5"	1.97	0.47
19:S:99:ARG:NH1	29:f:3275:U:O2'	2.48	0.47
29:f:912:G:OP2	32:j:9:ARG:NH2	2.45	0.47
29:f:1523:U:O4'	56:b0:123:TYR:HE2	1.96	0.47
29:f:1805:C:H2'	29:f:1806:A:H8	1.79	0.47
29:f:1833:G:P	56:b0:114:VAL:CG2	3.02	0.47
29:f:1907:C:O2	33:k:240:ARG:NH2	2.45	0.47
35:m:207:TYR:HA	35:m:210:GLU:HG2	1.97	0.47
43:u:38:ILE:HA	43:u:44:VAL:HG12	1.96	0.47
43:u:127:LYS:CD	55:a0:194:LEU:CD1	2.92	0.47
45:e:371:LEU:HB2	45:e:377:TRP:HE1	0.67	0.47
45:e:932:LEU:C	45:e:964:PHE:CE2	2.93	0.47
1:A:260:GLY:HA3	57:A:901:ATP:H5'2	1.94	0.47
1:D:694:GLY:HA3	57:D:901:ATP:N3	2.30	0.47
3:G:236:HIS:ND1	3:G:467:THR:O	2.47	0.47
7:6:167:ARG:NE	55:a0:119:VAL:HG11	2.30	0.47
29:f:627:U:H2'	29:f:628:A:C8	2.50	0.47
29:f:1477:A:OP1	29:f:3075:G:O2'	2.31	0.47
29:f:2239:G:O2'	44:a:867:GLY:O	2.30	0.47
33:k:219:ALA:HB2	33:k:336:VAL:HG23	1.96	0.47
40:r:66:GLU:OE1	40:r:69:ARG:NH2	2.47	0.47
42:t:76:THR:HG22	42:t:78:ALA:H	1.80	0.47
53:v:292:LEU:HD21	53:v:328:LYS:HB2	1.97	0.47
1:A:687:LYS:O	1:A:690:GLN:NE2	2.48	0.47
1:B:709:ILE:HG23	1:C:512:GLN:HE21	1.80	0.47
1:E:481:SER:HB2	1:E:543:THR:HG22	1.97	0.47
1:E:650:ASP:OD1	1:E:650:ASP:N	2.47	0.47
6:5:21:LYS:HE3	6:5:55:VAL:HA	1.97	0.47
20:T:95:ILE:HD11	29:f:2555:G:N7	2.30	0.47
24:Y:7:PHE:CZ	56:b0:88:MET:HE2	2.50	0.47
35:m:163:LEU:HD11	35:m:175:HIS:HB3	1.97	0.47
43:u:124:ARG:CA	55:a0:194:LEU:HD21	2.45	0.47
44:a:660:CYS:SG	44:a:661:PHE:N	2.88	0.47
51:w:122:ARG:HA	51:w:122:ARG:HD2	1.64	0.47
53:v:342:MET:HG2	53:v:681:ILE:HG23	1.96	0.47
2:J:207:THR:HA	2:J:269:LEU:HB3	1.97	0.47
13:M:22:LYS:NZ	13:M:132:SER:O	2.47	0.47
18:R:60:ASN:HB3	18:R:63:THR:HB	1.97	0.47
26:b:41:ARG:NH1	29:f:284:A:OP2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:2499:U:H2'	29:f:2500:A:C8	2.50	0.47
29:f:2874:G:O6	29:f:2945:G:H2'	2.15	0.47
45:e:1023:ARG:HA	45:e:1026:MET:HE3	1.97	0.47
46:g:219:GLU:HA	46:g:224:LEU:HD12	1.96	0.47
53:v:557:HIS:HE1	53:v:608:GLN:HE21	1.61	0.47
1:D:615:LEU:O	1:D:648:ARG:NH1	2.48	0.46
1:D:695:ALA:HA	1:D:698:LEU:HD12	1.96	0.46
1:E:452:LEU:HA	1:E:455:LEU:HD23	1.98	0.46
3:G:198:PHE:H	3:G:408:LEU:HD22	1.80	0.46
32:j:68:LYS:HE2	32:j:70:ARG:HH21	1.80	0.46
45:e:1505:PHE:CB	45:e:1514:ILE:HG12	2.40	0.46
53:v:374:GLN:NE2	54:2:10:GLY:CA	2.72	0.46
1:A:262:THR:HG23	57:A:901:ATP:O3B	2.15	0.46
57:D:901:ATP:O1B	1:E:645:ARG:NH2	2.48	0.46
1:E:430:MET:SD	1:F:375:ARG:NH2	2.87	0.46
29:f:1524:A:H5"	56:b0:111:ASN:CG	2.40	0.46
29:f:2444:C:H2'	29:f:2445:A:C8	2.41	0.46
33:k:96:PRO:HG3	55:a0:153:VAL:HG22	1.97	0.46
40:r:54:SER:OG	40:r:130:ASP:O	2.33	0.46
40:r:54:SER:HB3	40:r:135:ILE:HD11	1.97	0.46
45:e:876:PHE:HZ	45:e:963:MET:HB3	1.80	0.46
46:g:14:GLY:HA2	46:g:198:VAL:HG13	1.96	0.46
1:B:437:MET:HE2	1:B:437:MET:HB2	1.73	0.46
1:B:534:LYS:HB2	57:C:1001:ATP:PG	2.56	0.46
1:F:317:ASP:N	1:F:317:ASP:OD1	2.48	0.46
1:F:640:ASP:OD1	1:F:640:ASP:N	2.47	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
29:f:2384:A:H61	55:a0:96:LYS:HE3	1.78	0.46
29:f:2875[B]:U:O2'	47:x:76:A:H4'	2.15	0.46
29:f:3375:A:O2'	29:f:3378:C:OP2	2.26	0.46
45:e:844:LEU:HD23	45:e:844:LEU:O	2.16	0.46
45:e:992:LEU:HD22	45:e:1034:TRP:CE3	2.50	0.46
45:e:1498:VAL:O	45:e:1502:PHE:N	2.47	0.46
49:0:26:PHE:HZ	49:0:93:LEU:HA	1.80	0.46
52:X:5:ILE:CD1	52:X:14:LEU:HD12	2.45	0.46
1:A:529:PRO:HA	1:A:530:PRO:HD3	1.85	0.46
1:B:532:THR:HG21	57:C:1001:ATP:C6	2.51	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
29:f:40:A:OP1	61:f:3401:SPD:N10	2.48	0.46
29:f:1523:U:H4'	56:b0:113:LEU:CB	2.30	0.46
29:f:1717:U:H2'	29:f:1718:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:l:326:ARG:O	37:o:41:ARG:NH2	2.48	0.46
45:e:1181:ASP:O	45:e:1185:GLY:N	2.45	0.46
1:A:343:ASP:OD2	1:A:372:ARG:NH2	2.47	0.46
2:H:123:ILE:HB	2:H:152:ASP:HA	1.97	0.46
29:f:1612:A:OP2	52:X:46:ARG:NH1	2.48	0.46
32:j:104:LEU:HD12	32:j:158:ILE:HD11	1.98	0.46
8:7:116:ARG:NH2	29:f:1096:U:OP2	2.48	0.46
17:Q:75:ILE:HG12	17:Q:93:VAL:HG22	1.96	0.46
29:f:1949:G:H1	29:f:2097:U:H3	1.63	0.46
29:f:2094:C:H2'	29:f:2095:G:H8	1.81	0.46
29:f:2473:C:C4	29:f:2475:G:N3	2.83	0.46
29:f:3243:A:N1	55:a0:107:GLY:C	2.74	0.46
44:a:576:LYS:HB2	47:y:31:C:H5'	1.98	0.46
45:e:883:VAL:HG12	45:e:956:LEU:HD21	1.98	0.46
47:y:43:G:H3'	47:y:44:A:H8	1.80	0.46
1:B:430:MET:HG2	1:C:375:ARG:HH12	1.81	0.46
1:F:260:GLY:HA2	57:F:901:ATP:O2A	2.16	0.46
1:F:495:ILE:HD11	1:F:653:ILE:HD12	1.97	0.46
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
44:a:346:SER:HB2	44:a:564:VAL:HG13	1.98	0.46
4:3:67:ILE:HD11	4:3:80:LYS:HB3	1.97	0.46
29:f:571:U:H2'	29:f:572:A:H8	1.81	0.46
29:f:2451:G:H2'	29:f:2452:G:C8	2.50	0.46
29:f:3244:A:N7	55:a0:109:PRO:HB3	2.29	0.46
43:u:126:GLN:HB3	55:a0:190:VAL:HG11	1.96	0.46
53:v:233:VAL:HG21	53:v:278:ASP:CB	2.44	0.46
53:v:377:LEU:HD11	53:v:637:GLU:OE1	2.16	0.46
1:A:432:GLN:OE1	1:A:461:ASN:ND2	2.49	0.46
1:B:44:LEU:HD11	1:B:63:VAL:HG11	1.97	0.46
1:C:369:ARG:HH21	1:C:372:ARG:HH22	1.63	0.46
12:L:86:THR:OG1	12:L:95:VAL:O	2.34	0.46
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.46
19:S:49:ILE:HD11	19:S:71:VAL:HG22	1.96	0.46
29:f:2392:C:O2'	33:k:266:ARG:NH2	2.48	0.46
29:f:2498:U:H2'	29:f:2499:U:C6	2.51	0.46
44:a:618:SER:OG	44:a:646:SER:OG	2.26	0.46
45:e:1446:PRO:HD3	45:e:1454:ILE:HA	1.98	0.46
45:e:1477:GLN:CD	45:e:1477:GLN:O	2.59	0.46
54:2:42:ARG:HE	54:2:49:GLN:NE2	2.14	0.46
1:C:280:ASN:HB3	1:C:283:GLU:HB2	1.97	0.46
1:D:694:GLY:HA2	1:D:697:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:LEU:O	1:E:264:MET:C	2.59	0.46
1:F:647:GLY:H	1:F:650:ASP:HB3	1.81	0.46
26:b:30:ALA:O	29:f:2767:U:O2'	2.29	0.46
29:f:2218:G:H2'	29:f:2219:A:H8	1.80	0.46
37:o:86:VAL:O	37:o:114:GLY:HA2	2.16	0.46
45:e:930:ASN:O	45:e:933:LEU:HB3	2.15	0.46
1:B:286:SER:OG	1:C:290:GLY:O	2.33	0.45
1:C:536:LEU:HD12	57:C:1003:ATP:N7	2.29	0.45
1:E:562:TYR:CZ	1:E:609:ARG:CZ	2.99	0.45
2:H:115:LEU:HD11	2:H:129:LYS:HB3	1.98	0.45
4:3:22:LEU:HD12	4:3:146:ILE:HD12	1.97	0.45
29:f:2473:C:C6	29:f:2474:G:N3	2.84	0.45
35:m:83:LEU:HB3	35:m:88:ILE:HB	1.98	0.45
44:a:4:ARG:HD2	47:x:33:U:H4'	1.97	0.45
45:e:1017:VAL:HG12	45:e:1019:ILE:O	2.16	0.45
49:0:104:ARG:HA	49:0:104:ARG:HD2	1.85	0.45
53:v:341:MET:SD	53:v:368:HIS:HE1	2.38	0.45
1:C:383:ASP:O	1:C:387:ARG:NH2	2.49	0.45
1:E:499:LEU:HD11	1:E:524:VAL:HG11	1.97	0.45
10:I:18:PRO:HA	10:I:51:ALA:HA	1.97	0.45
29:f:1119:C:H2'	29:f:1120:A:H8	1.81	0.45
29:f:2676:A:OP1	44:a:652:LYS:NZ	2.46	0.45
29:f:3116:G:OP1	29:f:3116:G:N2	2.43	0.45
29:f:3379:C:H4'	33:k:315:GLY:HA2	1.98	0.45
34:l:8:VAL:HG23	34:l:151:VAL:HG12	1.98	0.45
43:u:123:LEU:HD21	55:a0:193:GLN:NE2	2.32	0.45
45:e:272:TYR:N	45:e:277:MET:CG	2.79	0.45
45:e:793:ASN:HD21	45:e:1005:ASN:HD21	1.63	0.45
45:e:1502:PHE:HE1	45:e:1515:LEU:HD21	1.80	0.45
46:g:11:ASN:ND2	46:g:209:ASP:OD2	2.49	0.45
1:B:117:ALA:HA	45:e:1029:ARG:NH2	2.30	0.45
1:D:531:GLY:N	57:D:901:ATP:O1B	2.46	0.45
5:4:35:PHE:HE1	29:f:1348:U:H5'	1.80	0.45
29:f:835:G:O2'	29:f:857:G:N2	2.37	0.45
29:f:2876:C:H2'	29:f:2877:G:O4'	2.16	0.45
29:f:3022:G:O2'	29:f:3031:G:O6	2.32	0.45
30:h:7:G:OP1	35:m:33:ARG:NH1	2.48	0.45
45:e:298:ILE:HD13	45:e:342:PHE:CE1	2.51	0.45
45:e:1269:LEU:HD23	45:e:1351:LEU:HB3	1.98	0.45
53:v:538:PHE:CE2	53:v:544:GLY:HA3	2.52	0.45
29:f:829:U:H3	29:f:895:A:H62	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:q:41:ILE:HD13	39:q:71:VAL:HB	1.99	0.45
43:u:127:LYS:HD3	55:a0:194:LEU:HD12	1.98	0.45
44:a:101:LEU:HB2	44:a:116:PHE:HE2	1.81	0.45
45:e:368:HIS:CE1	45:e:370:PHE:HB2	2.50	0.45
45:e:770:ILE:HD12	45:e:901:SER:HB2	1.98	0.45
47:x:6:U:H2'	47:x:7:G:C8	2.51	0.45
1:C:594:LYS:HE3	1:C:607:SER:HB3	1.99	0.45
1:F:343:ASP:OD1	1:F:343:ASP:N	2.45	0.45
2:K:44:ILE:HG22	2:K:45:PHE:N	2.32	0.45
17:Q:44:MET:O	17:Q:77:ARG:NH1	2.49	0.45
23:W:81:GLY:O	31:i:95:G:O2'	2.32	0.45
29:f:15:C:H5"	56:b0:42:ARG:HG3	1.95	0.45
29:f:2205:U:O4	44:a:854:GLN:NE2	2.42	0.45
29:f:2284:C:N4	29:f:2308:C:OP2	2.50	0.45
29:f:3092:C:O2'	29:f:3094:A:OP2	2.28	0.45
32:j:14:SER:OG	32:j:15:ILE:N	2.50	0.45
53:v:252:GLY:O	53:v:256:HIS:HA	2.16	0.45
1:A:262:THR:HG21	57:A:901:ATP:O3G	2.16	0.45
1:A:316:ILE:HD13	1:A:355:ALA:HB1	1.99	0.45
1:C:400:LEU:HA	1:C:457:VAL:HG22	1.99	0.45
1:C:561:TRP:CD2	2:K:8:LEU:CD1	2.98	0.45
1:F:527:TYR:HB3	1:F:633:THR:HG23	1.98	0.45
6:5:34:GLN:HG2	53:v:254:LYS:HE3	1.28	0.45
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.45
29:f:528:U:H2'	29:f:529:A:C8	2.51	0.45
29:f:1134:G:O2'	29:f:2642:A:N3	2.44	0.45
29:f:1497:C:H2'	29:f:1498:A:H8	1.81	0.45
29:f:3023:U:OP1	45:e:61:THR:HG21	2.16	0.45
44:a:4:ARG:NH1	44:a:118:SER:HA	2.30	0.45
45:e:272:TYR:HE1	45:e:323:TYR:HB2	1.81	0.45
45:e:917:LEU:HD12	45:e:959:ILE:CG2	2.47	0.45
1:F:263:LEU:HD22	57:F:901:ATP:C3'	2.43	0.45
29:f:19:U:H2'	29:f:20:A:C8	2.52	0.45
33:k:34:LYS:HE2	33:k:34:LYS:HB2	1.85	0.45
37:o:232:ARG:O	37:o:235:PHE:N	2.48	0.45
45:e:1079:LEU:HD23	45:e:1079:LEU:HA	1.61	0.45
46:g:106:ASN:OD1	46:g:150:SER:OG	2.34	0.45
47:x:29:C:H2'	47:x:30:C:C6	2.52	0.45
53:v:377:LEU:HD22	53:v:657:GLU:CB	2.47	0.45
1:B:59:ILE:HD11	1:B:69:ILE:HD11	1.98	0.45
1:C:591:SER:O	1:C:594:LYS:NZ	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:TYR:CD1	1:D:562:TYR:O	2.69	0.45
1:D:577:ARG:NH2	1:D:620:GLY:O	2.45	0.45
1:F:387:ARG:HA	1:F:390:VAL:HG22	1.98	0.45
10:I:129:VAL:O	10:I:133:SER:HB3	2.17	0.45
14:N:7:LYS:NZ	29:f:1373:A:OP2	2.40	0.45
26:b:7:THR:OG1	26:b:22:GLN:NE2	2.37	0.45
29:f:1750:A:OP2	52:X:42:LYS:HD2	2.15	0.45
43:u:55:ARG:NH2	43:u:76:ALA:O	2.48	0.45
45:e:1544:ARG:HD3	53:v:225:ILE:CG2	2.47	0.45
49:0:45:LEU:HB3	49:0:49:ALA:HB3	1.99	0.45
1:B:291:GLU:OE1	3:G:222:SER:OG	2.35	0.45
1:D:511:ASP:N	1:D:511:ASP:OD1	2.46	0.45
29:f:297:G:OP2	29:f:297:G:N2	2.41	0.45
29:f:307:A:H2'	29:f:308:A:C8	2.52	0.45
29:f:675:C:O2'	29:f:679:U:OP1	2.35	0.45
29:f:799:G:O2'	42:t:18:TRP:NE1	2.47	0.45
45:e:397:ASN:O	45:e:398:SER:C	2.60	0.45
45:e:1294:LEU:HB3	45:e:1300:ILE:HG12	1.99	0.45
1:B:52:LEU:HD11	1:B:58:ARG:HG3	1.99	0.45
1:B:677:GLU:HG3	1:B:679:GLY:H	1.82	0.45
1:C:437:MET:SD	1:C:437:MET:N	2.88	0.45
3:G:526:ASN:HB3	3:G:529:LEU:HB3	1.97	0.45
6:5:6:THR:OG1	29:f:1498:A:OP1	2.28	0.45
12:L:74:TYR:HB3	12:L:77:LYS:HB2	1.98	0.45
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.45
22:V:53:TYR:HA	22:V:56:ARG:HG2	1.99	0.45
29:f:358:G:N2	29:f:361:A:OP2	2.42	0.45
29:f:599:C:OP1	34:l:332:LYS:NZ	2.45	0.45
29:f:1307:G:H5'	55:a0:60:LYS:HE3	1.98	0.45
29:f:1523:U:C4	56:b0:75:LYS:HE3	2.51	0.45
29:f:2473:C:H2'	29:f:2474:G:C4'	2.47	0.45
38:p:52:TRP:CZ3	56:b0:32:PHE:CE1	3.05	0.45
43:u:48:GLY:HA3	43:u:53:VAL:HB	1.98	0.45
45:e:910:SER:OG	45:e:955:LEU:HD11	2.17	0.45
45:e:1196:THR:CG2	45:e:1197:LEU:N	2.80	0.45
45:e:1400:PHE:HE1	45:e:1428:VAL:HG22	1.81	0.45
46:g:2:ALA:HA	46:g:204:ALA:O	2.16	0.45
47:x:62:C:H2'	47:x:63:G:H8	1.82	0.45
1:C:282:PRO:HB3	1:D:332:ARG:HG2	1.98	0.44
1:D:557:LEU:HD21	1:D:569:ILE:HD12	1.99	0.44
1:E:325:LYS:HD3	1:E:325:LYS:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:VAL:HA	1:F:393:ILE:HD12	1.99	0.44
1:F:436:LYS:HD3	1:F:436:LYS:HA	1.79	0.44
3:G:255:THR:HG23	3:G:257:MET:H	1.82	0.44
29:f:86:G:O2'	29:f:98:G:O6	2.32	0.44
29:f:1523:U:N3	56:b0:123:TYR:CE1	2.84	0.44
31:i:134:G:O3'	56:b0:53:HIS:N	2.51	0.44
45:e:141:CYS:SG	45:e:221:LYS:CD	3.03	0.44
45:e:321:ASP:HA	45:e:328:ILE:HG12	1.99	0.44
1:B:536:LEU:HD13	57:C:1001:ATP:C8	2.50	0.44
1:C:587:ASP:N	1:C:587:ASP:OD1	2.51	0.44
1:E:262:THR:CG2	57:E:902:ATP:O1A	2.66	0.44
5:4:180:ARG:HH22	29:f:2719:U:H5"	1.82	0.44
29:f:2660:G:OP1	29:f:2750:U:O2'	2.35	0.44
35:m:65:ILE:HG12	35:m:74:VAL:HG22	1.99	0.44
38:p:53:PRO:CD	56:b0:32:PHE:CD2	2.95	0.44
45:e:1052:LEU:HB2	45:e:1079:LEU:HD11	1.99	0.44
45:e:1502:PHE:CE1	45:e:1515:LEU:HD21	2.52	0.44
53:v:345:TYR:CD2	53:v:349:ILE:HD12	2.53	0.44
1:B:328:GLY:HA3	2:K:15:LEU:HD23	2.00	0.44
4:3:179:GLN:HA	4:3:182:ILE:HG22	2.00	0.44
23:W:30:GLN:NE2	29:f:904:A:OP2	2.50	0.44
29:f:494:G:H2'	29:f:495:G:H8	1.82	0.44
44:a:199:ILE:HG12	44:a:212:LYS:HE3	1.99	0.44
45:e:378:LEU:O	45:e:379:PRO:C	2.60	0.44
45:e:1435:ASP:OD1	45:e:1514:ILE:HB	2.17	0.44
47:x:67:U:H2'	47:x:68:C:C6	2.52	0.44
1:E:301:GLU:O	1:E:305:LYS:NZ	2.49	0.44
1:F:605:GLY:HA2	1:F:609:ARG:HB2	1.99	0.44
15:O:14:ARG:NH2	29:f:1139:G:OP2	2.51	0.44
30:h:62:U:O2'	35:m:285:ARG:NH2	2.50	0.44
32:j:140:ASN:O	32:j:144:ASN:HA	2.16	0.44
35:m:205:SER:HB3	35:m:236:LEU:HD21	2.00	0.44
45:e:1059:LEU:HG	45:e:1065:VAL:HG11	2.00	0.44
1:A:262:THR:HG23	57:A:901:ATP:O3G	2.16	0.44
57:D:902:ATP:O1B	1:E:369:ARG:NH2	2.50	0.44
1:F:222:GLN:HE21	1:F:379:ILE:HD13	1.82	0.44
1:F:383:ASP:OD1	1:F:383:ASP:N	2.45	0.44
10:I:117:PRO:HA	10:I:135:VAL:HG13	2.00	0.44
13:M:133:LYS:NZ	29:f:1808:G:OP2	2.44	0.44
22:V:9:ILE:HD12	42:t:174:ARG:HB2	1.99	0.44
29:f:1786:G:H2'	29:f:1787:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:2116:G:OP1	29:f:2118:C:N4	2.50	0.44
29:f:2357:A:H2'	29:f:2358:A:C8	2.53	0.44
29:f:2514:U:H5'	38:p:68:ARG:HG3	2.00	0.44
32:j:135:ILE:HD12	32:j:149:ARG:HE	1.82	0.44
33:k:83:PRO:O	33:k:165:GLN:NE2	2.48	0.44
36:n:175:LYS:O	43:u:117:ARG:NH2	2.50	0.44
45:e:1540:TYR:HE1	53:v:210:PHE:CE2	2.36	0.44
52:X:21:LYS:C	52:X:73:LEU:HD12	2.43	0.44
1:C:336:SER:HA	1:C:339:LEU:HG	1.99	0.44
1:C:561:TRP:CE2	2:K:8:LEU:HD11	2.52	0.44
1:C:702:GLN:NE2	1:D:521:SER:OG	2.50	0.44
1:D:561:TRP:CD1	2:K:5:VAL:N	2.85	0.44
1:D:622:ASN:HB3	1:D:625:LYS:HD2	1.99	0.44
1:E:217:GLY:N	57:E:902:ATP:N6	2.66	0.44
2:H:155:THR:OG1	2:H:156:LEU:N	2.50	0.44
25:Z:124:LYS:NZ	29:f:2897:A:OP2	2.47	0.44
33:k:215:ILE:HD12	33:k:338:LEU:HD12	1.98	0.44
34:l:74:ILE:HD12	34:l:75:PRO:HD2	2.00	0.44
45:e:130:LYS:HE3	45:e:130:LYS:HB2	1.79	0.44
45:e:240:ILE:HG22	45:e:246:ILE:HD11	2.00	0.44
47:x:41:G:H2'	47:x:42:A:C8	2.53	0.44
53:v:479:TYR:OH	53:v:512:ARG:HD3	2.17	0.44
1:D:485:THR:OG1	1:D:486:TRP:N	2.51	0.44
1:D:559:SER:CB	1:E:562:TYR:CZ	2.88	0.44
1:F:680:LEU:HG	1:F:755:LYS:HG3	1.98	0.44
10:I:128:ARG:NE	46:g:12:GLU:OE2	2.50	0.44
29:f:1282:G:OP1	49:0:56:ASN:N	2.40	0.44
29:f:1888:U:H5"	33:k:247:ARG:HB2	2.00	0.44
29:f:2697:A:H2'	29:f:2698:G:C8	2.52	0.44
33:k:106:TRP:O	33:k:137:TYR:OH	2.24	0.44
37:o:83:LEU:HD11	37:o:116:PHE:HB3	1.99	0.44
38:p:50:VAL:HG22	56:b0:29:SER:O	2.17	0.44
47:x:26:G:C6	47:x:43:G:O6	2.69	0.44
53:v:211:LYS:CE	53:v:222:LEU:HD11	2.41	0.44
1:B:92:LEU:CD2	1:B:160:GLU:HB2	2.46	0.44
1:C:706:LYS:HB2	1:D:501:GLU:HG2	2.00	0.44
1:E:562:TYR:CD1	1:E:562:TYR:O	2.70	0.44
1:E:562:TYR:CB	2:K:2:GLN:HA	2.48	0.44
1:F:321:PRO:HD2	1:F:323:ARG:HH12	1.82	0.44
38:p:95:ASN:OD1	38:p:98:ARG:NH2	2.51	0.44
53:v:643:ALA:HB1	54:2:64:GLU:HG2	1.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ASN:OD1	1:C:332:ARG:NH1	2.51	0.44
1:C:663:ARG:HG2	1:C:666:ILE:HD12	2.00	0.44
1:F:622:ASN:O	1:F:624:LYS:NZ	2.42	0.44
1:F:671:LEU:HD13	1:F:676:LEU:HD22	1.99	0.44
3:G:495:MET:N	3:G:495:MET:SD	2.91	0.44
3:G:563:LEU:O	3:G:566:SER:OG	2.36	0.44
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.44
29:f:2768:U:H2'	29:f:2769:A:H8	1.83	0.44
29:f:3178:A:N6	55:a0:6:VAL:CG2	2.81	0.44
48:z:51:LYS:O	48:z:55:GLY:N	2.51	0.44
53:v:491:MET:HE2	53:v:502:PHE:CG	2.52	0.44
1:C:485:THR:OG1	1:C:486:TRP:N	2.48	0.43
1:E:571:ASP:O	1:E:575:LYS:NZ	2.47	0.43
2:H:172:ARG:O	2:H:174:ARG:NH2	2.51	0.43
3:G:413:MET:HG3	3:G:434:VAL:HG11	2.00	0.43
7:6:70:THR:OG1	43:u:55:ARG:NH1	2.51	0.43
18:R:3:SER:OG	18:R:4:LEU:N	2.51	0.43
29:f:1666:G:H2'	29:f:1667:A:H8	1.83	0.43
29:f:3007:U:H5"	55:a0:73:PHE:HA	1.99	0.43
29:f:3016:A:H2'	29:f:3017:A:H8	1.83	0.43
45:e:1508:CYS:O	45:e:1512:TYR:N	2.47	0.43
49:0:14:LYS:HE3	49:0:52:LEU:HD11	2.00	0.43
1:B:644:LEU:HA	1:B:649:LEU:HD12	2.00	0.43
1:F:259:THR:C	57:F:901:ATP:N1	2.76	0.43
3:G:325:ILE:HG22	3:G:384:CYS:HB3	2.00	0.43
7:6:164:SER:CB	55:a0:121:PRO:HG3	2.48	0.43
10:I:38:ALA:HB3	10:I:59:MET:HB2	1.99	0.43
12:L:112:ASP:OD2	31:i:85:G:N1	2.49	0.43
16:P:9:SER:OG	16:P:10:ILE:N	2.39	0.43
26:b:100:LYS:HE3	26:b:100:LYS:HB3	1.90	0.43
29:f:1524:A:H5"	56:b0:111:ASN:OD1	2.17	0.43
29:f:1675:G:H2'	29:f:1676:A:H8	1.83	0.43
29:f:2960:C:H2'	29:f:2961:G:C8	2.53	0.43
32:j:101:VAL:HG22	32:j:165:VAL:HG22	2.00	0.43
38:p:46:LEU:HD12	56:b0:28:THR:C	2.42	0.43
38:p:46:LEU:C	56:b0:27:ARG:O	2.61	0.43
45:e:773:PHE:HA	45:e:812:LEU:HD11	1.99	0.43
45:e:1240:LEU:HG	45:e:1290:PHE:CD1	2.54	0.43
45:e:1283:SER:OG	45:e:1286:MET:HG2	2.17	0.43
51:w:96:ASN:HD21	51:w:99:LEU:HD12	1.84	0.43
1:A:219:CYS:HB2	1:A:222:GLN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:LYS:HE3	1:F:464:PHE:HA	2.00	0.43
1:C:317:ASP:HA	1:C:363:ILE:HD13	2.00	0.43
1:D:561:TRP:HE1	2:K:5:VAL:C	2.26	0.43
1:F:504:GLU:HB3	1:F:545:VAL:HG12	2.00	0.43
23:W:63:ARG:NH1	31:i:58:G:O6	2.50	0.43
29:f:3295:A:H2'	29:f:3296:A:C8	2.53	0.43
45:e:932:LEU:C	45:e:933:LEU:HA	2.42	0.43
45:e:1075:LEU:HD23	45:e:1075:LEU:HA	1.80	0.43
49:0:15:LEU:O	49:0:19:LEU:HG	2.18	0.43
1:D:561:TRP:CD1	2:K:6:LYS:HD3	2.54	0.43
1:E:262:THR:HG21	57:E:902:ATP:O1A	2.18	0.43
1:E:535:THR:OG1	58:E:901:ADP:O3A	2.35	0.43
29:f:696:C:OP2	34:l:119:ARG:NH2	2.49	0.43
29:f:1222:G:N2	29:f:1285:G:O2'	2.51	0.43
29:f:1748:G:OP1	52:X:44:LYS:HE3	1.97	0.43
29:f:1748:G:OP1	52:X:44:LYS:NZ	2.41	0.43
31:i:134:G:H5"	56:b0:53:HIS:C	2.44	0.43
44:a:704:LEU:HD23	44:a:938:ILE:HD11	2.00	0.43
45:e:1498:VAL:HG13	45:e:1502:PHE:CD2	2.53	0.43
47:x:56:C:O2'	47:x:57:G:P	2.76	0.43
1:A:590:ASP:OD1	1:A:590:ASP:N	2.48	0.43
1:E:529:PRO:O	1:E:534:LYS:NZ	2.51	0.43
2:K:36:ILE:HG23	2:K:37:PRO:HD2	1.98	0.43
7:6:32:SER:HB2	7:6:36:ILE:HD12	2.01	0.43
13:M:64:LYS:NZ	29:f:1811:G:N7	2.64	0.43
29:f:710:A:H2'	29:f:711:A:C8	2.54	0.43
29:f:1524:A:OP1	56:b0:111:ASN:CA	2.67	0.43
29:f:1750:A:H4'	52:X:26:LYS:HZ3	1.84	0.43
29:f:2160:G:H2'	29:f:2161:G:H8	1.84	0.43
29:f:2840:C:N4	29:f:2845:A:O2'	2.50	0.43
45:e:1303:MET:CA	45:e:1303:MET:HE3	2.40	0.43
45:e:1435:ASP:OD2	45:e:1514:ILE:CB	2.67	0.43
46:g:38:PHE:O	46:g:42:LEU:HB2	2.19	0.43
47:y:61:C:H2'	47:y:62:C:C6	2.54	0.43
53:v:501:GLY:HA2	53:v:567:TYR:CE1	2.53	0.43
57:C:1003:ATP:PB	1:D:645:ARG:CZ	3.00	0.43
1:D:689:THR:HB	1:D:692:PHE:HB2	2.00	0.43
1:D:696:ASP:HA	1:E:646:PRO:HG2	2.00	0.43
2:H:139:ASP:O	2:H:174:ARG:NH1	2.52	0.43
7:6:80:ARG:HG3	7:6:124:LEU:HD21	1.99	0.43
8:7:133:ALA:HB3	37:o:121:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:20:SER:HA	9:8:23:THR:HG22	2.00	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43
24:Y:37:TYR:O	29:f:351:A:N6	2.48	0.43
26:b:28:TYR:HB3	26:b:69:VAL:HB	2.01	0.43
29:f:2459:A:H61	29:f:2487:U:H3	1.67	0.43
38:p:44:ARG:O	56:b0:28:THR:CB	2.66	0.43
38:p:82:LEU:HD13	38:p:222:PHE:HE2	1.84	0.43
45:e:1407:MET:HB2	45:e:1407:MET:HE2	1.68	0.43
45:e:1477:GLN:OE1	45:e:1477:GLN:O	2.36	0.43
46:g:119:PRO:O	46:g:139:ARG:NH1	2.50	0.43
51:w:43:PRO:HD3	51:w:163:LEU:HD21	2.01	0.43
1:E:520:PRO:O	1:E:522:LYS:NZ	2.45	0.43
2:J:255:THR:OG1	2:J:256:LEU:N	2.52	0.43
8:7:102:ARG:HA	8:7:102:ARG:HD2	1.77	0.43
29:f:595:G:OP2	37:o:30:ARG:NH1	2.51	0.43
29:f:1831:U:P	56:b0:92:LYS:HG3	2.58	0.43
29:f:2270:A:H2'	29:f:2271:A:C8	2.53	0.43
29:f:2468:A:H4'	29:f:2469:G:H4'	2.00	0.43
29:f:3358:U:H2'	29:f:3359:A:H8	1.84	0.43
40:r:106:ALA:CB	47:x:74:C:H5"	2.49	0.43
45:e:272:TYR:CB	45:e:277:MET:CE	2.97	0.43
45:e:272:TYR:CG	45:e:277:MET:SD	3.12	0.43
52:X:30:LYS:HB2	52:X:38:PHE:CZ	2.53	0.43
1:A:530:PRO:HB3	1:A:634:ASN:HB3	2.00	0.43
1:B:1:LEU:HD12	1:B:77:ILE:CD1	2.49	0.43
57:F:901:ATP:H5'1	57:F:901:ATP:N3	2.32	0.43
3:G:327:THR:HG22	3:G:386:ILE:HD12	2.00	0.43
7:6:80:ARG:HD2	8:7:155:PRO:HA	2.00	0.43
10:I:80:ARG:HB2	10:I:99:ALA:HB3	2.00	0.43
14:N:36:GLY:HA3	14:N:40:HIS:CE1	2.53	0.43
27:c:44:LYS:NZ	29:f:1727:G:OP1	2.51	0.43
29:f:1523:U:C5	56:b0:123:TYR:OH	2.65	0.43
29:f:1666:G:H2'	29:f:1667:A:C8	2.54	0.43
29:f:1825:G:P	52:X:49:SER:HG	2.32	0.43
29:f:2745:G:N2	29:f:2748:A:OP2	2.47	0.43
29:f:3244:A:O2'	55:a0:111:PRO:CG	2.63	0.43
29:f:3245:A:O2'	55:a0:110:PRO:CB	2.67	0.43
38:p:104:GLU:HA	38:p:107:GLU:HG3	2.00	0.43
39:q:9:GLN:HB3	39:q:52:LEU:HD11	2.01	0.43
53:v:381:ARG:NH2	54:2:6:LYS:CD	2.60	0.43
1:B:52:LEU:HD21	1:B:58:ARG:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:ASP:OD1	1:D:672:ARG:NH1	2.52	0.43
3:G:241:LYS:HG3	3:G:243:GLU:H	1.83	0.43
9:8:42:LYS:NZ	29:f:1686:U:OP1	2.44	0.43
23:W:45:ARG:NH2	29:f:361:A:O3'	2.52	0.43
26:b:10:THR:HG21	26:b:72:LEU:HD13	2.01	0.43
29:f:1558:A:H1'	56:b0:34:LEU:CD1	2.48	0.43
29:f:2213:A:H2'	29:f:2214:A:C8	2.54	0.43
29:f:2383:C:N3	55:a0:91:LYS:HG2	2.32	0.43
35:m:95:TRP:CE3	35:m:198:TYR:HB3	2.54	0.43
38:p:86:THR:HA	38:p:89:GLU:HG2	2.00	0.43
38:p:239:GLY:O	38:p:243:GLN:HB2	2.19	0.43
45:e:1164:LEU:HG	45:e:1165:LYS:HD3	2.00	0.43
49:0:75:LYS:O	49:0:78:PRO:HD2	2.19	0.43
1:B:531:GLY:HA2	1:B:695:ALA:HB2	2.00	0.43
1:B:587:ASP:OD1	1:B:587:ASP:N	2.52	0.43
2:J:243:LEU:HD11	2:J:267:LEU:HB3	1.99	0.43
27:c:66:GLY:HA2	32:j:80:GLU:HG3	2.00	0.43
29:f:520:U:O4	34:l:347:THR:OG1	2.34	0.43
29:f:2129:U:H2'	29:f:2130:G:C8	2.54	0.43
34:l:22:LEU:HA	34:l:23:PRO:HD3	1.85	0.43
45:e:1193:LEU:HD23	45:e:1193:LEU:HA	1.63	0.43
47:y:37:A:H3'	47:y:38:U:H4'	2.01	0.43
53:v:289:MET:HE2	53:v:327:TYR:CG	2.54	0.43
53:v:541:LYS:HE2	53:v:568:MET:HE3	2.00	0.43
1:A:387:ARG:NH1	1:A:413:THR:O	2.52	0.42
1:A:399:LYS:NZ	1:B:242:ALA:O	2.46	0.42
22:V:18:THR:HG23	42:t:106:GLN:HB3	2.01	0.42
29:f:417:A:H2'	29:f:418:A:C8	2.54	0.42
29:f:1522:U:C5	56:b0:116:PRO:CG	2.94	0.42
29:f:2268:U:H3	29:f:2272:G:H22	1.65	0.42
33:k:94:GLU:HG3	55:a0:152:VAL:CG2	2.49	0.42
38:p:183:LYS:HB2	38:p:194:THR:HG23	2.01	0.42
44:a:117:PHE:CD1	44:a:118:SER:N	2.86	0.42
45:e:1083:SER:O	45:e:1087:CYS:SG	2.70	0.42
45:e:1189:ASN:ND2	45:e:1337:PHE:HB3	2.34	0.42
45:e:1446:PRO:HD2	45:e:1449:TYR:HD1	1.84	0.42
1:A:279:ILE:HB	1:A:313:ILE:HG22	2.01	0.42
1:A:490:GLY:H	1:A:666:ILE:HG12	1.83	0.42
1:E:259:THR:CG2	1:E:261:LYS:HD2	2.49	0.42
1:E:391:LEU:HD13	1:E:406:LEU:HB3	2.01	0.42
1:F:258:GLY:CA	57:F:901:ATP:O1B	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:417:VAL:HG13	1:F:419:ALA:H	1.85	0.42
29:f:2711:C:O2'	29:f:2744:U:OP1	2.38	0.42
29:f:3178:A:N6	55:a0:6:VAL:HG21	2.34	0.42
29:f:3322:A:H2'	29:f:3323:A:C8	2.53	0.42
33:k:284:ARG:HB3	33:k:323:MET:HB3	2.02	0.42
38:p:51:LYS:O	56:b0:32:PHE:CB	2.68	0.42
44:a:45:LYS:HG2	44:a:46:PRO:HD2	2.00	0.42
48:z:54:LYS:O	48:z:56:ILE:N	2.52	0.42
1:A:663:ARG:HD2	1:A:686:ALA:HB1	2.00	0.42
1:D:436:LYS:HA	1:D:436:LYS:HD3	1.94	0.42
2:K:37:PRO:HB3	2:K:38:PRO:CD	2.25	0.42
7:6:95:ARG:HB2	7:6:140:VAL:HG23	2.00	0.42
29:f:2218:G:H2'	29:f:2219:A:C8	2.54	0.42
31:i:136:G:P	56:b0:48:SER:HG	2.42	0.42
35:m:234:ASP:OD1	35:m:234:ASP:N	2.47	0.42
43:u:113:THR:OG1	43:u:114:ASP:N	2.52	0.42
45:e:254:ASN:OD1	45:e:254:ASN:N	2.49	0.42
45:e:1099:ARG:HE	45:e:1099:ARG:HB3	1.48	0.42
1:B:1:LEU:N	1:B:75:VAL:O	2.48	0.42
8:7:68:THR:OG1	8:7:69:LYS:N	2.51	0.42
14:N:27:LYS:NZ	29:f:801:A:OP1	2.37	0.42
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.42
29:f:531:G:H2'	29:f:532:A:C8	2.55	0.42
29:f:3243:A:N1	55:a0:107:GLY:CA	2.82	0.42
38:p:178:ALA:HB2	38:p:218:ILE:HG23	2.02	0.42
41:s:96:PHE:HB2	41:s:156:LYS:HE3	2.01	0.42
45:e:227:LYS:HA	45:e:227:LYS:HD3	1.85	0.42
45:e:1057:THR:CG2	45:e:1108:THR:HG21	2.49	0.42
1:A:239:LEU:HD13	1:F:433:ILE:HD13	2.01	0.42
1:C:489:VAL:CG2	57:C:1003:ATP:N6	2.83	0.42
1:D:359:ARG:HD2	1:D:360:PRO:HD2	2.01	0.42
3:G:129:ILE:HB	3:G:151:LEU:HB3	2.02	0.42
26:b:34:SER:OG	26:b:35:LEU:O	2.32	0.42
29:f:1221:A:C4	49:0:12:PHE:HZ	2.38	0.42
29:f:3218:A:H5"	29:f:3219:G:C5	2.55	0.42
33:k:262:TRP:HD1	55:a0:64:PHE:C	2.27	0.42
34:l:261:VAL:HG23	34:l:262:TRP:CD1	2.55	0.42
35:m:144:VAL:HG11	35:m:171:LEU:HD13	2.02	0.42
37:o:129:LEU:HD23	37:o:129:LEU:HA	1.89	0.42
44:a:113:VAL:HB	44:a:123:ILE:HB	2.01	0.42
45:e:704:THR:O	45:e:707:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:1068:MET:CE	45:e:1070:ILE:HD11	2.49	0.42
53:v:451:LYS:HE3	53:v:473:PHE:CE1	2.54	0.42
1:A:391:LEU:HD13	1:A:409:LEU:HD13	2.01	0.42
2:K:39:ASP:O	3:G:472:ASN:N	2.53	0.42
5:4:124:LEU:HD13	5:4:127:LEU:HD23	2.01	0.42
6:5:102:LEU:HD22	6:5:138:LEU:HD22	2.01	0.42
11:9:34:SER:OG	29:f:3085:G:OP1	2.32	0.42
29:f:219:A:HO2'	29:f:220:G:H21	1.66	0.42
29:f:1203:A:H2'	29:f:1204:A:C8	2.55	0.42
29:f:1825:G:OP2	52:X:49:SER:CB	2.68	0.42
29:f:2772:C:H4'	29:f:2773:C:H5'	2.02	0.42
29:f:3016:A:H2'	29:f:3017:A:C8	2.55	0.42
44:a:54:VAL:HG22	44:a:60:ILE:HG13	2.00	0.42
45:e:1083:SER:HA	45:e:1086:MET:HG2	2.00	0.42
47:y:68:C:H2'	47:y:69:G:C8	2.54	0.42
52:X:5:ILE:HD11	52:X:14:LEU:HD12	2.00	0.42
53:v:374:GLN:NE2	54:2:10:GLY:N	2.66	0.42
53:v:399:PHE:CE1	53:v:426:PHE:HB2	2.54	0.42
1:F:511:ASP:OD1	1:F:511:ASP:N	2.51	0.42
29:f:1831:U:OP2	56:b0:92:LYS:HG3	2.20	0.42
29:f:2876:C:H5'	47:x:76:A:H4'	2.01	0.42
1:F:322:LYS:HA	1:F:322:LYS:HD3	1.91	0.42
29:f:158:G:H2'	29:f:159:A:H8	1.85	0.42
29:f:760:G:O2'	29:f:770:G:N2	2.43	0.42
29:f:1660:C:H2'	29:f:1661:G:H8	1.85	0.42
31:i:26:U:O2'	34:l:51:ALA:O	2.37	0.42
38:p:46:LEU:H	56:b0:28:THR:HA	1.85	0.42
38:p:228:GLU:O	38:p:232:HIS:ND1	2.43	0.42
56:b0:142:ILE:HD12	56:b0:142:ILE:HA	1.83	0.42
1:D:249:ARG:NH1	1:D:349:SER:O	2.49	0.42
26:b:10:THR:HA	26:b:20:HIS:HD2	1.84	0.42
29:f:16:A:O3'	56:b0:45:LYS:HG2	2.19	0.42
29:f:1194:G:H2'	29:f:1195:A:C8	2.55	0.42
29:f:3023:U:H2'	29:f:3024:A:H8	1.84	0.42
29:f:3183:A:P	55:a0:12:LYS:HE3	2.60	0.42
44:a:601:TYR:HA	44:a:605:ILE:HB	2.02	0.42
45:e:1429:LYS:HE2	45:e:1429:LYS:HB3	1.85	0.42
46:g:199:VAL:HG23	46:g:204:ALA:HB2	2.02	0.42
51:w:37:GLY:O	51:w:202:GLY:N	2.52	0.42
53:v:345:TYR:CE2	53:v:349:ILE:HD12	2.54	0.42
1:C:529:PRO:HG2	1:C:532:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:560:MET:O	2:K:6:LYS:NZ	2.50	0.42
1:F:413:THR:HB	1:F:416:TYR:HB2	2.02	0.42
29:f:240:U:H4'	29:f:241:G:H5'	2.02	0.42
29:f:716:A:OP1	29:f:752:C:O2'	2.37	0.42
29:f:1237:G:H22	29:f:1251:A:H2	1.66	0.42
29:f:1751:G:H5"	52:X:26:LYS:HE3	2.01	0.42
29:f:3180:A:C6	55:a0:167:TYR:CZ	3.08	0.42
39:q:90:MET:HE3	39:q:179:ILE:HG22	2.01	0.42
44:a:967:LEU:HD13	44:a:1005:LEU:HB2	2.01	0.42
45:e:1172:LYS:HB3	45:e:1173:ARG:NH2	2.35	0.42
47:y:12:G:H2'	47:y:13:U:O4'	2.20	0.42
51:w:25:LYS:HD2	51:w:25:LYS:HA	1.88	0.42
53:v:186:PRO:HG2	53:v:189:CYS:SG	2.60	0.42
54:2:45:PHE:HB3	54:2:50:LEU:HD21	2.02	0.42
1:B:532:THR:HG22	57:C:1001:ATP:H5'2	2.02	0.41
1:C:222:GLN:NE2	1:C:378:ASP:O	2.53	0.41
1:D:666:ILE:CD1	57:D:901:ATP:N1	2.82	0.41
2:J:222:THR:HA	2:J:255:THR:HA	2.02	0.41
4:3:116:HIS:HB3	4:3:149:VAL:HB	2.02	0.41
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.01	0.41
29:f:129:U:H2'	29:f:130:A:C8	2.54	0.41
29:f:2268:U:H3	29:f:2272:G:H1	1.68	0.41
29:f:2514:U:OP2	29:f:2586:G:N2	2.49	0.41
35:m:200:PHE:HB3	35:m:237:GLU:HG2	2.02	0.41
36:n:112:THR:HG23	36:n:115:GLU:H	1.85	0.41
44:a:246:ASP:HB2	44:a:249:GLU:HB2	2.02	0.41
45:e:735:GLN:HG2	45:e:815:TYR:HB2	2.01	0.41
45:e:1193:LEU:O	45:e:1196:THR:HG22	2.20	0.41
45:e:1521:LYS:NZ	53:v:216:ASP:O	2.53	0.41
1:A:677:GLU:HG2	1:A:679:GLY:H	1.84	0.41
1:C:490:GLY:HA3	1:C:666:ILE:HG12	2.02	0.41
13:M:121:ARG:HA	13:M:121:ARG:HD2	1.93	0.41
29:f:443:G:O6	29:f:490:C:N4	2.53	0.41
29:f:2500:A:H4'	29:f:2501:U:OP1	2.20	0.41
29:f:3163:A:N6	29:f:3288:G:O6	2.53	0.41
33:k:236:LYS:HE2	33:k:236:LYS:HB2	1.90	0.41
40:r:72:ALA:HB2	40:r:155:ALA:HB2	2.01	0.41
40:r:144:ASN:HD22	40:r:144:ASN:N	2.18	0.41
41:s:131:MET:HE3	41:s:131:MET:HB3	1.81	0.41
45:e:1544:ARG:HH22	53:v:276:ARG:NH1	1.76	0.41
1:A:777:TYR:HA	1:A:780:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:GLN:NE2	1:B:456:GLY:O	2.54	0.41
1:D:493:ASP:N	1:D:493:ASP:OD1	2.48	0.41
1:E:209:ASN:OD1	1:E:209:ASN:N	2.53	0.41
1:E:466:LEU:HA	1:E:469:SER:HB3	2.02	0.41
1:E:561:TRP:CD1	1:E:564:GLU:HG3	2.54	0.41
11:9:17:ARG:HD3	11:9:17:ARG:HA	1.91	0.41
20:T:60:ARG:NH1	29:f:1593:A:OP1	2.53	0.41
29:f:1579:C:H2'	29:f:1580:A:C8	2.55	0.41
29:f:3007:U:O2'	55:a0:71:PHE:CD1	2.73	0.41
30:h:38:U:N3	30:h:41:G:OP2	2.41	0.41
39:q:86:TYR:CE2	39:q:151:VAL:HB	2.56	0.41
45:e:178:LEU:HA	45:e:178:LEU:HD12	1.66	0.41
45:e:1477:GLN:CD	45:e:1477:GLN:C	2.88	0.41
1:A:317:ASP:OD1	1:A:317:ASP:N	2.46	0.41
1:A:470:ASN:OD1	1:A:470:ASN:N	2.53	0.41
1:B:111:LYS:HB3	1:B:112:PRO:HD3	2.02	0.41
1:B:492:LEU:HD23	1:B:495:ILE:HD12	2.02	0.41
1:B:608:ASP:OD1	1:B:608:ASP:N	2.54	0.41
13:M:9:LYS:HB3	13:M:9:LYS:HE3	1.91	0.41
29:f:2471:U:O3'	29:f:2472:U:H6	2.03	0.41
29:f:2871:G:H5"	29:f:2872:A:H5'	2.02	0.41
29:f:3233:C:H2'	29:f:3234:A:C8	2.55	0.41
34:l:34:ILE:HG21	34:l:120:TYR:HD2	1.85	0.41
43:u:47:ASP:HB2	43:u:55:ARG:HG3	2.02	0.41
44:a:956:ILE:HG12	44:a:1016:VAL:HG12	2.03	0.41
45:e:858:LEU:HD12	45:e:858:LEU:HA	1.92	0.41
48:z:51:LYS:O	48:z:54:LYS:N	2.54	0.41
1:A:214:ASP:OD1	1:A:214:ASP:N	2.52	0.41
1:A:311:ILE:HB	1:A:353:VAL:HG12	2.02	0.41
1:B:275:PHE:HE2	1:B:277:PHE:HD2	1.67	0.41
1:C:476:GLU:HG3	1:C:479:VAL:HB	2.02	0.41
1:E:256:PRO:HA	1:E:257:PRO:HD3	1.96	0.41
3:G:168:SER:O	3:G:171:SER:OG	2.39	0.41
3:G:284:ILE:HG21	3:G:325:ILE:HD11	2.02	0.41
4:3:122:ALA:HB3	4:3:143:PRO:HB2	2.01	0.41
10:I:135:VAL:HG23	46:g:102:SER:HB3	2.03	0.41
19:S:16:TYR:OH	19:S:89:LEU:O	2.31	0.41
26:b:61:LYS:NZ	26:b:63:LYS:O	2.53	0.41
29:f:1404:G:N2	29:f:1407:A:OP2	2.43	0.41
29:f:1831:U:C5'	56:b0:91:ASN:HB3	2.40	0.41
29:f:2523:A:H3'	56:b0:30:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:3198:U:H1'	39:q:21:LYS:HB2	2.01	0.41
40:r:52:LEU:HB3	40:r:136:PHE:HB2	2.02	0.41
45:e:1165:LYS:HB2	45:e:1165:LYS:HE2	1.81	0.41
1:A:314:ASP:OD2	57:A:901:ATP:O3G	2.38	0.41
1:B:387:ARG:NE	1:B:413:THR:O	2.54	0.41
1:D:650:ASP:OD1	1:D:650:ASP:N	2.46	0.41
1:F:697:LEU:HD22	1:F:700:ILE:HD11	2.02	0.41
3:G:169:PHE:HA	3:G:172:TYR:HB3	2.01	0.41
29:f:3121:U:H1'	29:f:3122:A:H5"	2.01	0.41
35:m:266:ALA:O	35:m:270:LYS:HB2	2.20	0.41
44:a:98:ASP:HA	47:x:34:A:H61	1.84	0.41
45:e:759:ASP:O	45:e:762:GLN:HG3	2.20	0.41
45:e:964:PHE:CD2	45:e:968:ASN:ND2	2.89	0.41
45:e:1273:HIS:HA	45:e:1276:LEU:HG	2.02	0.41
45:e:1496:LYS:O	45:e:1500:LEU:HG	2.21	0.41
45:e:1514:ILE:O	45:e:1535:HIS:NE2	2.29	0.41
49:0:67:LEU:HD22	49:0:67:LEU:HA	1.85	0.41
1:A:246:LYS:HB2	1:A:246:LYS:HE2	1.88	0.41
1:B:666:ILE:HD13	57:C:1001:ATP:C2	2.55	0.41
1:E:485:THR:OG1	1:E:487:ASP:OD1	2.34	0.41
1:E:619:ASP:OD1	1:E:619:ASP:N	2.44	0.41
1:F:276:PHE:HE2	1:F:278:LEU:HD12	1.85	0.41
1:F:648:ARG:HG2	1:F:649:LEU:HD12	2.01	0.41
29:f:673:U:H2'	29:f:674:G:C8	2.55	0.41
29:f:1083:G:H2'	29:f:1084:A:C8	2.56	0.41
29:f:2747:A:H2'	29:f:2748:A:C8	2.54	0.41
38:p:46:LEU:H	56:b0:27:ARG:C	2.09	0.41
53:v:191:ARG:HA	53:v:412:LEU:HD11	2.03	0.41
1:A:364:ASP:HA	1:A:365:PRO:HD3	1.94	0.41
1:C:583:VAL:HG13	1:C:628:PHE:HZ	1.84	0.41
1:D:216:ILE:HG22	57:D:902:ATP:N7	2.32	0.41
1:D:531:GLY:N	57:D:901:ATP:PB	2.94	0.41
1:F:574:ASP:OD1	1:F:574:ASP:N	2.52	0.41
6:5:31:GLU:HA	6:5:34:GLN:HB2	2.03	0.41
29:f:182:U:H2'	29:f:183:G:H8	1.85	0.41
29:f:745:C:H2'	29:f:746:A:H8	1.85	0.41
29:f:1288:U:H2'	29:f:1289:G:C8	2.54	0.41
29:f:1497:C:H2'	29:f:1498:A:C8	2.56	0.41
29:f:2357:A:H2'	29:f:2358:A:H8	1.85	0.41
29:f:2536:A:H2'	29:f:2537:U:C4	2.56	0.41
29:f:3008:A:P	55:a0:72:HIS:H	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:h:84:A:H2'	30:h:85:G:C8	2.56	0.41
32:j:52:SER:HB3	32:j:191:LEU:HD23	2.02	0.41
35:m:279:LYS:HE2	35:m:279:LYS:HB3	1.89	0.41
36:n:176:PHE:O	43:u:113:THR:OG1	2.33	0.41
44:a:117:PHE:HD1	44:a:118:SER:O	2.02	0.41
45:e:875:ASN:O	45:e:879:ILE:HG13	2.21	0.41
45:e:1435:ASP:CG	45:e:1514:ILE:HB	2.45	0.41
53:v:304:GLU:HG3	53:v:620:PHE:CZ	2.56	0.41
53:v:540:GLU:OE2	53:v:568:MET:HE1	2.20	0.41
1:B:531:GLY:O	57:C:1001:ATP:C5'	2.63	0.41
1:C:465:ALA:O	1:C:469:SER:OG	2.32	0.41
1:D:499:LEU:HD21	1:D:526:PHE:HZ	1.86	0.41
9:8:92:TRP:CZ2	45:e:1474:MET:HB2	2.55	0.41
10:I:66:LYS:HA	10:I:67:PRO:HD3	1.94	0.41
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	0.41
20:T:19:LYS:HA	20:T:19:LYS:HD3	1.93	0.41
20:T:92:ALA:O	20:T:96:GLU:HG2	2.21	0.41
20:T:93:PHE:HD2	20:T:94:LEU:HD22	1.86	0.41
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
29:f:20:A:H2'	29:f:21:G:C8	2.56	0.41
29:f:352:A:H61	29:f:365:A:H5"	1.86	0.41
29:f:1833:G:OP2	56:b0:114:VAL:HG21	2.14	0.41
29:f:2208:A:H62	44:a:843:LYS:NZ	2.18	0.41
29:f:2413:A:H2'	29:f:2414:G:H8	1.85	0.41
29:f:2457:G:H2'	29:f:2459:A:C2	2.55	0.41
29:f:2473:C:C2'	29:f:2474:G:H4'	2.50	0.41
29:f:3217:C:C5	29:f:3220:G:H1'	2.56	0.41
29:f:3243:A:C2'	55:a0:110:PRO:CD	2.98	0.41
30:h:53:U:O2'	30:h:55:A:N7	2.53	0.41
35:m:191:ASP:HA	35:m:192:PRO:HD3	1.94	0.41
41:s:75:LYS:O	41:s:79:ILE:HG13	2.20	0.41
43:u:93:LYS:HB2	43:u:93:LYS:HE3	1.87	0.41
43:u:124:ARG:CG	55:a0:194:LEU:HD22	2.35	0.41
44:a:90:THR:CG2	44:a:107:ASP:OD1	2.66	0.41
44:a:574:PHE:HB2	44:a:589:MET:HE1	2.03	0.41
44:a:632:PRO:HA	44:a:635:LEU:HD12	2.02	0.41
45:e:251:ASN:HD21	45:e:253:LYS:HB2	1.85	0.41
45:e:308:PRO:O	45:e:311:PRO:HD2	2.20	0.41
45:e:854:GLU:HA	45:e:855:PRO:HD3	1.91	0.41
45:e:1057:THR:HG23	45:e:1105:LEU:HA	2.03	0.41
45:e:1237:LYS:HB2	45:e:1237:LYS:HE3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:e:1400:PHE:CE1	45:e:1428:VAL:HG22	2.55	0.41
45:e:1447:LYS:HB2	45:e:1447:LYS:HE2	1.89	0.41
45:e:1511:CYS:SG	45:e:1535:HIS:CE1	3.14	0.41
49:0:70:LEU:HB3	49:0:73:PHE:CD1	2.55	0.41
51:w:9:VAL:HG12	51:w:180:VAL:HG22	2.03	0.41
51:w:204:LEU:HB2	51:w:216:LEU:O	2.21	0.41
1:B:111:LYS:HG3	1:B:115:VAL:HG21	2.01	0.41
1:B:533:GLY:N	57:C:1001:ATP:O2A	2.54	0.41
1:C:608:ASP:OD1	1:C:608:ASP:N	2.54	0.41
1:D:666:ILE:HD11	57:D:901:ATP:C6	2.48	0.41
7:6:14:LEU:HA	7:6:15:PRO:HD3	1.96	0.41
12:L:48:LEU:HD23	12:L:48:LEU:HA	1.92	0.41
19:S:37:THR:OG1	19:S:39:GLN:OE1	2.39	0.41
29:f:596:C:N3	29:f:608:A:O2'	2.54	0.41
29:f:824:C:H5"	32:j:21:ARG:HG3	2.03	0.41
29:f:1421:G:H2'	29:f:1422:G:H8	1.86	0.41
29:f:1596:C:H2'	29:f:1597:C:C6	2.56	0.41
29:f:2508:U:H2'	29:f:2509:U:C6	2.56	0.41
42:t:57:VAL:HG23	42:t:147:ILE:HD12	2.03	0.41
44:a:597:THR:HG23	44:a:621:TRP:HE1	1.86	0.41
46:g:49:VAL:HG21	46:g:88:LEU:HD22	2.03	0.41
52:X:8:ILE:HG23	53:v:131:ILE:HG21	2.03	0.41
54:2:36:ILE:HG21	54:2:71:LEU:HD22	2.03	0.41
1:A:431:GLN:HA	1:A:434:ARG:HG2	2.02	0.40
1:A:706:LYS:HD2	1:A:706:LYS:HA	1.94	0.40
1:B:703:ARG:HA	1:B:703:ARG:HD2	1.89	0.40
1:F:640:ASP:HA	1:F:641:PRO:HD3	1.90	0.40
1:F:689:THR:HA	1:F:692:PHE:HD2	1.86	0.40
2:K:21:ASP:OD2	3:G:227:GLN:NE2	2.43	0.40
8:7:73:GLY:HA2	8:7:89:LEU:O	2.21	0.40
25:Z:113:ARG:NH2	29:f:1190:A:H4'	2.36	0.40
28:d:21:ARG:HD2	28:d:21:ARG:HA	1.80	0.40
45:e:1094:TYR:O	45:e:1098:LEU:HG	2.21	0.40
45:e:1410:LEU:HG	45:e:1417:LEU:HD11	2.03	0.40
53:v:196:PHE:HA	53:v:481:TYR:HE2	1.86	0.40
53:v:331:PRO:HG3	53:v:422:PHE:CE2	2.56	0.40
53:v:368:HIS:CD2	53:v:371:GLY:H	2.39	0.40
1:C:685:ILE:HD11	1:C:700:ILE:HD13	2.04	0.40
1:F:529:PRO:HA	1:F:530:PRO:HD3	1.85	0.40
5:4:161:LYS:HA	5:4:161:LYS:HD3	1.82	0.40
7:6:137:ARG:HH21	29:f:1213:G:H5'	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:10:LYS:HZ1	56:b0:114:VAL:C	2.27	0.40
29:f:1152:G:OP2	29:f:1152:G:N2	2.44	0.40
40:r:181:TYR:CE2	40:r:185:ARG:HD2	2.56	0.40
44:a:26:LEU:HD21	44:a:29:ILE:HD11	2.04	0.40
45:e:59:GLU:HG2	45:e:103:TYR:CG	2.57	0.40
45:e:129:LEU:HD23	45:e:129:LEU:HA	1.77	0.40
47:y:1:G:C5	47:y:73:G:N2	2.90	0.40
1:E:314:ASP:HA	1:E:356:ALA:HB3	2.04	0.40
5:4:126:GLN:HA	5:4:129:VAL:HG22	2.04	0.40
9:8:41:ILE:HG21	9:8:54:VAL:HG21	2.02	0.40
14:N:96:LYS:HE2	14:N:96:LYS:HB2	1.70	0.40
29:f:656:A:H2'	29:f:657:A:C8	2.57	0.40
29:f:1565:G:H1	29:f:1574:C:H42	1.69	0.40
29:f:2207:A:H1'	29:f:2208:A:H5'	2.04	0.40
29:f:2264:U:H2'	29:f:2265:C:C6	2.56	0.40
33:k:323:MET:HE3	33:k:323:MET:HB2	1.90	0.40
34:l:166:VAL:O	34:l:170:LYS:HG2	2.22	0.40
45:e:819:LEU:O	45:e:823:LEU:HG	2.21	0.40
45:e:1204:LYS:HA	45:e:1204:LYS:HD3	1.95	0.40
53:v:470:ASP:HB2	53:v:505:ALA:HB2	2.04	0.40
1:B:430:MET:HE1	1:C:240:PHE:HE1	1.87	0.40
1:C:694:GLY:C	57:C:1003:ATP:N3	2.79	0.40
1:E:551:SER:HA	1:E:585:PHE:HB3	2.02	0.40
1:F:527:TYR:HE2	1:F:652:LEU:HB2	1.87	0.40
1:F:663:ARG:HD2	1:F:697:LEU:HD12	2.04	0.40
3:G:263:MET:HG2	3:G:284:ILE:HG12	2.02	0.40
4:3:182:ILE:HD12	4:3:182:ILE:HA	1.85	0.40
12:L:51:ARG:NH2	31:i:83:C:O2	2.54	0.40
14:N:41:HIS:CE1	42:t:2:ALA:HB3	2.56	0.40
14:N:114:GLY:O	14:N:137:LYS:NZ	2.54	0.40
29:f:129:U:H3	29:f:139:G:H1	1.69	0.40
29:f:1238:C:C4'	48:z:139:VAL:CB	2.98	0.40
29:f:2836:C:H5	29:f:2852:C:N4	2.16	0.40
35:m:108:ARG:CZ	35:m:253:PHE:HB2	2.51	0.40
40:r:191:LYS:HB3	40:r:213:PHE:HE1	1.87	0.40
44:a:90:THR:CG2	44:a:107:ASP:H	2.35	0.40
44:a:185:ILE:HD12	44:a:258:THR:HG23	2.04	0.40
44:a:601:TYR:HA	44:a:605:ILE:HD12	2.03	0.40
45:e:371:LEU:HB3	45:e:377:TRP:NE1	2.16	0.40
45:e:1544:ARG:NH1	53:v:207:HIS:HE1	2.17	0.40
53:v:211:LYS:CE	53:v:222:LEU:HD13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLY:HA3	1:A:474:LEU:HD11	2.02	0.40
1:B:402:ASP:OD1	1:B:402:ASP:N	2.54	0.40
1:C:399:LYS:HG3	1:C:456:GLY:HA2	2.04	0.40
1:D:561:TRP:NE1	2:K:5:VAL:N	2.56	0.40
1:E:570:ARG:HA	1:E:573:PHE:HD2	1.87	0.40
3:G:291:ASP:OD1	3:G:291:ASP:N	2.48	0.40
9:8:35:LYS:HA	9:8:38:ILE:HG12	2.04	0.40
19:S:37:THR:HG23	19:S:40:ASP:H	1.86	0.40
29:f:94:G:H2'	29:f:95:A:C8	2.57	0.40
29:f:448:U:O2	29:f:488:U:O2'	2.33	0.40
29:f:946:U:H2'	29:f:947:G:H8	1.86	0.40
29:f:1577:G:H2'	29:f:1578:C:H6	1.86	0.40
29:f:1827:C:H2'	29:f:1828:A:C8	2.57	0.40
29:f:3178:A:C6	55:a0:6:VAL:CG2	3.05	0.40
29:f:3178:A:H5'	55:a0:4:GLU:OE1	2.22	0.40
30:h:112:G:H2'	30:h:113:C:C6	2.57	0.40
34:l:145:ILE:HD13	34:l:145:ILE:HA	1.97	0.40
40:r:182:LEU:HD23	40:r:182:LEU:HA	1.98	0.40
42:t:46:ILE:HD11	42:t:51:LEU:HA	2.04	0.40
44:a:576:LYS:HD3	47:y:31:C:H5"	2.03	0.40
44:a:702:GLY:HA2	44:a:952:TYR:O	2.21	0.40
45:e:373:TYR:OH	45:e:416:SER:HB3	2.22	0.40
45:e:911:ARG:O	45:e:915:LYS:HG2	2.20	0.40
45:e:1196:THR:HG23	45:e:1197:LEU:N	2.35	0.40
45:e:1464:ILE:HG22	45:e:1468:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	543/835 (65%)	522 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	648/835 (78%)	612 (94%)	36 (6%)	0	100	100
1	C	488/835 (58%)	448 (92%)	40 (8%)	0	100	100
1	D	485/835 (58%)	449 (93%)	36 (7%)	0	100	100
1	E	492/835 (59%)	463 (94%)	27 (6%)	2 (0%)	30	61
1	F	527/835 (63%)	501 (95%)	26 (5%)	0	100	100
2	H	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	J	74/76 (97%)	74 (100%)	0	0	100	100
2	K	46/76 (60%)	31 (67%)	10 (22%)	5 (11%)	0	1
3	G	466/580 (80%)	421 (90%)	44 (9%)	1 (0%)	44	72
4	3	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
5	4	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
6	5	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
7	6	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
8	7	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
9	8	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
10	I	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
11	9	61/155 (39%)	61 (100%)	0	0	100	100
12	L	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	31
16	P	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
17	Q	107/113 (95%)	98 (92%)	9 (8%)	0	100	100
18	R	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
19	S	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
20	T	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
21	U	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
22	V	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
23	W	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
24	Y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
25	Z	50/128 (39%)	48 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	b	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
27	c	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
28	d	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
32	j	244/254 (96%)	226 (93%)	18 (7%)	0	100	100
33	k	384/387 (99%)	363 (94%)	21 (6%)	0	100	100
34	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	37	66
35	m	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
36	n	163/176 (93%)	154 (94%)	9 (6%)	0	100	100
37	o	220/244 (90%)	207 (94%)	13 (6%)	0	100	100
38	p	231/256 (90%)	220 (95%)	11 (5%)	0	100	100
39	q	189/191 (99%)	174 (92%)	14 (7%)	1 (0%)	25	57
40	r	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
41	s	167/174 (96%)	161 (96%)	5 (3%)	1 (1%)	22	54
42	t	191/199 (96%)	174 (91%)	16 (8%)	1 (0%)	25	57
43	u	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
44	a	842/1038 (81%)	827 (98%)	15 (2%)	0	100	100
45	e	1518/1562 (97%)	1486 (98%)	30 (2%)	2 (0%)	48	77
46	g	223/245 (91%)	215 (96%)	8 (4%)	0	100	100
48	z	144/165 (87%)	135 (94%)	7 (5%)	2 (1%)	9	36
49	0	117/312 (38%)	116 (99%)	0	1 (1%)	14	45
51	w	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
52	X	74/78 (95%)	74 (100%)	0	0	100	100
53	v	527/753 (70%)	510 (97%)	16 (3%)	1 (0%)	44	72
54	2	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
55	a0	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
56	b0	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
All	All	13416/16565 (81%)	12793 (95%)	604 (4%)	19 (0%)	50	77

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	561	TRP
2	K	37	PRO

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Mol	Chain	Res	Type
2	K	38	PRO
2	K	41	GLN
48	z	88	PRO
53	v	615	ASN
1	E	262	THR
45	e	437	LYS
2	K	45	PHE
3	G	169	PHE
45	e	855	PRO
34	l	4	PRO
39	q	107	ASP
41	s	108	GLU
49	0	93	LEU
15	O	21	ILE
2	K	44	ILE
42	t	47	ALA
48	z	55	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	448/695 (64%)	447 (100%)	1 (0%)	92 96
1	B	545/695 (78%)	543 (100%)	2 (0%)	89 94
1	C	401/695 (58%)	399 (100%)	2 (0%)	86 92
1	D	398/695 (57%)	397 (100%)	1 (0%)	91 95
1	E	403/695 (58%)	399 (99%)	4 (1%)	73 85
1	F	434/695 (62%)	433 (100%)	1 (0%)	92 96
2	H	69/69 (100%)	69 (100%)	0	100 100
2	J	69/69 (100%)	69 (100%)	0	100 100
2	K	44/69 (64%)	42 (96%)	2 (4%)	23 52
3	G	420/516 (81%)	419 (100%)	1 (0%)	92 96
4	3	138/146 (94%)	138 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	150/151 (99%)	150 (100%)	0	100	100
6	5	129/154 (84%)	129 (100%)	0	100	100
7	6	155/156 (99%)	155 (100%)	0	100	100
8	7	135/137 (98%)	135 (100%)	0	100	100
9	8	87/107 (81%)	87 (100%)	0	100	100
10	I	104/105 (99%)	104 (100%)	0	100	100
11	9	54/129 (42%)	54 (100%)	0	100	100
12	L	108/110 (98%)	108 (100%)	0	100	100
13	M	112/116 (97%)	112 (100%)	0	100	100
14	N	117/119 (98%)	117 (100%)	0	100	100
15	O	46/47 (98%)	46 (100%)	0	100	100
16	P	81/88 (92%)	81 (100%)	0	100	100
17	Q	92/97 (95%)	92 (100%)	0	100	100
18	R	107/111 (96%)	107 (100%)	0	100	100
19	S	90/91 (99%)	90 (100%)	0	100	100
20	T	95/103 (92%)	95 (100%)	0	100	100
21	U	104/105 (99%)	104 (100%)	0	100	100
22	V	80/82 (98%)	80 (100%)	0	100	100
23	W	67/71 (94%)	67 (100%)	0	100	100
24	Y	45/46 (98%)	45 (100%)	0	100	100
25	Z	45/116 (39%)	45 (100%)	0	100	100
26	b	87/91 (96%)	87 (100%)	0	100	100
27	c	71/72 (99%)	71 (100%)	0	100	100
28	d	20/23 (87%)	20 (100%)	0	100	100
32	j	189/196 (96%)	189 (100%)	0	100	100
33	k	320/323 (99%)	320 (100%)	0	100	100
34	l	288/289 (100%)	288 (100%)	0	100	100
35	m	241/245 (98%)	241 (100%)	0	100	100
36	n	139/155 (90%)	139 (100%)	0	100	100
37	o	186/205 (91%)	186 (100%)	0	100	100
38	p	187/208 (90%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	q	168/171 (98%)	168 (100%)	0	100 100
40	r	185/187 (99%)	184 (100%)	1 (0%)	86 92
41	s	145/150 (97%)	145 (100%)	0	100 100
42	t	154/159 (97%)	154 (100%)	0	100 100
43	u	107/109 (98%)	107 (100%)	0	100 100
44	a	677/949 (71%)	676 (100%)	1 (0%)	92 97
45	e	1157/1451 (80%)	1102 (95%)	55 (5%)	21 50
46	g	180/211 (85%)	180 (100%)	0	100 100
49	0	104/254 (41%)	94 (90%)	10 (10%)	7 25
51	w	197/198 (100%)	197 (100%)	0	100 100
52	X	68/69 (99%)	68 (100%)	0	100 100
53	v	492/686 (72%)	484 (98%)	8 (2%)	58 77
54	2	68/68 (100%)	68 (100%)	0	100 100
55	a0	160/162 (99%)	160 (100%)	0	100 100
56	b0	104/118 (88%)	104 (100%)	0	100 100
All	All	11066/14029 (79%)	10977 (99%)	89 (1%)	77 89

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	B	436	LYS
1	B	437	MET
1	C	259	THR
1	C	562	TYR
1	D	330	VAL
1	E	261	LYS
1	E	262	THR
1	E	263	LEU
1	E	562	TYR
1	F	479	VAL
2	K	40	GLN
2	K	44	ILE
3	G	477	THR
40	r	112	GLN
44	a	98	ASP
45	e	8	THR

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Mol	Chain	Res	Type
45	e	105	VAL
45	e	125	ILE
45	e	169	LEU
45	e	205	GLU
45	e	230	SER
45	e	254	ASN
45	e	271	LEU
45	e	277	MET
45	e	283	ILE
45	e	299	THR
45	e	309	VAL
45	e	319	THR
45	e	327	THR
45	e	400	GLU
45	e	731	LEU
45	e	733	HIS
45	e	754	ILE
45	e	763	ILE
45	e	770	ILE
45	e	780	ILE
45	e	797	LEU
45	e	799	THR
45	e	806	LEU
45	e	826	LEU
45	e	853	GLU
45	e	867	PHE
45	e	904	VAL
45	e	910	SER
45	e	924	VAL
45	e	1102	CYS
45	e	1142	GLU
45	e	1149	THR
45	e	1164	LEU
45	e	1179	LEU
45	e	1184	ILE
45	e	1269	LEU
45	e	1294	LEU
45	e	1300	ILE
45	e	1303	MET
45	e	1363	VAL
45	e	1367	THR
45	e	1372	LEU

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Mol	Chain	Res	Type
45	e	1379	LEU
45	e	1384	GLU
45	e	1400	PHE
45	e	1407	MET
45	e	1421	LEU
45	e	1428	VAL
45	e	1441	ILE
45	e	1454	ILE
45	e	1464	ILE
45	e	1480	ILE
45	e	1508	CYS
45	e	1514	ILE
49	0	30	VAL
49	0	51	VAL
49	0	52	LEU
49	0	67	LEU
49	0	76	LEU
49	0	80	VAL
49	0	93	LEU
49	0	95	GLU
49	0	105	VAL
49	0	189	GLN
53	v	238	LEU
53	v	258	LEU
53	v	269	HIS
53	v	332	LEU
53	v	336	LEU
53	v	403	LEU
53	v	529	HIS
53	v	616	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	A	509	HIS
1	A	588	GLN
1	A	651	GLN
1	A	757	HIS
1	B	78	HIS
1	B	135	GLN
1	B	153	GLN

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Mol	Chain	Res	Type
1	B	327	ASN
1	B	394	HIS
1	B	432	GLN
1	B	509	HIS
1	B	626	ASN
1	B	690	GLN
1	C	222	GLN
1	C	236	HIS
1	C	280	ASN
1	C	306	ASN
1	C	337	GLN
1	C	350	ASN
1	C	394	HIS
1	C	461	ASN
1	C	483	ASN
1	C	512	GLN
1	C	612	ASN
1	C	702	GLN
1	D	295	ASN
1	D	306	ASN
1	D	337	GLN
1	D	431	GLN
1	D	588	GLN
1	D	670	GLN
1	D	702	GLN
1	E	209	ASN
1	E	222	GLN
1	E	350	ASN
1	E	461	ASN
1	E	512	GLN
1	E	548	ASN
1	E	568	ASN
1	E	588	GLN
1	E	626	ASN
1	E	651	GLN
1	F	295	ASN
1	F	306	ASN
1	F	337	GLN
1	F	394	HIS
1	F	468	ASN
1	F	651	GLN
2	K	25	ASN

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Mol	Chain	Res	Type
2	K	31	GLN
3	G	162	ASN
3	G	179	ASN
3	G	181	ASN
3	G	250	GLN
3	G	491	ASN
3	G	521	HIS
4	3	55	GLN
4	3	97	ASN
5	4	158	HIS
6	5	150	GLN
8	7	66	ASN
8	7	149	GLN
9	8	87	ASN
9	8	101	ASN
13	M	103	GLN
13	M	122	HIS
13	M	127	ASN
14	N	38	GLN
15	O	12	GLN
15	O	17	HIS
17	Q	15	ASN
17	Q	21	HIS
18	R	35	GLN
18	R	49	ASN
21	U	16	GLN
21	U	59	ASN
21	U	99	GLN
23	W	12	HIS
23	W	13	ASN
24	Y	4	GLN
24	Y	20	ASN
26	b	3	ASN
26	b	102	GLN
33	k	139	GLN
33	k	198	HIS
33	k	224	HIS
34	l	5	GLN
34	l	196	ASN
34	l	316	ASN
36	n	61	ASN
37	o	64	GLN

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Mol	Chain	Res	Type
37	o	244	ASN
39	q	49	ASN
39	q	169	ASN
39	q	183	HIS
40	r	51	HIS
40	r	208	ASN
41	s	43	GLN
41	s	62	ASN
41	s	90	GLN
41	s	109	HIS
43	u	62	GLN
44	a	51	ASN
44	a	121	ASN
44	a	382	GLN
44	a	395	ASN
44	a	417	ASN
44	a	438	ASN
44	a	562	HIS
44	a	624	ASN
44	a	689	GLN
45	e	79	ASN
45	e	160	ASN
45	e	174	GLN
45	e	189	ASN
45	e	226	ASN
45	e	233	ASN
45	e	251	ASN
45	e	397	ASN
45	e	403	ASN
45	e	408	ASN
45	e	795	HIS
45	e	805	ASN
45	e	869	HIS
45	e	888	ASN
45	e	902	ASN
45	e	968	ASN
45	e	1005	ASN
45	e	1111	GLN
45	e	1141	GLN
45	e	1189	ASN
45	e	1288	GLN
45	e	1455	GLN

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Mol	Chain	Res	Type
45	e	1457	ASN
45	e	1477	GLN
45	e	1478	HIS
45	e	1499	HIS
45	e	1516	HIS
45	e	1532	ASN
46	g	9	ASN
46	g	75	GLN
49	0	36	GLN
53	v	198	GLN
53	v	359	ASN
53	v	368	HIS
53	v	374	GLN
53	v	389	ASN
53	v	476	ASN
53	v	608	GLN
53	v	610	HIS
54	2	40	GLN
55	a0	55	HIS
55	a0	193	GLN
56	b0	65	GLN
56	b0	85	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	f	3211/3395 (94%)	601 (18%)	0
30	h	120/121 (99%)	12 (10%)	0
31	i	157/158 (99%)	32 (20%)	0
47	x	72/76 (94%)	26 (36%)	0
47	y	71/76 (93%)	26 (36%)	0
All	All	3631/3826 (94%)	697 (19%)	0

All (697) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	f	6	A
29	f	13	A
29	f	14	U
29	f	26	A
29	f	40	A

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Mol	Chain	Res	Type
29	f	43	A
29	f	49	A
29	f	59	G
29	f	60	A
29	f	65	A
29	f	66	A
29	f	92	G
29	f	99	A
29	f	109	A
29	f	110	G
29	f	111	C
29	f	116	A
29	f	120	G
29	f	121	A
29	f	122	A
29	f	133	U
29	f	134	U
29	f	135	C
29	f	136	G
29	f	156	G
29	f	157	A
29	f	165	A
29	f	166	C
29	f	172	G
29	f	173	G
29	f	187	A
29	f	190	U
29	f	191	U
29	f	200	C
29	f	206	G
29	f	210	U
29	f	211	A
29	f	213	A
29	f	218	G
29	f	219	A
29	f	234	G
29	f	240	U
29	f	241	G
29	f	242	C
29	f	243	G
29	f	245	U
29	f	249	U

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Mol	Chain	Res	Type
29	f	252	U
29	f	269	G
29	f	283	G
29	f	286	U
29	f	295	A
29	f	305	U
29	f	323	A
29	f	329	U
29	f	339	C
29	f	350	C
29	f	374	A
29	f	376	G
29	f	398	A
29	f	399	A
29	f	401	U
29	f	402	A
29	f	403	C
29	f	421	G
29	f	422	A
29	f	439	C
29	f	440	A
29	f	441	U
29	f	442	G
29	f	443	G
29	f	445	G
29	f	446	U
29	f	447	U
29	f	448	U
29	f	450	G
29	f	487	U
29	f	488	U
29	f	489	U
29	f	490	C
29	f	494	G
29	f	518	G
29	f	520	U
29	f	521	A
29	f	523	A
29	f	535	G
29	f	536	U
29	f	543	C
29	f	544	C

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Mol	Chain	Res	Type
29	f	546	C
29	f	547	G
29	f	548	G
29	f	551	A
29	f	552	G
29	f	555	U
29	f	557	A
29	f	559	A
29	f	578	A
29	f	579	G
29	f	589	A
29	f	597	G
29	f	604	G
29	f	608	A
29	f	609	G
29	f	611	A
29	f	620	U
29	f	621	A
29	f	622	A
29	f	637	C
29	f	638	C
29	f	649	A
29	f	660	A
29	f	677	A
29	f	681	U
29	f	684	G
29	f	690	A
29	f	691	A
29	f	705	A
29	f	712	G
29	f	715	A
29	f	716	A
29	f	719	U
29	f	720	A
29	f	758	C
29	f	763	G
29	f	764	U
29	f	765	C
29	f	766	U
29	f	767	U
29	f	776	U
29	f	777	U

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Mol	Chain	Res	Type
29	f	780	A
29	f	781	G
29	f	785	G
29	f	786	A
29	f	806	A
29	f	817	A
29	f	830	A
29	f	846	A
29	f	849	C
29	f	850	U
29	f	861	C
29	f	874	U
29	f	879	U
29	f	896	A
29	f	907	G
29	f	908	G
29	f	914	A
29	f	916	G
29	f	917	A
29	f	920	A
29	f	921	A
29	f	924	G
29	f	925	A
29	f	937	G
29	f	944	C
29	f	959	C
29	f	960	U
29	f	981	U
29	f	982	C
29	f	991	G
29	f	994	G
29	f	1001	G
29	f	1002	A
29	f	1010	G
29	f	1015	U
29	f	1016	C
29	f	1017	C
29	f	1018	G
29	f	1021	G
29	f	1024	G
29	f	1025	A
29	f	1028	U

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Mol	Chain	Res	Type
29	f	1036	A
29	f	1041	U
29	f	1047	A
29	f	1049	C
29	f	1063	G
29	f	1064	A
29	f	1065	A
29	f	1072	G
29	f	1081	U
29	f	1087	G
29	f	1093	A
29	f	1094	U
29	f	1095	U
29	f	1097	G
29	f	1098	A
29	f	1103	A
29	f	1104	G
29	f	1117	G
29	f	1131	G
29	f	1144	U
29	f	1153	A
29	f	1159	A
29	f	1160	C
29	f	1177	G
29	f	1180	A
29	f	1181	U
29	f	1192	C
29	f	1193	A
29	f	1196	C
29	f	1197	A
29	f	1201	C
29	f	1202	A
29	f	1208	U
29	f	1217	A
29	f	1218	U
29	f	1219	C
29	f	1222	G
29	f	1225	A
29	f	1227	C
29	f	1235	U
29	f	1236	G
29	f	1238	C

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Mol	Chain	Res	Type
29	f	1241	U
29	f	1242	G
29	f	1244	A
29	f	1245	A
29	f	1251	A
29	f	1252	A
29	f	1254	C
29	f	1258	U
29	f	1259	A
29	f	1263	A
29	f	1264	G
29	f	1265	U
29	f	1269	U
29	f	1272	C
29	f	1277	C
29	f	1278	A
29	f	1279	C
29	f	1282	G
29	f	1285	G
29	f	1286	A
29	f	1287	A
29	f	1295	G
29	f	1307	G
29	f	1308	A
29	f	1309	U
29	f	1313	G
29	f	1330	A
29	f	1348	U
29	f	1349	G
29	f	1351	U
29	f	1352	A
29	f	1354	G
29	f	1355	A
29	f	1356	U
29	f	1357	G
29	f	1386	A
29	f	1392	G
29	f	1399	A
29	f	1400	G
29	f	1419	A
29	f	1434	G
29	f	1437	C

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Mol	Chain	Res	Type
29	f	1446	A
29	f	1450	G
29	f	1481	A
29	f	1482	A
29	f	1483	G
29	f	1487	G
29	f	1488	G
29	f	1502	C
29	f	1508	C
29	f	1536	G
29	f	1539	A
29	f	1555	U
29	f	1556	C
29	f	1557	A
29	f	1560	G
29	f	1562	C
29	f	1563	C
29	f	1566	A
29	f	1568	U
29	f	1569	U
29	f	1572	U
29	f	1573	G
29	f	1575	A
29	f	1576	G
29	f	1580	A
29	f	1581	C
29	f	1582	C
29	f	1583	A
29	f	1589	A
29	f	1590	G
29	f	1605	A
29	f	1607	U
29	f	1620	U
29	f	1629	U
29	f	1639	C
29	f	1642	A
29	f	1643	A
29	f	1645	U
29	f	1657	C
29	f	1683	A
29	f	1716	U
29	f	1717	U

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Mol	Chain	Res	Type
29	f	1724	U
29	f	1725	C
29	f	1736	G
29	f	1741	A
29	f	1750	A
29	f	1751	G
29	f	1760	A
29	f	1761	C
29	f	1764	U
29	f	1765	U
29	f	1766	G
29	f	1770	G
29	f	1775	G
29	f	1780	G
29	f	1797	A
29	f	1814	A
29	f	1816	A
29	f	1819	U
29	f	1820	U
29	f	1821	U
29	f	1835	A
29	f	1839	A
29	f	1840	U
29	f	1841	A
29	f	1842	A
29	f	1846	C
29	f	1849	C
29	f	1850	A
29	f	1866	C
29	f	1867	A
29	f	1880	U
29	f	1881	A
29	f	1893	A
29	f	1906	G
29	f	1943	C
29	f	1952	G
29	f	1953	G
29	f	1954	G
29	f	2094	C
29	f	2101	C
29	f	2102	U
29	f	2111	G

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Mol	Chain	Res	Type
29	f	2112	U
29	f	2113	A
29	f	2114	C
29	f	2121	G
29	f	2122	G
29	f	2131	A
29	f	2134	G
29	f	2140	U
29	f	2144	A
29	f	2158	A
29	f	2160	G
29	f	2169	G
29	f	2176	U
29	f	2201	G
29	f	2206	G
29	f	2207	A
29	f	2208	A
29	f	2209	U
29	f	2222	A
29	f	2223	A
29	f	2225	U
29	f	2228	A
29	f	2251	G
29	f	2252	A
29	f	2267	C
29	f	2272	G
29	f	2273	G
29	f	2274	U
29	f	2281	A
29	f	2282	U
29	f	2288	G
29	f	2307	G
29	f	2308	C
29	f	2310	U
29	f	2313	A
29	f	2314	U
29	f	2315	G
29	f	2334	U
29	f	2335	G
29	f	2336	U
29	f	2373	A
29	f	2374	C

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Mol	Chain	Res	Type
29	f	2375	G
29	f	2385	G
29	f	2388	U
29	f	2393	G
29	f	2397	A
29	f	2402	A
29	f	2403	G
29	f	2404	A
29	f	2411	U
29	f	2419	A
29	f	2435	G
29	f	2437	G
29	f	2439	A
29	f	2440	G
29	f	2445	A
29	f	2446	U
29	f	2447	A
29	f	2448	G
29	f	2449	A
29	f	2450	G
29	f	2451	G
29	f	2452	G
29	f	2453	U
29	f	2460	U
29	f	2461	A
29	f	2465	G
29	f	2468	A
29	f	2469	G
29	f	2471	U
29	f	2473	C
29	f	2474	G
29	f	2476	C
29	f	2479	C
29	f	2480	A
29	f	2482	U
29	f	2484	A
29	f	2486	A
29	f	2487	U
29	f	2494	A
29	f	2495	C
29	f	2499	U
29	f	2501	U

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Mol	Chain	Res	Type
29	f	2503	G
29	f	2505	U
29	f	2506	U
29	f	2511	A
29	f	2514	U
29	f	2515	A
29	f	2522	G
29	f	2526	C
29	f	2531	C
29	f	2537	U
29	f	2538	U
29	f	2539	C
29	f	2540	A
29	f	2541	U
29	f	2542	U
29	f	2544	U
29	f	2547	A
29	f	2548	C
29	f	2549	G
29	f	2552	C
29	f	2554	A
29	f	2555	G
29	f	2561	A
29	f	2569	A
29	f	2570	U
29	f	2571	U
29	f	2572	C
29	f	2573	G
29	f	2581	U
29	f	2585	G
29	f	2593	A
29	f	2594	C
29	f	2606	G
29	f	2607	G
29	f	2614	G
29	f	2648	G
29	f	2651	G
29	f	2652	U
29	f	2656	A
29	f	2674	A
29	f	2677	G
29	f	2678	A

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Mol	Chain	Res	Type
29	f	2689	A
29	f	2691	A
29	f	2694	A
29	f	2696	A
29	f	2704	A
29	f	2714	G
29	f	2719	U
29	f	2728	G
29	f	2729	U
29	f	2740	A
29	f	2752	U
29	f	2753	G
29	f	2755	C
29	f	2772	C
29	f	2773	C
29	f	2777	G
29	f	2778	G
29	f	2788	C
29	f	2796	G
29	f	2800	G
29	f	2801	A
29	f	2803	A
29	f	2810	C
29	f	2814	G
29	f	2817	A
29	f	2818	U
29	f	2821	C
29	f	2822	U
29	f	2842	U
29	f	2844	C
29	f	2845	A
29	f	2846	U
29	f	2849	C
29	f	2867	C
29	f	2871	G
29	f	2872	A
29	f	2876	C
29	f	2887	A
29	f	2898	G
29	f	2899	C
29	f	2911	A
29	f	2914	G

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Mol	Chain	Res	Type
29	f	2923	U
29	f	2935	U
29	f	2936	A
29	f	2941	A
29	f	2942	C
29	f	2947	G
29	f	2971	A
29	f	2983	C
29	f	2990	G
29	f	2992	U
29	f	2996	U
29	f	2997	G
29	f	3006	A
29	f	3012	A
29	f	3056	U
29	f	3059	G
29	f	3078	U
29	f	3079	U
29	f	3080	G
29	f	3086	A
29	f	3092	C
29	f	3104	U
29	f	3113	A
29	f	3122	A
29	f	3130	A
29	f	3131	U
29	f	3142	A
29	f	3143	C
29	f	3151	U
29	f	3154	C
29	f	3155	U
29	f	3156	U
29	f	3157	U
29	f	3165	A
29	f	3170	A
29	f	3173	G
29	f	3174	A
29	f	3175	U
29	f	3176	G
29	f	3179	U
29	f	3181	C
29	f	3186	A

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Mol	Chain	Res	Type
29	f	3187	A
29	f	3196	U
29	f	3207	U
29	f	3209	A
29	f	3217	C
29	f	3218	A
29	f	3219	G
29	f	3228	C
29	f	3229	G
29	f	3243	A
29	f	3245	A
29	f	3247	G
29	f	3259	U
29	f	3263	G
29	f	3269	U
29	f	3270	U
29	f	3273	A
29	f	3276	G
29	f	3281	U
29	f	3287	U
29	f	3288	G
29	f	3289	G
29	f	3294	A
29	f	3295	A
29	f	3303	G
29	f	3304	U
29	f	3307	A
29	f	3313	U
29	f	3316	A
29	f	3317	U
29	f	3318	G
29	f	3319	U
29	f	3320	A
29	f	3341	U
29	f	3342	A
29	f	3345	G
29	f	3351	U
29	f	3352	U
29	f	3353	G
29	f	3354	U
29	f	3355	U
29	f	3369	G

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Mol	Chain	Res	Type
29	f	3375	A
29	f	3378	C
29	f	3382	U
29	f	3383	G
29	f	3386	G
29	f	3389	U
29	f	3390	G
29	f	3396	U
30	h	7	G
30	h	29	C
30	h	53	U
30	h	54	U
30	h	55	A
30	h	65	G
30	h	73	C
30	h	74	C
30	h	95	A
30	h	102	A
30	h	112	G
30	h	121	U
31	i	23	U
31	i	34	U
31	i	35	C
31	i	39	G
31	i	48	A
31	i	52	A
31	i	53	A
31	i	59	A
31	i	62	C
31	i	63	G
31	i	80	A
31	i	81	U
31	i	82	U
31	i	83	C
31	i	84	C
31	i	85	G
31	i	86	U
31	i	87	G
31	i	90	U
31	i	95	G
31	i	104	A
31	i	105	A

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Mol	Chain	Res	Type
31	i	106	C
31	i	111	A
31	i	113	U
31	i	125	U
31	i	126	A
31	i	138	A
31	i	151	C
31	i	152	G
31	i	157	U
31	i	158	U
47	x	5	G
47	x	7	G
47	x	10	G
47	x	13	U
47	x	16	U
47	x	17	C
47	x	18	G
47	x	22	G
47	x	28	U
47	x	33	U
47	x	34	A
47	x	35	G
47	x	36	C
47	x	37	A
47	x	38	U
47	x	42	A
47	x	43	G
47	x	46	G
47	x	48	C
47	x	49	U
47	x	56	C
47	x	57	G
47	x	58	A
47	x	60	U
47	x	61	C
47	x	74	C
47	y	5	G
47	y	7	G
47	y	8	U
47	y	9	G
47	y	13	U
47	y	16	U

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Mol	Chain	Res	Type
47	y	17	C
47	y	22	G
47	y	23	C
47	y	36	C
47	y	38	U
47	y	43	G
47	y	44	A
47	y	46	G
47	y	47	U
47	y	48	C
47	y	51	C
47	y	52	G
47	y	53	G
47	y	56	C
47	y	57	G
47	y	58	A
47	y	59	U
47	y	61	C
47	y	75	C
47	y	76	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 19 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
57	ATP	C	1001	-	28,33,33	0.99	0	34,52,52	1.21	3 (8%)
57	ATP	D	902	-	28,33,33	0.98	0	34,52,52	1.22	3 (8%)
58	ADP	E	901	-	24,29,29	0.92	0	29,45,45	1.26	3 (10%)
57	ATP	C	1003	-	28,33,33	0.99	0	34,52,52	1.22	3 (8%)
57	ATP	E	902	-	28,33,33	0.99	1 (3%)	34,52,52	1.23	3 (8%)
57	ATP	F	901	-	28,33,33	0.99	1 (3%)	34,52,52	1.21	3 (8%)
57	ATP	A	901	-	28,33,33	0.98	0	34,52,52	1.22	3 (8%)
57	ATP	B	901	-	28,33,33	0.99	0	34,52,52	1.23	3 (8%)
57	ATP	D	901	-	28,33,33	0.99	0	34,52,52	1.23	3 (8%)
61	SPD	f	3401	-	9,9,9	0.31	0	8,8,8	0.85	0
57	ATP	C	1002	-	28,33,33	0.99	0	34,52,52	1.22	3 (8%)

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
57	ATP	C	1001	-	-	5/18/38/38	0/3/3/3
57	ATP	D	902	-	-	5/18/38/38	0/3/3/3
58	ADP	E	901	-	-	3/12/32/32	0/3/3/3
57	ATP	C	1003	-	-	5/18/38/38	0/3/3/3
57	ATP	E	902	-	-	5/18/38/38	0/3/3/3
57	ATP	F	901	-	-	1/18/38/38	0/3/3/3
57	ATP	A	901	-	-	5/18/38/38	0/3/3/3
57	ATP	B	901	-	-	3/18/38/38	0/3/3/3
57	ATP	D	901	-	-	4/18/38/38	0/3/3/3
61	SPD	f	3401	-	-	5/7/7/7	-
57	ATP	C	1002	-	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	F	901	ATP	O4'-C1'	2.06	1.43	1.40
57	E	902	ATP	O4'-C1'	2.02	1.43	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	D	901	ATP	N3-C2-N1	-3.70	123.65	128.67
57	E	902	ATP	N3-C2-N1	-3.70	123.65	128.67
57	B	901	ATP	N3-C2-N1	-3.69	123.66	128.67
57	C	1002	ATP	N3-C2-N1	-3.68	123.68	128.67
57	C	1003	ATP	N3-C2-N1	-3.67	123.70	128.67
57	A	901	ATP	N3-C2-N1	-3.64	123.74	128.67
57	F	901	ATP	N3-C2-N1	-3.62	123.76	128.67
58	E	901	ADP	N3-C2-N1	-3.61	123.77	128.67
57	D	902	ATP	N3-C2-N1	-3.59	123.80	128.67
57	C	1001	ATP	N3-C2-N1	-3.58	123.81	128.67
57	C	1001	ATP	C4-C5-N7	-2.65	106.54	109.34
57	D	902	ATP	C4-C5-N7	-2.65	106.54	109.34
57	A	901	ATP	C4-C5-N7	-2.63	106.56	109.34
57	B	901	ATP	C4-C5-N7	-2.62	106.57	109.34
57	E	902	ATP	C4-C5-N7	-2.61	106.58	109.34
57	D	901	ATP	C4-C5-N7	-2.61	106.58	109.34
57	C	1002	ATP	C4-C5-N7	-2.60	106.59	109.34
57	C	1003	ATP	C4-C5-N7	-2.60	106.59	109.34
58	E	901	ADP	C4-C5-N7	-2.58	106.62	109.34
57	F	901	ATP	C4-C5-N7	-2.57	106.62	109.34
57	E	902	ATP	C4'-O4'-C1'	2.17	111.91	109.92
57	B	901	ATP	C4'-O4'-C1'	2.17	111.91	109.92
57	D	902	ATP	C4'-O4'-C1'	2.16	111.90	109.92
57	D	901	ATP	C4'-O4'-C1'	2.15	111.89	109.92
58	E	901	ADP	C4'-O4'-C1'	2.14	111.88	109.92
57	C	1001	ATP	C4'-O4'-C1'	2.13	111.88	109.92
57	A	901	ATP	C4'-O4'-C1'	2.10	111.85	109.92
57	C	1003	ATP	C4'-O4'-C1'	2.09	111.84	109.92
57	C	1002	ATP	C4'-O4'-C1'	2.08	111.83	109.92
57	F	901	ATP	C4'-O4'-C1'	2.04	111.80	109.92

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	901	ATP	O4'-C4'-C5'-O5'
57	A	901	ATP	C3'-C4'-C5'-O5'
57	C	1001	ATP	O4'-C4'-C5'-O5'
57	C	1001	ATP	C3'-C4'-C5'-O5'
57	C	1002	ATP	O4'-C4'-C5'-O5'
57	C	1002	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
57	C	1003	ATP	O4'-C4'-C5'-O5'
57	C	1003	ATP	C3'-C4'-C5'-O5'
57	D	901	ATP	O4'-C4'-C5'-O5'
57	D	902	ATP	O4'-C4'-C5'-O5'
57	D	902	ATP	C3'-C4'-C5'-O5'
57	E	902	ATP	O4'-C4'-C5'-O5'
57	E	902	ATP	C3'-C4'-C5'-O5'
58	E	901	ADP	C5'-O5'-PA-O3A
58	E	901	ADP	C4'-C5'-O5'-PA
57	D	901	ATP	C3'-C4'-C5'-O5'
61	f	3401	SPD	C3-C4-C5-N6
61	f	3401	SPD	N6-C7-C8-C9
57	A	901	ATP	PB-O3A-PA-O2A
57	B	901	ATP	PB-O3A-PA-O2A
57	C	1002	ATP	PB-O3A-PA-O2A
57	D	901	ATP	PG-O3B-PB-O2B
57	D	902	ATP	PB-O3A-PA-O2A
57	E	902	ATP	PB-O3A-PA-O2A
61	f	3401	SPD	C2-C3-C4-C5
57	A	901	ATP	C5'-O5'-PA-O1A
57	B	901	ATP	C5'-O5'-PA-O2A
57	C	1001	ATP	C5'-O5'-PA-O1A
57	C	1002	ATP	C5'-O5'-PA-O1A
57	C	1003	ATP	C5'-O5'-PA-O1A
57	D	902	ATP	C5'-O5'-PA-O1A
57	E	902	ATP	C5'-O5'-PA-O1A
58	E	901	ADP	C5'-O5'-PA-O1A
57	C	1001	ATP	PB-O3A-PA-O2A
57	C	1003	ATP	PB-O3A-PA-O2A
57	F	901	ATP	C4'-C5'-O5'-PA
57	D	901	ATP	PG-O3B-PB-O1B
61	f	3401	SPD	C4-C5-N6-C7
61	f	3401	SPD	C8-C7-N6-C5
57	A	901	ATP	PB-O3A-PA-O1A
57	B	901	ATP	PB-O3A-PA-O1A
57	C	1001	ATP	PB-O3A-PA-O1A
57	C	1002	ATP	PB-O3A-PA-O1A
57	C	1003	ATP	PB-O3A-PA-O1A
57	D	902	ATP	PB-O3A-PA-O1A
57	E	902	ATP	PB-O3A-PA-O1A

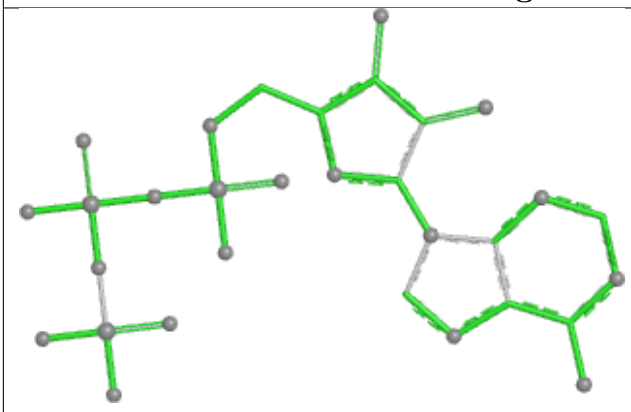
There are no ring outliers.

11 monomers are involved in 194 short contacts:

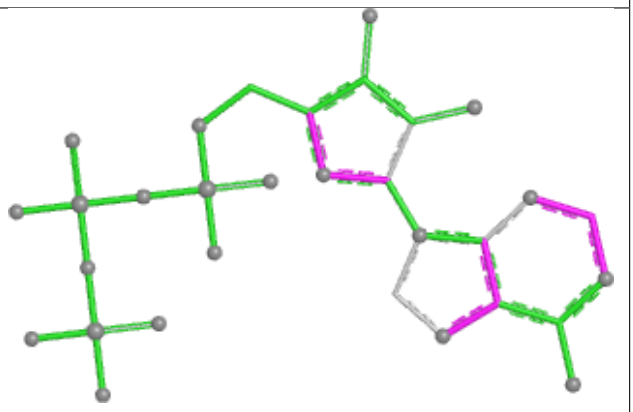
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	C	1001	ATP	42	0
57	D	902	ATP	29	0
58	E	901	ADP	23	0
57	C	1003	ATP	18	0
57	E	902	ATP	14	0
57	F	901	ATP	18	0
57	A	901	ATP	23	0
57	B	901	ATP	2	0
57	D	901	ATP	20	0
61	f	3401	SPD	1	0
57	C	1002	ATP	4	0

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

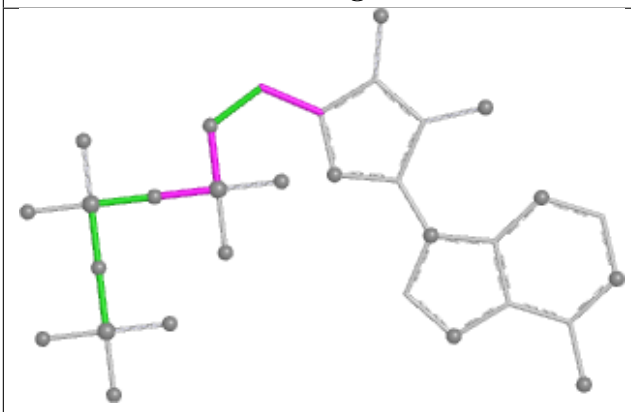
Ligand ATP C 1001



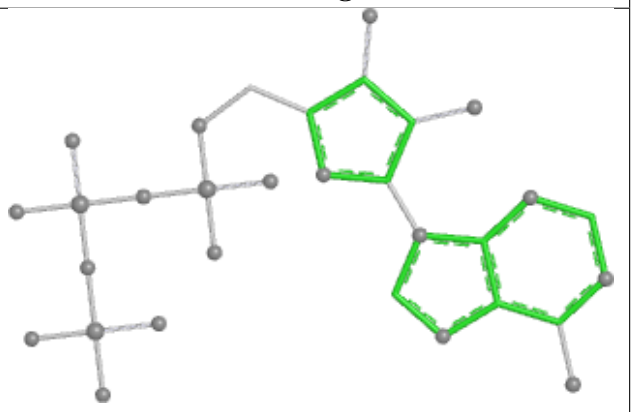
Bond lengths



Bond angles

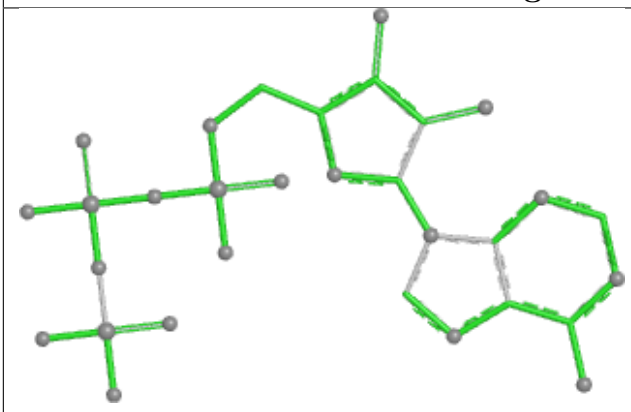


Torsions



Rings

Ligand ATP D 902



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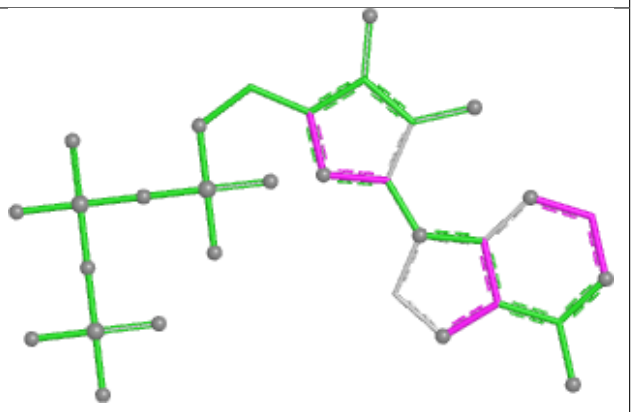

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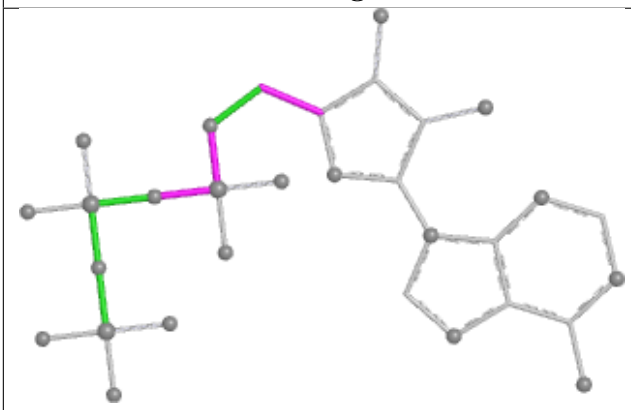

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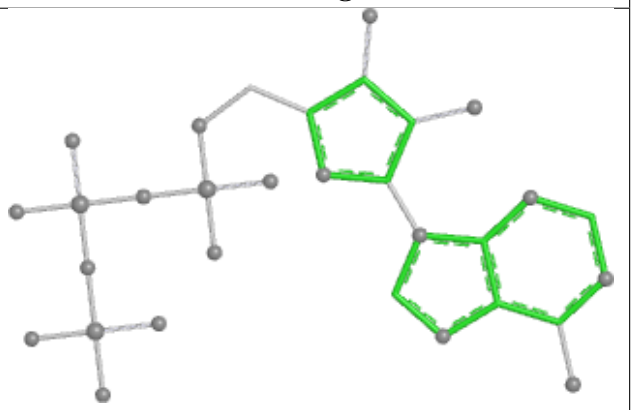
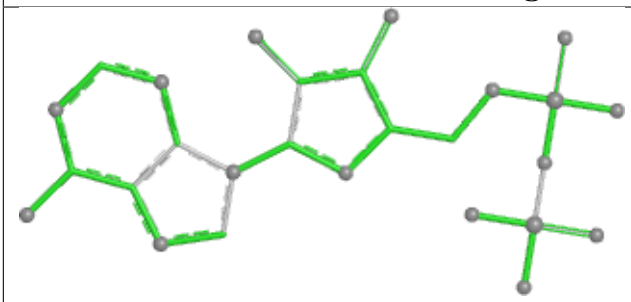


Rings

Ligand ADP E 901



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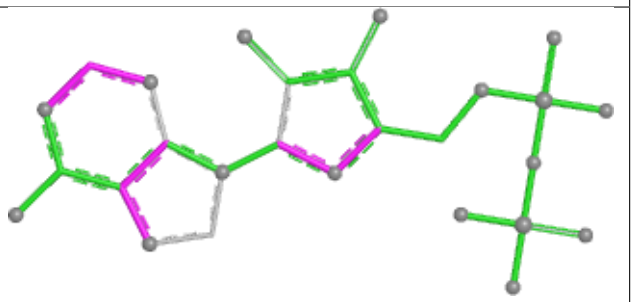
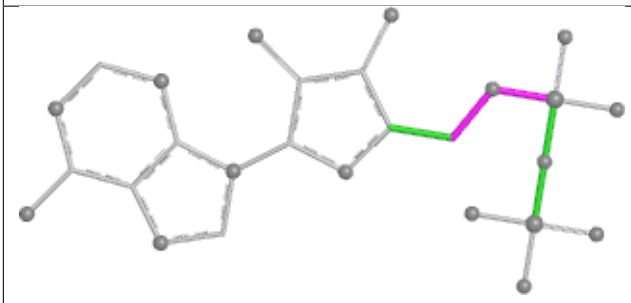
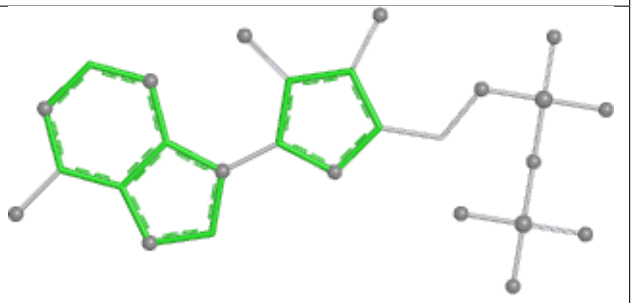


Bond angles

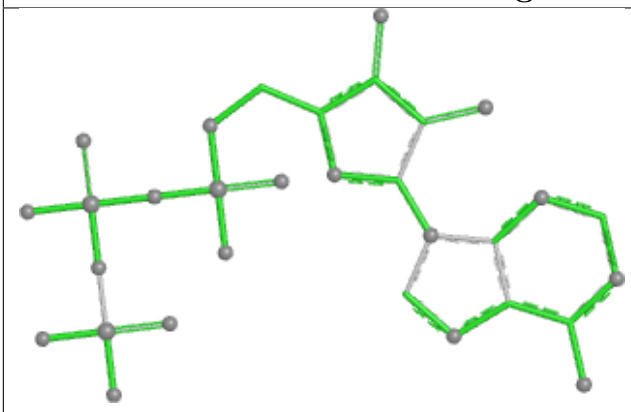


Torsions

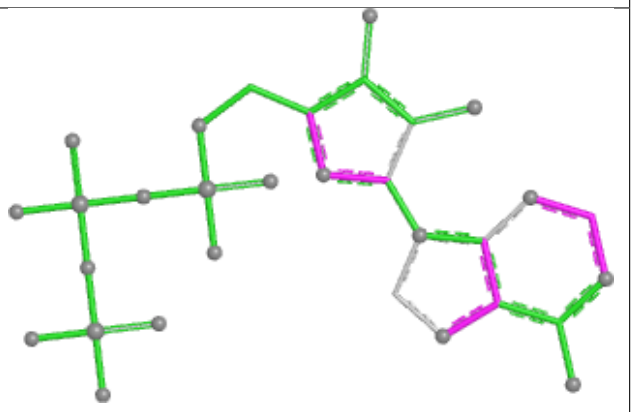


Rings

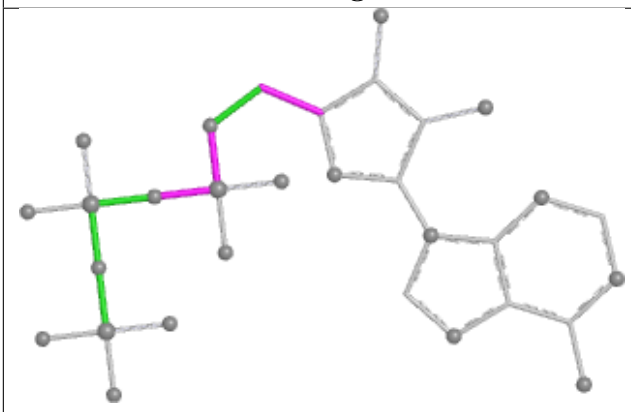
Ligand ATP C 1003



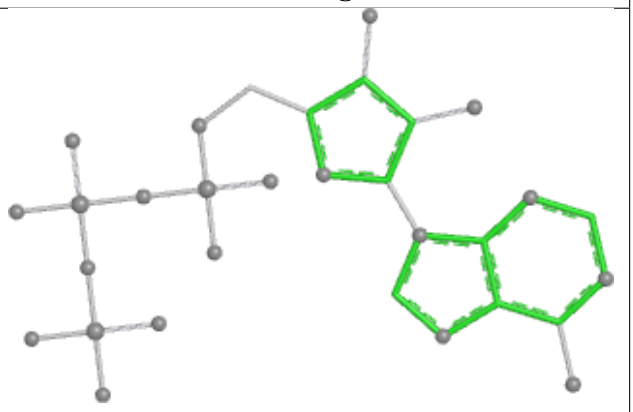
Bond lengths



Bond angles

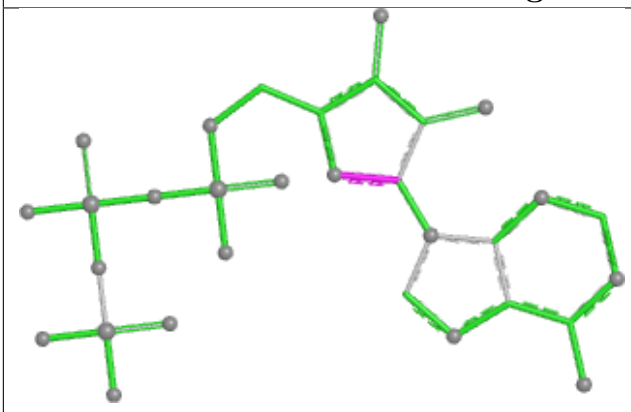


Torsions

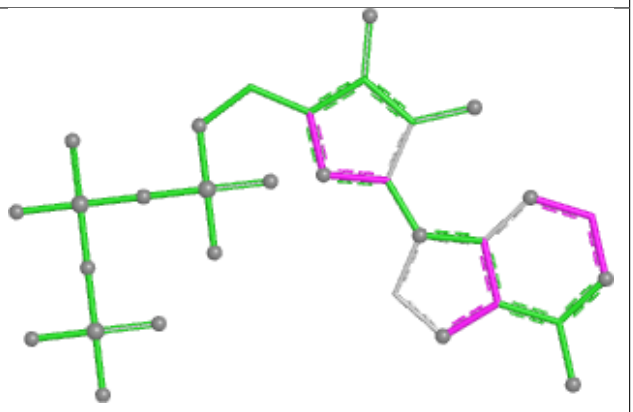


Rings

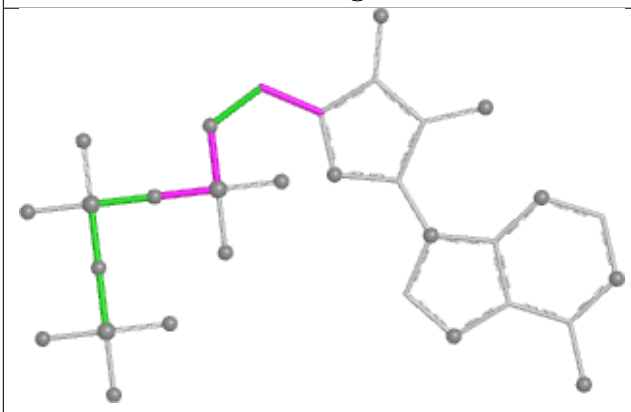
Ligand ATP E 902



Bond lengths



Bond angles



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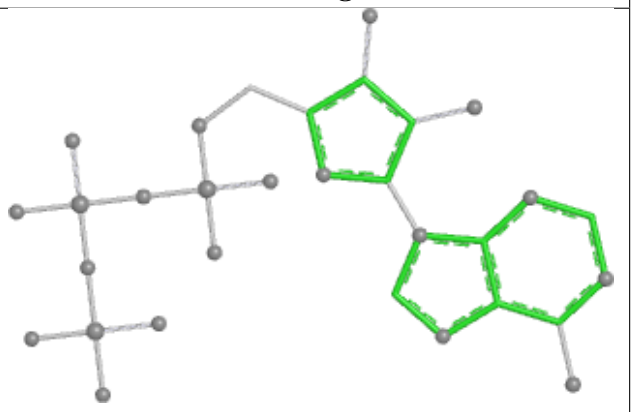
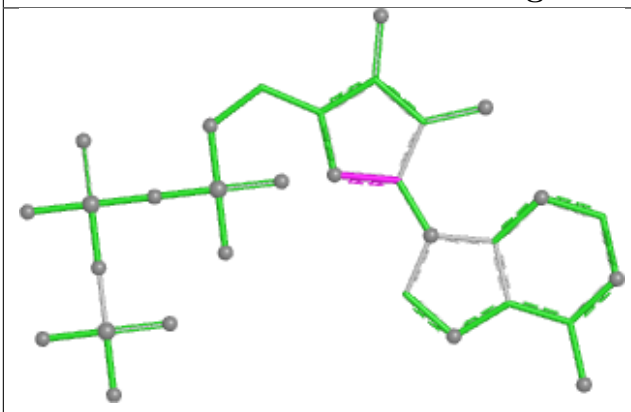


Rings

Ligand ATP F 901



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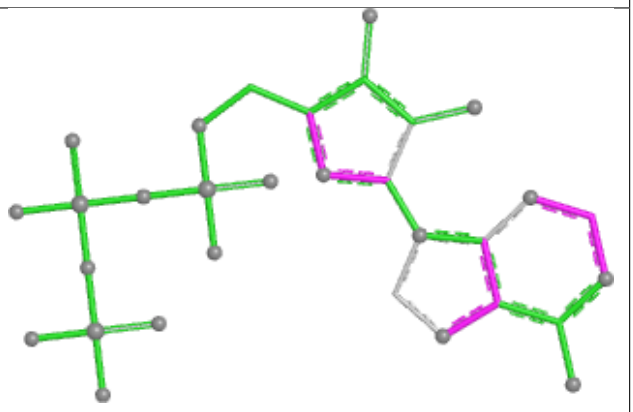

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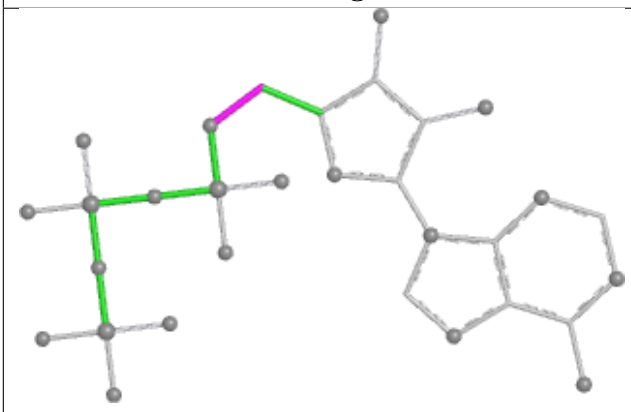

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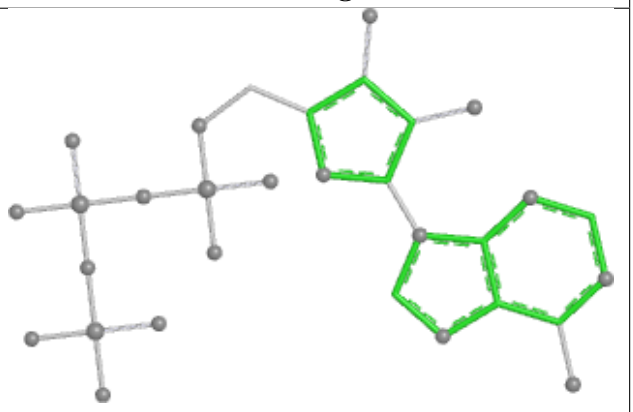
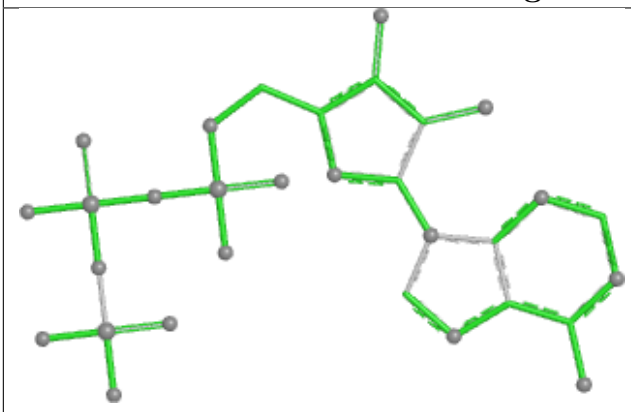
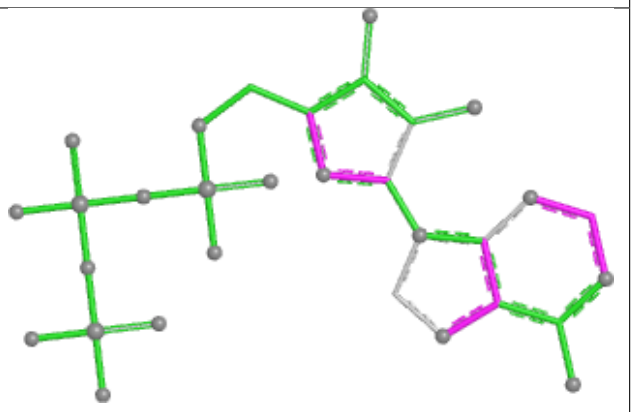


Rings

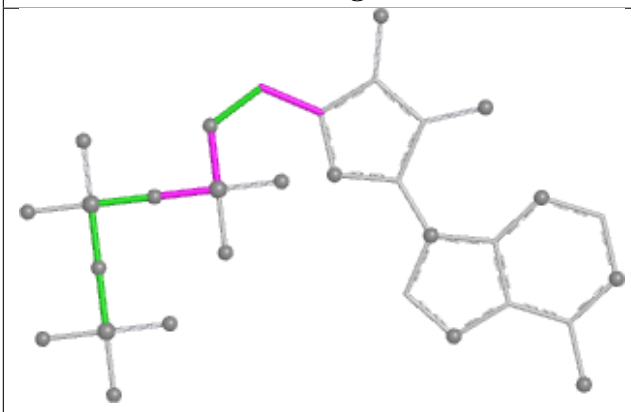
Ligand ATP A 901



Bond lengths



Bond angles



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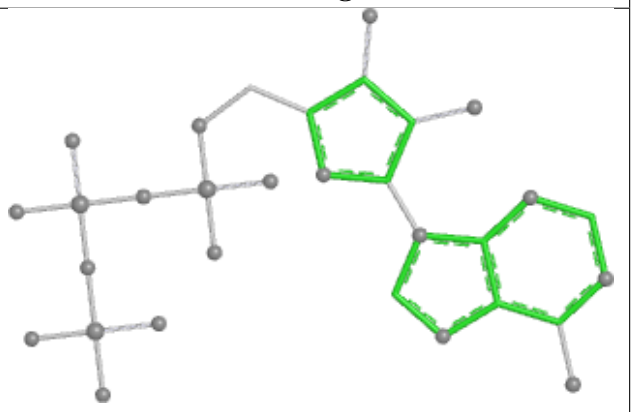
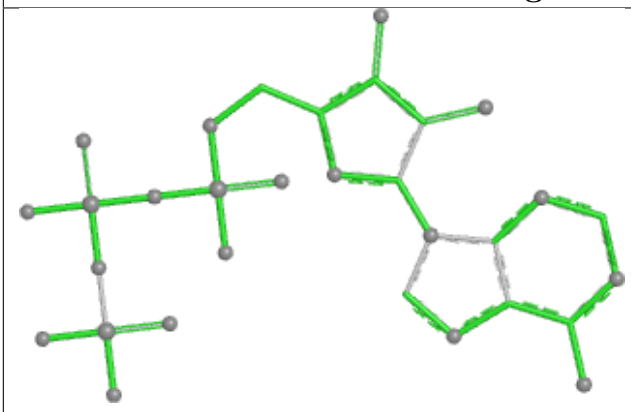
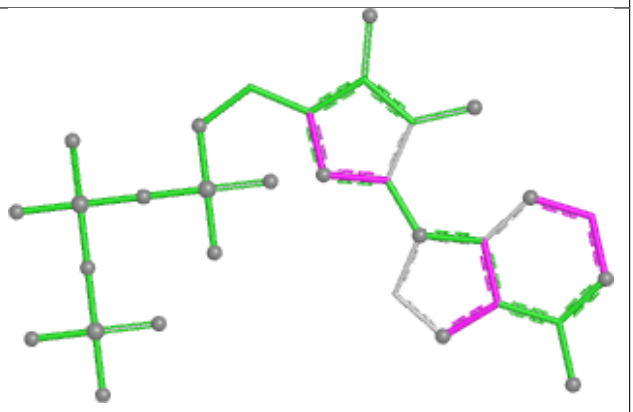


Rings

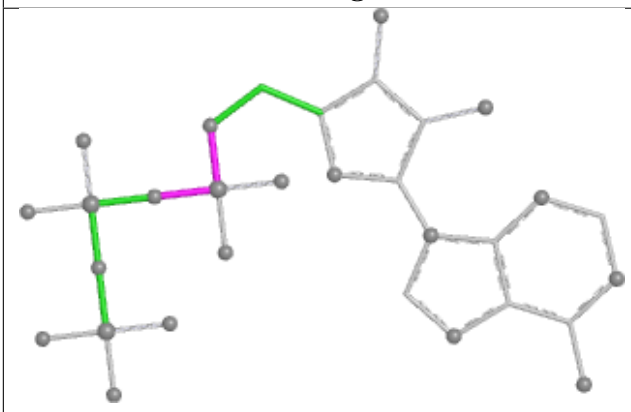
Ligand ATP B 901



Bond lengths



Bond angles



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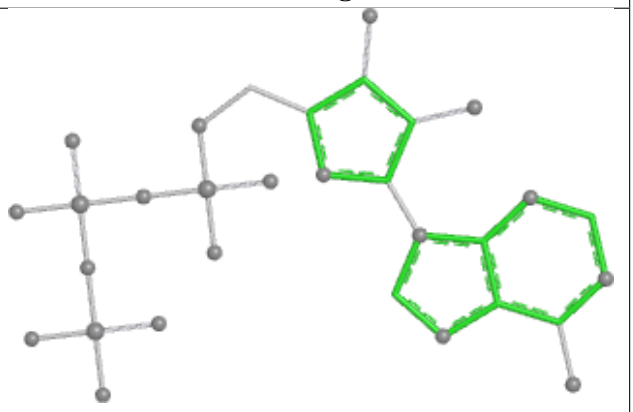
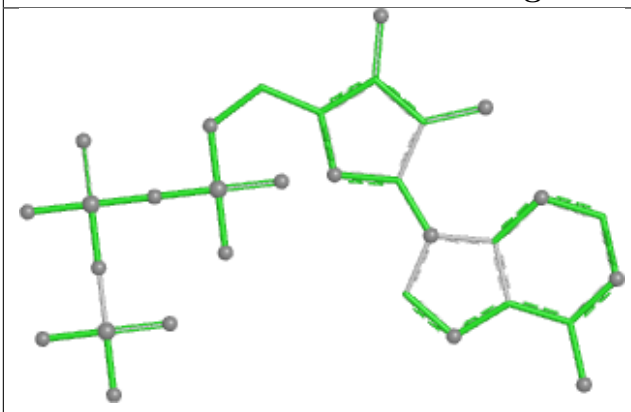
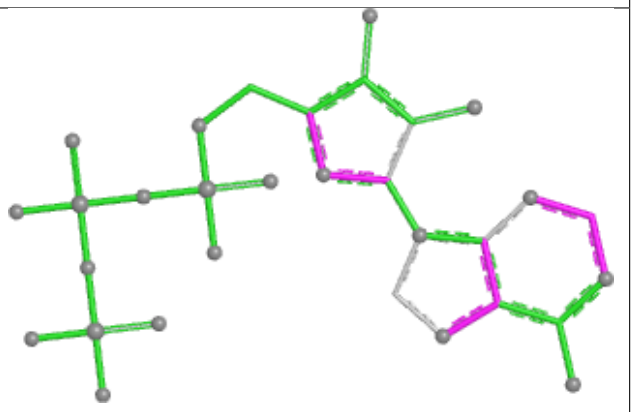


Rings

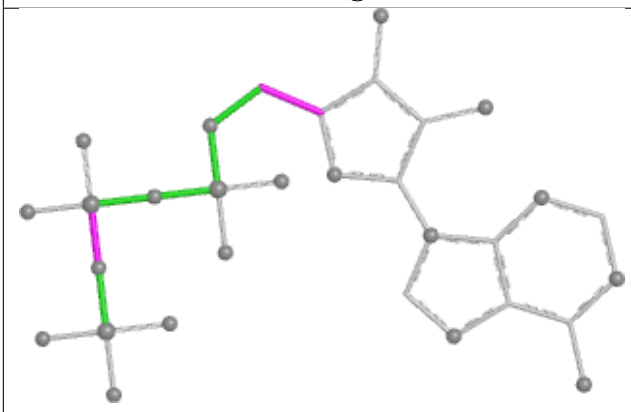
Ligand ATP D 901



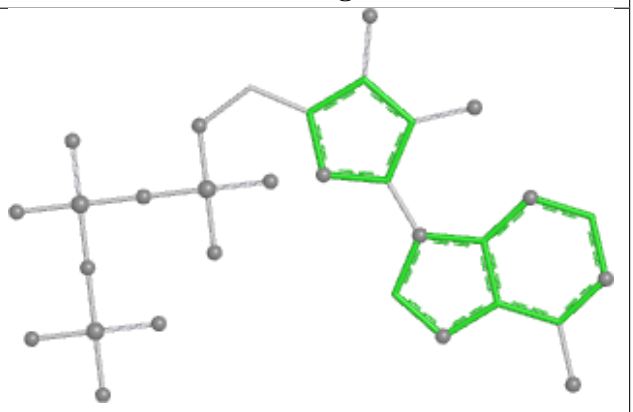
Bond lengths



Bond angles

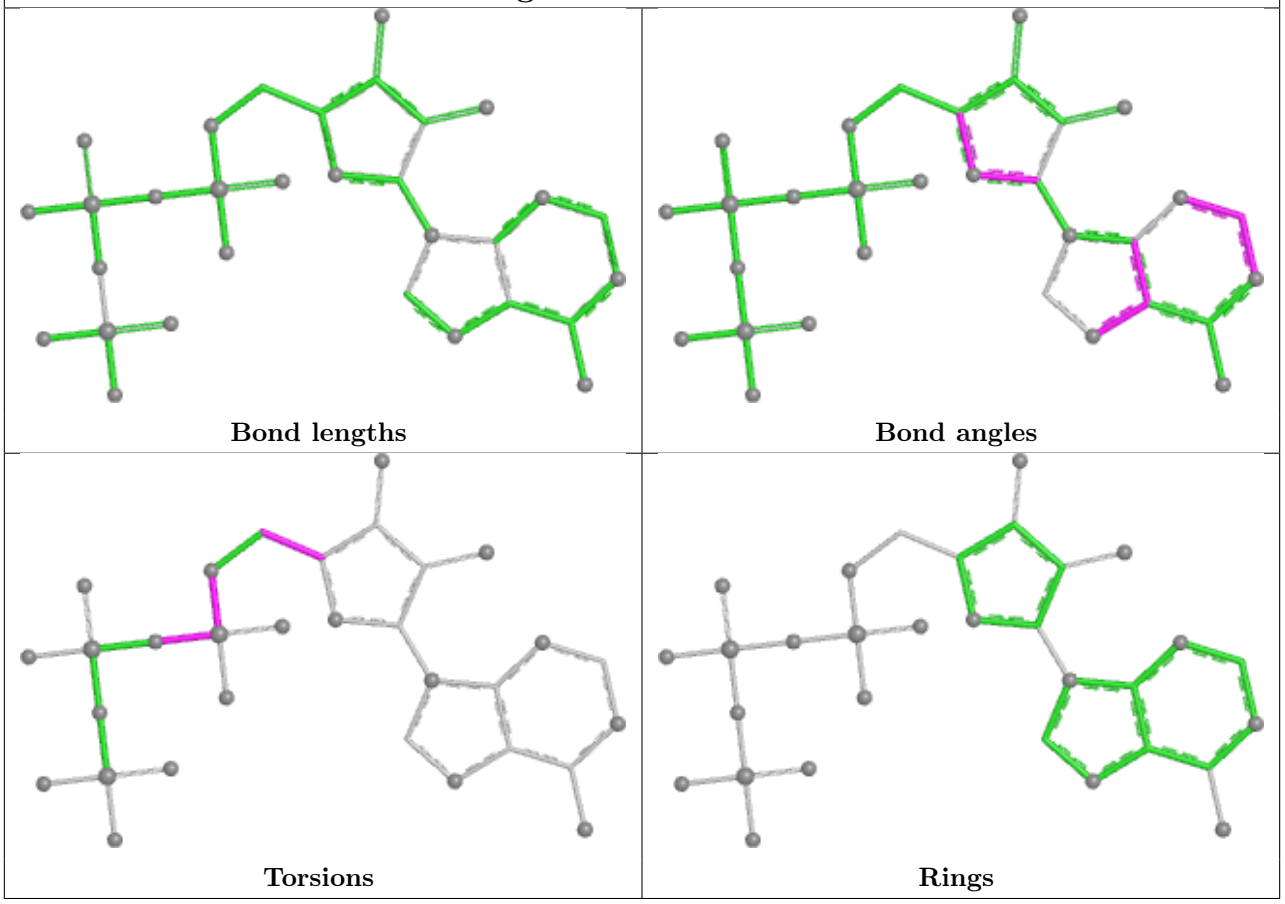


Torsions



Rings

Ligand ATP C 1002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	e	2
53	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	1071:THR	C	1072:ALA	N	3.98
1	e	932:LEU	C	933:LEU	N	2.01
1	v	439:GLN	C	440:ARG	N	1.62

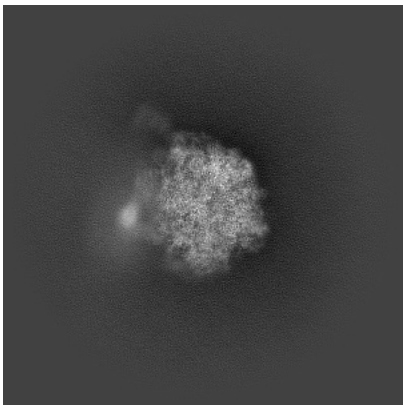
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70444. These allow visual inspection of the internal detail of the map and identification of artifacts.

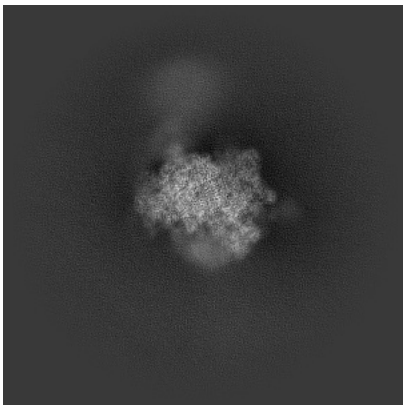
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

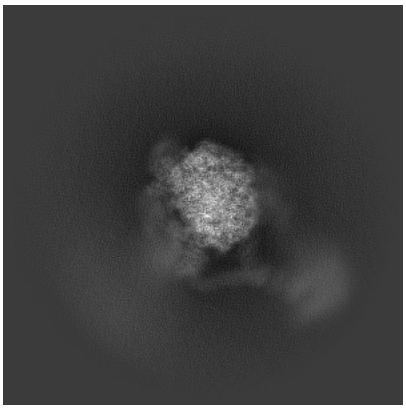
6.1.1 Primary map



X

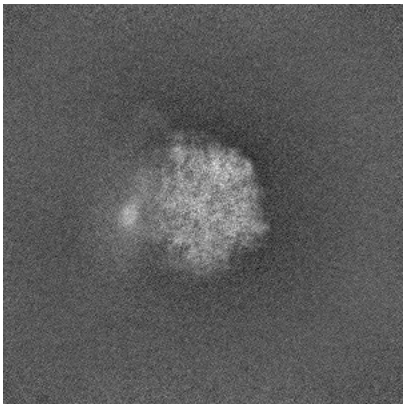


Y

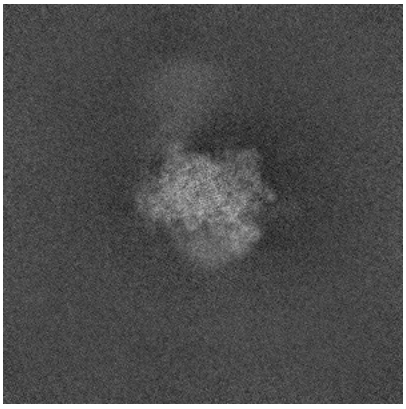


Z

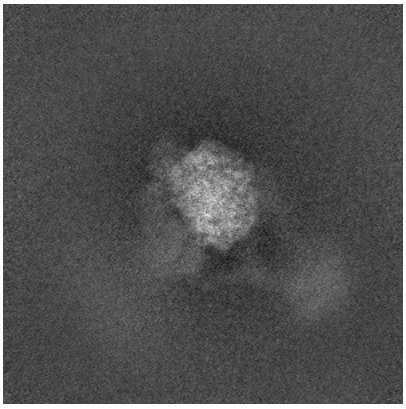
6.1.2 Raw map



X



Y

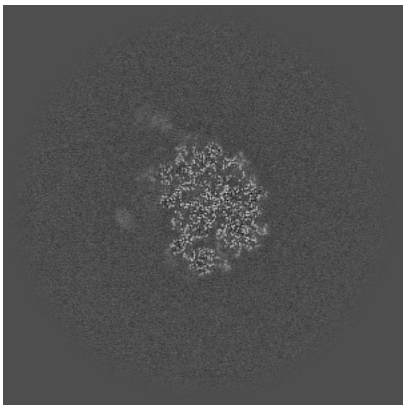


Z

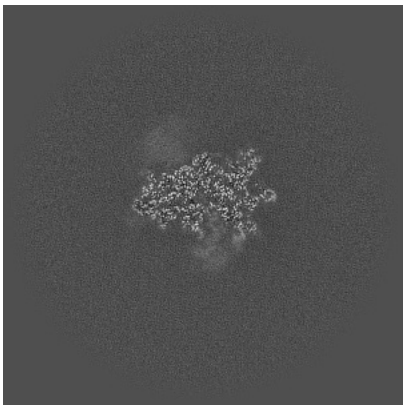
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

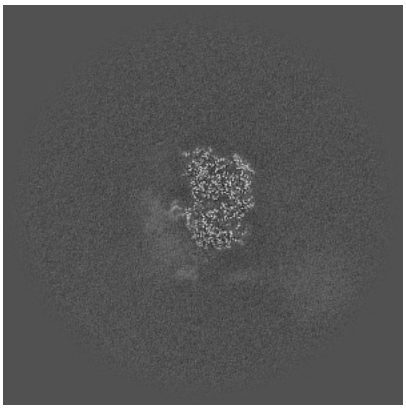
6.2.1 Primary map



X Index: 320

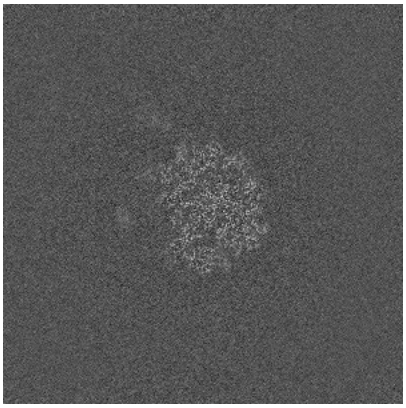


Y Index: 320

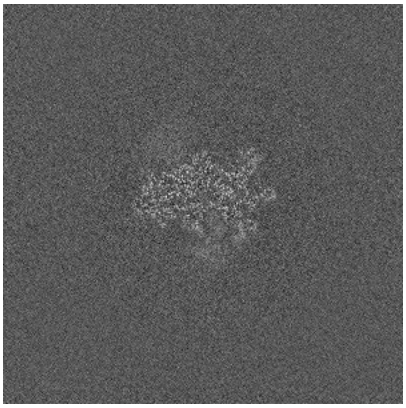


Z Index: 320

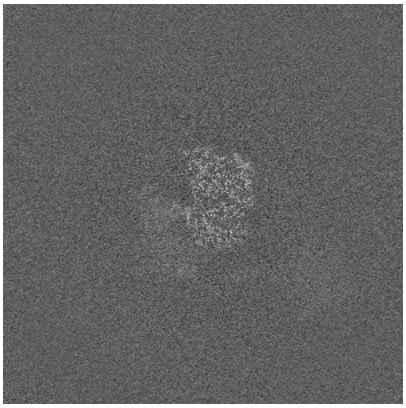
6.2.2 Raw map



X Index: 320



Y Index: 320

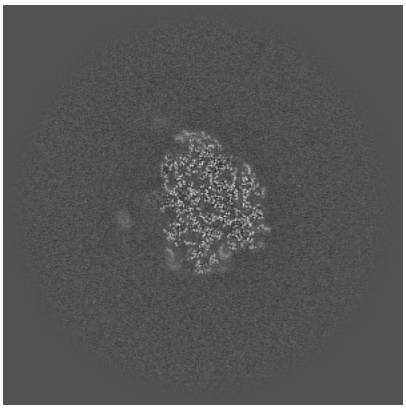


Z Index: 320

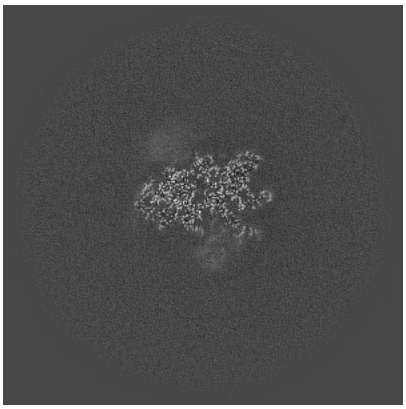
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

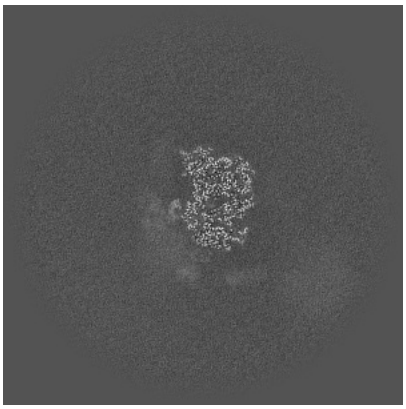
6.3.1 Primary map



X Index: 331

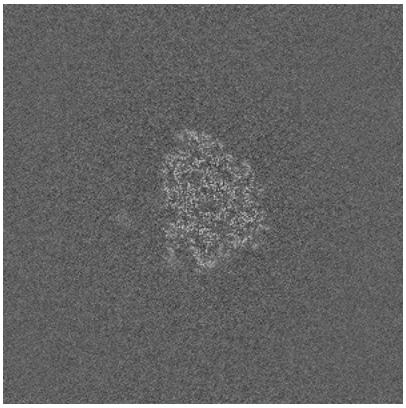


Y Index: 325

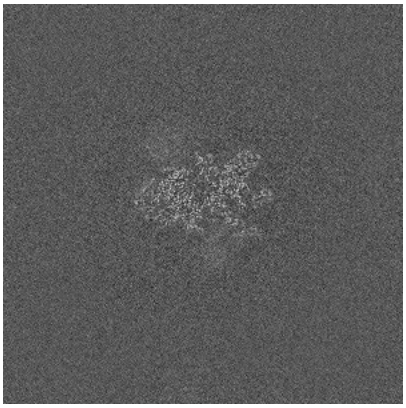


Z Index: 318

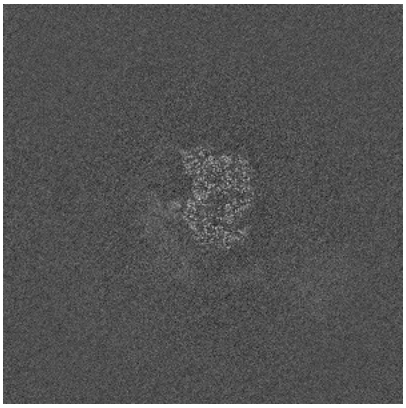
6.3.2 Raw map



X Index: 333



Y Index: 326

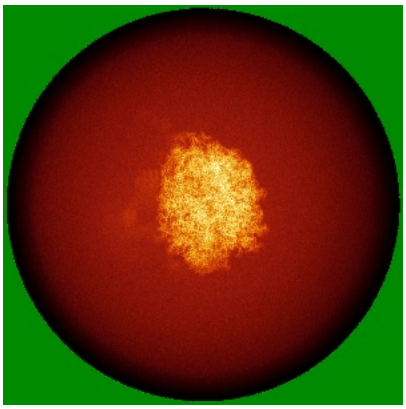


Z Index: 317

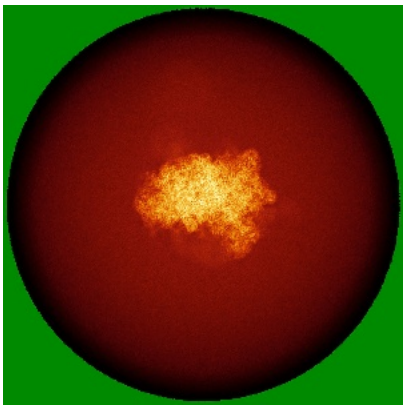
The images above show the largest variance slices of the map in three orthogonal directions.

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

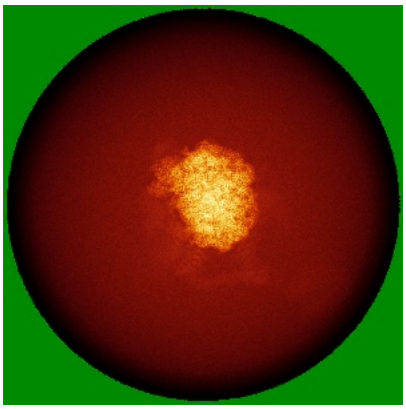
6.4.1 Primary map



X

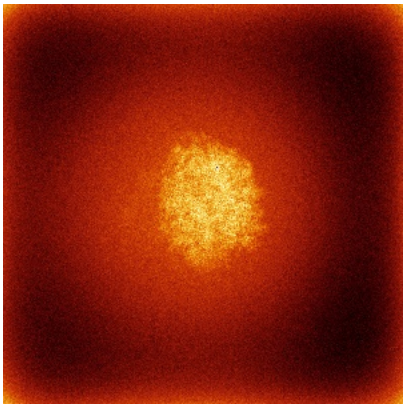


Y

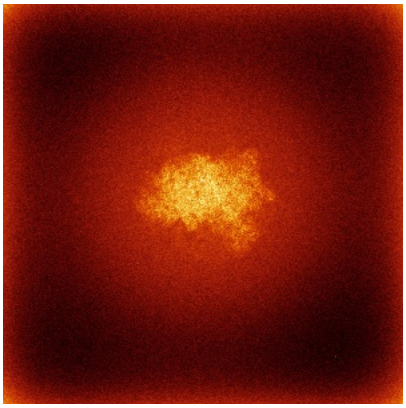


Z

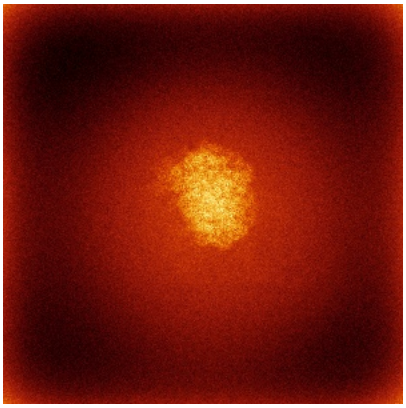
6.4.2 Raw map



X



Y

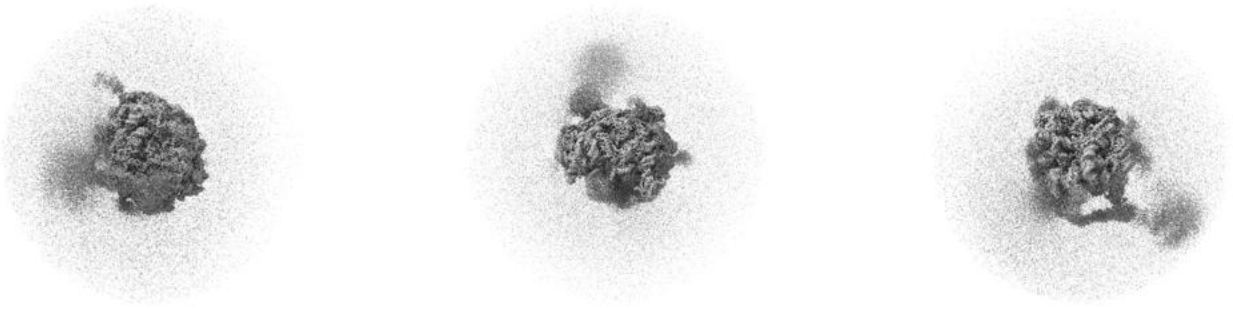


Z

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

6.5 Orthogonal surface views (i)

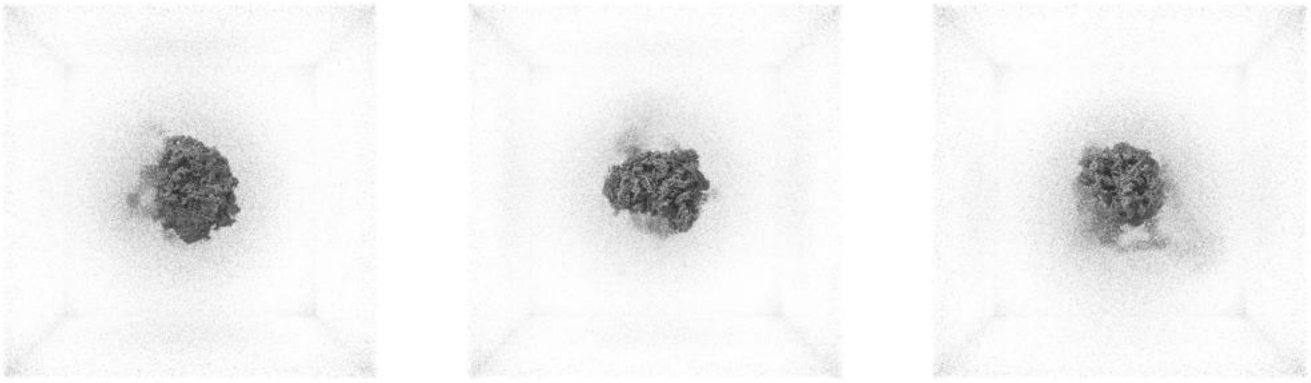
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

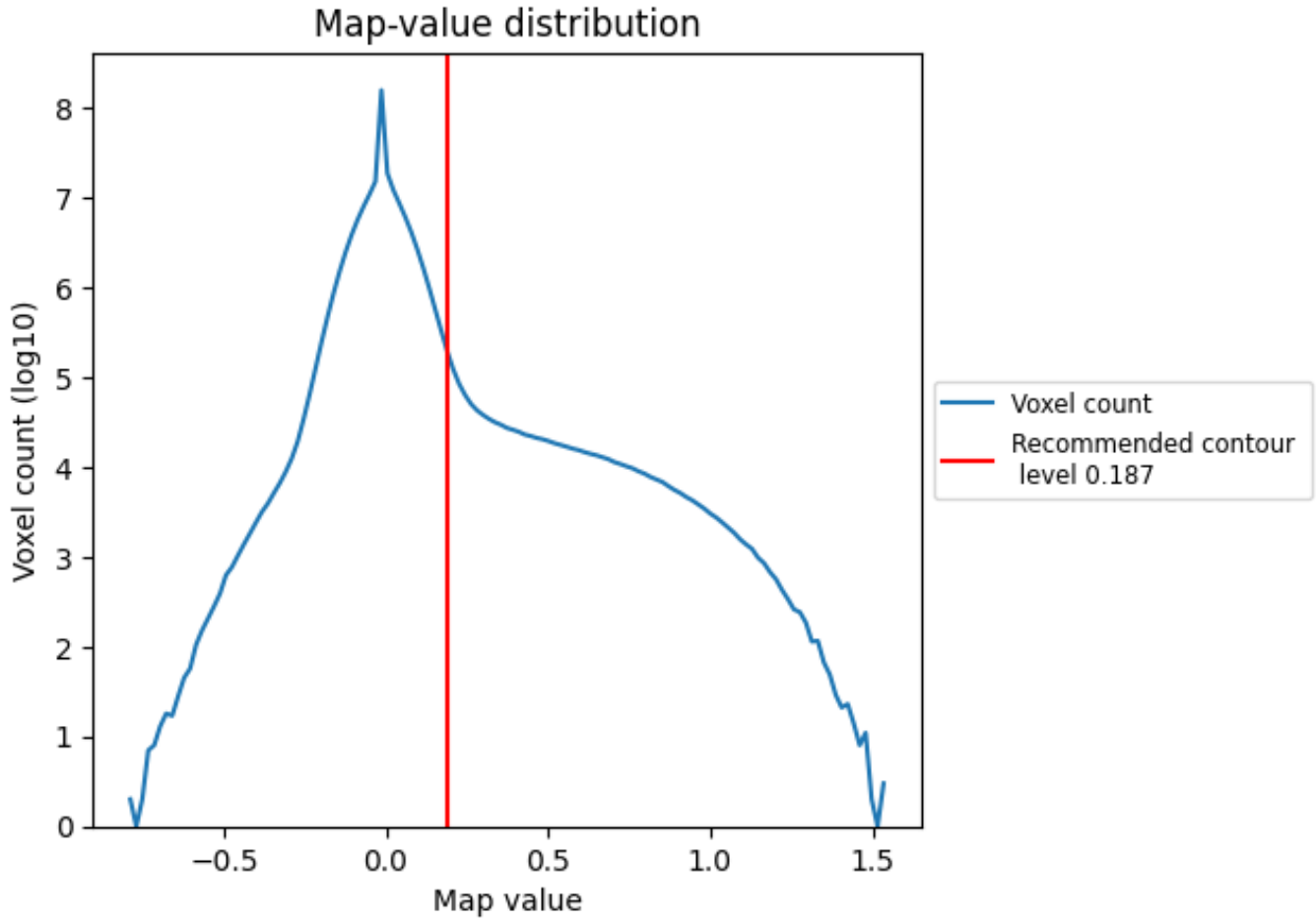
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

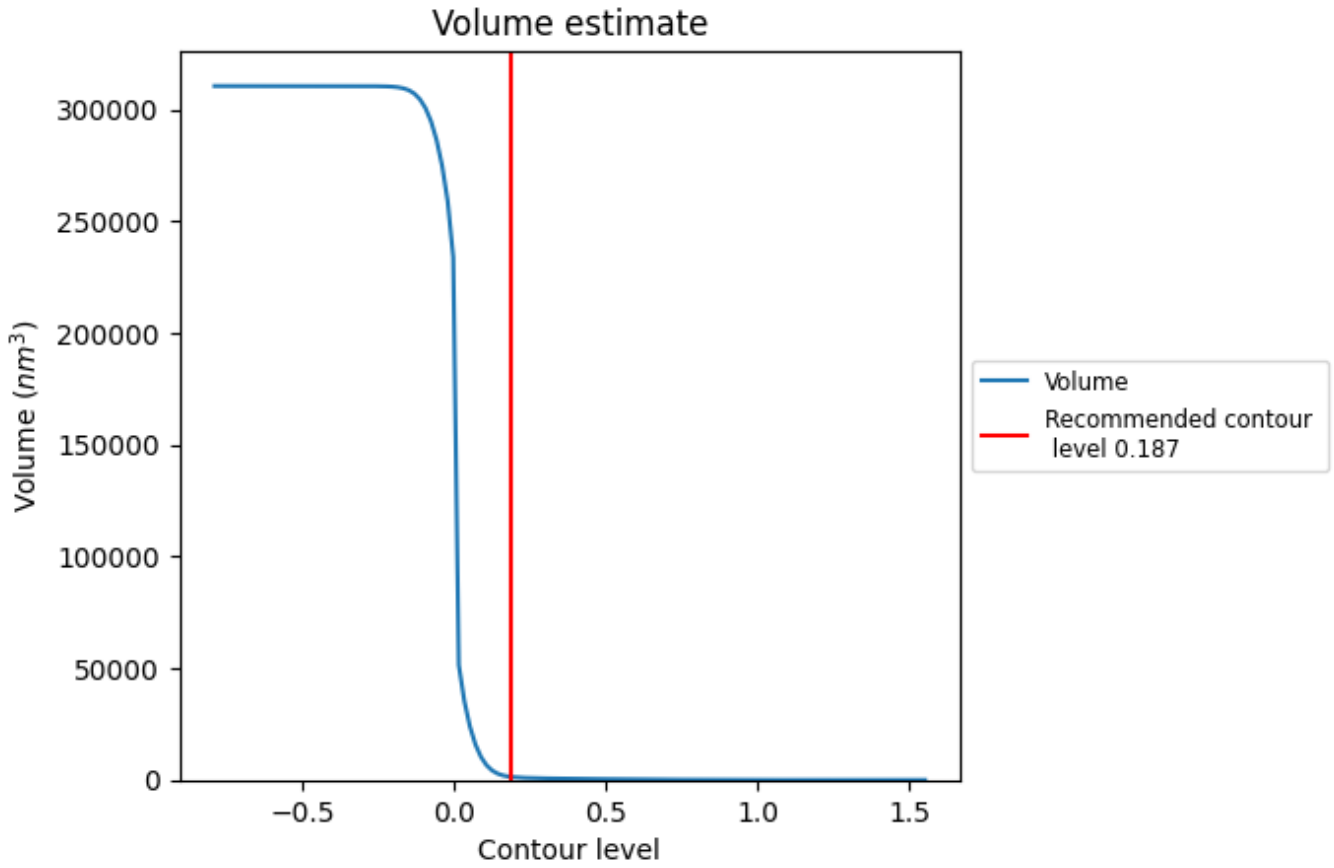
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

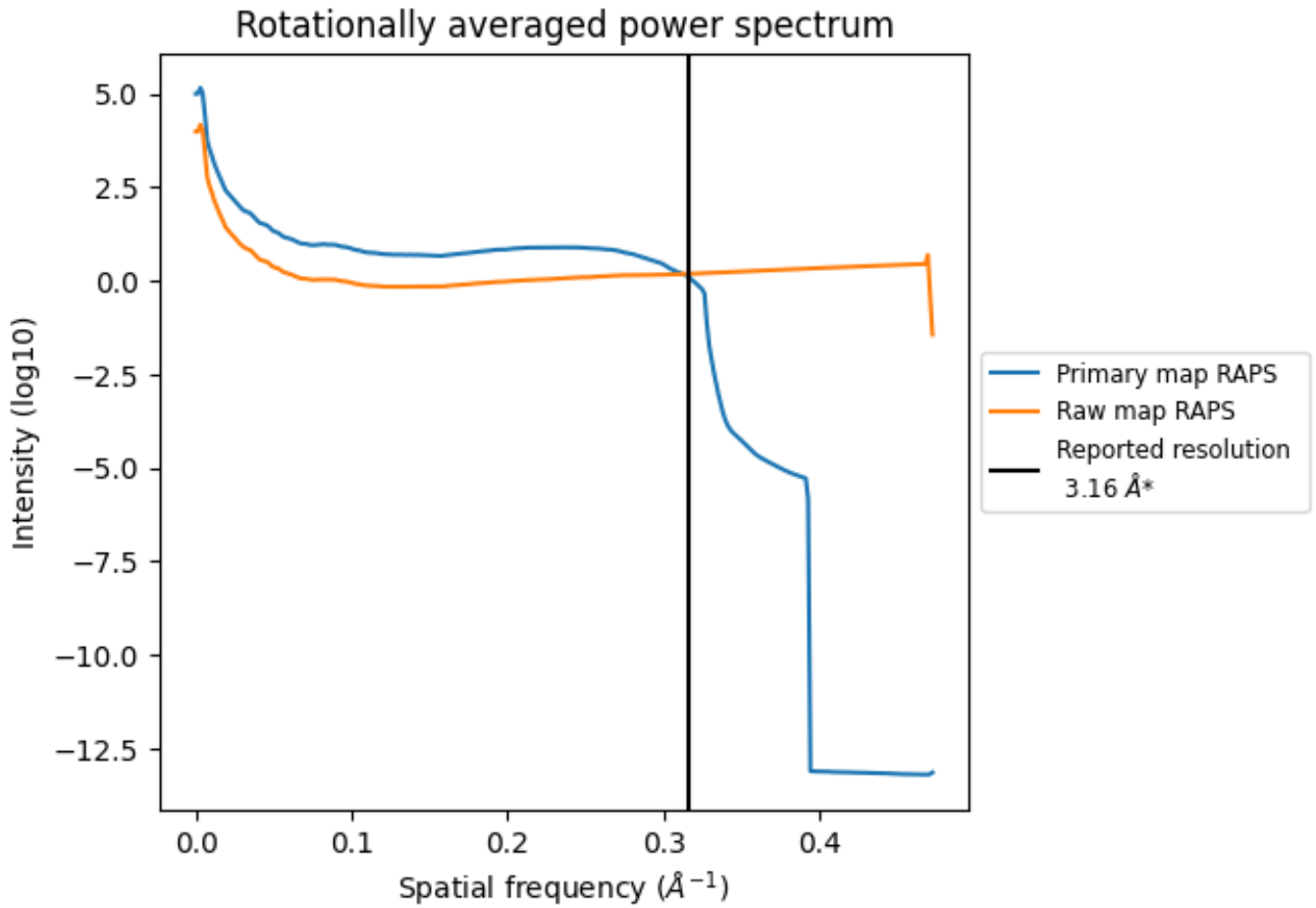
7.2 Volume estimate



The volume at the recommended contour level is 1424 nm^3; this corresponds to an approximate mass of 1287 kDa.

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

7.3 Rotationally averaged power spectrum (i)

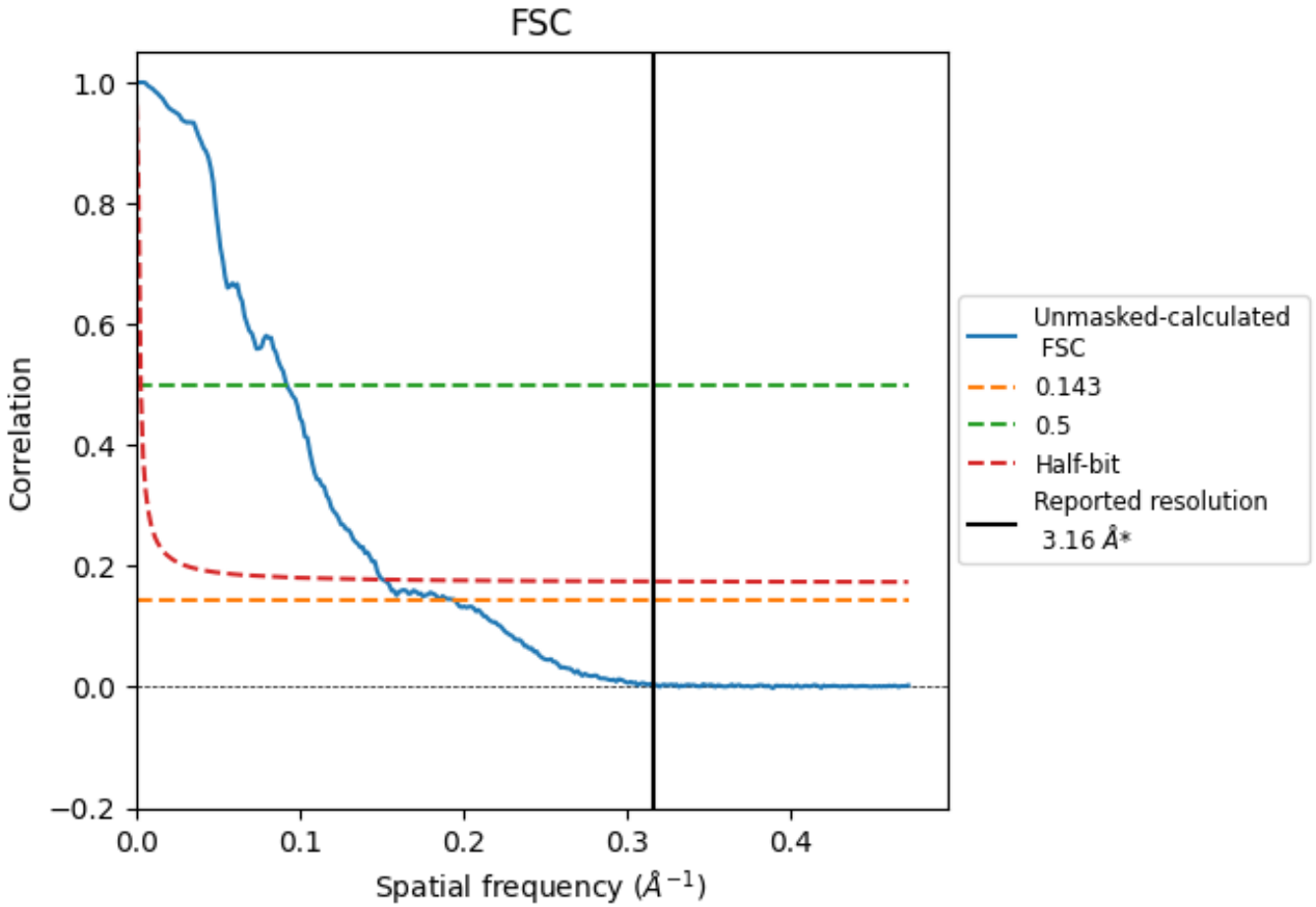


*Reported resolution corresponds to spatial frequency of 0.316 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

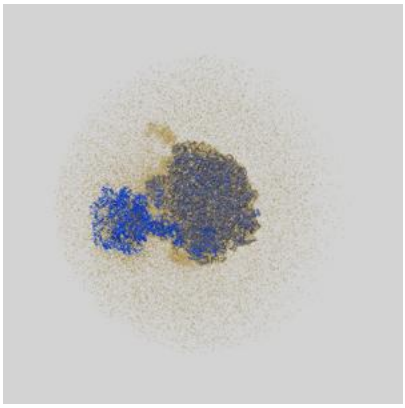
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.12	10.83	6.62

*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 5.12 differs from the reported value 3.16 by more than 10 %

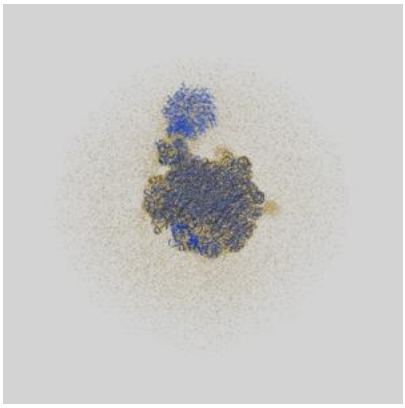
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70444 and PDB model 9OFV. Per-residue inclusion information can be found in section 3 on page 19.

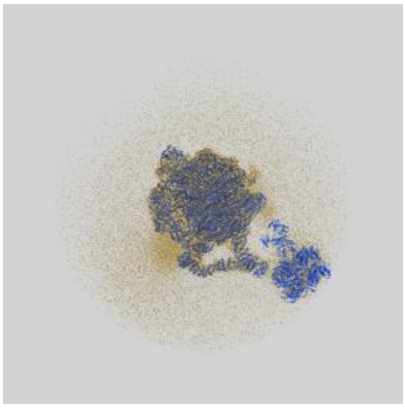
9.1 Map-model overlay



X



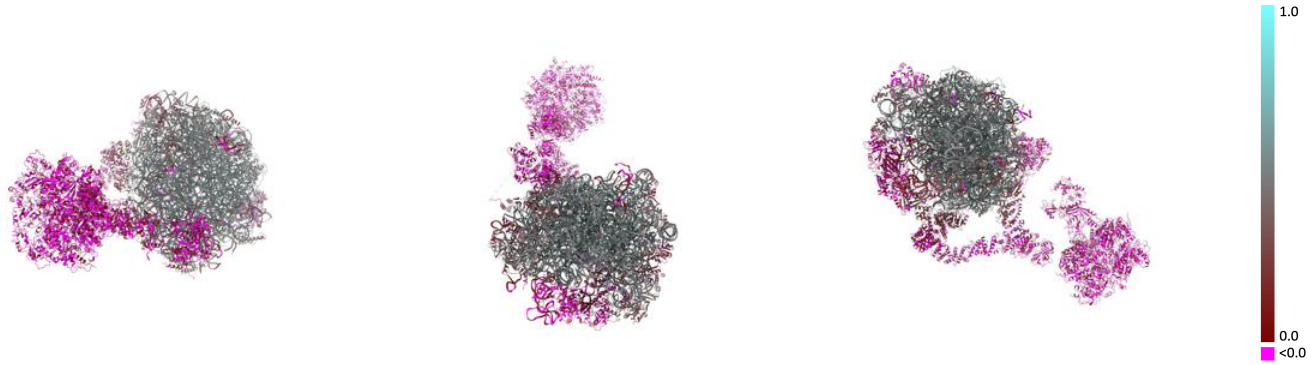
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.187 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.

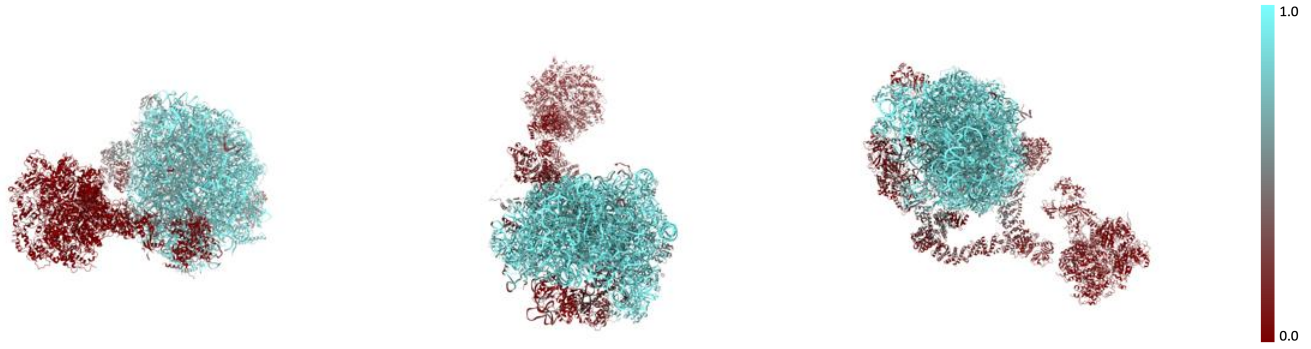
9.2 Q-score mapped to coordinate model



X Y Z

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

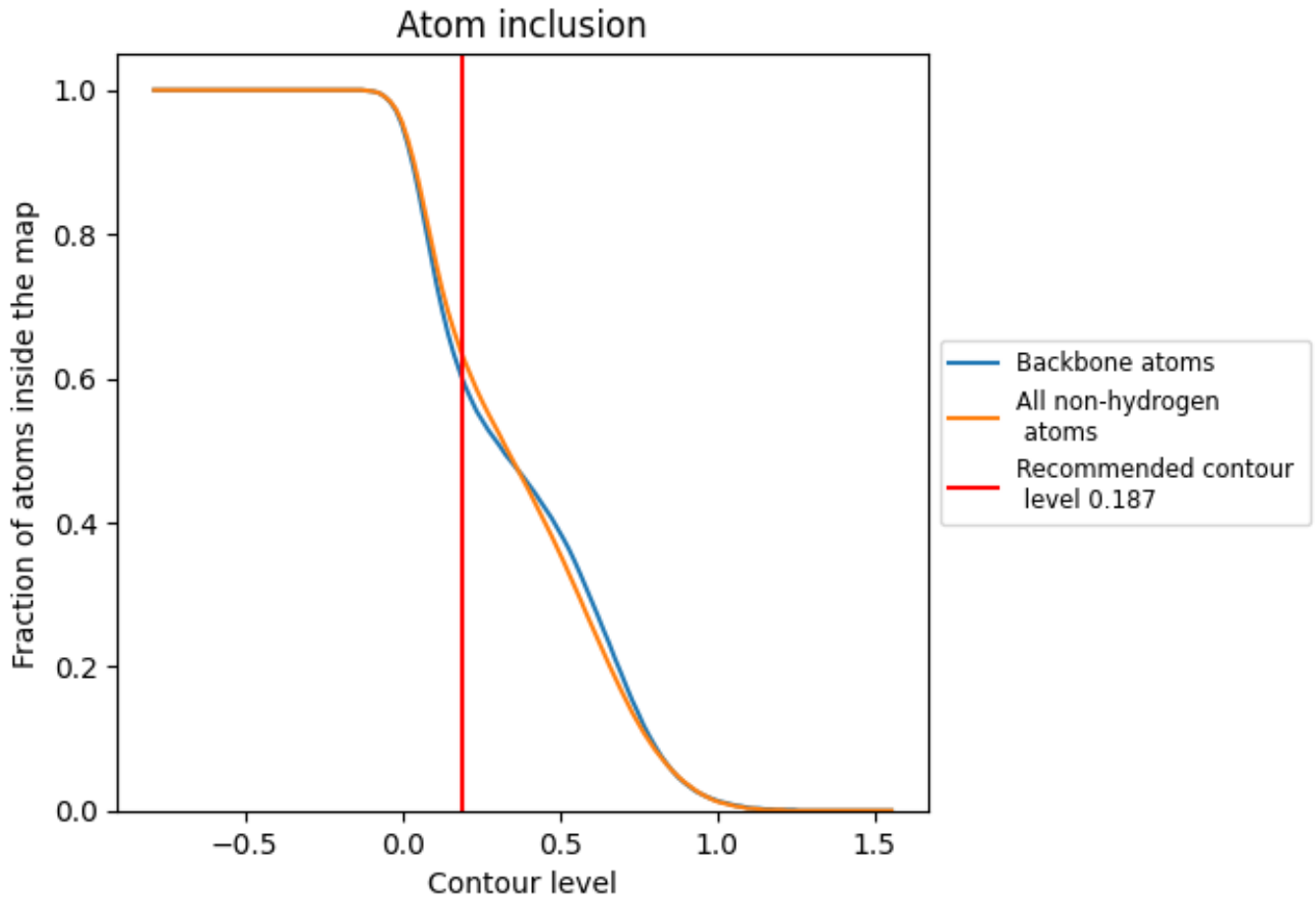
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.187).

9.4 Atom inclusion (i)



At the recommended contour level, 60% 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 (0.187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.3290
0	0.5700	0.2150
1	0.5770	0.3690
2	0.0370	-0.0080
3	0.8750	0.5180
4	0.9070	0.5240
5	0.8230	0.4600
6	0.8890	0.5070
7	0.8730	0.5020
8	0.7950	0.4250
9	0.8670	0.4790
A	0.0140	0.0070
B	0.0140	0.0020
C	0.0070	-0.0160
D	0.0080	-0.0000
E	0.0070	0.0060
F	0.0070	0.0010
G	0.0030	0.0110
H	0.0000	0.0090
I	0.8320	0.4920
J	0.0020	0.0010
K	0.0000	0.0050
L	0.8780	0.4980
M	0.8280	0.4230
N	0.9090	0.5300
O	0.8500	0.4870
P	0.8180	0.4310
Q	0.8330	0.4800
R	0.8980	0.5310
S	0.9000	0.5270
T	0.8420	0.4740
U	0.8560	0.4850
V	0.8450	0.4450
W	0.9210	0.5440
X	0.7280	0.3320

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.9060	0.5280
Z	0.8720	0.4990
a	0.1590	0.0670
a0	0.7390	0.3180
b	0.8670	0.5000
b0	0.6670	0.2380
c	0.8510	0.4680
d	0.2180	0.2700
e	0.2610	0.0850
f	0.9320	0.4770
g	0.0740	0.2270
h	0.9720	0.4930
i	0.9530	0.4990
j	0.8840	0.5060
k	0.8870	0.5090
l	0.8930	0.5050
m	0.8370	0.4270
n	0.8270	0.4420
o	0.8820	0.4900
p	0.8250	0.4280
q	0.8530	0.4740
r	0.8410	0.4820
s	0.8110	0.3930
t	0.8930	0.4940
u	0.8530	0.4610
v	0.0890	0.0090
w	0.0490	0.0010
x	0.1830	0.0950
y	0.2690	0.0980
z	0.4600	0.1380