



Full wwPDB EM Validation Report ⓘ

Aug 25, 2026 – 02:00 pm BST

PDB ID : 7A09 / pdb_00007a09
EMDB ID : EMD-11602
Title : Structure of a human ABCE1-bound 43S pre-initiation complex - State III
Authors : Kratzat, H.; Mackens-Kiani, T.; Ameismeier, A.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-08-07
Resolution : 3.50 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

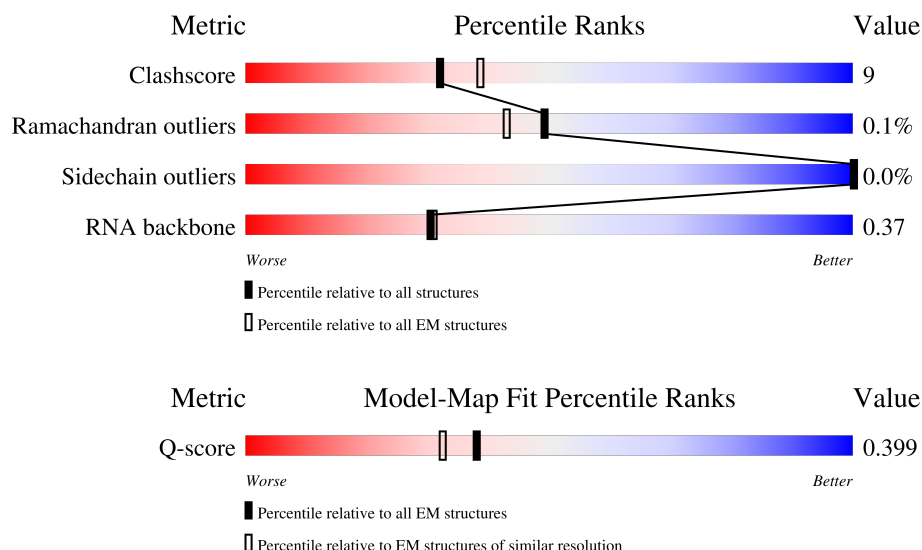
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	a	295	
2	p	264	
3	d	293	

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Mol	Chain	Length	Quality of chain
4	Q	115	
5	q	263	
6	W	25	
7	r	249	
8	s	194	
9	t	208	
10	c	194	
11	n	158	
12	m	151	
13	y	83	
14	D	130	
15	z	131	
16	R	84	
17	T	59	
18	2	1721	
19	w	135	
20	b	243	
21	e	204	
22	u	165	
23	v	132	
24	o	145	
25	g	146	
26	k	152	
27	x	145	
28	h	119	

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Mol	Chain	Length	Quality of chain
29	P	125	
30	S	69	
31	l	56	
32	U	156	
33	V	317	
34	i	151	
35	j	143	
36	G	112	
37	I	325	
38	B	814	
39	A	1382	
40	C	921	
41	E	445	
42	F	357	
43	H	352	
44	K	218	
45	L	564	
46	M	374	
47	J	599	
48	N	548	
49	X	78	
50	f	75	
51	4	333	
52	O	315	
53	Y	472	

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Mol	Chain	Length	Quality of chain
54	Z	113	<div><div></div><div>16%</div><div>75%</div><div>22%</div><div></div></div>

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 122168 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 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	216	Total	C	N	O	S	0	0
			1674	1085	287	292	10		

- Molecule 4 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	q	255	Total	C	N	O	S	0	0
			2031	1299	377	347	8		

- Molecule 6 is a protein called 60S ribosomal protein L41.

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

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	222	Total	C	N	O	S	0	0
			1794	1123	357	308	6		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	s	173	Total	C	N	O	S	0	0
			1399	898	256	244	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	t	199	Total	C	N	O	S	0	0
			1638	1027	322	284	5		

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	135	Total	C	N	O	S	0	0
			1119	715	211	187	6		

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	y	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	z	122	Total	C	N	O	S	0	0
			999	633	196	165	5		

- Molecule 16 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 17 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	44	Total	C	N	O	S	0	0
			354	216	81	56	1		

- Molecule 18 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	1721	Total	C	N	O	P	0	0
			36717	16400	6603	12003	1711		

- Molecule 19 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	w	128	Total	C	N	O	S	0	0
			1011	641	182	184	4		

- Molecule 20 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 21 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 22 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	u	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 23 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	111	Total	C	N	O	S	0	0
			861	544	151	159	7		

- Molecule 24 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	o	119	Total	C	N	O	S	0	0
			980	623	183	167	7		

- Molecule 25 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	g	138	Total	C	N	O	S	0	0
			1100	699	208	190	3		

- Molecule 26 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	k	140	Total	C	N	O	S	0	0
			1162	731	234	196	1		

- Molecule 27 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	x	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 28 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	98	Total	C	N	O	S	0	0
			780	489	148	139	4		

- Molecule 29 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	70	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 30 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	l	54	Total	C	N	O	S	0	0
			450	282	93	70	5		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	296	Total	C	N	O	S	0	0
			2314	1464	404	434	12		

- Molecule 34 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	125	Total	C	N	O	S	0	0
			939	574	187	172	6		

- Molecule 35 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	G	88	Total	C	N	O	S	0	0
			712	451	129	128	4		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	305	Total	C	N	O	S	0	0
			1497	887	305	305			

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A	692	Total	C	N	O	S	0	0
			5385	3379	980	1004	22		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit C, Eukaryotic translation initiation factor 3 subunit C, Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	C	633	Total	C	N	O	S	0	0
			5113	3229	907	942	35		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	E	416	Total	C	N	O	S	0	0
			3437	2202	585	630	20		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	F	269	Total	C	N	O	S	0	0
			2090	1317	356	405	12		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	H	295	Total	C	N	O	S	0	0
			2413	1532	417	449	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	K	217	Total	C	N	O	S	0	0
			1750	1116	288	334	12		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L	372	Total	C	N	O	S	0	0
			3111	2011	520	563	17		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	M	340	Total	C	N	O	S	0	0
			2718	1734	459	508	17		

- Molecule 47 is a protein called ATP-binding cassette sub-family E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	J	576	Total	C	N	O	S	0	0
			4541	2899	779	835	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N	447	Total	C	N	O	S	0	0
			3617	2279	625	691	22		

- Molecule 49 is a protein called RNA recognition motif.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	X	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 50 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	f	75	Total	C	N	O	P	0	0
			1603	717	298	514	74		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	144	Total	C	N	O	S	0	0
			1080	679	202	192	7		

- Molecule 52 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

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

- Molecule 53 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Y	414	Total	C	N	O	0	0
			2156	1296	433	427		

- Molecule 54 is a protein called Eukaryotic translation initiation factor 1.

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

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

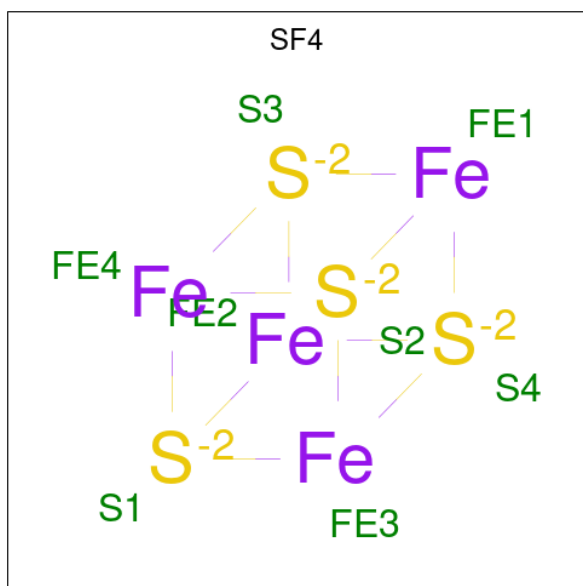
Mol	Chain	Residues	Atoms		AltConf
55	Q	1	Total	Zn	0
			1	1	
55	l	1	Total	Zn	0
			1	1	
55	U	1	Total	Zn	0
			1	1	

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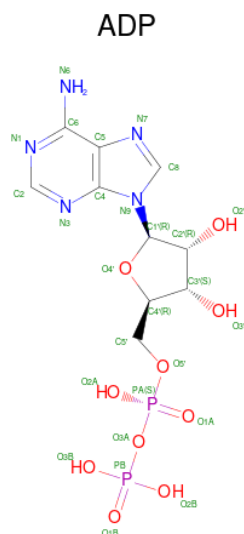
Mol	Chain	Residues	Atoms		AltConf
55	4	1	Total	Zn	0
			1	1	

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
56	J	1	Total	Fe	S	0
			8	4	4	
56	J	1	Total	Fe	S	0
			8	4	4	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

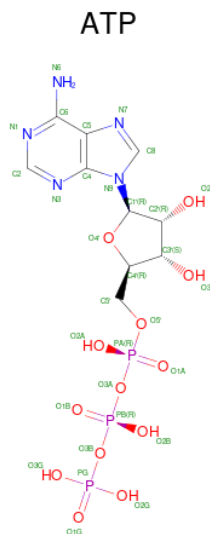


Mol	Chain	Residues	Atoms					AltConf
57	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

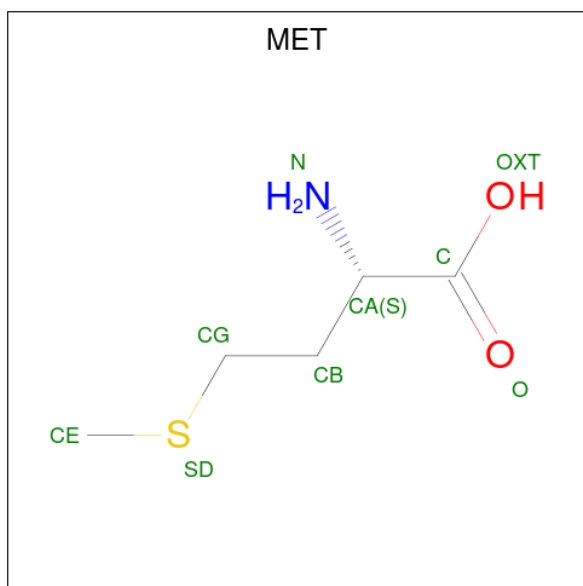
Mol	Chain	Residues	Atoms	AltConf
58	J	2	Total Mg 2 2	0
58	Y	1	Total Mg 1 1	0

- Molecule 59 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



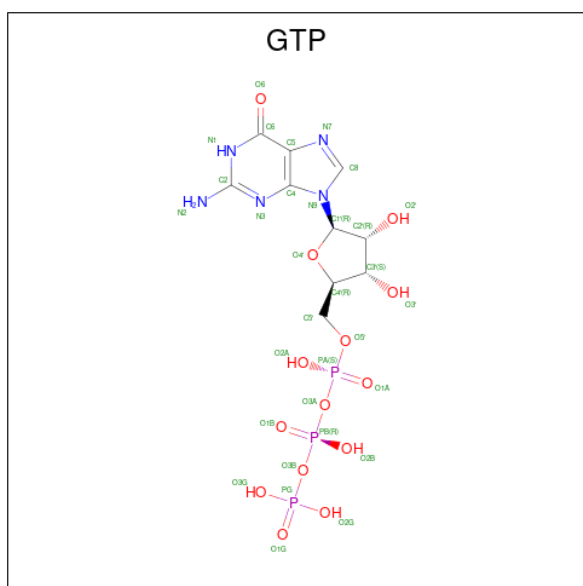
Mol	Chain	Residues	Atoms					AltConf
59	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 60 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).

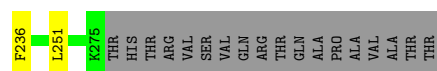


Mol	Chain	Residues	Atoms					AltConf
60	f	1	Total	C	N	O	S	0
			8	5	1	1	1	

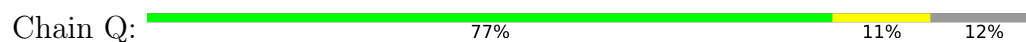
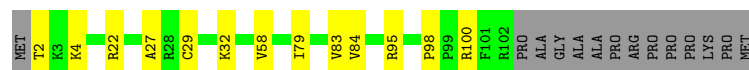
- Molecule 61 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



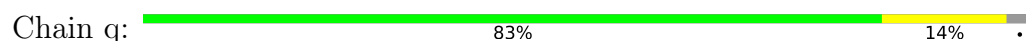
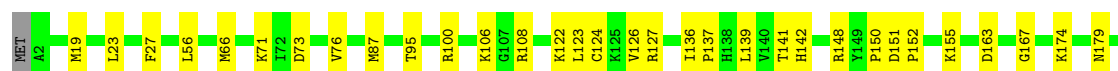
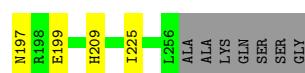
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
61	Y	1	32	10	5	14	3	0



- Molecule 4: 40S ribosomal protein S26



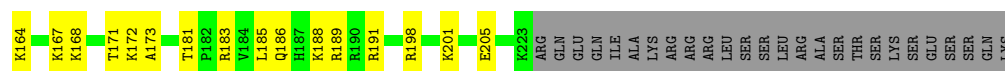
- Molecule 5: 40S ribosomal protein S4, X isoform



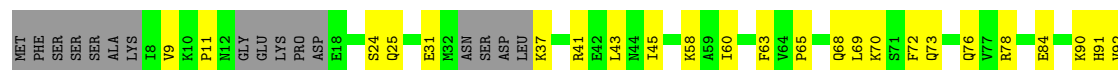
- Molecule 6: 60S ribosomal protein L41



- Molecule 7: 40S ribosomal protein S6

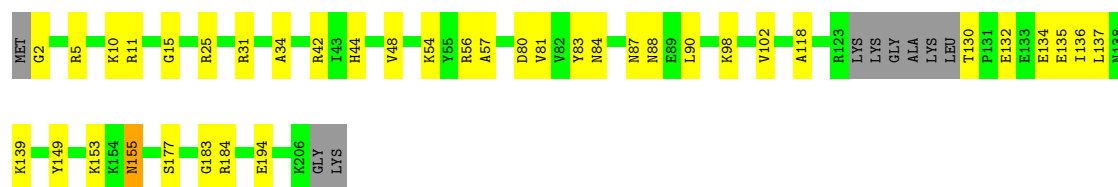


- Molecule 8: 40S ribosomal protein S7



- Molecule 9: 40S ribosomal protein S8

Chain t:  77% 18% .



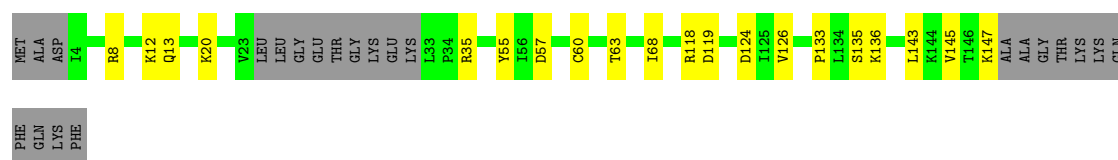
- Molecule 10: 40S ribosomal protein S9

Chain c:  76% 16% 7% .



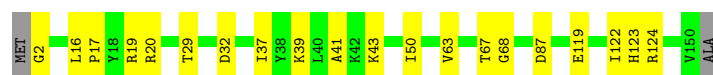
- Molecule 11: 40S ribosomal protein S11

Chain n:  73% 13% 15% .



- Molecule 12: 40S ribosomal protein S13

Chain m:  85% 13% .



- Molecule 13: 40S ribosomal protein S21

Chain y:  86% 13% .



- Molecule 14: 40S ribosomal protein S15a

Chain D:  85% 14% .



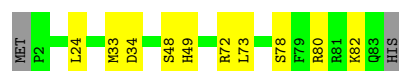
- Molecule 15: 40S ribosomal protein S24

Chain z:  71% 22% 7%



- Molecule 16: 40S ribosomal protein S27

Chain R:  86% 12% .



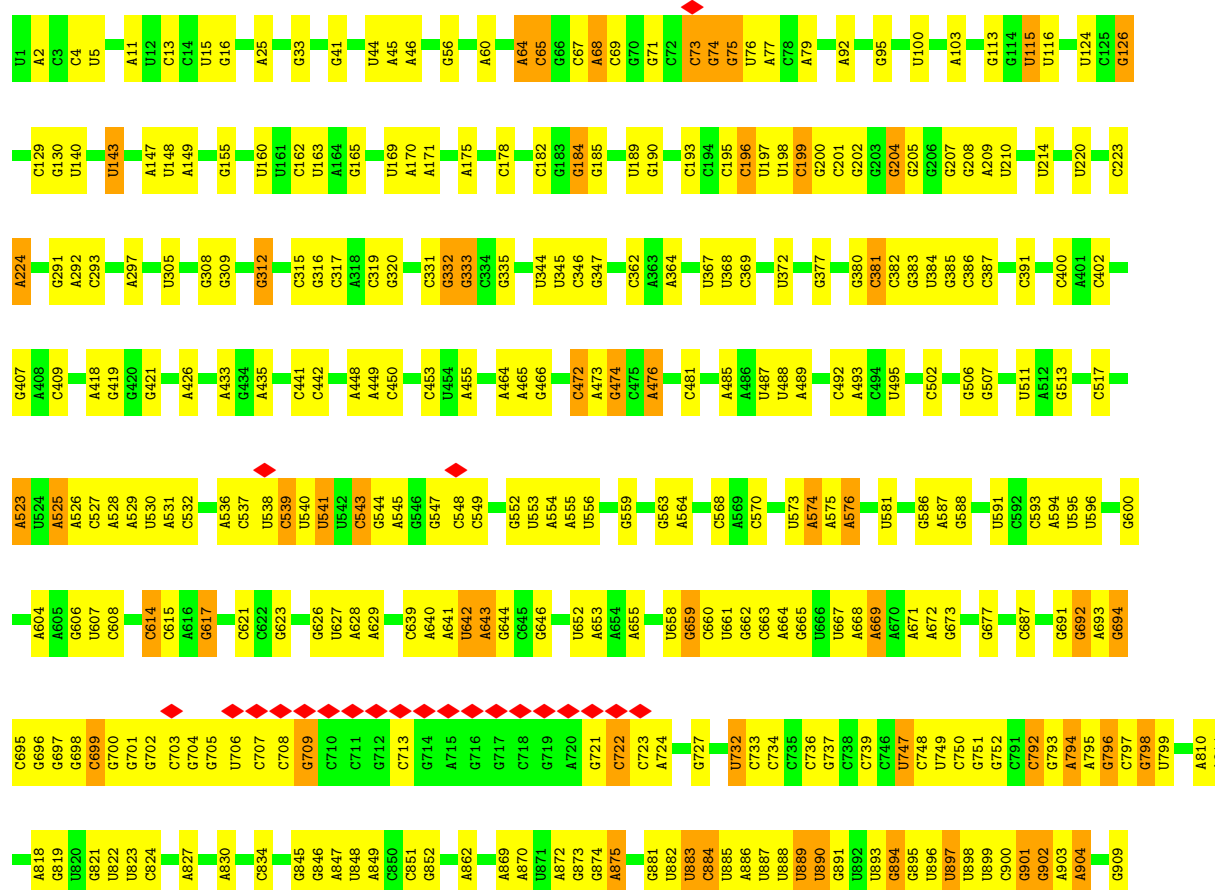
- Molecule 17: 40S ribosomal protein S30

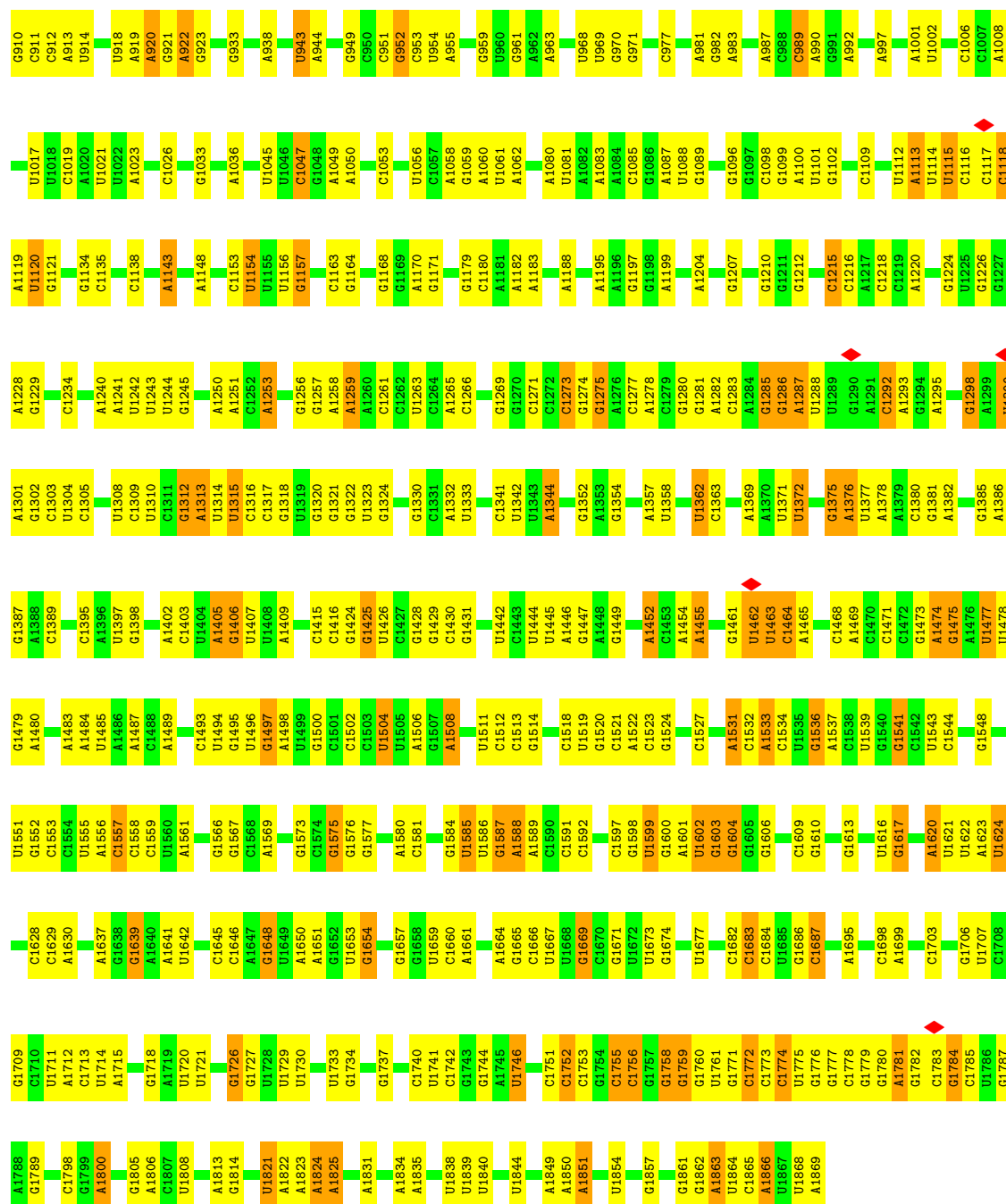
Chain T:  69% 5% 25%



- Molecule 18: 18S ribosomal RNA

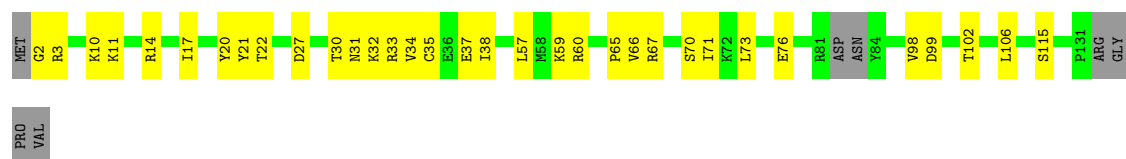
Chain 2:  55% 37% 8%



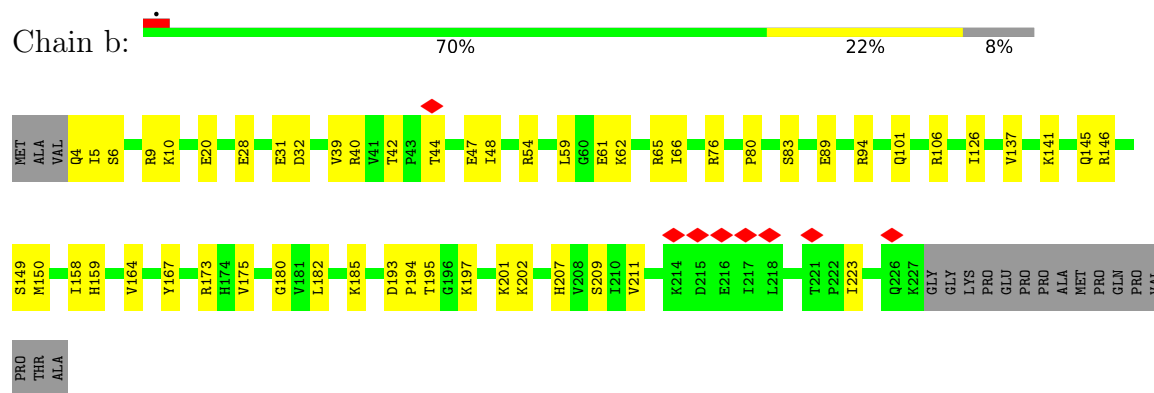


• Molecule 19: 40S ribosomal protein S17

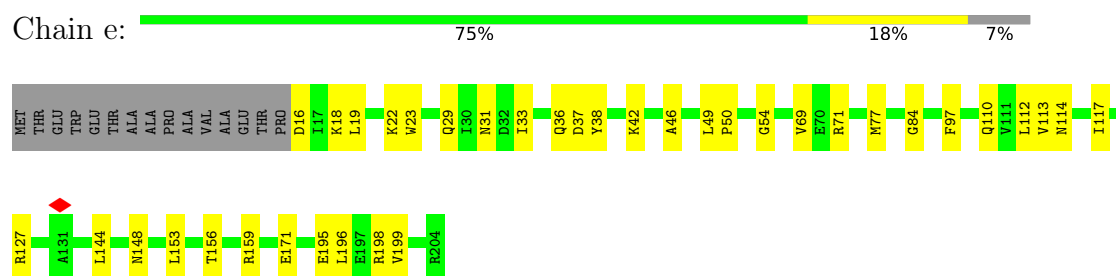
Chain w: 70% 24% 5%



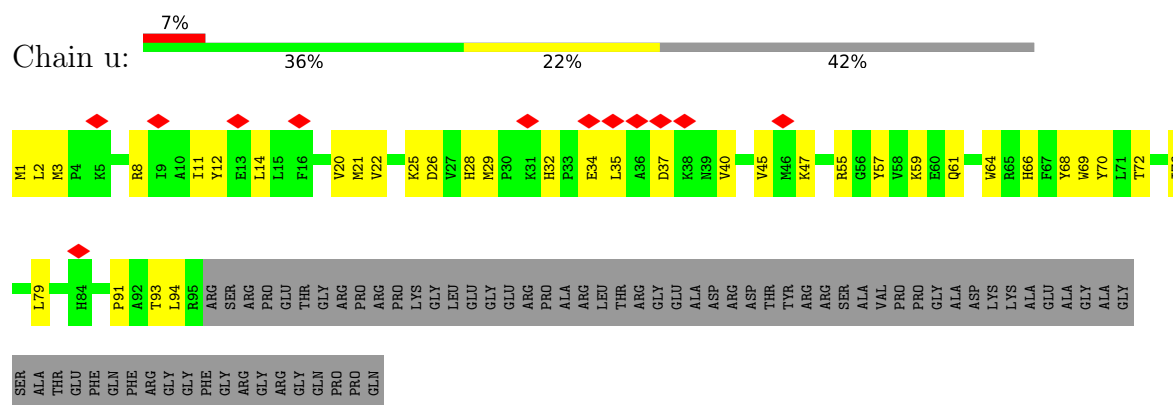
• Molecule 20: 40S ribosomal protein S3



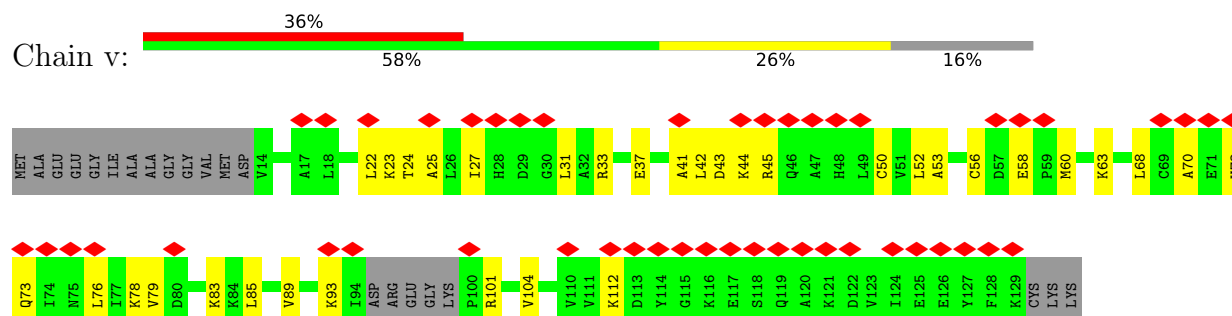
- Molecule 21: 40S ribosomal protein S5



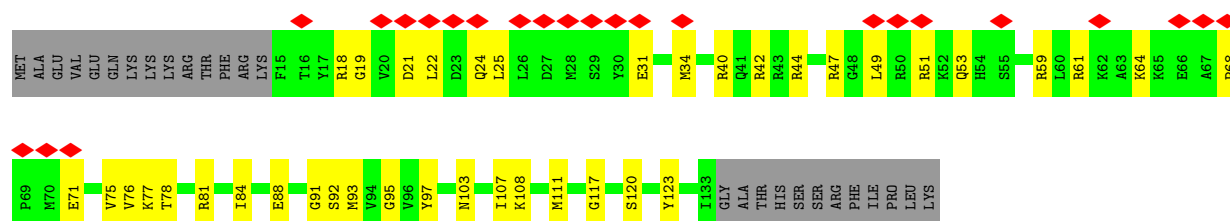
- Molecule 22: 40S ribosomal protein S10



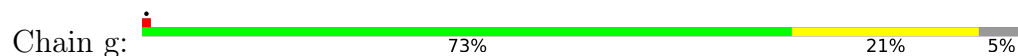
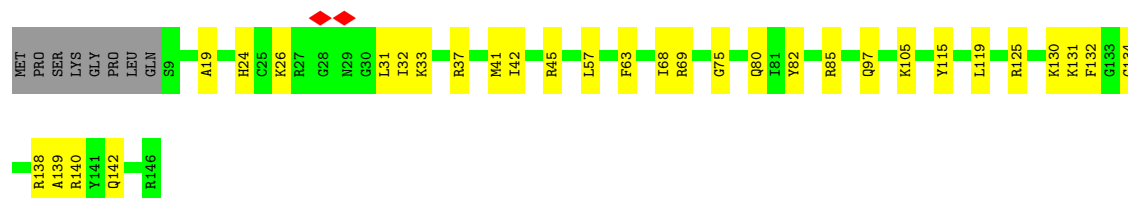
- Molecule 23: 40S ribosomal protein S12



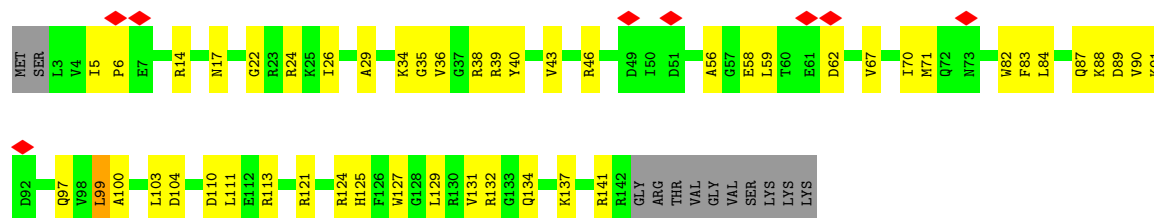
- Molecule 24: 40S ribosomal protein S15



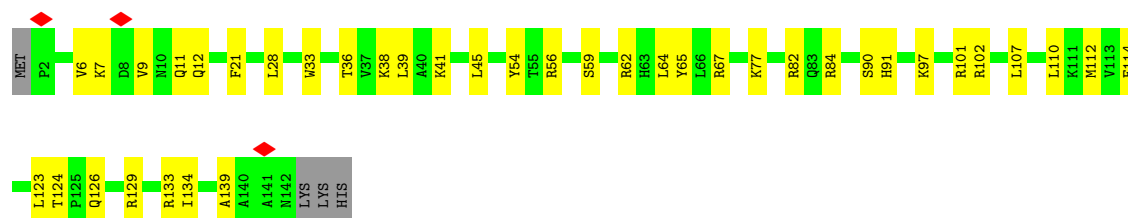
• Molecule 25: 40S ribosomal protein S16



• Molecule 26: 40S ribosomal protein S18



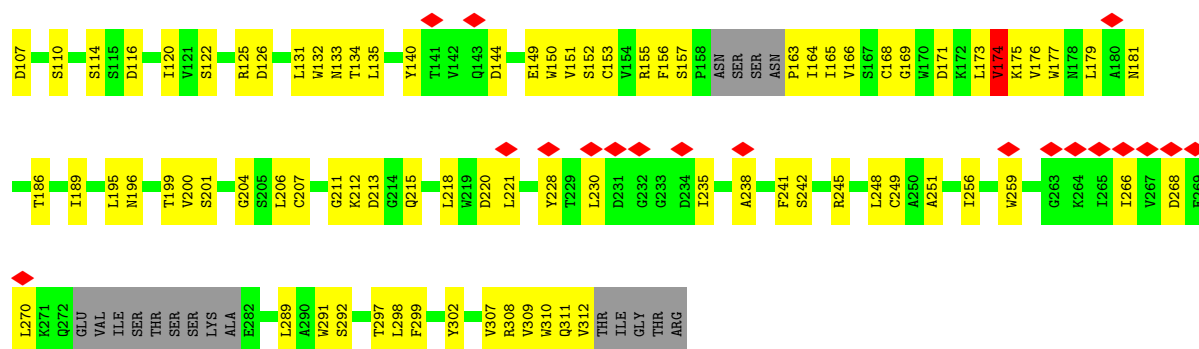
• Molecule 27: 40S ribosomal protein S19



• Molecule 28: 40S ribosomal protein S20

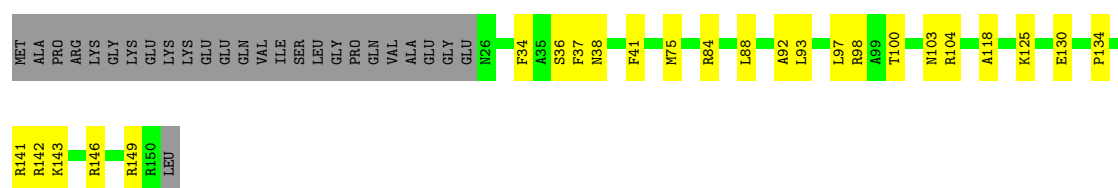






• Molecule 34: 40S ribosomal protein S14

Chain i: 67% 16% 17%



• Molecule 35: 40S ribosomal protein S23

Chain j: 80% 17% 3%



• Molecule 36: Eukaryotic translation initiation factor 1A, X-chromosomal

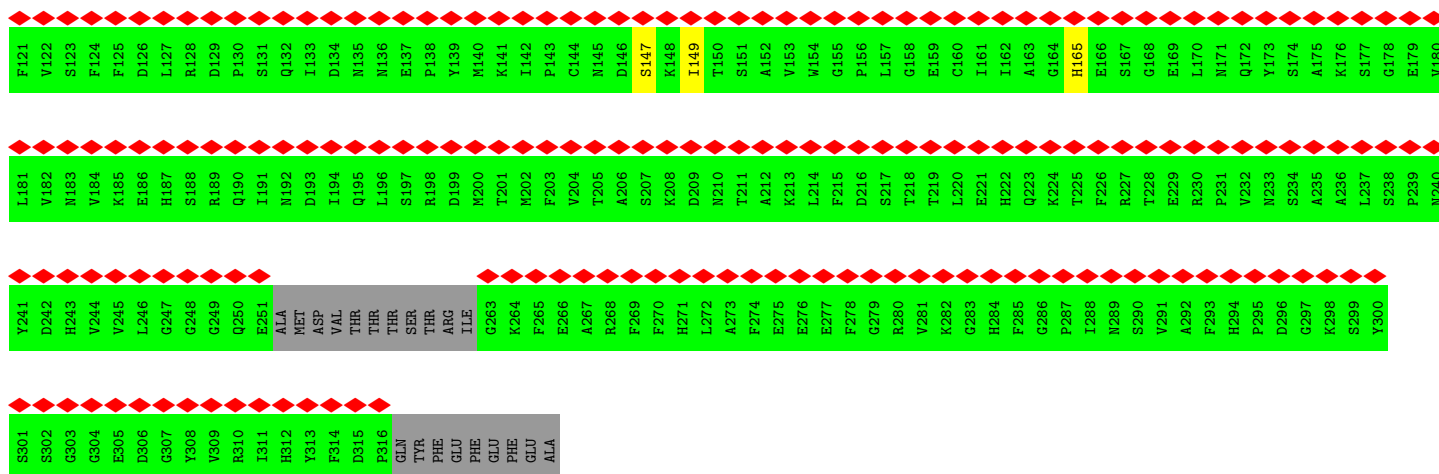
Chain G: 62% 17% 21%



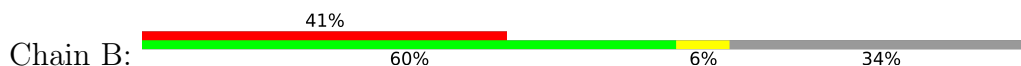
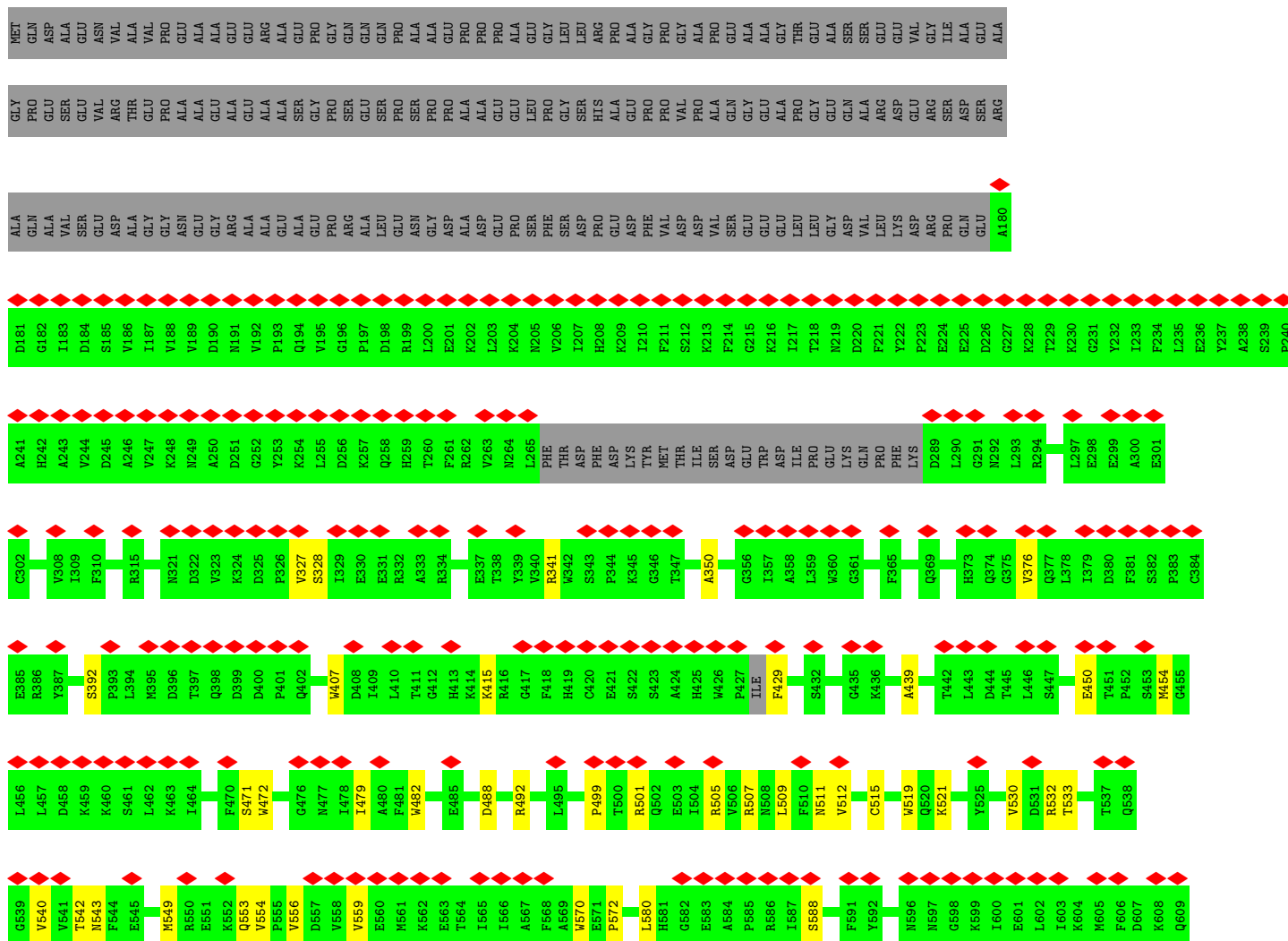
• Molecule 37: Eukaryotic translation initiation factor 3 subunit I

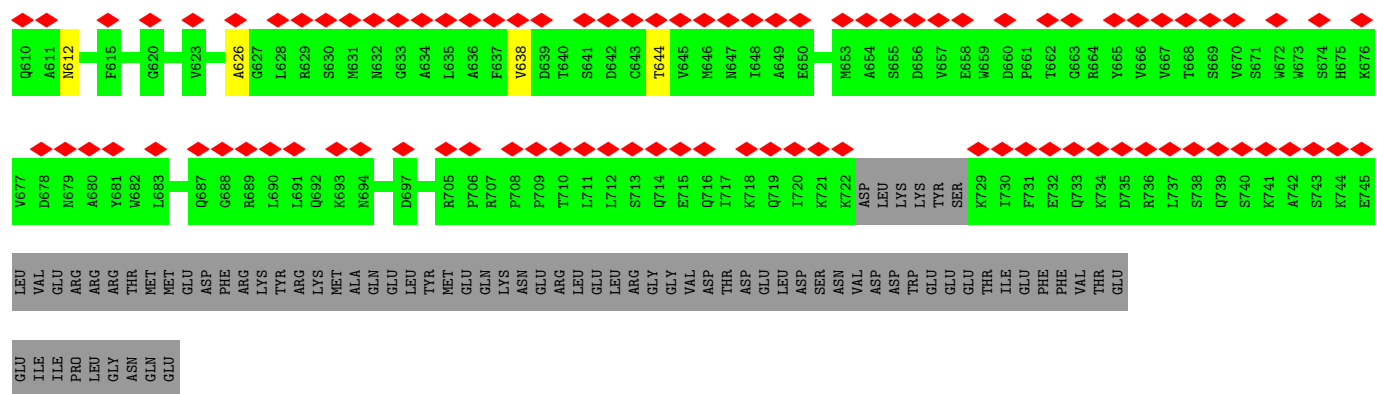
Chain I: 94% 93% 6%



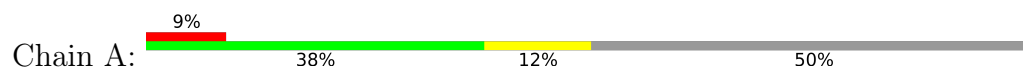
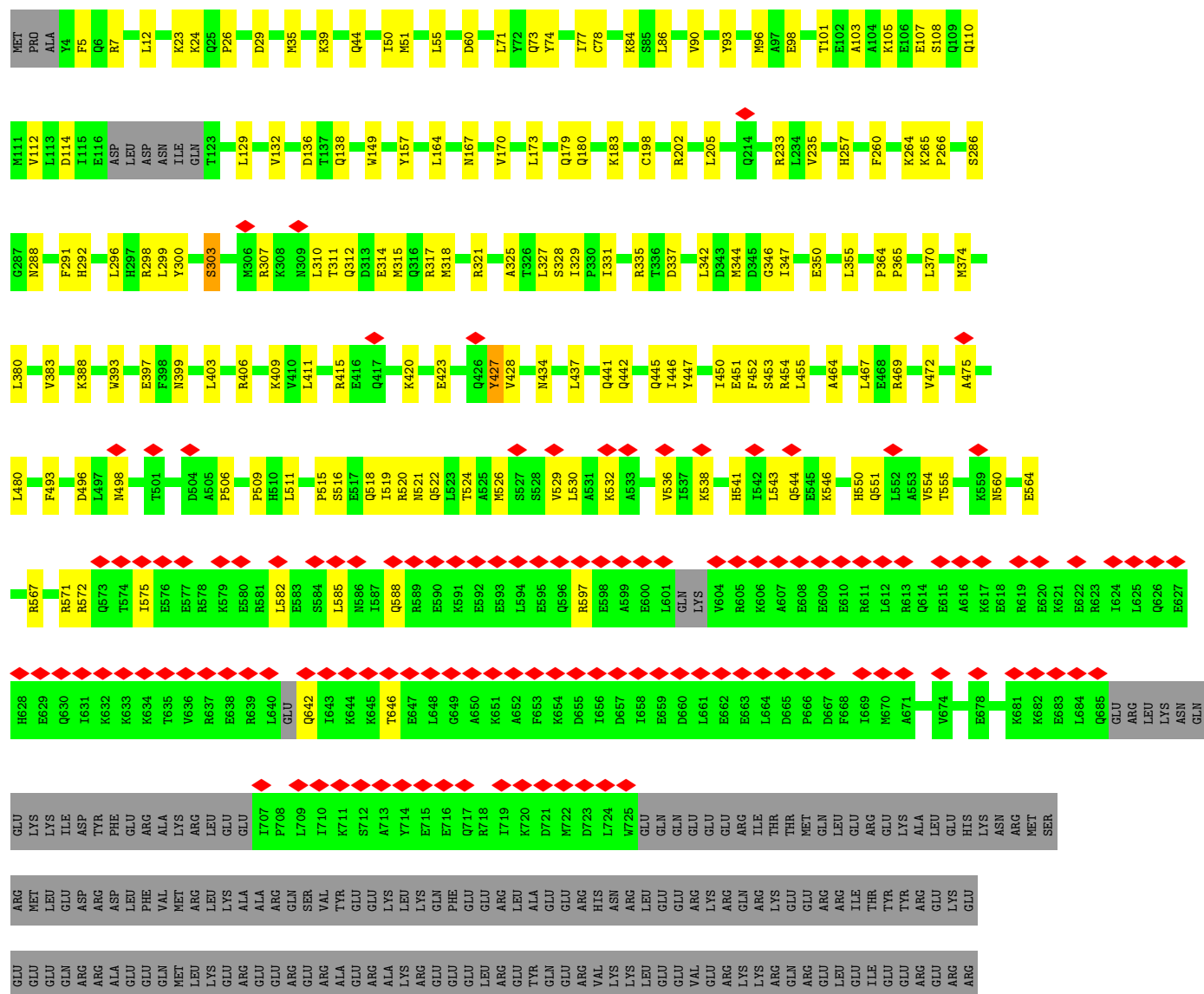


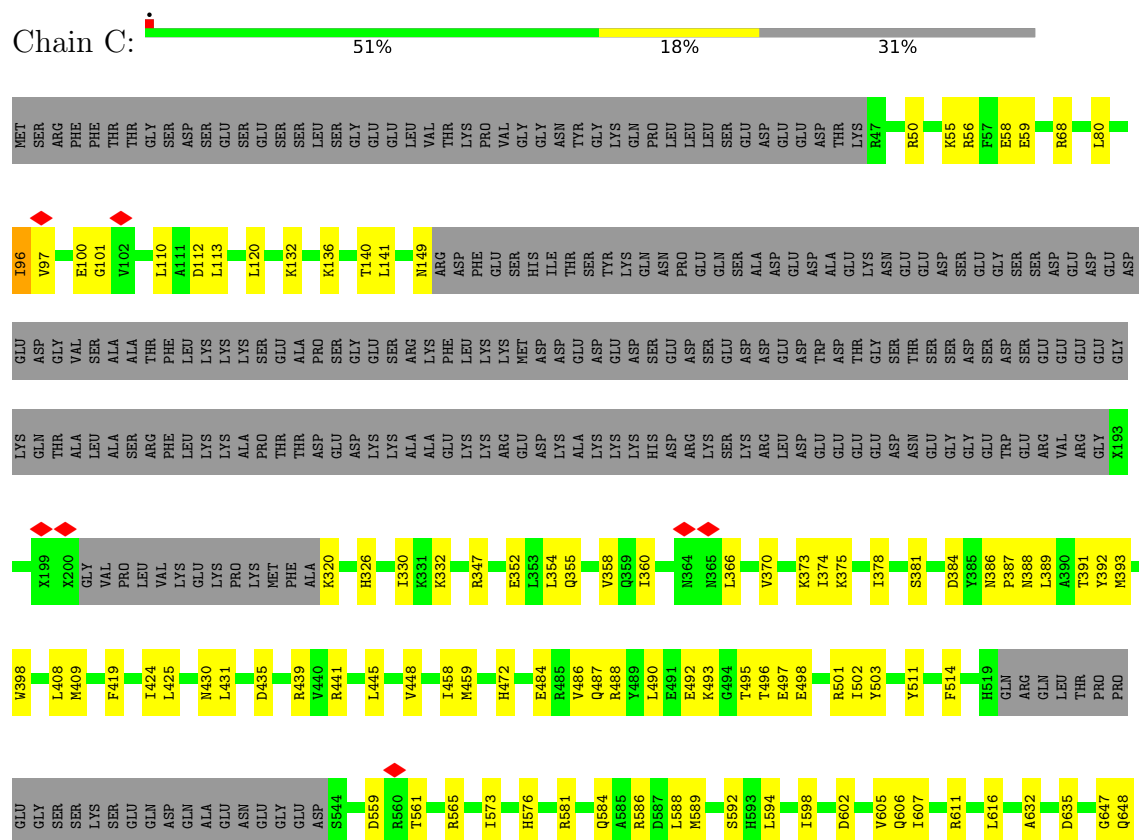
• Molecule 38: Eukaryotic translation initiation factor 3 subunit B

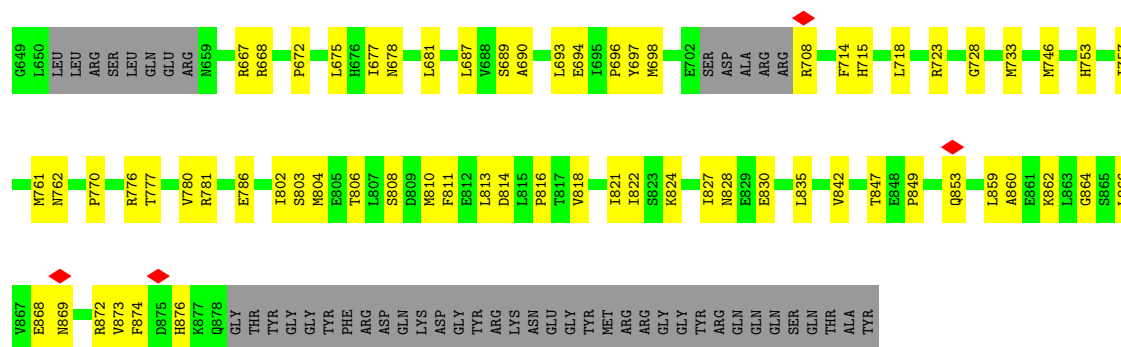




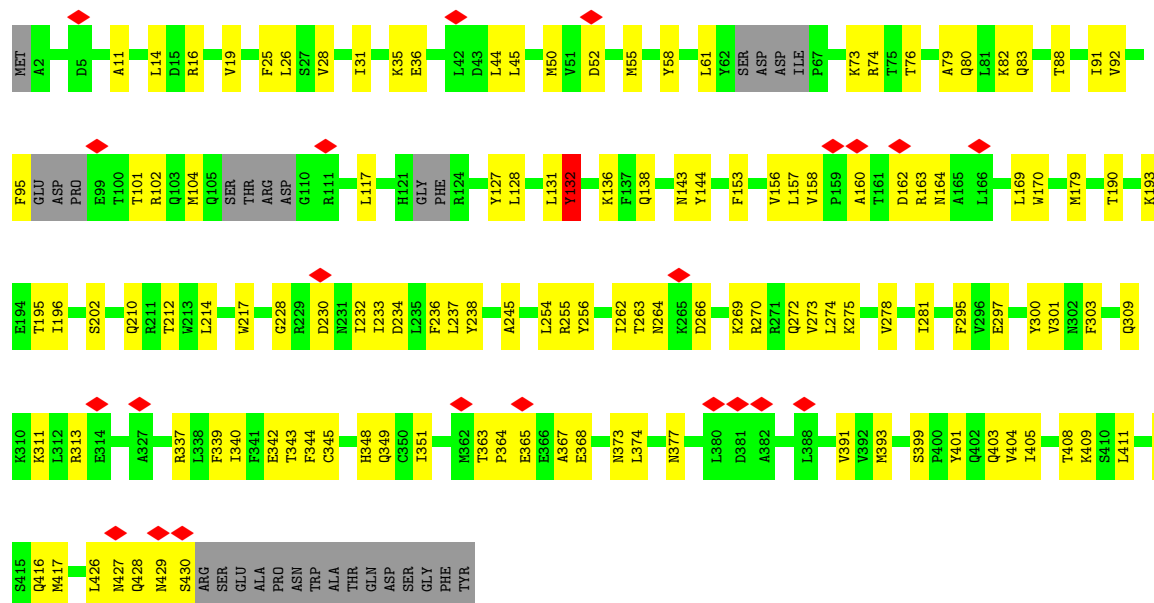
• Molecule 39: Eukaryotic translation initiation factor 3 subunit A



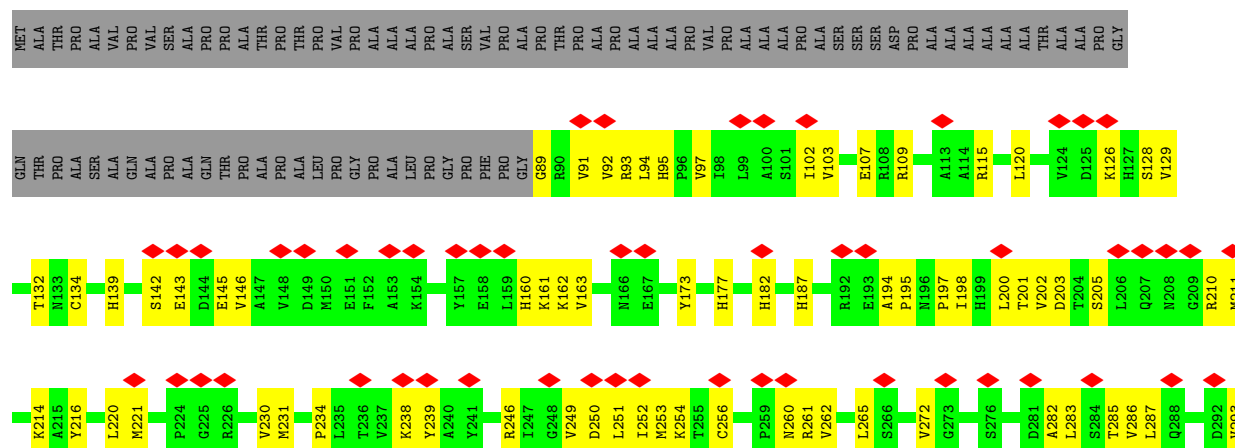


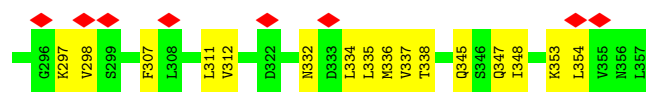


• Molecule 41: Eukaryotic translation initiation factor 3 subunit E

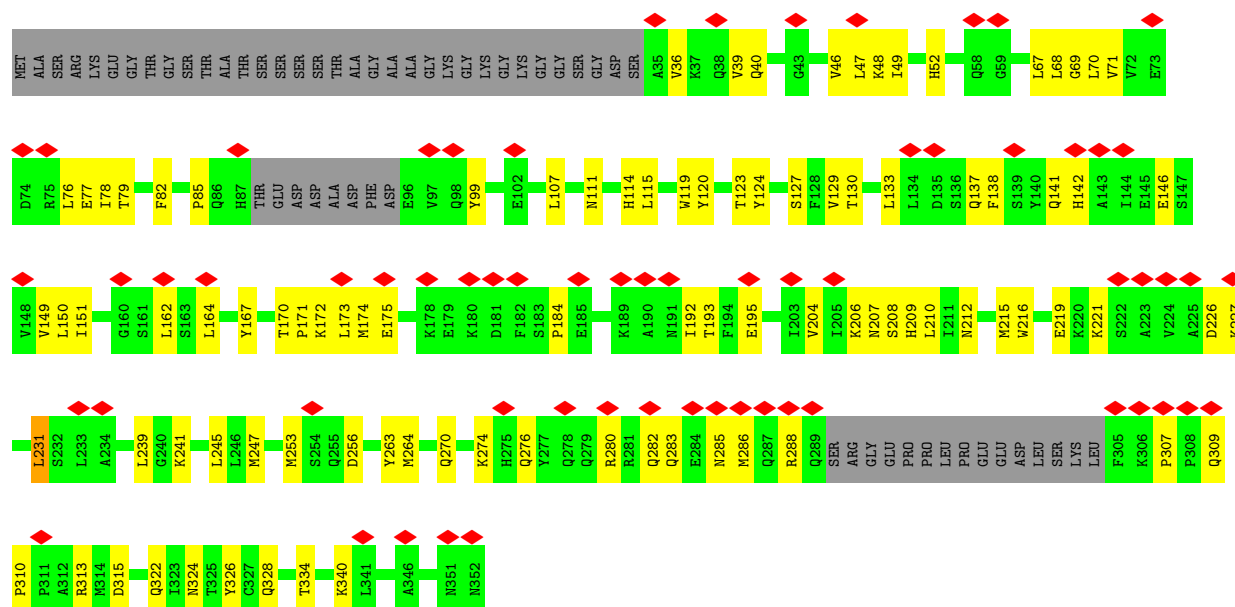


• Molecule 42: Eukaryotic translation initiation factor 3 subunit F

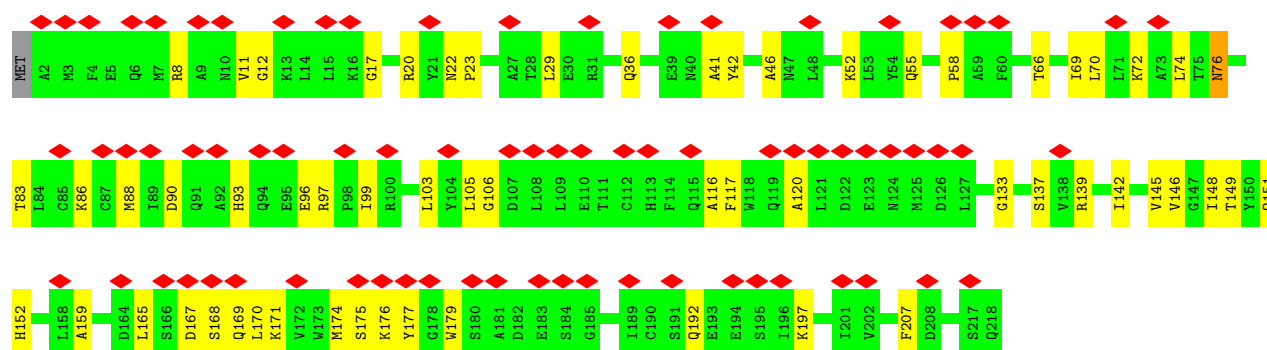




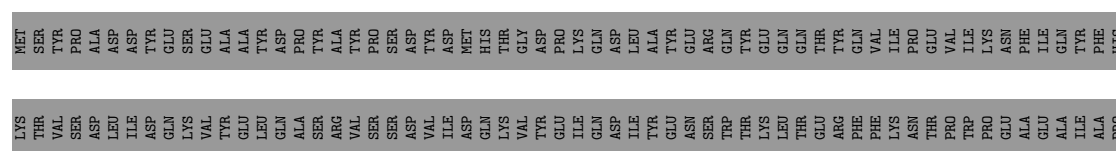
• Molecule 43: Eukaryotic translation initiation factor 3 subunit H

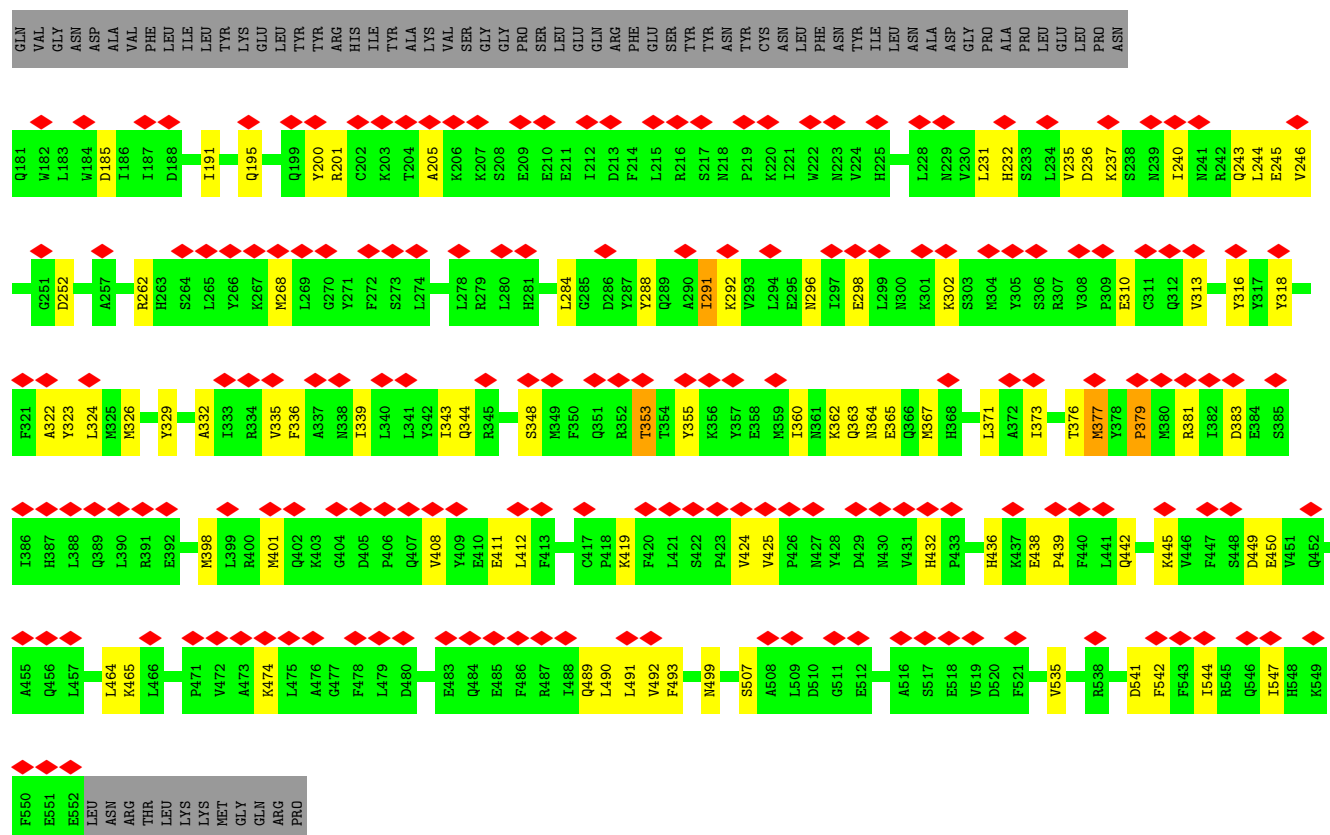


• Molecule 44: Eukaryotic translation initiation factor 3 subunit K

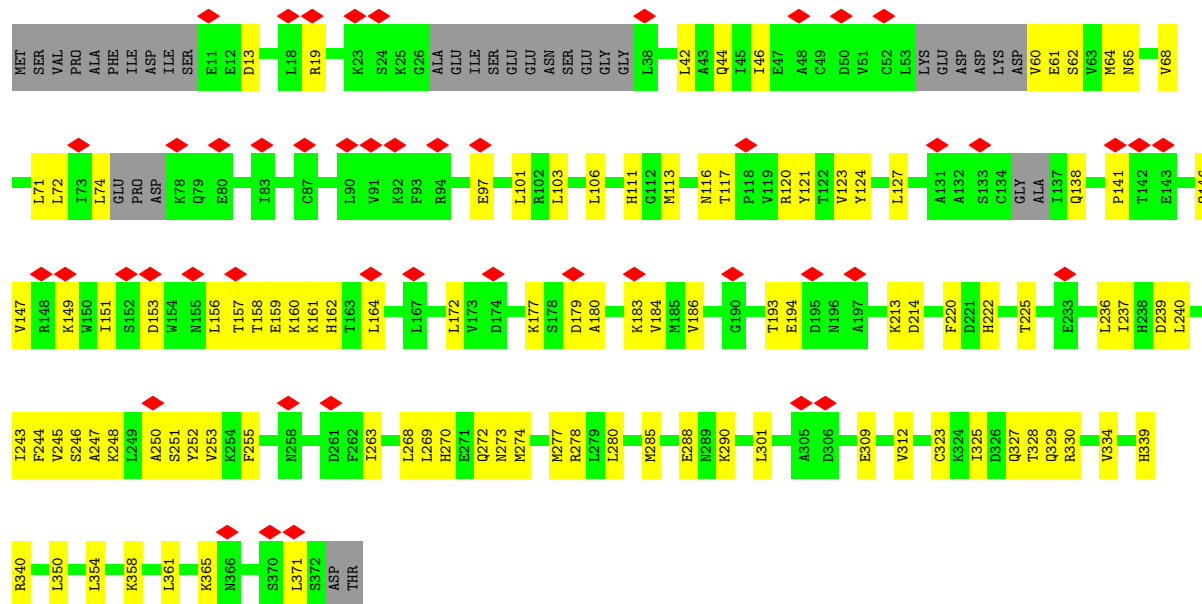


• Molecule 45: Eukaryotic translation initiation factor 3 subunit L



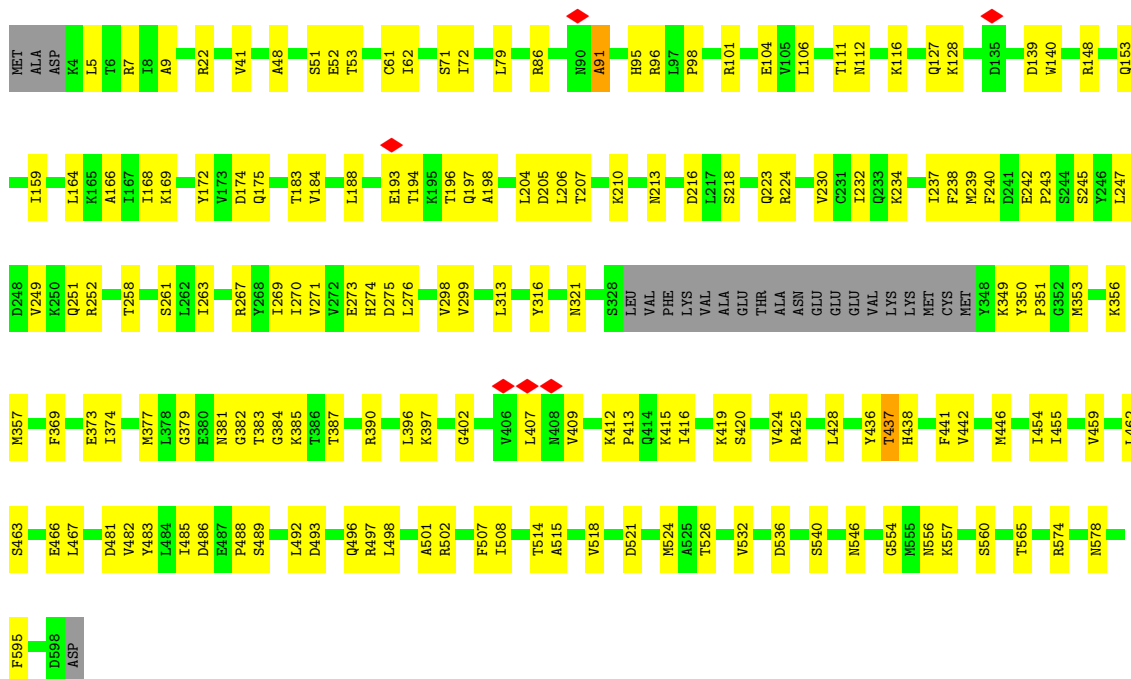


- Molecule 46: Eukaryotic translation initiation factor 3 subunit M

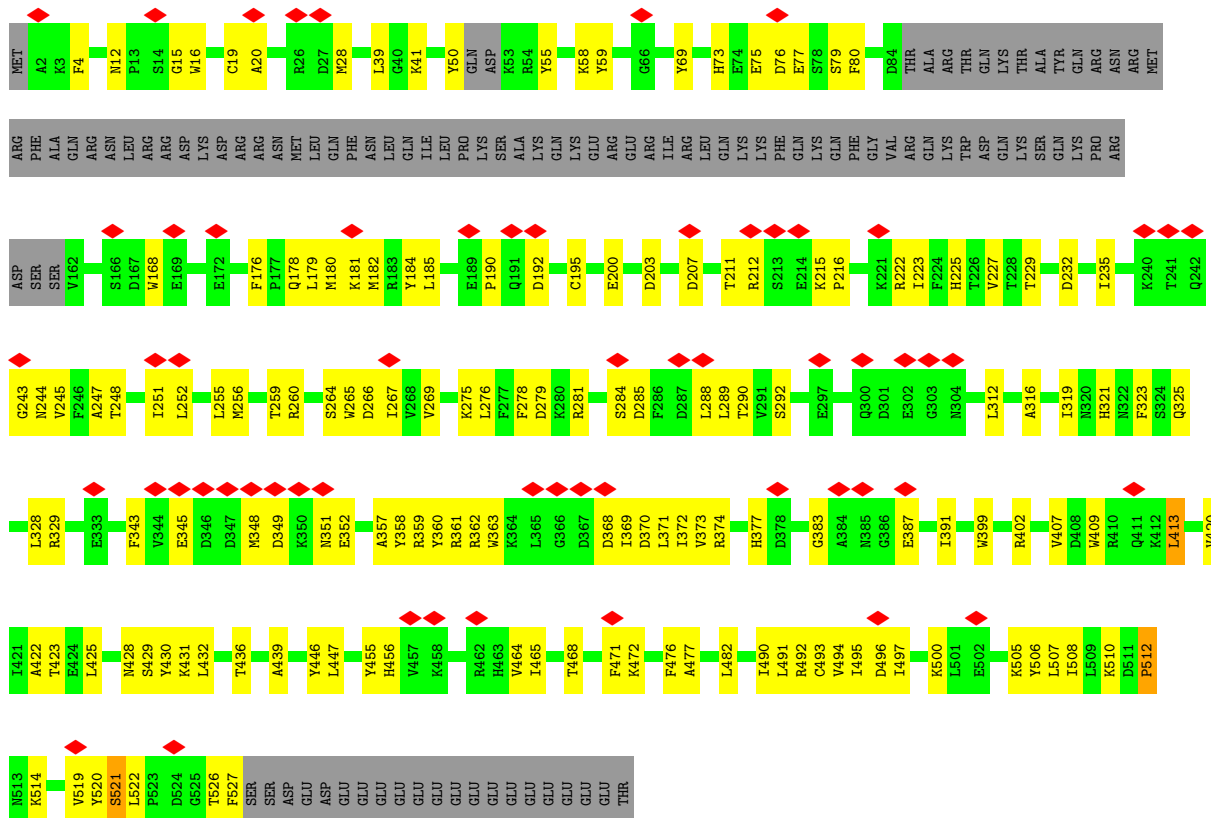


- Molecule 47: ATP-binding cassette sub-family E member 1

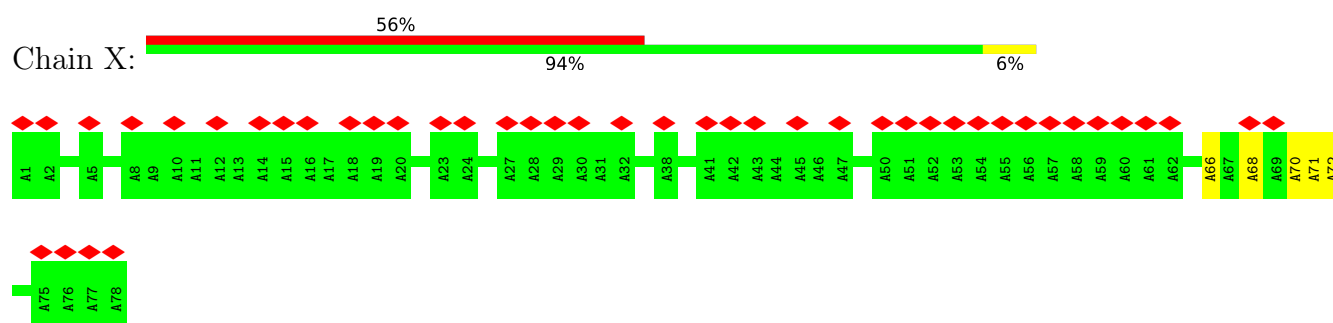




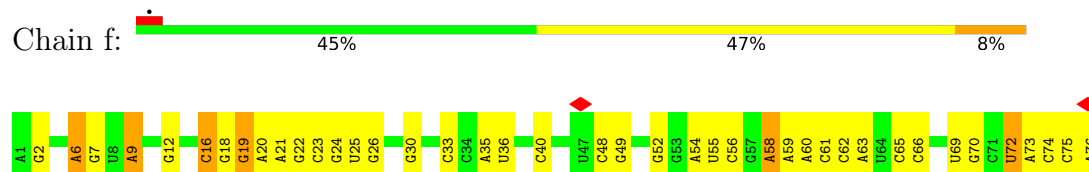
• Molecule 48: Eukaryotic translation initiation factor 3 subunit D



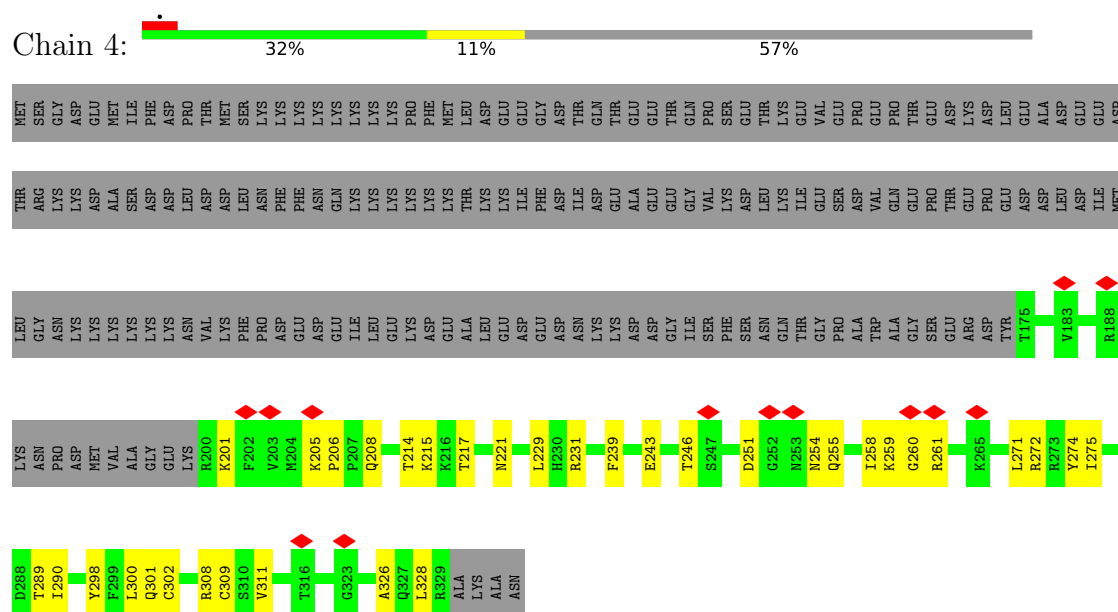
• Molecule 49: RNA recognition motif



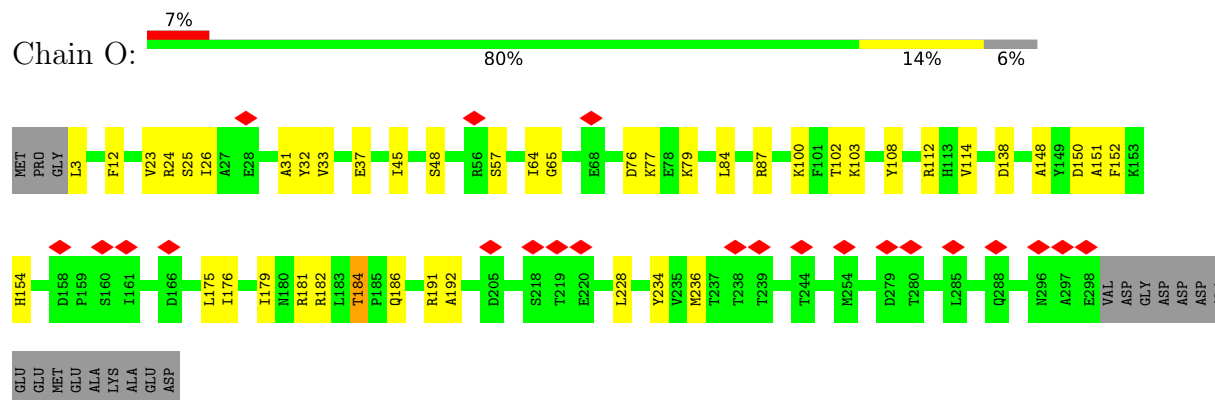
- Molecule 50: tRNA



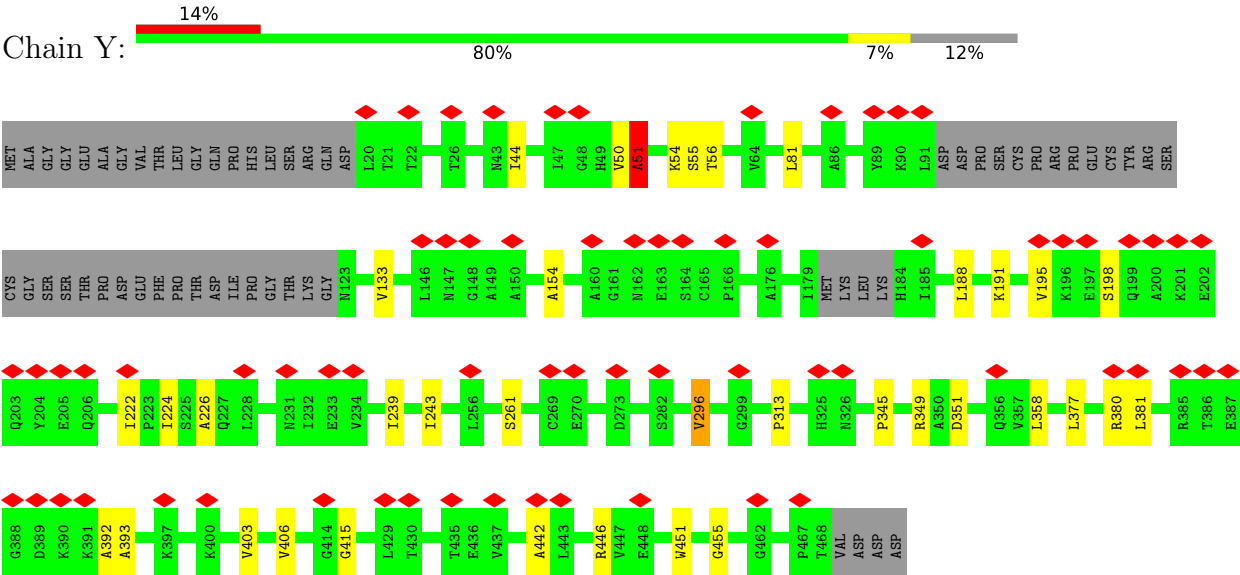
- Molecule 51: Eukaryotic translation initiation factor 2 subunit 2



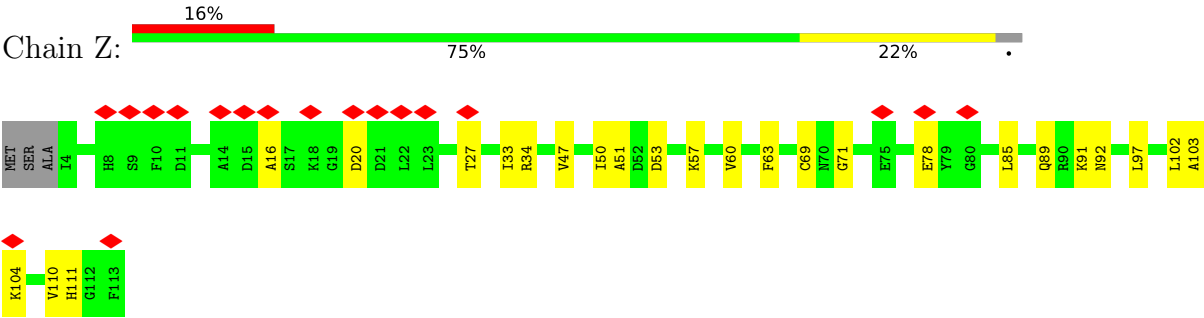
- Molecule 52: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 53: Eukaryotic translation initiation factor 2 subunit 3



• Molecule 54: Eukaryotic translation initiation factor 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ADP, SF4, ZN, MG, ATP

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	0.62	0/1742	0.71	0/2367
2	p	0.58	0/1742	0.68	0/2330
3	d	0.65	0/1710	0.75	0/2310
4	Q	0.64	0/828	0.74	0/1109
5	q	0.62	0/2073	0.67	0/2791
6	W	0.59	0/231	0.81	0/294
7	r	0.48	0/1817	0.68	1/2421 (0.0%)
8	s	0.49	0/1418	0.69	0/1895
9	t	0.56	0/1666	0.70	0/2223
10	c	0.62	0/1524	0.71	0/2035
11	n	0.64	0/1139	0.67	0/1524
12	m	0.59	0/1226	0.64	0/1649
13	y	0.55	0/631	0.70	0/844
14	D	0.73	1/1051 (0.1%)	0.75	0/1406
15	z	0.55	0/1016	0.73	0/1349
16	R	0.60	0/653	0.75	0/876
17	T	0.56	0/356	0.69	0/466
18	2	0.56	0/41057	0.53	0/63987
19	w	0.43	0/1024	0.74	0/1377
20	b	0.37	0/1773	0.66	0/2387
21	e	0.37	0/1516	0.72	0/2037
22	u	0.39	0/823	0.75	0/1111
23	v	0.28	0/870	0.68	2/1168 (0.2%)
24	o	0.33	0/999	0.73	0/1336
25	g	0.40	0/1117	0.67	0/1494
26	k	0.36	0/1180	0.71	0/1581
27	x	0.34	0/1113	0.64	0/1493
28	h	0.37	0/789	0.76	0/1059
29	P	0.33	0/563	0.69	0/758
30	S	0.44	0/481	0.80	0/643
31	l	0.39	0/461	0.73	0/612
32	U	0.29	0/474	0.75	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	V	0.38	0/2369	0.78	3/3221 (0.1%)
34	i	0.54	0/951	0.70	0/1275
35	j	0.61	0/1097	0.75	1/1464 (0.1%)
36	G	0.41	0/721	0.62	0/963
37	I	0.13	0/1495	0.39	0/2073
38	B	0.26	0/2981	0.63	0/4115
39	A	0.35	0/5469	0.70	3/7403 (0.0%)
40	C	0.39	0/5157	0.76	1/6946 (0.0%)
41	E	0.33	0/3503	0.74	1/4728 (0.0%)
42	F	0.33	0/2126	0.77	1/2890 (0.0%)
43	H	0.34	0/2458	0.77	1/3313 (0.0%)
44	K	0.37	1/1785 (0.1%)	0.82	0/2414
45	L	0.31	0/3187	0.79	10/4299 (0.2%)
46	M	0.32	0/2756	0.82	3/3714 (0.1%)
47	J	0.42	0/4626	0.74	2/6247 (0.0%)
48	N	0.42	3/3699 (0.1%)	0.85	8/5001 (0.2%)
49	X	0.16	0/389	0.50	0/543
50	f	0.29	0/1794	0.47	0/2796
51	4	0.35	0/1095	0.83	0/1477
52	O	0.30	0/2167	0.68	0/2943
53	Y	0.27	0/2161	0.69	2/2985 (0.1%)
54	Z	0.40	0/843	0.75	0/1134
All	All	0.48	5/127892 (0.0%)	0.66	39/181502 (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
13	y	0	1
14	D	0	1
15	z	0	1
19	w	0	1
21	e	0	1
24	o	0	1
25	g	0	1
26	k	0	1
28	h	0	1
33	V	0	3
37	I	0	1
39	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	C	0	2
41	E	0	2
42	F	0	1
43	H	0	1
44	K	0	1
45	L	0	1
46	M	0	1
47	J	0	1
48	N	0	3
52	O	0	1
53	Y	0	3
54	Z	0	2
All	All	0	33

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N	512	PRO	CG-CD	-11.77	1.10	1.50
14	D	93	LEU	C-N	-8.05	1.21	1.33
44	K	76	ASN	C-N	-6.57	1.25	1.33
48	N	512	PRO	CB-CG	-6.55	1.16	1.49
48	N	521	SER	C-N	6.22	1.42	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	512	PRO	N-CD-CG	-17.68	76.69	103.20
48	N	512	PRO	CB-CG-CD	13.13	148.11	106.10
48	N	512	PRO	CA-CB-CG	-12.84	80.10	104.50
45	L	379	PRO	CA-C-N	8.42	136.86	121.70
45	L	379	PRO	C-N-CA	8.42	136.86	121.70
45	L	377	MET	CA-C-N	7.87	130.97	120.58
45	L	377	MET	C-N-CA	7.87	130.97	120.58
23	v	58	GLU	N-CA-C	-7.76	99.30	110.40
42	F	298	VAL	N-CA-C	-7.16	105.53	111.91
35	j	113	GLY	N-CA-C	-7.10	96.35	113.18
48	N	521	SER	CA-C-N	6.95	133.05	121.92
48	N	521	SER	C-N-CA	6.95	133.05	121.92
48	N	512	PRO	CA-N-CD	-6.77	102.52	112.00
53	Y	296	VAL	CA-C-N	6.44	127.72	120.06
53	Y	296	VAL	C-N-CA	6.44	127.72	120.06
45	L	348	SER	CA-C-N	6.22	132.90	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	L	348	SER	C-N-CA	6.22	132.90	121.70
45	L	291	ILE	CB-CA-C	6.07	121.25	111.29
39	A	427	TYR	CA-C-N	6.07	125.19	120.33
39	A	427	TYR	C-N-CA	6.07	125.19	120.33
46	M	113	MET	CA-CB-CG	5.94	125.97	114.10
33	V	174	VAL	CA-C-N	5.83	132.67	121.54
33	V	174	VAL	C-N-CA	5.83	132.67	121.54
46	M	339	HIS	CA-C-N	5.82	128.08	120.28
46	M	339	HIS	C-N-CA	5.82	128.08	120.28
47	J	437	THR	CA-C-N	-5.69	108.99	122.31
47	J	437	THR	C-N-CA	-5.69	108.99	122.31
48	N	185	LEU	CA-C-N	5.60	132.25	121.54
48	N	185	LEU	C-N-CA	5.60	132.25	121.54
45	L	353	THR	CA-C-N	5.50	131.61	121.70
45	L	353	THR	C-N-CA	5.50	131.61	121.70
45	L	291	ILE	N-CA-CB	-5.48	102.19	111.23
7	r	130	PRO	CA-N-CD	-5.43	104.39	112.00
39	A	374	MET	CB-CG-SD	-5.43	96.42	112.70
41	E	132	TYR	N-CA-C	-5.39	105.40	111.28
23	v	60	MET	CA-CB-CG	5.38	124.85	114.10
43	H	231	LEU	CA-CB-CG	5.08	134.08	116.30
33	V	5	MET	CB-CG-SD	5.05	127.86	112.70
40	C	605	VAL	N-CA-C	-5.05	107.91	112.96

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	A	303	SER	Peptide
40	C	847	THR	Peptide
40	C	96	ILE	Peptide
14	D	54	ASP	Peptide
41	E	202	SER	Peptide
41	E	263	THR	Peptide
42	F	194	ALA	Peptide
43	H	221	LYS	Peptide
37	I	147	SER	Peptide
47	J	91	ALA	Peptide
44	K	97	ARG	Peptide
45	L	432	HIS	Peptide
46	M	236	LEU	Peptide
48	N	402	ARG	Peptide

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Mol	Chain	Res	Type	Group
48	N	413	LEU	Peptide
48	N	75	GLU	Peptide
52	O	184	THR	Peptide
33	V	134	THR	Peptide
33	V	174	VAL	Peptide
33	V	74	ASP	Peptide
53	Y	50	VAL	Peptide
53	Y	51	ALA	Peptide
53	Y	55	SER	Peptide
54	Z	103	ALA	Peptide
54	Z	78	GLU	Peptide
21	e	77	MET	Peptide
25	g	42	ILE	Peptide
28	h	93	SER	Peptide
26	k	99	LEU	Peptide
24	o	47	ARG	Peptide
19	w	115	SER	Peptide
13	y	50	PHE	Peptide
15	z	29	HIS	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	1705	0	1706	20	0
2	p	1715	0	1785	29	0
3	d	1674	0	1764	25	0
4	Q	814	0	863	12	0
5	q	2031	0	2133	26	0
6	W	230	0	276	7	0
7	r	1794	0	1942	37	0
8	s	1399	0	1492	30	0
9	t	1638	0	1710	30	0
10	c	1499	0	1618	26	0
11	n	1119	0	1186	14	0
12	m	1202	0	1289	15	0
13	y	625	0	628	8	0
14	D	1034	0	1080	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	z	999	0	1071	19	0
16	R	640	0	665	10	0
17	T	354	0	388	3	0
18	2	36717	0	18572	345	0
19	w	1011	0	1053	24	0
20	b	1745	0	1839	37	0
21	e	1495	0	1549	26	0
22	u	799	0	823	29	0
23	v	861	0	895	23	0
24	o	980	0	1025	30	0
25	g	1100	0	1166	22	0
26	k	1162	0	1221	37	0
27	x	1094	0	1120	31	0
28	h	780	0	850	22	0
29	P	557	0	610	12	0
30	S	479	0	507	9	0
31	l	450	0	448	9	0
32	U	465	0	482	15	0
33	V	2314	0	2273	76	0
34	i	939	0	965	17	0
35	j	1080	0	1147	17	0
36	G	712	0	736	14	0
37	I	1497	0	676	1	0
38	B	2966	0	1764	31	0
39	A	5385	0	5173	111	0
40	C	5113	0	5124	126	0
41	E	3437	0	3433	100	0
42	F	2090	0	2092	66	0
43	H	2413	0	2411	76	0
44	K	1750	0	1717	43	0
45	L	3111	0	3085	63	0
46	M	2718	0	2768	66	0
47	J	4541	0	4658	110	0
48	N	3617	0	3495	115	0
49	X	390	0	392	4	0
50	f	1603	0	816	16	0
51	4	1080	0	1047	25	0
52	O	2138	0	1930	29	0
53	Y	2156	0	1161	19	0
54	Z	830	0	793	15	0
55	4	1	0	0	0	0
55	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	U	1	0	0	0	0
55	l	1	0	0	0	0
56	J	16	0	0	1	0
57	J	27	0	12	1	0
58	J	2	0	0	0	0
58	Y	1	0	0	0	0
59	J	31	0	11	4	0
60	f	8	0	8	0	0
61	Y	32	0	12	2	0
All	All	122168	0	101455	1874	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 9.

All (1874) 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)
41:E:132:TYR:CE2	41:E:164:ASN:ND2	1.93	1.36
41:E:132:TYR:CD2	41:E:164:ASN:ND2	2.01	1.28
47:J:493:ASP:O	47:J:497:ARG:HB2	1.61	1.01
40:C:697:TYR:HH	40:C:708:ARG:N	1.60	0.98
18:2:1533:A:H62	18:2:1602:U:H3	1.01	0.97
45:L:232:HIS:O	45:L:236:ASP:HB2	1.64	0.97
18:2:1273:C:H42	18:2:1508:A:H62	1.06	0.96
18:2:1273:C:N4	18:2:1508:A:H62	1.65	0.95
47:J:424:VAL:O	47:J:428:LEU:HB3	1.72	0.90
18:2:698:G:H1	18:2:732:U:H3	0.89	0.87
45:L:489:GLN:O	45:L:493:PHE:HB2	1.73	0.87
18:2:1287:A:H62	18:2:1312:G:N2	1.73	0.87
20:b:137:VAL:HB	20:b:185:LYS:O	1.77	0.84
38:B:580:LEU:HA	38:B:588:SER:O	1.78	0.83
18:2:1273:C:H42	18:2:1508:A:N6	1.76	0.83
18:2:1324:G:H1	18:2:1504:U:H3	1.27	0.82
18:2:1287:A:N6	18:2:1312:G:H21	1.78	0.81
41:E:132:TYR:HH	48:N:16:TRP:CD1	1.98	0.81
18:2:1455:A:H61	18:2:1471:C:H42	1.28	0.81
40:C:110:LEU:HD13	40:C:149:ASN:OD1	1.80	0.81
8:s:68:GLN:O	8:s:72:PHE:HB2	1.81	0.81
46:M:97:GLU:O	46:M:101:LEU:HB2	1.81	0.80
40:C:110:LEU:HB3	40:C:149:ASN:ND2	1.96	0.80
18:2:694:G:N2	18:2:736:C:O2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:E:132:TYR:HD2	41:E:164:ASN:ND2	1.74	0.79
39:A:642:GLN:O	39:A:646:THR:HG23	1.83	0.78
46:M:312:VAL:HG11	46:M:325:ILE:HD11	1.66	0.77
48:N:357:ALA:HB3	48:N:377:HIS:HB2	1.66	0.77
48:N:252:LEU:HG	48:N:256:MET:HE3	1.65	0.77
41:E:132:TYR:HE2	41:E:164:ASN:HD21	0.82	0.77
18:2:694:G:N1	18:2:736:C:N3	2.32	0.77
54:Z:69:CYS:SG	54:Z:89:GLN:NE2	2.59	0.76
51:4:251:ASP:HB2	51:4:254:ASN:HB2	1.66	0.76
18:2:1286:G:H21	18:2:1313:A:H62	1.35	0.74
43:H:212:ASN:HA	43:H:215:MET:HG3	1.70	0.74
21:e:110:GLN:NE2	21:e:114:ASN:OD1	2.20	0.74
48:N:222:ARG:HG3	48:N:325:GLN:HG2	1.70	0.74
40:C:430:ASN:ND2	40:C:435:ASP:OD1	2.21	0.74
23:v:22:LEU:HD13	23:v:89:VAL:HB	1.69	0.74
45:L:284:LEU:O	45:L:288:TYR:HB2	1.88	0.73
7:r:189:ARG:NH1	18:2:332:G:N7	2.37	0.72
42:F:337:VAL:HG11	43:H:239:LEU:HD21	1.71	0.72
44:K:8:ARG:HH12	44:K:12:GLY:HA3	1.55	0.72
18:2:1287:A:H62	18:2:1312:G:H21	1.33	0.72
40:C:667:ARG:HG3	40:C:668:ARG:HE	1.54	0.72
42:F:353:LYS:HD2	45:L:544:ILE:HD13	1.73	0.71
47:J:249:VAL:HG12	47:J:252:ARG:HH21	1.55	0.71
48:N:281:ARG:HE	48:N:284:SER:HB2	1.55	0.71
33:V:120:ILE:HB	33:V:132:TRP:HB2	1.73	0.71
39:A:411:LEU:HD13	39:A:428:VAL:HG13	1.72	0.71
52:O:26:ILE:HG12	52:O:64:ILE:HD13	1.73	0.71
25:g:97:GLN:HB2	25:g:105:LYS:HG3	1.72	0.71
7:r:140:ARG:NH1	18:2:170:A:OP2	2.24	0.70
15:z:20:ARG:HE	15:z:22:GLN:HE21	1.39	0.70
39:A:526:MET:HE1	42:F:312:VAL:HG12	1.72	0.70
18:2:810:A:N6	18:2:851:C:N3	2.39	0.70
23:v:41:ALA:HB1	23:v:112:LYS:HD3	1.72	0.70
40:C:459:MET:HE1	40:C:472:HIS:HB3	1.73	0.69
24:o:91:GLY:H	24:o:107:ILE:HB	1.56	0.69
47:J:407:LEU:HD23	47:J:481:ASP:HB2	1.74	0.69
18:2:1416:C:N3	18:2:1424:G:N1	2.40	0.69
40:C:849:PRO:HB3	40:C:853:GLN:HE21	1.58	0.69
40:C:862:LYS:NZ	43:H:247:MET:SD	2.62	0.69
39:A:51:MET:HE3	39:A:74:TYR:HB2	1.75	0.69
20:b:61:GLU:HG2	20:b:62:LYS:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:O:24:ARG:H	52:O:33:VAL:HA	1.57	0.68
33:V:165:ILE:HB	33:V:177:TRP:HB2	1.75	0.68
11:n:136:LYS:NZ	18:2:372:U:OP1	2.26	0.68
42:F:312:VAL:HG11	46:M:354:LEU:HD11	1.75	0.68
18:2:617:G:N7	35:j:67:ARG:NH1	2.40	0.68
33:V:168:CYS:SG	33:V:169:GLY:N	2.66	0.68
41:E:132:TYR:HE1	48:N:16:TRP:HE1	1.40	0.68
15:z:51:THR:HG23	15:z:53:ASP:H	1.59	0.68
18:2:13:C:HO2'	18:2:1143:A:HO2'	1.40	0.68
18:2:1286:G:N2	18:2:1313:A:H62	1.92	0.68
33:V:163:PRO:O	33:V:179:LEU:HB3	1.94	0.68
40:C:375:LYS:HB3	40:C:408:LEU:HD21	1.76	0.68
40:C:864:GLY:HA2	41:E:411:LEU:HD21	1.76	0.68
24:o:81:ARG:HH12	24:o:120:SER:HB3	1.59	0.68
39:A:447:TYR:HB2	39:A:493:PHE:HD2	1.59	0.68
40:C:559:ASP:O	40:C:565:ARG:NH2	2.27	0.68
18:2:1497:G:N7	22:u:25:LYS:NZ	2.34	0.68
33:V:4:GLN:N	33:V:268:ASP:OD2	2.27	0.68
39:A:179:GLN:HG3	39:A:235:VAL:HG11	1.76	0.68
39:A:564:GLU:HG2	39:A:567:ARG:HE	1.59	0.68
10:c:79:ARG:NH2	18:2:819:G:OP1	2.27	0.67
18:2:1752:C:N3	18:2:1781:A:N6	2.42	0.67
41:E:144:TYR:HB2	41:E:179:MET:HE3	1.75	0.67
51:4:229:LEU:HD22	51:4:231:ARG:HH21	1.58	0.67
18:2:1533:A:N6	18:2:1602:U:H3	1.85	0.67
41:E:408:THR:HG22	41:E:411:LEU:HD12	1.77	0.67
14:D:71:LYS:NZ	18:2:1156:U:OP1	2.28	0.67
18:2:698:G:O6	18:2:732:U:O4	2.13	0.67
8:s:68:GLN:O	8:s:72:PHE:CB	2.43	0.67
25:g:132:PHE:O	25:g:140:ARG:NH1	2.28	0.67
47:J:501:ALA:HB2	47:J:524:MET:HG3	1.77	0.67
3:d:203:GLY:O	3:d:221:ASP:HA	1.95	0.67
47:J:532:VAL:HG21	47:J:554:GLY:HA3	1.76	0.67
7:r:159:ARG:HD2	7:r:171:THR:HB	1.77	0.67
18:2:1709:G:N2	36:G:42:LEU:O	2.28	0.67
33:V:164:ILE:HD11	33:V:221:LEU:HB3	1.76	0.66
48:N:195:CYS:SG	48:N:359:ARG:NH1	2.68	0.66
40:C:859:LEU:HD13	43:H:247:MET:HG3	1.77	0.66
42:F:234:PRO:HG2	46:M:111:HIS:HB3	1.77	0.66
43:H:71:VAL:HG11	43:H:146:GLU:HG3	1.77	0.66
39:A:464:ALA:HA	39:A:467:LEU:HD12	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:H:141:GLN:NE2	43:H:174:MET:SD	2.69	0.66
1:a:124:VAL:HG21	1:a:134:LEU:HD11	1.78	0.66
38:B:505:ARG:HG3	38:B:554:VAL:HB	1.76	0.66
44:K:159:ALA:HB2	44:K:170:LEU:HD11	1.76	0.66
48:N:363:TRP:O	48:N:370:ASP:HA	1.96	0.66
1:a:141:ASN:ND2	13:y:31:SER:O	2.29	0.66
8:s:24:SER:OG	8:s:25:GLN:NE2	2.29	0.66
45:L:245:GLU:OE2	45:L:436:HIS:ND1	2.28	0.66
21:e:171:GLU:OE2	29:P:106:GLN:NE2	2.29	0.66
24:o:64:LYS:HD3	24:o:92:SER:HB2	1.78	0.66
40:C:648:GLN:HE22	40:C:677:ILE:H	1.44	0.66
44:K:151:GLN:HE22	44:K:192:GLN:HA	1.61	0.66
9:t:42:ARG:NH1	18:2:1741:U:OP1	2.28	0.66
16:R:78:SER:HB3	48:N:80:PHE:HB3	1.78	0.66
40:C:419:PHE:HB2	40:C:439:ARG:HG2	1.77	0.66
2:p:214:LYS:NZ	18:2:943:U:OP1	2.29	0.65
28:h:46:LYS:HD3	28:h:97:ILE:HG23	1.77	0.65
38:B:407:TRP:HA	38:B:415:LYS:H	1.62	0.65
38:B:533:THR:HG23	38:B:540:VAL:HA	1.76	0.65
48:N:290:THR:HB	48:N:431:LYS:HD2	1.77	0.65
7:r:198:ARG:NH1	18:2:126:G:OP2	2.29	0.65
18:2:1445:U:H4'	28:h:57:PRO:HG3	1.78	0.65
22:u:59:LYS:HB2	22:u:70:TYR:HB2	1.78	0.65
39:A:575:ILE:HG12	43:H:70:LEU:HD12	1.78	0.65
41:E:399:SER:O	41:E:403:GLN:NE2	2.29	0.65
23:v:68:LEU:O	23:v:72:HIS:ND1	2.27	0.65
43:H:67:LEU:HD13	43:H:78:ILE:HD13	1.77	0.65
42:F:347:GLN:HG3	43:H:253:MET:HE1	1.77	0.65
48:N:360:TYR:HA	48:N:373:VAL:O	1.97	0.65
53:Y:446:ARG:HA	53:Y:451:TRP:HA	1.78	0.65
36:G:57:ARG:NH1	36:G:86:ASP:O	2.29	0.65
41:E:132:TYR:HE2	41:E:164:ASN:ND2	1.59	0.65
40:C:424:ILE:HG13	40:C:439:ARG:HB3	1.77	0.65
44:K:88:MET:HG3	45:L:291:ILE:HG23	1.79	0.65
7:r:191:ARG:NH1	18:2:312:G:O2'	2.30	0.65
18:2:894:G:N7	18:2:895:G:N2	2.45	0.64
46:M:60:VAL:HG12	46:M:64:MET:HE1	1.79	0.64
33:V:173:LEU:HD22	33:V:189:ILE:HG13	1.77	0.64
43:H:208:SER:O	43:H:212:ASN:ND2	2.30	0.64
18:2:1275:G:N2	18:2:1506:A:OP2	2.24	0.64
18:2:511:U:O2'	18:2:576:A:N6	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:C:511:TYR:OH	40:C:611:ARG:NH2	2.31	0.64
47:J:240:PHE:HB2	47:J:271:VAL:HG23	1.79	0.64
50:f:40:C:H5''	52:O:57:SER:HB2	1.79	0.64
54:Z:51:ALA:O	54:Z:57:LYS:NZ	2.29	0.64
18:2:747:U:O2	18:2:796:G:O6	2.15	0.64
19:w:65:PRO:HA	19:w:73:LEU:HD21	1.77	0.64
23:v:31:LEU:HD21	23:v:33:ARG:HD3	1.80	0.64
45:L:288:TYR:OH	45:L:318:TYR:O	2.12	0.64
40:C:110:LEU:HB3	40:C:149:ASN:CG	2.22	0.64
33:V:120:ILE:O	33:V:131:LEU:HA	1.98	0.63
40:C:409:MET:HE2	40:C:486:VAL:HG12	1.80	0.63
47:J:420:SER:HB2	47:J:459:VAL:HG11	1.81	0.63
18:2:196:C:O2'	18:2:204:G:N2	2.30	0.63
18:2:1369:A:N7	19:w:2:GLY:N	2.46	0.63
39:A:12:LEU:HG	39:A:50:ILE:HG22	1.79	0.63
41:E:278:VAL:HA	41:E:281:ILE:HG22	1.80	0.63
40:C:50:ARG:HH12	40:C:58:GLU:HG3	1.63	0.63
52:O:48:SER:O	52:O:87:ARG:NH2	2.32	0.63
18:2:1261:C:OP1	18:2:1518:C:N4	2.32	0.63
18:2:1524:G:OP2	26:k:141:ARG:NH1	2.31	0.63
51:4:251:ASP:OD2	51:4:255:GLN:NE2	2.32	0.63
5:q:197:ASN:HB3	5:q:209:HIS:HB2	1.81	0.62
22:u:3:MET:HB2	22:u:8:ARG:HH21	1.61	0.62
18:2:1654:G:OP1	27:x:82:ARG:NH1	2.32	0.62
19:w:22:THR:O	33:V:212:LYS:NZ	2.30	0.62
7:r:14:LYS:HE3	7:r:124:LEU:HG	1.80	0.62
33:V:72:SER:HB3	33:V:75:GLY:HA2	1.82	0.62
43:H:69:GLY:HA3	43:H:78:ILE:HA	1.81	0.62
18:2:1376:A:OP2	19:w:67:ARG:NE	2.33	0.62
42:F:338:THR:HG23	43:H:334:THR:HG21	1.82	0.62
51:4:229:LEU:HD23	51:4:279:VAL:HG11	1.81	0.62
18:2:885:U:O2	18:2:901:G:N2	2.33	0.62
18:2:1324:G:O6	18:2:1504:U:O4	2.17	0.62
39:A:498:ASN:OD1	39:A:520:ARG:NH2	2.33	0.62
41:E:153:PHE:HA	41:E:156:VAL:HG12	1.82	0.62
2:p:71:LEU:HD21	2:p:189:ILE:HG23	1.80	0.62
11:n:13:GLN:HE21	11:n:35:ARG:HD2	1.64	0.62
53:Y:296:VAL:HA	53:Y:358:LEU:HA	1.80	0.62
15:z:86:GLU:OE2	15:z:90:ARG:NH1	2.32	0.62
18:2:1314:U:O2'	22:u:8:ARG:NH2	2.33	0.62
4:Q:2:THR:HB	18:2:1199:A:H5''	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:z:102:THR:H	15:z:103:SER:HA	1.65	0.62
18:2:1536:G:H2'	18:2:1537:A:H8	1.64	0.62
40:C:448:VAL:HG11	40:C:486:VAL:HG11	1.81	0.62
59:J:605:ATP:H5'1	59:J:605:ATP:H8	1.64	0.62
18:2:1452:A:H61	18:2:1473:G:H21	1.47	0.61
45:L:360:ILE:O	45:L:364:ASN:ND2	2.33	0.61
53:Y:406:VAL:HA	53:Y:442:ALA:O	2.00	0.61
18:2:1629:C:O2'	26:k:83:PHE:O	2.14	0.61
43:H:36:VAL:HG21	43:H:76:LEU:HB2	1.82	0.61
45:L:243:GLN:HG2	45:L:252:ASP:H	1.65	0.61
48:N:243:GLY:O	48:N:275:LYS:NZ	2.32	0.61
48:N:269:VAL:HB	48:N:506:TYR:HB2	1.81	0.61
18:2:1377:U:O4	19:w:67:ARG:NH2	2.33	0.61
30:S:31:ARG:NH2	30:S:41:SER:OG	2.33	0.61
52:O:37:GLU:OE2	52:O:100:LYS:NZ	2.27	0.61
5:q:87:MET:HE1	5:q:123:LEU:HB2	1.81	0.61
40:C:330:ILE:HD11	40:C:431:LEU:HD11	1.82	0.61
47:J:5:LEU:HG	47:J:79:LEU:HD11	1.83	0.61
3:d:105:GLU:HB2	3:d:216:MET:HE1	1.81	0.61
12:m:20:ARG:NH2	18:2:918:U:O3'	2.32	0.61
23:v:24:THR:HA	23:v:27:ILE:HG12	1.82	0.61
28:h:21:ARG:O	28:h:114:VAL:HA	2.00	0.61
33:V:249:CYS:SG	33:V:291:TRP:NE1	2.72	0.61
41:E:117:LEU:HD12	41:E:157:LEU:HD21	1.81	0.61
41:E:127:TYR:O	41:E:131:LEU:HB2	2.00	0.61
41:E:297:GLU:O	41:E:301:VAL:N	2.31	0.61
48:N:77:GLU:HB3	48:N:79:SER:H	1.65	0.61
48:N:251:ILE:HB	48:N:267:ILE:HD12	1.83	0.61
42:F:92:VAL:HG11	42:F:198:ILE:HG21	1.83	0.61
47:J:276:LEU:O	47:J:574:ARG:NH1	2.34	0.61
18:2:1259:A:N6	18:2:1519:U:OP1	2.32	0.61
48:N:312:LEU:HD11	48:N:399:TRP:HB3	1.82	0.61
48:N:508:ILE:HG12	48:N:519:VAL:HG22	1.81	0.61
18:2:1228:A:H2'	18:2:1229:G:C8	2.36	0.61
18:2:1569:A:H5'	27:x:41:LYS:HD3	1.83	0.61
40:C:804:MET:HE3	40:C:822:ILE:HD12	1.83	0.61
47:J:169:LYS:HB2	47:J:230:VAL:HG21	1.82	0.61
18:2:1534:C:O2'	18:2:1598:G:N2	2.34	0.61
39:A:454:ARG:HH21	46:M:327:GLN:HG3	1.66	0.61
39:A:454:ARG:HH12	46:M:309:GLU:HG3	1.66	0.61
47:J:204:LEU:O	47:J:224:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:201:LYS:NZ	18:2:124:U:OP1	2.31	0.60
22:u:64:TRP:O	22:u:66:HIS:ND1	2.34	0.60
39:A:317:ARG:NH1	39:A:420:LYS:O	2.31	0.60
43:H:40:GLN:O	43:H:77:GLU:HA	2.00	0.60
47:J:172:TYR:CD2	47:J:175:GLN:HB3	2.36	0.60
52:O:23:VAL:HG23	52:O:65:GLY:H	1.65	0.60
5:q:174:LYS:O	5:q:179:ASN:ND2	2.34	0.60
14:D:28:ARG:NH2	18:2:922:A:OP2	2.34	0.60
18:2:1426:U:OP2	25:g:69:ARG:NH2	2.34	0.60
21:e:49:LEU:HD12	21:e:50:PRO:HD2	1.82	0.60
33:V:72:SER:HB2	33:V:77:PHE:HB2	1.82	0.60
41:E:344:PHE:O	41:E:348:HIS:HB2	2.00	0.60
41:E:373:ASN:O	41:E:377:ASN:ND2	2.28	0.60
45:L:324:LEU:HD21	45:L:371:LEU:HD12	1.82	0.60
47:J:263:ILE:HD13	47:J:269:ILE:HD13	1.83	0.60
16:R:72:ARG:HH22	18:2:1120:U:H5'	1.65	0.60
21:e:29:GLN:OE1	48:N:472:LYS:NZ	2.32	0.60
24:o:123:TYR:OH	26:k:124:ARG:NH1	2.33	0.60
39:A:327:LEU:O	39:A:434:ASN:ND2	2.33	0.60
39:A:347:ILE:HD11	40:C:723:ARG:HA	1.84	0.60
48:N:182:MET:HE1	48:N:493:CYS:HB2	1.83	0.60
53:Y:188:LEU:HA	53:Y:222:ILE:H	1.66	0.60
34:i:36:SER:OG	34:i:37:PHE:N	2.33	0.60
41:E:101:THR:OG1	41:E:102:ARG:NH1	2.33	0.60
44:K:86:LYS:HD2	45:L:450:GLU:HB2	1.83	0.60
47:J:252:ARG:NH1	47:J:275:ASP:OD1	2.34	0.60
48:N:496:ASP:HA	48:N:500:LYS:HE2	1.83	0.60
52:O:184:THR:O	52:O:186:GLN:NE2	2.35	0.60
20:b:39:VAL:HG13	20:b:48:ILE:HG12	1.84	0.60
23:v:70:ALA:O	23:v:73:GLN:NE2	2.34	0.60
42:F:160:HIS:HA	42:F:163:VAL:HG12	1.83	0.60
3:d:199:PRO:HG2	10:c:58:ARG:HD2	1.83	0.60
10:c:176:LYS:NZ	18:2:586:G:OP1	2.30	0.60
18:2:1616:U:O2'	18:2:1661:A:N3	2.31	0.60
18:2:1825:A:OP1	36:G:66:ARG:NH2	2.35	0.60
23:v:83:LYS:NZ	23:v:104:VAL:O	2.31	0.60
10:c:39:ASN:ND2	18:2:643:A:OP1	2.34	0.60
11:n:35:ARG:HH21	11:n:63:THR:HG21	1.65	0.60
38:B:471:SER:OG	38:B:519:TRP:NE1	2.33	0.60
42:F:262:VAL:HG13	43:H:206:LYS:HZ3	1.67	0.60
47:J:381:ASN:ND2	59:J:605:ATP:O1G	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:f:9:A:H62	50:f:23:C:H5	1.50	0.60
54:Z:27:THR:HG22	54:Z:51:ALA:HB2	1.83	0.60
18:2:1454:A:N6	18:2:1477:U:OP2	2.33	0.60
21:e:156:THR:OG1	21:e:159:ARG:NH2	2.35	0.60
25:g:41:MET:SD	25:g:45:ARG:NH2	2.75	0.60
42:F:120:LEU:HD13	42:F:134:CYS:HB2	1.84	0.60
48:N:227:VAL:O	48:N:374:ARG:NH2	2.32	0.60
1:a:36:GLN:O	1:a:53:ARG:NH1	2.34	0.59
9:t:31:ARG:NH1	18:2:380:G:OP1	2.31	0.59
18:2:1714:U:H2'	18:2:1715:A:H8	1.67	0.59
20:b:167:TYR:OH	20:b:202:LYS:O	2.19	0.59
39:A:93:TYR:HA	39:A:96:MET:HE2	1.82	0.59
40:C:594:LEU:O	40:C:598:ILE:HB	2.02	0.59
42:F:202:VAL:HA	42:F:211:MET:HE1	1.83	0.59
47:J:111:THR:O	47:J:116:LYS:NZ	2.35	0.59
47:J:224:ARG:NE	47:J:251:GLN:OE1	2.34	0.59
48:N:245:VAL:O	48:N:371:LEU:HA	2.02	0.59
5:q:27:PHE:O	18:2:495:U:O2'	2.19	0.59
9:t:34:ALA:HB2	9:t:56:ARG:HD2	1.84	0.59
21:e:54:GLY:O	25:g:125:ARG:NH1	2.35	0.59
44:K:116:ALA:HA	44:K:120:ALA:HB3	1.84	0.59
10:c:32:ILE:HD11	10:c:40:LYS:HG2	1.84	0.59
26:k:35:GLY:O	26:k:97:GLN:NE2	2.35	0.59
40:C:56:ARG:NH1	40:C:59:GLU:OE1	2.36	0.59
40:C:484:GLU:OE1	40:C:488:ARG:NH2	2.36	0.59
41:E:158:VAL:HG22	41:E:160:ALA:H	1.65	0.59
43:H:68:LEU:HD22	43:H:114:HIS:HA	1.84	0.59
44:K:11:VAL:HG21	44:K:46:ALA:HB2	1.83	0.59
26:k:39:ARG:NH2	27:x:36:THR:O	2.35	0.59
26:k:132:ARG:HB2	26:k:134:GLN:HE22	1.66	0.59
34:i:84:ARG:HH12	34:i:88:LEU:HD21	1.67	0.59
38:B:530:VAL:O	38:B:542:THR:OG1	2.17	0.59
41:E:351:ILE:HB	41:E:391:VAL:HB	1.83	0.59
47:J:412:LYS:NZ	47:J:413:PRO:O	2.34	0.59
18:2:1300:U:O2'	24:o:51:ARG:NH2	2.36	0.59
20:b:28:GLU:OE2	22:u:70:TYR:OH	2.20	0.59
40:C:589:MET:HE1	48:N:39:LEU:HD22	1.84	0.59
41:E:416:GLN:OE1	45:L:344:GLN:NE2	2.33	0.59
46:M:124:TYR:HA	46:M:127:LEU:HD12	1.83	0.59
47:J:497:ARG:NH1	47:J:521:ASP:OD1	2.36	0.59
18:2:1113:A:O2'	18:2:1119:A:N6	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:F:246:ARG:O	42:F:250:ASP:HB2	2.01	0.59
47:J:62:ILE:HD11	47:J:72:ILE:HG13	1.84	0.59
7:r:92:ARG:O	18:2:453:C:O2'	2.19	0.59
20:b:94:ARG:O	20:b:101:GLN:NE2	2.36	0.59
33:V:166:VAL:HB	33:V:221:LEU:HD21	1.83	0.59
33:V:256:ILE:HB	33:V:270:LEU:HB2	1.83	0.59
38:B:507:ARG:HG3	38:B:556:VAL:HG11	1.84	0.59
41:E:132:TYR:HD2	41:E:164:ASN:HD22	1.41	0.59
47:J:463:SER:N	47:J:466:GLU:OE2	2.32	0.59
18:2:207:G:H3'	18:2:208:G:H8	1.66	0.59
31:l:20:SER:OG	31:l:21:CYS:N	2.35	0.59
40:C:824:LYS:NZ	41:E:301:VAL:O	2.36	0.59
52:O:76:ASP:OD2	52:O:79:LYS:NZ	2.31	0.59
4:Q:4:LYS:NZ	18:2:1863:A:OP2	2.36	0.59
18:2:476:A:N3	18:2:488:U:O2'	2.29	0.59
18:2:701:G:H2'	18:2:702:G:H8	1.68	0.59
18:2:1758:G:N2	18:2:1759:G:N7	2.51	0.59
20:b:31:GLU:O	20:b:54:ARG:NH1	2.36	0.59
27:x:90:SER:O	27:x:91:HIS:ND1	2.36	0.59
31:l:22:ARG:NH1	31:l:36:LEU:O	2.35	0.59
39:A:101:THR:HG22	39:A:149:TRP:HB3	1.84	0.59
18:2:1287:A:N6	18:2:1312:G:N2	2.39	0.59
18:2:1452:A:H61	18:2:1473:G:N2	2.00	0.58
18:2:1746:U:O4	18:2:1789:G:N2	2.36	0.58
46:M:120:ARG:HA	46:M:123:VAL:HG12	1.85	0.58
48:N:391:ILE:HA	48:N:446:TYR:O	2.03	0.58
39:A:321:ARG:NH2	39:A:423:GLU:OE2	2.36	0.58
42:F:287:LEU:HD11	46:M:358:LYS:HE2	1.85	0.58
46:M:277:MET:HA	46:M:280:LEU:HG	1.85	0.58
47:J:239:MET:HE3	47:J:270:ILE:HD11	1.84	0.58
47:J:379:GLY:HA3	47:J:383:THR:HG21	1.84	0.58
18:2:952:G:O2'	18:2:953:C:O2	2.21	0.58
44:K:167:ASP:HA	44:K:170:LEU:HB2	1.85	0.58
18:2:1036:A:N3	18:2:1844:U:O2'	2.37	0.58
18:2:1730:U:H5''	40:C:132:LYS:HG3	1.84	0.58
28:h:98:VAL:HA	28:h:101:ILE:HG22	1.83	0.58
33:V:201:SER:HB2	33:V:206:LEU:HB2	1.84	0.58
48:N:55:TYR:HA	48:N:58:LYS:HG3	1.85	0.58
12:m:39:LYS:O	12:m:43:LYS:NZ	2.35	0.58
43:H:231:LEU:HB2	43:H:340:LYS:HE2	1.86	0.58
47:J:172:TYR:HD2	47:J:175:GLN:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N:264:SER:HB3	48:N:512:PRO:HD3	1.85	0.58
18:2:1452:A:O2'	18:2:1475:G:N2	2.37	0.58
42:F:332:ASN:HA	42:F:335:LEU:HD12	1.84	0.58
42:F:345:GLN:NE2	43:H:324:ASN:OD1	2.37	0.58
48:N:225:HIS:HB3	48:N:227:VAL:HG23	1.84	0.58
47:J:207:THR:HA	47:J:210:LYS:HG3	1.85	0.58
5:q:56:LEU:HD11	15:z:74:MET:HE1	1.85	0.58
7:r:49:VAL:HG22	7:r:115:LYS:HB3	1.86	0.58
18:2:722:C:O2'	18:2:724:A:N7	2.36	0.58
25:g:85:ARG:HH21	25:g:119:LEU:HG	1.69	0.58
41:E:88:THR:HG22	41:E:91:ILE:HD12	1.86	0.58
18:2:1628:C:OP1	27:x:38:LYS:NZ	2.36	0.58
48:N:413:LEU:HB3	48:N:420:VAL:HG21	1.86	0.58
38:B:505:ARG:HH11	38:B:507:ARG:HH12	1.51	0.58
23:v:93:LYS:HD3	23:v:101:ARG:HA	1.86	0.57
26:k:36:VAL:HG23	26:k:40:TYR:HD2	1.68	0.57
33:V:10:THR:HG22	33:V:308:ARG:HG2	1.86	0.57
41:E:230:ASP:OD1	41:E:264:ASN:ND2	2.37	0.57
41:E:363:THR:HG22	41:E:365:GLU:H	1.68	0.57
44:K:133:GLY:O	44:K:137:SER:OG	2.19	0.57
46:M:361:LEU:O	46:M:365:LYS:HB2	2.03	0.57
47:J:61:CYS:HB3	56:J:601:SF4:S2	2.44	0.57
48:N:360:TYR:CZ	48:N:374:ARG:HB2	2.39	0.57
16:R:33:MET:HE1	16:R:73:LEU:HD21	1.86	0.57
18:2:663:C:OP2	35:j:3:LYS:NZ	2.28	0.57
27:x:33:TRP:HE1	27:x:102:ARG:HH12	1.50	0.57
39:A:538:LYS:HE3	39:A:543:LEU:HD13	1.85	0.57
18:2:1617:G:O6	24:o:40:ARG:NH2	2.37	0.57
21:e:144:LEU:O	21:e:148:ASN:ND2	2.37	0.57
42:F:201:THR:HB	42:F:214:LYS:HG3	1.85	0.57
42:F:256:CYS:HA	42:F:261:ARG:HH22	1.69	0.57
18:2:1584:G:H4'	18:2:1585:U:H5'	1.86	0.57
35:j:93:PHE:O	35:j:140:ARG:NH1	2.37	0.57
40:C:110:LEU:HB3	40:C:149:ASN:HD21	1.67	0.57
42:F:334:LEU:HD12	43:H:334:THR:HA	1.85	0.57
44:K:17:GLY:O	45:L:262:ARG:NH2	2.31	0.57
46:M:117:THR:H	46:M:120:ARG:HD2	1.67	0.57
48:N:192:ASP:OD1	48:N:359:ARG:NH1	2.37	0.57
18:2:573:U:H1'	18:2:576:A:H2	1.70	0.57
20:b:106:ARG:HD2	20:b:173:ARG:HB3	1.86	0.57
30:S:15:THR:OG1	30:S:31:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:C:687:LEU:HD12	40:C:733:MET:HE1	1.86	0.57
44:K:152:HIS:HB2	45:L:507:SER:HA	1.86	0.57
4:Q:84:VAL:HG13	18:2:1866:A:H62	1.69	0.57
18:2:792:C:N3	18:2:794:A:N6	2.53	0.57
22:u:61:GLN:HB3	22:u:68:TYR:HB2	1.86	0.57
40:C:607:ILE:HD11	40:C:647:GLY:HA3	1.86	0.57
42:F:92:VAL:HG12	42:F:129:VAL:HB	1.87	0.57
42:F:220:LEU:HD23	42:F:230:VAL:HA	1.86	0.57
47:J:437:THR:HG23	47:J:441:PHE:HB2	1.87	0.57
18:2:1536:G:H2'	18:2:1537:A:C8	2.40	0.57
40:C:326:HIS:HB3	40:C:366:LEU:HB3	1.87	0.57
48:N:349:ASP:O	48:N:351:ASN:ND2	2.38	0.57
4:Q:100:ARG:NH1	18:2:1868:U:O2	2.38	0.57
39:A:571:ARG:HD3	43:H:70:LEU:HD13	1.86	0.57
41:E:128:LEU:HD13	41:E:158:VAL:HG23	1.85	0.57
46:M:280:LEU:O	46:M:340:ARG:NH1	2.38	0.57
48:N:289:LEU:HD23	48:N:289:LEU:H	1.69	0.57
54:Z:60:VAL:HA	54:Z:63:PHE:HB2	1.86	0.57
1:a:113:GLN:NE2	18:2:1380:C:O2	2.38	0.57
9:t:136:ILE:HG13	9:t:137:LEU:HD12	1.87	0.57
13:y:80:SER:OG	13:y:81:LYS:N	2.35	0.57
20:b:32:ASP:OD2	20:b:65:ARG:NH1	2.38	0.57
33:V:6:THR:N	33:V:311:GLN:O	2.37	0.57
41:E:80:GLN:HA	41:E:83:GLN:HG2	1.86	0.57
46:M:278:ARG:HD3	46:M:301:LEU:HB3	1.87	0.57
18:2:693:A:H2	18:2:737:G:H22	1.53	0.56
18:2:1033:G:N1	18:2:1080:A:O2'	2.32	0.56
40:C:573:ILE:HB	40:C:588:LEU:HD23	1.87	0.56
43:H:226:ASP:OD1	43:H:227:LYS:N	2.38	0.56
22:u:1:MET:HE2	22:u:3:MET:HG2	1.86	0.56
46:M:213:LYS:HZ3	46:M:269:LEU:H	1.53	0.56
48:N:260:ARG:NH1	48:N:429:SER:OG	2.37	0.56
2:p:28:LYS:HB3	2:p:48:LEU:HD11	1.87	0.56
8:s:159:ASP:OD2	12:m:19:ARG:NH2	2.38	0.56
11:n:68:ILE:HG21	11:n:143:LEU:HD11	1.88	0.56
28:h:22:ILE:HG23	28:h:112:VAL:HG13	1.87	0.56
33:V:11:LEU:HB2	33:V:307:VAL:HB	1.86	0.56
33:V:114:SER:HA	33:V:156:PHE:HD2	1.69	0.56
39:A:110:GLN:NE2	39:A:114:ASP:OD1	2.37	0.56
44:K:42:TYR:OH	44:K:76:ASN:OD1	2.16	0.56
47:J:223:GLN:NE2	47:J:245:SER:OG	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:J:409:VAL:HG22	47:J:482:VAL:HB	1.86	0.56
50:f:19:G:O6	52:O:182:ARG:NH1	2.38	0.56
5:q:148:ARG:NH2	7:r:205:GLU:OE1	2.38	0.56
15:z:37:LYS:HA	15:z:40:ILE:HD12	1.87	0.56
21:e:144:LEU:HD23	30:S:49:PRO:HG2	1.88	0.56
24:o:92:SER:OG	24:o:93:MET:N	2.39	0.56
33:V:149:GLU:HG2	33:V:150:TRP:H	1.69	0.56
39:A:447:TYR:HE2	39:A:450:ILE:HD12	1.70	0.56
43:H:123:THR:OG1	43:H:124:TYR:N	2.37	0.56
48:N:506:TYR:HA	48:N:521:SER:HA	1.87	0.56
53:Y:54:LYS:NZ	53:Y:133:VAL:O	2.30	0.56
7:r:164:LYS:NZ	18:2:68:A:OP2	2.39	0.56
10:c:166:GLY:O	38:B:492:ARG:NH1	2.38	0.56
24:o:61:ARG:NH2	24:o:88:GLU:O	2.38	0.56
28:h:33:GLU:OE2	28:h:55:ARG:NH2	2.37	0.56
41:E:36:GLU:OE1	48:N:4:PHE:N	2.39	0.56
46:M:42:LEU:HD13	46:M:74:LEU:HD11	1.86	0.56
11:n:135:SER:OG	11:n:136:LYS:N	2.36	0.56
33:V:245:ARG:HH12	33:V:312:VAL:HG21	1.70	0.56
40:C:694:GLU:HB3	40:C:698:MET:SD	2.46	0.56
42:F:187:HIS:HE1	42:F:197:PRO:HG2	1.71	0.56
45:L:240:ILE:O	45:L:244:LEU:HB2	2.06	0.56
3:d:221:ASP:N	3:d:221:ASP:OD1	2.35	0.56
14:D:30:CYS:HA	14:D:34:ILE:HD12	1.88	0.56
17:T:11:LYS:NZ	18:2:615:C:O2	2.29	0.56
18:2:1287:A:N6	18:2:1312:G:C2	2.72	0.56
27:x:11:GLN:HB3	27:x:62:ARG:HD2	1.88	0.56
40:C:635:ASP:OD2	48:N:59:TYR:OH	2.16	0.56
46:M:285:MET:HA	46:M:288:GLU:HB3	1.88	0.56
47:J:159:ILE:HD13	47:J:164:LEU:HB2	1.88	0.56
48:N:41:LYS:HG3	48:N:50:TYR:HE1	1.70	0.56
53:Y:239:ILE:O	53:Y:243:ILE:N	2.38	0.56
7:r:37:ALA:HA	7:r:49:VAL:HG12	1.88	0.56
26:k:127:TRP:HB3	26:k:129:LEU:HG	1.88	0.56
34:i:97:LEU:HD12	34:i:98:ARG:H	1.69	0.56
46:M:116:ASN:OD1	46:M:120:ARG:NH1	2.39	0.56
3:d:94:ILE:HG21	3:d:162:ILE:HD12	1.86	0.56
40:C:388:ASN:OD1	40:C:389:LEU:N	2.39	0.56
52:O:148:ALA:O	52:O:152:PHE:HB2	2.05	0.56
1:a:34:MET:HE1	1:a:162:PRO:HB3	1.88	0.56
8:s:73:GLN:HA	8:s:76:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:z:41:ARG:HA	15:z:55:ILE:HD11	1.88	0.56
18:2:1650:A:H5''	25:g:139:ALA:HB2	1.88	0.56
47:J:416:ILE:HG21	47:J:467:LEU:HD12	1.88	0.56
40:C:869:ASN:OD1	40:C:872:ARG:NH1	2.39	0.55
44:K:168:SER:OG	44:K:169:GLN:OE1	2.24	0.55
47:J:353:MET:HE1	47:J:397:LYS:HG3	1.87	0.55
51:4:289:THR:HG22	51:4:302:CYS:HA	1.87	0.55
21:e:38:TYR:HE2	21:e:144:LEU:HB2	1.70	0.55
24:o:81:ARG:NH1	24:o:97:TYR:O	2.39	0.55
38:B:530:VAL:HG22	38:B:543:ASN:H	1.71	0.55
39:A:441:GLN:NE2	39:A:506:PRO:O	2.40	0.55
40:C:611:ARG:NH1	40:C:675:LEU:O	2.39	0.55
41:E:428:GLN:NE2	41:E:429:ASN:OD1	2.39	0.55
42:F:93:ARG:HA	42:F:238:LYS:O	2.06	0.55
52:O:102:THR:HG23	52:O:103:LYS:HE3	1.88	0.55
1:a:67:ALA:HB2	13:y:37:ALA:HB2	1.87	0.55
3:d:116:THR:OG1	3:d:119:GLY:O	2.23	0.55
15:z:108:LYS:NZ	18:2:506:G:OP1	2.39	0.55
18:2:513:G:H4'	47:J:148:ARG:HD3	1.87	0.55
18:2:1253:A:HO2'	18:2:1666:C:HO2'	1.51	0.55
18:2:1599:U:O2	18:2:1600:G:N2	2.40	0.55
26:k:82:TRP:O	26:k:87:GLN:NE2	2.40	0.55
43:H:40:GLN:HA	43:H:204:VAL:O	2.06	0.55
5:q:95:THR:HG22	15:z:16:ARG:HD3	1.88	0.55
6:W:9:ARG:NH1	18:2:1851:A:OP1	2.40	0.55
7:r:9:ALA:O	7:r:131:ARG:NH2	2.40	0.55
18:2:955:A:N1	18:2:968:U:O2'	2.39	0.55
40:C:424:ILE:HD12	40:C:439:ARG:HE	1.72	0.55
48:N:203:ASP:HB2	48:N:329:ARG:HG2	1.87	0.55
7:r:12:CYS:SG	7:r:13:GLN:N	2.80	0.55
18:2:1157:G:H8	35:j:5:ARG:HD3	1.72	0.55
18:2:1513:C:OP1	31:l:12:ARG:NH2	2.38	0.55
18:2:1531:A:OP1	27:x:84:ARG:NH2	2.37	0.55
41:E:234:ASP:HA	41:E:238:TYR:HB2	1.88	0.55
44:K:36:GLN:HA	44:K:41:ALA:HB3	1.88	0.55
8:s:163:GLN:O	8:s:167:GLU:HB2	2.06	0.55
39:A:307:ARG:HD2	39:A:310:LEU:HA	1.89	0.55
47:J:96:ARG:NH2	47:J:299:VAL:O	2.40	0.55
48:N:244:ASN:ND2	48:N:368:ASP:O	2.40	0.55
51:4:208:GLN:NE2	51:4:221:ASN:OD1	2.40	0.55
6:W:11:ARG:NH2	18:2:1844:U:OP1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:c:80:ARG:NH2	18:2:818:A:OP1	2.37	0.55
18:2:1597:C:OP2	29:P:85:ARG:NH2	2.36	0.55
33:V:171:ASP:OD1	33:V:171:ASP:N	2.40	0.55
41:E:414:ARG:HA	41:E:417:MET:HB2	1.88	0.55
47:J:194:THR:OG1	47:J:232:ILE:O	2.25	0.55
47:J:218:SER:OG	59:J:605:ATP:O2G	2.24	0.55
9:t:130:THR:HG23	9:t:134:GLU:HG2	1.88	0.55
24:o:75:VAL:HA	24:o:93:MET:O	2.07	0.55
32:U:141:CYS:SG	32:U:146:LEU:N	2.71	0.55
33:V:238:ALA:O	33:V:251:ALA:HB3	2.07	0.55
44:K:29:LEU:HD13	44:K:46:ALA:HB1	1.88	0.55
47:J:242:GLU:OE1	47:J:274:HIS:N	2.39	0.55
11:n:57:ASP:OD2	11:n:60:CYS:N	2.39	0.55
30:S:40:ARG:NH2	30:S:61:SER:O	2.39	0.55
52:O:45:ILE:HG12	52:O:84:LEU:HB2	1.89	0.55
33:V:218:LEU:HB2	33:V:228:TYR:HB2	1.89	0.54
39:A:564:GLU:OE2	39:A:567:ARG:NH1	2.38	0.54
40:C:110:LEU:HD22	40:C:149:ASN:OD1	2.06	0.54
51:4:300:LEU:HB3	51:4:309:CYS:HB2	1.89	0.54
3:d:66:LEU:HD21	3:d:81:ILE:HD12	1.89	0.54
18:2:1447:G:OP1	28:h:85:HIS:ND1	2.38	0.54
26:k:34:LYS:NZ	26:k:104:ASP:OD1	2.34	0.54
28:h:67:LYS:HG3	28:h:78:ASP:HB2	1.89	0.54
18:2:1587:G:OP1	27:x:77:LYS:NZ	2.40	0.54
18:2:1648:G:O2'	18:2:1674:G:O6	2.22	0.54
18:2:1857:G:OP2	34:i:146:ARG:NH2	2.41	0.54
19:w:27:ASP:OD2	19:w:30:THR:N	2.33	0.54
22:u:26:ASP:OD2	22:u:29:MET:N	2.40	0.54
24:o:59:ARG:HH21	24:o:76:VAL:HA	1.72	0.54
29:P:57:LYS:O	29:P:61:GLU:HB2	2.07	0.54
39:A:582:LEU:HD23	39:A:585:LEU:HD21	1.89	0.54
7:r:116:LYS:NZ	7:r:119:LYS:O	2.35	0.54
21:e:33:ILE:O	21:e:36:GLN:NE2	2.40	0.54
39:A:529:VAL:HA	39:A:532:LYS:HD2	1.89	0.54
41:E:349:GLN:HA	41:E:393:MET:HB2	1.89	0.54
43:H:138:PHE:O	43:H:142:HIS:HB3	2.07	0.54
46:M:141:PRO:O	46:M:146:GLN:NE2	2.39	0.54
51:4:214:THR:HB	51:4:261:ARG:HH12	1.73	0.54
18:2:1464:C:O3'	19:w:60:ARG:NH1	2.40	0.54
18:2:1610:G:H5''	26:k:121:ARG:HH12	1.72	0.54
20:b:89:GLU:HB2	49:X:72:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:o:19:GLY:N	26:k:91:LYS:O	2.36	0.54
40:C:393:MET:HE3	40:C:398:TRP:HD1	1.72	0.54
41:E:35:LYS:HG3	41:E:36:GLU:HG3	1.88	0.54
41:E:427:ASN:OD1	41:E:430:SER:OG	2.26	0.54
42:F:250:ASP:OD2	42:F:254:LYS:NZ	2.40	0.54
43:H:307:PRO:O	43:H:309:GLN:NE2	2.39	0.54
46:M:213:LYS:HD3	46:M:268:LEU:HA	1.88	0.54
53:Y:191:LYS:H	53:Y:226:ALA:H	1.55	0.54
8:s:9:VAL:HG22	8:s:11:PRO:HD3	1.90	0.54
39:A:292:HIS:NE2	39:A:427:TYR:OH	2.34	0.54
43:H:208:SER:OG	43:H:209:HIS:N	2.41	0.54
18:2:1659:U:OP2	18:2:1660:C:N4	2.35	0.54
41:E:55:MET:HE1	41:E:74:ARG:HG3	1.90	0.54
48:N:19:CYS:SG	48:N:20:ALA:N	2.81	0.54
18:2:961:G:OP1	34:i:149:ARG:NH2	2.40	0.54
40:C:592:SER:HB3	40:C:594:LEU:HG	1.89	0.54
1:a:205:ARG:HE	1:a:210:ILE:HD13	1.73	0.54
40:C:68:ARG:NH1	40:C:112:ASP:OD2	2.39	0.54
41:E:11:ALA:HA	41:E:14:LEU:HD12	1.89	0.54
18:2:223:C:H2'	18:2:224:A:C8	2.42	0.54
18:2:693:A:H2'	18:2:694:G:C8	2.43	0.54
28:h:38:ASP:OD1	28:h:41:ARG:NH2	2.40	0.54
32:U:119:ARG:HH21	32:U:139:HIS:HB2	1.72	0.54
43:H:138:PHE:O	43:H:142:HIS:CB	2.56	0.54
48:N:216:PRO:HA	48:N:464:VAL:HA	1.90	0.54
33:V:73:SER:OG	33:V:74:ASP:N	2.42	0.53
39:A:518:GLN:O	39:A:522:GLN:NE2	2.28	0.53
41:E:345:CYS:HA	41:E:393:MET:HE1	1.90	0.53
43:H:39:VAL:HG12	43:H:76:LEU:HB3	1.90	0.53
45:L:243:GLN:HA	45:L:246:VAL:HG12	1.90	0.53
46:M:46:ILE:HD11	46:M:71:LEU:HD21	1.90	0.53
48:N:248:THR:HA	48:N:373:VAL:HG13	1.89	0.53
48:N:284:SER:OG	48:N:285:ASP:N	2.40	0.53
7:r:181:THR:HG23	7:r:183:ARG:H	1.74	0.53
18:2:1726:G:O6	18:2:1808:U:O2	2.27	0.53
38:B:429:PHE:N	38:B:439:ALA:O	2.42	0.53
39:A:469:ARG:HA	39:A:472:VAL:HG22	1.90	0.53
41:E:170:TRP:HZ2	41:E:210:GLN:HG3	1.73	0.53
41:E:266:ASP:HB3	41:E:269:LYS:HB2	1.90	0.53
47:J:258:THR:O	47:J:261:SER:OG	2.22	0.53
53:Y:56:THR:OG1	61:Y:501:GTP:O1A	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:106:THR:OG1	34:i:130:GLU:OE1	2.25	0.53
6:W:18:ARG:NH2	18:2:1182:A:OP1	2.37	0.53
42:F:142:SER:HB3	42:F:145:GLU:HB3	1.88	0.53
43:H:184:PRO:HB3	43:H:313:ARG:HB2	1.90	0.53
6:W:1:MET:HE2	18:2:1851:A:H5'	1.89	0.53
40:C:110:LEU:CB	40:C:149:ASN:HD21	2.21	0.53
41:E:138:GLN:O	41:E:143:ASN:N	2.41	0.53
18:2:1544:C:O2'	25:g:80:GLN:OE1	2.26	0.53
41:E:132:TYR:CE2	41:E:164:ASN:CG	2.80	0.53
43:H:324:ASN:OD1	43:H:328:GLN:NE2	2.42	0.53
46:M:149:LYS:O	46:M:153:ASP:HB2	2.08	0.53
47:J:565:THR:O	47:J:578:ASN:ND2	2.42	0.53
48:N:73:HIS:HD2	48:N:76:ASP:HA	1.71	0.53
11:n:126:VAL:HG12	11:n:145:VAL:HG22	1.89	0.53
47:J:101:ARG:NH1	47:J:104:GLU:OE2	2.41	0.53
48:N:12:ASN:OD1	48:N:15:GLY:N	2.42	0.53
1:a:157:VAL:O	13:y:65:SER:OG	2.27	0.53
7:r:77:LEU:HD13	7:r:95:LYS:HB2	1.90	0.53
18:2:665:G:N2	18:2:1163:C:O2	2.41	0.53
18:2:1362:U:H5''	18:2:1363:C:H5	1.74	0.53
18:2:1446:A:H5''	28:h:58:THR:HG23	1.90	0.53
41:E:255:ARG:NH2	41:E:256:TYR:OH	2.25	0.53
42:F:173:TYR:HB3	42:F:200:LEU:HB3	1.91	0.53
16:R:80:ARG:NH2	48:N:79:SER:OG	2.39	0.53
18:2:1226:G:N1	18:2:1639:G:OP2	2.42	0.53
18:2:1332:A:H2	20:b:180:GLY:HA2	1.74	0.53
18:2:1575:G:H2'	18:2:1576:G:H8	1.74	0.53
24:o:31:GLU:HA	24:o:34:MET:HE1	1.90	0.53
44:K:20:ARG:HH21	45:L:292:LYS:HE2	1.74	0.53
44:K:207:PHE:HZ	46:M:371:LEU:HD12	1.74	0.53
18:2:160:U:O2'	18:2:162:C:OP2	2.26	0.53
18:2:920:A:O2'	18:2:922:A:OP1	2.27	0.53
39:A:551:GLN:HA	39:A:554:VAL:HG22	1.89	0.53
41:E:270:ARG:HD2	41:E:339:PHE:HE2	1.73	0.53
47:J:483:TYR:O	47:J:515:ALA:HA	2.09	0.53
52:O:114:VAL:HG21	52:O:175:LEU:HD13	1.89	0.53
9:t:87:ASN:OD1	9:t:88:ASN:N	2.42	0.52
18:2:1714:U:H2'	18:2:1715:A:C8	2.43	0.52
21:e:29:GLN:NE2	21:e:31:ASN:OD1	2.42	0.52
23:v:44:LYS:HA	32:U:128:ALA:HB1	1.91	0.52
39:A:112:VAL:HG21	39:A:138:GLN:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:C:808:SER:OG	40:C:813:LEU:O	2.24	0.52
18:2:667:U:O4	18:2:1143:A:N6	2.42	0.52
29:P:50:PHE:HE1	29:P:79:ILE:HD13	1.74	0.52
47:J:442:VAL:HA	47:J:446:MET:HB2	1.92	0.52
48:N:526:THR:HG23	48:N:527:PHE:HD1	1.74	0.52
51:4:217:THR:OG1	51:4:260:GLY:O	2.27	0.52
1:a:106:GLY:N	1:a:136:GLU:OE2	2.42	0.52
8:s:69:LEU:HD22	8:s:96:ALA:HB2	1.91	0.52
16:R:72:ARG:NH2	18:2:1120:U:H5''	2.24	0.52
18:2:626:G:N2	36:G:63:GLY:O	2.42	0.52
25:g:31:LEU:HD11	25:g:33:LYS:HE2	1.89	0.52
26:k:14:ARG:HE	26:k:17:ASN:HA	1.75	0.52
38:B:543:ASN:HA	38:B:559:VAL:O	2.09	0.52
43:H:82:PHE:HB3	43:H:107:LEU:HD11	1.92	0.52
51:4:290:ILE:HG13	51:4:301:GLN:HB3	1.91	0.52
2:p:28:LYS:HD2	2:p:48:LEU:HG	1.91	0.52
3:d:114:LYS:HD3	3:d:121:ARG:HH21	1.74	0.52
10:c:38:ARG:HG3	17:T:31:ARG:HB2	1.90	0.52
18:2:1813:A:N3	47:J:22:ARG:NH1	2.49	0.52
28:h:20:ILE:HG22	28:h:116:ILE:HB	1.92	0.52
33:V:195:LEU:HA	33:V:211:GLY:HA3	1.91	0.52
42:F:97:VAL:HA	43:H:47:LEU:HD23	1.91	0.52
45:L:329:TYR:HA	45:L:332:ALA:HB3	1.92	0.52
45:L:489:GLN:O	45:L:493:PHE:CB	2.51	0.52
46:M:248:LYS:O	46:M:251:SER:OG	2.26	0.52
26:k:39:ARG:HH12	26:k:46:ARG:HH22	1.56	0.52
27:x:6:VAL:HG12	27:x:11:GLN:HE22	1.73	0.52
42:F:272:VAL:HG21	43:H:340:LYS:HD3	1.92	0.52
18:2:1409:A:OP1	25:g:26:LYS:NZ	2.35	0.52
20:b:59:LEU:HD11	49:X:71:ALA:HB2	1.91	0.52
35:j:4:CYS:SG	35:j:9:THR:OG1	2.62	0.52
39:A:445:GLN:HB3	39:A:511:LEU:HB3	1.91	0.52
41:E:79:ALA:HA	41:E:82:LYS:HD2	1.92	0.52
18:2:959:G:OP2	34:i:38:ASN:ND2	2.42	0.52
18:2:1551:U:OP1	20:b:9:ARG:NH1	2.34	0.52
18:2:1771:G:O2'	18:2:1774:C:N4	2.38	0.52
39:A:24:LYS:NZ	39:A:60:ASP:OD2	2.30	0.52
43:H:130:THR:HG23	43:H:133:LEU:H	1.74	0.52
46:M:350:LEU:O	46:M:354:LEU:HB2	2.10	0.52
20:b:149:SER:OG	20:b:150:MET:N	2.42	0.52
39:A:546:LYS:NZ	43:H:219:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:E:132:TYR:HD1	41:E:132:TYR:O	1.93	0.52
43:H:46:VAL:HA	43:H:49:ILE:HG22	1.92	0.52
47:J:377:MET:HB2	47:J:518:VAL:HG22	1.92	0.52
53:Y:81:LEU:HG	53:Y:133:VAL:HA	1.90	0.52
9:t:149:TYR:O	9:t:153:LYS:HG3	2.10	0.52
10:c:64:ASP:OD1	10:c:66:LYS:N	2.39	0.52
39:A:325:ALA:O	39:A:328:SER:OG	2.24	0.52
39:A:415:ARG:HH12	39:A:428:VAL:HG11	1.75	0.52
1:a:158:ASP:OD2	13:y:32:ILE:HD13	2.10	0.52
2:p:155:TYR:OH	18:2:989:C:OP2	2.25	0.52
18:2:1569:A:OP2	27:x:97:LYS:NZ	2.43	0.52
52:O:191:ARG:HA	52:O:236:MET:O	2.10	0.52
53:Y:380:ARG:HA	53:Y:393:ALA:HA	1.92	0.52
3:d:85:SER:O	3:d:85:SER:OG	2.27	0.51
11:n:124:ASP:HB2	11:n:147:LYS:HA	1.92	0.51
18:2:1286:G:N1	23:v:37:GLU:OE1	2.36	0.51
33:V:242:SER:OG	33:V:248:LEU:N	2.37	0.51
51:4:217:THR:HB	51:4:258:ILE:HB	1.91	0.51
54:Z:16:ALA:O	54:Z:20:ASP:CB	2.58	0.51
15:z:55:ILE:HG22	15:z:75:ILE:HG23	1.93	0.51
20:b:207:HIS:NE2	20:b:209:SER:OG	2.43	0.51
21:e:19:LEU:HD21	21:e:69:VAL:HG11	1.91	0.51
33:V:176:VAL:HB	33:V:186:THR:HB	1.93	0.51
40:C:835:LEU:HA	40:C:842:VAL:HA	1.92	0.51
46:M:193:THR:HG22	46:M:194:GLU:H	1.74	0.51
48:N:321:HIS:O	48:N:325:GLN:NE2	2.43	0.51
18:2:1452:A:N6	18:2:1473:G:H21	2.07	0.51
18:2:1587:G:N7	27:x:67:ARG:HD2	2.24	0.51
33:V:31:ILE:HB	33:V:43:TRP:HD1	1.75	0.51
45:L:408:VAL:HA	45:L:411:GLU:HG3	1.91	0.51
47:J:205:ASP:O	47:J:224:ARG:NH1	2.41	0.51
48:N:176:PHE:HA	48:N:179:LEU:HD12	1.92	0.51
18:2:851:C:H5''	18:2:852:G:H5'	1.92	0.51
22:u:21:MET:O	22:u:68:TYR:HA	2.10	0.51
36:G:38:VAL:HG22	36:G:47:LEU:HD13	1.92	0.51
41:E:270:ARG:O	41:E:274:LEU:HB2	2.10	0.51
46:M:68:VAL:HA	46:M:71:LEU:HB2	1.93	0.51
2:p:131:ASP:OD1	2:p:131:ASP:N	2.40	0.51
10:c:88:ASP:HB3	10:c:91:LYS:HG2	1.91	0.51
23:v:22:LEU:HA	23:v:25:ALA:HB3	1.93	0.51
28:h:22:ILE:HG13	28:h:114:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:h:60:THR:O	28:h:60:THR:OG1	2.27	0.51
4:Q:83:VAL:HG12	4:Q:84:VAL:HG23	1.91	0.51
8:s:159:ASP:OD1	8:s:160:LYS:N	2.44	0.51
19:w:31:ASN:HA	19:w:34:VAL:HG12	1.91	0.51
19:w:70:SER:OG	19:w:71:ILE:N	2.41	0.51
21:e:18:LYS:HB3	21:e:23:TRP:H	1.75	0.51
24:o:44:ARG:HH12	24:o:49:LEU:HD23	1.74	0.51
33:V:116:ASP:N	33:V:116:ASP:OD1	2.43	0.51
35:j:68:LYS:HB3	35:j:91:LEU:HD22	1.93	0.51
45:L:491:LEU:HD12	45:L:492:VAL:HG13	1.91	0.51
47:J:489:SER:OG	47:J:521:ASP:OD2	2.26	0.51
7:r:136:LYS:NZ	18:2:64:A:OP1	2.40	0.51
41:E:262:ILE:HA	41:E:270:ARG:HG2	1.93	0.51
4:Q:22:ARG:NH2	4:Q:27:ALA:O	2.44	0.51
9:t:84:ASN:HD22	9:t:90:LEU:HB2	1.76	0.51
18:2:949:G:H1	18:2:977:C:H5	1.57	0.51
19:w:20:TYR:OH	20:b:211:VAL:O	2.27	0.51
20:b:40:ARG:HB3	20:b:47:GLU:HB2	1.93	0.51
20:b:42:THR:HG22	20:b:44:THR:H	1.76	0.51
33:V:213:ASP:HB3	33:V:215:GLN:HG2	1.93	0.51
43:H:151:ILE:HG13	43:H:167:TYR:CE2	2.46	0.51
18:2:1513:C:H2'	18:2:1514:G:H8	1.76	0.51
22:u:11:ILE:HD11	22:u:40:VAL:HG11	1.93	0.51
38:B:450:GLU:O	38:B:454:MET:N	2.38	0.51
38:B:511:ASN:O	38:B:532:ARG:NE	2.36	0.51
40:C:386:ASN:ND2	40:C:391:THR:OG1	2.35	0.51
41:E:132:TYR:CD1	41:E:132:TYR:C	2.86	0.51
48:N:215:LYS:O	48:N:465:ILE:N	2.37	0.51
48:N:247:ALA:HB2	48:N:278:PHE:HD2	1.75	0.51
48:N:359:ARG:HD2	48:N:361:ARG:HD2	1.92	0.51
9:t:11:ARG:NH1	9:t:15:GLY:O	2.41	0.51
10:c:6:SER:O	10:c:6:SER:OG	2.28	0.51
18:2:694:G:O2'	18:2:695:C:O4'	2.25	0.51
18:2:1706:G:H21	18:2:1850:A:H1'	1.75	0.51
36:G:47:LEU:HD21	36:G:91:VAL:HG21	1.93	0.51
41:E:52:ASP:HA	41:E:55:MET:HE3	1.93	0.51
45:L:438:GLU:HG3	45:L:439:PRO:HD3	1.92	0.51
47:J:184:VAL:O	47:J:188:LEU:HB2	2.11	0.51
52:O:138:ASP:OD1	52:O:138:ASP:N	2.43	0.51
5:q:106:LYS:HD2	5:q:108:ARG:HH12	1.76	0.50
6:W:9:ARG:HH22	18:2:1707:U:H5'	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:87:ASP:N	12:m:87:ASP:OD1	2.41	0.50
14:D:90:GLN:OE1	14:D:113:HIS:ND1	2.40	0.50
18:2:1454:A:H5'	19:w:3:ARG:HD3	1.92	0.50
18:2:1657:G:H1	18:2:1667:U:H3	1.59	0.50
33:V:152:SER:OG	33:V:196:ASN:O	2.22	0.50
39:A:23:LYS:HB3	39:A:26:PRO:HD2	1.93	0.50
40:C:487:GLN:HE21	40:C:503:TYR:HE1	1.59	0.50
47:J:556:ASN:O	47:J:560:SER:OG	2.25	0.50
18:2:419:G:N2	18:2:661:U:O2	2.44	0.50
18:2:981:A:H2'	18:2:982:G:C8	2.46	0.50
33:V:179:LEU:O	33:V:181:ASN:N	2.45	0.50
42:F:177:HIS:N	42:F:203:ASP:OD1	2.44	0.50
44:K:142:ILE:HA	44:K:145:VAL:HG12	1.92	0.50
50:f:62:C:H2'	50:f:63:A:C8	2.46	0.50
8:s:37:LYS:HE2	8:s:78:ARG:HE	1.76	0.50
40:C:381:SER:HA	40:C:384:ASP:HB2	1.92	0.50
47:J:373:GLU:O	47:J:514:THR:OG1	2.23	0.50
48:N:345:GLU:HG2	48:N:348:MET:HB2	1.93	0.50
48:N:471:PHE:HB3	48:N:476:PHE:HB2	1.92	0.50
18:2:1285:G:H1	23:v:56:CYS:HA	1.76	0.50
33:V:156:PHE:HE1	33:V:165:ILE:HG12	1.76	0.50
47:J:424:VAL:O	47:J:428:LEU:CB	2.54	0.50
53:Y:261:SER:O	53:Y:351:ASP:N	2.41	0.50
18:2:1617:G:N1	18:2:1620:A:OP2	2.44	0.50
18:2:1782:G:H2'	18:2:1784:G:C8	2.47	0.50
41:E:405:ILE:O	41:E:409:LYS:HB2	2.11	0.50
46:M:121:TYR:HD1	46:M:164:LEU:HD12	1.77	0.50
48:N:281:ARG:HG2	48:N:527:PHE:HE2	1.76	0.50
48:N:432:LEU:HD12	48:N:476:PHE:CZ	2.46	0.50
18:2:1310:U:H4'	32:U:143:LYS:HE3	1.94	0.50
29:P:49:LEU:HD13	29:P:83:LEU:HD13	1.93	0.50
48:N:176:PHE:HB3	48:N:180:MET:HE3	1.92	0.50
18:2:695:C:H2'	18:2:696:G:H8	1.77	0.50
18:2:1771:G:H4'	18:2:1772:C:H5	1.77	0.50
20:b:141:LYS:HE3	20:b:145:GLN:HA	1.94	0.50
30:S:46:VAL:HG21	30:S:50:VAL:HG11	1.93	0.50
39:A:451:GLU:HG3	39:A:453:SER:H	1.76	0.50
18:2:441:C:H2'	18:2:442:C:C6	2.47	0.50
21:e:38:TYR:CE2	21:e:144:LEU:HB2	2.47	0.50
34:i:142:ARG:HG2	34:i:143:LYS:H	1.77	0.50
40:C:373:LYS:HZ3	40:C:431:LEU:HD13	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L:332:ALA:HA	45:L:335:VAL:HG12	1.94	0.50
3:d:183:LYS:HA	3:d:195:LEU:O	2.11	0.50
15:z:105:LYS:NZ	18:2:507:G:O6	2.45	0.50
18:2:875:A:H61	18:2:911:C:H42	1.60	0.50
33:V:62:HIS:ND1	33:V:84:ASP:OD2	2.41	0.50
39:A:105:LYS:O	39:A:108:SER:OG	2.29	0.50
40:C:715:HIS:HA	40:C:718:LEU:HD12	1.93	0.50
43:H:48:LYS:O	43:H:52:HIS:HB2	2.11	0.50
48:N:245:VAL:HG22	48:N:276:LEU:HD23	1.93	0.50
54:Z:33:ILE:HG22	54:Z:47:VAL:HG12	1.94	0.50
8:s:65:PRO:O	8:s:69:LEU:N	2.44	0.49
22:u:32:HIS:CE1	22:u:34:GLU:HB2	2.47	0.49
27:x:6:VAL:O	27:x:11:GLN:NE2	2.45	0.49
48:N:178:GLN:O	48:N:181:LYS:N	2.45	0.49
52:O:31:ALA:HB3	52:O:45:ILE:HB	1.94	0.49
18:2:573:U:N3	18:2:576:A:OP2	2.37	0.49
40:C:97:VAL:O	40:C:101:GLY:N	2.44	0.49
43:H:71:VAL:HG12	43:H:76:LEU:HG	1.94	0.49
43:H:119:TRP:O	43:H:149:VAL:HA	2.12	0.49
48:N:244:ASN:ND2	48:N:370:ASP:H	2.10	0.49
48:N:292:SER:N	48:N:428:ASN:OD1	2.37	0.49
12:m:67:THR:OG1	12:m:68:GLY:N	2.45	0.49
15:z:38:THR:O	15:z:42:GLU:HG2	2.12	0.49
16:R:34:ASP:OD1	16:R:80:ARG:HG2	2.12	0.49
9:t:5:ARG:NH2	18:2:384:U:O4	2.40	0.49
10:c:144:ILE:HG22	10:c:146:SER:H	1.77	0.49
27:x:21:PHE:CD2	27:x:134:ILE:HD11	2.46	0.49
33:V:79:LEU:HB2	33:V:89:LEU:HD23	1.93	0.49
39:A:5:PHE:O	39:A:39:LYS:NZ	2.34	0.49
39:A:546:LYS:O	39:A:550:HIS:HB2	2.13	0.49
47:J:557:LYS:O	47:J:557:LYS:NZ	2.42	0.49
20:b:158:ILE:HG13	20:b:164:VAL:HG12	1.93	0.49
26:k:22:GLY:HA2	26:k:56:ALA:HB3	1.95	0.49
30:S:60:GLU:OE2	30:S:63:ARG:NH2	2.46	0.49
47:J:486:ASP:HB2	47:J:518:VAL:HB	1.95	0.49
18:2:73:C:H4'	18:2:74:G:O4'	2.13	0.49
18:2:703:C:H2'	18:2:704:G:C8	2.48	0.49
20:b:223:ILE:HG23	33:V:189:ILE:HB	1.95	0.49
21:e:42:LYS:O	21:e:46:ALA:N	2.46	0.49
22:u:21:MET:HB3	22:u:69:TRP:HE3	1.77	0.49
25:g:32:ILE:HD11	25:g:63:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:329:ILE:HD11	39:A:370:LEU:HD23	1.93	0.49
39:A:452:PHE:HA	39:A:455:LEU:HB3	1.95	0.49
40:C:352:GLU:HA	40:C:355:GLN:HG2	1.95	0.49
46:M:183:LYS:HA	46:M:186:VAL:HG22	1.95	0.49
48:N:422:ALA:HA	48:N:425:LEU:HD12	1.95	0.49
50:f:16:C:H5'	50:f:60:A:H2	1.77	0.49
53:Y:345:PRO:O	53:Y:349:ARG:CB	2.60	0.49
33:V:151:VAL:HA	33:V:169:GLY:HA2	1.95	0.49
44:K:105:LEU:HG	44:K:117:PHE:HE1	1.77	0.49
50:f:6:A:H2'	50:f:7:G:C8	2.48	0.49
18:2:140:U:O2'	18:2:143:U:OP1	2.31	0.49
26:k:71:MET:HB3	26:k:99:LEU:HD11	1.95	0.49
26:k:110:ASP:HA	26:k:113:ARG:HB3	1.95	0.49
28:h:94:PRO:HD2	28:h:97:ILE:HD12	1.95	0.49
41:E:401:TYR:HA	41:E:404:VAL:HG12	1.95	0.49
43:H:127:SER:HG	43:H:326:TYR:HH	1.52	0.49
47:J:196:THR:HG23	47:J:197:GLN:H	1.77	0.49
1:a:77:ILE:HB	1:a:124:VAL:HG12	1.95	0.49
18:2:1464:C:H2'	18:2:1465:A:N3	2.27	0.49
33:V:199:THR:OG1	33:V:200:VAL:N	2.46	0.49
34:i:34:PHE:HB3	34:i:41:PHE:HB2	1.95	0.49
39:A:585:LEU:HA	39:A:588:GLN:HG2	1.94	0.49
45:L:353:THR:OG1	45:L:355:TYR:N	2.42	0.49
8:s:43:LEU:HB3	8:s:72:PHE:HD1	1.78	0.48
18:2:537:C:O2	18:2:539:C:N4	2.42	0.48
26:k:125:HIS:HD2	26:k:131:VAL:HG21	1.78	0.48
40:C:586:ARG:HG3	40:C:589:MET:HE2	1.94	0.48
41:E:45:LEU:HD22	41:E:50:MET:HB3	1.95	0.48
43:H:270:GLN:OE1	43:H:274:LYS:NZ	2.29	0.48
45:L:201:ARG:HB3	45:L:268:MET:HE1	1.95	0.48
51:4:298:TYR:HB2	51:4:311:VAL:HG13	1.94	0.48
2:p:128:LYS:HE3	2:p:132:GLY:HA2	1.95	0.48
3:d:132:ASP:HB3	3:d:136:HIS:HB2	1.95	0.48
18:2:1212:G:H1	18:2:1687:C:H42	1.61	0.48
22:u:37:ASP:N	22:u:37:ASP:OD1	2.42	0.48
41:E:337:ARG:HA	41:E:340:ILE:HG22	1.96	0.48
45:L:185:ASP:N	45:L:185:ASP:OD1	2.44	0.48
47:J:98:PRO:HD3	47:J:299:VAL:HG21	1.94	0.48
7:r:126:ASP:OD1	7:r:126:ASP:N	2.45	0.48
47:J:316:TYR:OH	47:J:321:ASN:OD1	2.24	0.48
5:q:66:MET:HE2	18:2:502:C:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:164:LYS:NZ	18:2:69:C:OP2	2.46	0.48
10:c:110:LEU:HB2	10:c:147:PHE:HB3	1.95	0.48
45:L:288:TYR:HE1	45:L:322:ALA:HB2	1.77	0.48
48:N:207:ASP:HA	48:N:468:THR:HB	1.95	0.48
52:O:3:LEU:O	52:O:112:ARG:NH1	2.46	0.48
8:s:63:PHE:HA	8:s:95:ILE:O	2.13	0.48
9:t:48:VAL:HG11	9:t:54:LYS:HE2	1.94	0.48
9:t:155:ASN:HD22	9:t:155:ASN:C	2.19	0.48
18:2:541:U:OP1	18:2:543:C:N4	2.44	0.48
18:2:1288:U:O2'	18:2:1315:U:O2'	2.20	0.48
21:e:196:LEU:HA	21:e:199:VAL:HG22	1.96	0.48
26:k:84:LEU:O	26:k:87:GLN:NE2	2.42	0.48
27:x:28:LEU:HD23	27:x:54:TYR:HD1	1.77	0.48
41:E:342:GLU:HB2	41:E:374:LEU:HD11	1.95	0.48
46:M:220:PHE:HB2	46:M:245:VAL:HG22	1.95	0.48
46:M:328:THR:OG1	46:M:329:GLN:OE1	2.30	0.48
59:J:605:ATP:H5'1	59:J:605:ATP:C8	2.48	0.48
48:N:510:LYS:NZ	48:N:514:LYS:O	2.32	0.48
53:Y:381:LEU:N	53:Y:392:ALA:O	2.47	0.48
1:a:12:GLU:HG3	1:a:16:LEU:HD23	1.96	0.48
2:p:142:PHE:HB2	2:p:208:HIS:HB3	1.94	0.48
14:D:87:GLU:HA	14:D:90:GLN:HG2	1.94	0.48
18:2:1711:U:H2'	18:2:1712:A:H8	1.78	0.48
18:2:1730:U:OP1	40:C:132:LYS:NZ	2.45	0.48
39:A:205:LEU:HD13	39:A:233:ARG:HH22	1.77	0.48
46:M:158:THR:O	46:M:161:LYS:HG2	2.14	0.48
15:z:66:GLY:HA2	18:2:581:U:H4'	1.96	0.48
18:2:1598:G:H3'	29:P:80:ARG:HH11	1.78	0.48
18:2:1727:G:N2	18:2:1808:U:H1'	2.27	0.48
48:N:362:ARG:HA	48:N:372:ILE:HD13	1.95	0.48
54:Z:33:ILE:HD11	54:Z:110:VAL:HG22	1.96	0.48
15:z:12:PHE:HZ	15:z:21:LYS:HD2	1.79	0.48
18:2:694:G:O6	18:2:736:C:N4	2.46	0.48
39:A:288:ASN:HD21	39:A:291:PHE:HD2	1.61	0.48
41:E:426:LEU:HD21	45:L:547:ILE:HG21	1.96	0.48
47:J:106:LEU:HB3	47:J:270:ILE:HG22	1.96	0.48
48:N:190:PRO:HG2	48:N:361:ARG:HB3	1.94	0.48
52:O:150:ASP:O	52:O:154:HIS:ND1	2.35	0.48
12:m:119:GLU:O	12:m:123:HIS:ND1	2.46	0.48
18:2:472:C:O2'	18:2:474:G:OP1	2.29	0.48
18:2:525:A:H2'	18:2:526:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:614:C:O2'	18:2:626:G:N2	2.47	0.48
25:g:19:ALA:HB2	25:g:75:GLY:HA3	1.94	0.48
32:U:98:VAL:HG21	32:U:104:LYS:HE3	1.96	0.48
44:K:74:LEU:HD12	44:K:106:GLY:HA2	1.95	0.48
46:M:244:PHE:HE1	46:M:273:ASN:HB3	1.79	0.48
9:t:177:SER:OG	9:t:184:ARG:O	2.28	0.48
12:m:16:LEU:HD23	12:m:17:PRO:HD2	1.95	0.48
18:2:701:G:H2'	18:2:702:G:C8	2.47	0.48
18:2:708:C:H2'	18:2:709:G:C8	2.49	0.48
18:2:848:U:H2'	18:2:849:A:H8	1.79	0.48
18:2:1372:U:OP1	18:2:1385:G:N2	2.32	0.48
18:2:1462:U:H5''	18:2:1464:C:H41	1.79	0.48
38:B:519:TRP:HZ3	38:B:549:MET:HE3	1.79	0.48
40:C:589:MET:SD	40:C:616:LEU:HD13	2.54	0.48
41:E:58:TYR:HE1	41:E:61:LEU:HD22	1.79	0.48
41:E:254:LEU:HD12	41:E:281:ILE:HG13	1.95	0.48
48:N:269:VAL:O	48:N:505:LYS:HA	2.14	0.48
7:r:10:THR:OG1	7:r:127:THR:O	2.21	0.47
22:u:57:TYR:O	22:u:72:THR:OG1	2.27	0.47
33:V:106:LYS:HD3	33:V:126:ASP:HB3	1.96	0.47
43:H:129:VAL:HB	43:H:322:GLN:HE21	1.78	0.47
47:J:238:PHE:HE2	47:J:267:ARG:HD3	1.79	0.47
5:q:124:CYS:HB3	5:q:141:THR:HB	1.96	0.47
5:q:163:ASP:O	5:q:167:GLY:N	2.46	0.47
7:r:186:GLN:NE2	18:2:333:G:O6	2.47	0.47
18:2:797:C:O2'	18:2:798:G:N2	2.47	0.47
22:u:21:MET:HE3	22:u:22:VAL:H	1.78	0.47
26:k:26:ILE:HG12	26:k:59:LEU:HD11	1.96	0.47
32:U:132:MET:SD	32:U:141:CYS:HB3	2.54	0.47
34:i:75:MET:HG3	34:i:118:ALA:HB2	1.96	0.47
36:G:29:LYS:N	36:G:35:TYR:OH	2.47	0.47
39:A:167:ASN:HB3	39:A:170:VAL:HG22	1.96	0.47
40:C:425:LEU:HA	40:C:441:ARG:HD2	1.96	0.47
40:C:802:ILE:O	40:C:842:VAL:N	2.45	0.47
40:C:803:SER:O	40:C:806:THR:OG1	2.26	0.47
42:F:162:LYS:HG3	43:H:85:PRO:HB3	1.96	0.47
50:f:54:A:N6	50:f:61:C:N3	2.62	0.47
5:q:136:ILE:HG21	5:q:148:ARG:HD2	1.97	0.47
9:t:98:LYS:HB3	18:2:377:G:H5'	1.95	0.47
18:2:1468:C:H2'	18:2:1469:A:H8	1.79	0.47
18:2:1677:U:OP1	21:e:71:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:1821:U:H2'	18:2:1822:A:C8	2.49	0.47
25:g:82:TYR:HA	25:g:85:ARG:HG2	1.96	0.47
27:x:126:GLN:HA	27:x:129:ARG:HG2	1.96	0.47
34:i:103:ASN:ND2	34:i:141:ARG:O	2.47	0.47
39:A:164:LEU:HD21	39:A:173:LEU:HD23	1.95	0.47
40:C:445:LEU:HD21	40:C:501:ARG:HG3	1.95	0.47
44:K:146:VAL:HA	44:K:149:THR:HG22	1.95	0.47
48:N:316:ALA:HA	48:N:319:ILE:HD12	1.96	0.47
30:S:21:THR:HG23	30:S:67:ARG:NH2	2.29	0.47
35:j:114:ASP:OD1	35:j:114:ASP:N	2.39	0.47
42:F:345:GLN:HE21	43:H:324:ASN:HA	1.80	0.47
46:M:179:ASP:OD1	46:M:180:ALA:N	2.45	0.47
4:Q:79:ILE:HD11	18:2:1864:U:H5'	1.96	0.47
18:2:184:G:H2'	18:2:185:G:C8	2.50	0.47
18:2:481:C:OP2	47:J:7:ARG:NH2	2.42	0.47
19:w:35:CYS:HA	19:w:38:ILE:HG12	1.96	0.47
33:V:107:ASP:HB2	33:V:125:ARG:HD2	1.95	0.47
40:C:80:LEU:HA	40:C:141:LEU:HD13	1.95	0.47
46:M:323:CYS:HB3	46:M:334:VAL:HG12	1.96	0.47
47:J:148:ARG:HA	47:J:153:GLN:OE1	2.14	0.47
50:f:25:U:H2'	50:f:26:G:H8	1.79	0.47
52:O:192:ALA:HB3	52:O:236:MET:HB2	1.95	0.47
18:2:1101:U:H2'	18:2:1102:G:C8	2.49	0.47
18:2:1774:C:O2'	18:2:1775:U:N3	2.47	0.47
19:w:14:ARG:HA	19:w:17:ILE:HG22	1.95	0.47
23:v:76:LEU:O	23:v:78:LYS:NZ	2.46	0.47
34:i:92:ALA:HA	34:i:125:LYS:O	2.13	0.47
39:A:475:ALA:HA	39:A:480:LEU:HB2	1.95	0.47
41:E:233:ILE:HG21	41:E:269:LYS:HE2	1.96	0.47
41:E:349:GLN:O	41:E:393:MET:N	2.45	0.47
43:H:263:TYR:CZ	43:H:310:PRO:HB3	2.50	0.47
7:r:172:LYS:HD3	18:2:65:C:H4'	1.96	0.47
9:t:83:TYR:OH	11:n:8:ARG:O	2.27	0.47
14:D:87:GLU:HG3	14:D:88:LYS:HE2	1.96	0.47
18:2:1047:C:H5'	34:i:143:LYS:HA	1.94	0.47
18:2:1317:C:H2'	18:2:1318:G:C8	2.50	0.47
23:v:52:LEU:HB2	23:v:76:LEU:HD23	1.97	0.47
23:v:85:LEU:O	23:v:89:VAL:HG12	2.14	0.47
26:k:89:ASP:OD1	26:k:90:VAL:N	2.47	0.47
30:S:38:THR:OG1	30:S:39:SER:N	2.48	0.47
39:A:257:HIS:HA	39:A:260:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:346:GLY:O	39:A:350:GLU:HB2	2.15	0.47
40:C:687:LEU:HD23	40:C:687:LEU:HA	1.74	0.47
42:F:205:SER:HA	42:F:211:MET:HA	1.97	0.47
45:L:288:TYR:CE1	45:L:322:ALA:HB2	2.50	0.47
48:N:407:VAL:HG22	48:N:423:THR:HG21	1.95	0.47
8:s:98:ARG:HB3	8:s:125:VAL:HG22	1.97	0.47
18:2:148:U:N3	18:2:169:U:O4	2.48	0.47
18:2:1567:G:OP2	27:x:102:ARG:NH2	2.48	0.47
18:2:1603:G:H22	26:k:24:ARG:HD3	1.79	0.47
19:w:59:LYS:HE2	19:w:59:LYS:HB3	1.79	0.47
33:V:89:LEU:HD12	33:V:99:ARG:HG3	1.97	0.47
43:H:283:GLN:HA	43:H:286:MET:HE3	1.96	0.47
54:Z:47:VAL:HG23	54:Z:50:ILE:HD11	1.97	0.47
2:p:71:LEU:HD12	2:p:71:LEU:HA	1.77	0.47
7:r:121:ILE:HG22	7:r:123:GLY:H	1.79	0.47
8:s:58:LYS:HB2	8:s:90:LYS:HG2	1.97	0.47
18:2:909:G:H2'	18:2:910:G:C8	2.49	0.47
18:2:1533:A:N6	18:2:1602:U:C2	2.83	0.47
20:b:66:ILE:HD13	49:X:70:ALA:HB1	1.96	0.47
20:b:101:GLN:HG3	20:b:126:ILE:HD11	1.97	0.47
36:G:26:LEU:HD11	36:G:103:LEU:HG	1.97	0.47
41:E:14:LEU:HA	41:E:217:TRP:HE1	1.80	0.47
41:E:416:GLN:NE2	41:E:417:MET:HG2	2.30	0.47
2:p:68:GLU:HG3	2:p:85:LYS:HG2	1.97	0.47
18:2:1119:A:H2'	18:2:1120:U:C2	2.50	0.47
21:e:113:VAL:O	21:e:117:ILE:HG12	2.15	0.47
39:A:403:LEU:HA	39:A:406:ARG:HD2	1.97	0.47
41:E:190:THR:O	41:E:193:LYS:HG3	2.15	0.47
43:H:162:LEU:HB3	43:H:164:LEU:HD23	1.96	0.47
43:H:285:ASN:HA	43:H:288:ARG:HD2	1.97	0.47
45:L:329:TYR:HB3	45:L:371:LEU:HD21	1.97	0.47
45:L:363:GLN:O	45:L:367:MET:HG2	2.15	0.47
47:J:369:PHE:HZ	47:J:514:THR:HG21	1.79	0.47
52:O:150:ASP:OD1	52:O:151:ALA:N	2.41	0.47
5:q:87:MET:HG2	5:q:100:ARG:HD3	1.97	0.46
8:s:31:GLU:OE2	8:s:41:ARG:NH1	2.48	0.46
18:2:944:A:H5''	34:i:134:PRO:HB3	1.96	0.46
18:2:1098:C:H2'	18:2:1099:G:C8	2.51	0.46
18:2:1278:A:OP1	22:u:55:ARG:NH1	2.48	0.46
18:2:1711:U:H2'	18:2:1712:A:C8	2.49	0.46
22:u:76:ILE:HD13	22:u:91:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:393:TRP:CD1	39:A:406:ARG:HD3	2.50	0.46
46:M:121:TYR:CG	46:M:156:LEU:HD21	2.50	0.46
2:p:106:THR:HG23	2:p:109:LYS:H	1.79	0.46
5:q:199:GLU:OE2	5:q:209:HIS:NE2	2.48	0.46
7:r:164:LYS:HD3	7:r:167:LYS:HD2	1.98	0.46
19:w:98:VAL:HG22	19:w:102:THR:HB	1.96	0.46
32:U:119:ARG:HG3	32:U:132:MET:HG3	1.96	0.46
40:C:374:ILE:O	40:C:378:ILE:HD12	2.14	0.46
40:C:632:ALA:HB2	48:N:39:LEU:HD11	1.97	0.46
46:M:270:HIS:CE1	46:M:274:MET:HE3	2.50	0.46
46:M:327:GLN:O	46:M:330:ARG:NH2	2.47	0.46
47:J:357:MET:HG3	47:J:396:LEU:HD21	1.97	0.46
1:a:42:LYS:NZ	19:w:99:ASP:OD2	2.34	0.46
11:n:20:LYS:NZ	18:2:223:C:OP1	2.36	0.46
18:2:199:C:O2'	18:2:200:G:N2	2.49	0.46
18:2:890:U:O2'	18:2:896:U:O4	2.23	0.46
18:2:1112:U:N3	18:2:1113:A:N7	2.63	0.46
38:B:482:TRP:NE1	38:B:515:CYS:HB2	2.30	0.46
39:A:35:MET:HE3	39:A:35:MET:HB3	1.63	0.46
40:C:733:MET:HG2	40:C:761:MET:HE1	1.98	0.46
41:E:170:TRP:CZ2	41:E:210:GLN:HG3	2.50	0.46
48:N:222:ARG:HA	48:N:352:GLU:HB3	1.98	0.46
10:c:18:ARG:O	10:c:24:ARG:NH2	2.46	0.46
10:c:162:ARG:HB2	10:c:162:ARG:NH2	2.31	0.46
39:A:526:MET:HA	42:F:311:LEU:HD11	1.97	0.46
40:C:96:ILE:HG22	40:C:97:VAL:H	1.80	0.46
41:E:272:GLN:HG3	41:E:273:VAL:HG23	1.97	0.46
43:H:282:GLN:HG2	43:H:286:MET:HE2	1.96	0.46
52:O:103:LYS:HA	52:O:103:LYS:HD3	1.71	0.46
2:p:109:LYS:HE3	2:p:211:PHE:CE2	2.51	0.46
5:q:137:PRO:HG2	5:q:150:PRO:HD2	1.97	0.46
18:2:1604:G:OP1	26:k:38:ARG:NH2	2.49	0.46
20:b:4:GLN:HG3	20:b:5:ILE:HG12	1.98	0.46
25:g:24:HIS:O	25:g:68:ILE:HA	2.15	0.46
34:i:100:THR:HG21	34:i:104:ARG:HE	1.80	0.46
39:A:560:ASN:HD22	43:H:209:HIS:CD2	2.33	0.46
42:F:231:MET:HE3	46:M:72:LEU:HD11	1.98	0.46
42:F:250:ASP:HA	42:F:253:MET:HB2	1.96	0.46
47:J:382:GLY:O	47:J:540:SER:N	2.49	0.46
9:t:194:GLU:OE1	11:n:12:LYS:NZ	2.44	0.46
16:R:48:SER:HG	16:R:49:HIS:HD1	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:952:G:O2'	18:2:953:C:O4'	2.32	0.46
26:k:39:ARG:NH1	26:k:46:ARG:HH22	2.13	0.46
28:h:74:SER:O	28:h:74:SER:OG	2.31	0.46
32:U:121:CYS:HB3	32:U:126:CYS:HB3	1.97	0.46
39:A:103:ALA:O	39:A:107:GLU:HG2	2.15	0.46
41:E:237:LEU:HD22	41:E:273:VAL:HG13	1.96	0.46
43:H:171:PRO:O	43:H:175:GLU:HG2	2.16	0.46
45:L:490:LEU:HA	45:L:493:PHE:HB3	1.97	0.46
47:J:127:GLN:NE2	47:J:128:LYS:O	2.49	0.46
48:N:200:GLU:HB2	48:N:328:LEU:HD13	1.96	0.46
53:Y:377:LEU:HA	53:Y:455:GLY:HA2	1.97	0.46
8:s:84:GLU:OE2	8:s:91:HIS:ND1	2.49	0.46
18:2:889:U:H2'	18:2:897:U:H3	1.80	0.46
18:2:951:C:H2'	18:2:952:G:H5'	1.97	0.46
40:C:860:ALA:HB2	41:E:404:VAL:HG23	1.96	0.46
40:C:876:HIS:CE1	43:H:264:MET:HB3	2.51	0.46
45:L:200:TYR:HB3	45:L:205:ALA:HB2	1.97	0.46
46:M:156:LEU:HB3	46:M:157:THR:H	1.51	0.46
47:J:194:THR:HG23	47:J:234:LYS:HB2	1.98	0.46
48:N:232:ASP:OD2	48:N:360:TYR:OH	2.34	0.46
51:4:301:GLN:HB2	51:4:308:ARG:HH11	1.81	0.46
2:p:202:GLN:O	18:2:1121:G:N2	2.48	0.46
8:s:145:ARG:NE	14:D:51:GLU:OE2	2.41	0.46
22:u:12:TYR:HB3	22:u:79:LEU:HD11	1.98	0.46
23:v:53:ALA:HA	23:v:79:VAL:HG22	1.97	0.46
28:h:37:ALA:HA	28:h:40:ILE:HG22	1.98	0.46
33:V:299:PHE:HD1	33:V:309:VAL:HG12	1.80	0.46
40:C:810:MET:HG3	40:C:811:PHE:HD1	1.80	0.46
46:M:246:SER:HA	46:M:340:ARG:HD3	1.98	0.46
49:X:66:ALA:O	49:X:68:ALA:N	2.49	0.46
18:2:190:G:H1'	18:2:209:A:H61	1.80	0.46
18:2:1661:A:OP2	31:l:32:ARG:NH1	2.33	0.46
36:G:29:LYS:HG3	36:G:34:GLU:HA	1.96	0.46
39:A:335:ARG:HD3	40:C:746:MET:HE3	1.97	0.46
41:E:275:LYS:HA	41:E:278:VAL:HG22	1.97	0.46
48:N:281:ARG:NE	48:N:284:SER:HB2	2.29	0.46
9:t:184:ARG:NH2	18:2:305:U:O4	2.49	0.46
18:2:641:A:H2'	18:2:642:U:O4'	2.16	0.46
18:2:1468:C:H2'	18:2:1469:A:C8	2.51	0.46
24:o:91:GLY:N	24:o:107:ILE:HB	2.27	0.46
29:P:69:THR:H	29:P:72:VAL:HG22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B:488:ASP:OD1	38:B:488:ASP:N	2.48	0.46
38:B:521:LYS:NZ	38:B:570:TRP:O	2.49	0.46
38:B:549:MET:N	38:B:549:MET:SD	2.89	0.46
41:E:196:ILE:HG12	41:E:210:GLN:HG2	1.97	0.46
42:F:249:VAL:HA	42:F:252:ILE:HG22	1.98	0.46
46:M:361:LEU:O	46:M:365:LYS:CB	2.63	0.46
47:J:243:PRO:HD2	47:J:273:GLU:HG2	1.98	0.46
52:O:176:ILE:HA	52:O:179:ILE:HG22	1.98	0.46
7:r:183:ARG:NH2	18:2:317:C:OP2	2.47	0.45
9:t:25:ARG:NH2	18:2:433:A:OP1	2.37	0.45
10:c:81:LEU:HD12	10:c:97:ILE:HD12	1.98	0.45
15:z:13:MET:HB3	15:z:13:MET:HE2	1.81	0.45
22:u:14:LEU:HG	22:u:35:LEU:HD21	1.99	0.45
28:h:60:THR:HG22	28:h:83:ARG:HD3	1.97	0.45
39:A:265:LYS:HG2	39:A:266:PRO:HD2	1.98	0.45
42:F:334:LEU:HD12	43:H:334:THR:HG23	1.97	0.45
48:N:229:THR:HB	48:N:279:ASP:HA	1.98	0.45
51:4:246:THR:HB	51:4:259:LYS:HD3	1.98	0.45
5:q:73:ASP:OD2	5:q:122:LYS:NZ	2.35	0.45
18:2:1298:G:H4'	24:o:78:THR:HA	1.99	0.45
20:b:80:PRO:HG2	20:b:83:SER:HB3	1.98	0.45
20:b:159:HIS:C	20:b:164:VAL:HG11	2.40	0.45
24:o:53:GLN:OE1	24:o:53:GLN:N	2.48	0.45
26:k:67:VAL:HA	26:k:70:ILE:HG22	1.98	0.45
30:S:62:GLU:HG3	30:S:63:ARG:HG3	1.98	0.45
31:l:8:TRP:CZ2	31:l:12:ARG:HG3	2.51	0.45
31:l:20:SER:HB2	31:l:27:ARG:HG2	1.98	0.45
41:E:196:ILE:HD13	41:E:214:LEU:HD12	1.98	0.45
42:F:265:LEU:HD23	43:H:204:VAL:HA	1.98	0.45
45:L:231:LEU:O	45:L:235:VAL:HG22	2.15	0.45
47:J:41:VAL:HG12	47:J:48:ALA:HA	1.99	0.45
48:N:168:TRP:CE3	48:N:520:TYR:HB3	2.51	0.45
5:q:71:LYS:HG2	5:q:76:VAL:HG22	1.98	0.45
7:r:137:ARG:NH2	18:2:171:A:OP2	2.30	0.45
18:2:1683:C:H2'	18:2:1684:C:H6	1.82	0.45
20:b:193:ASP:OD2	20:b:197:LYS:N	2.48	0.45
33:V:32:LEU:HD12	33:V:71:ILE:HG22	1.98	0.45
33:V:302:TYR:CD2	33:V:308:ARG:HD2	2.51	0.45
46:M:222:HIS:O	46:M:225:THR:OG1	2.32	0.45
54:Z:71:GLY:HA3	54:Z:85:LEU:HD13	1.99	0.45
24:o:68:PRO:HG2	24:o:71:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:196:ASN:H	33:V:211:GLY:HA2	1.82	0.45
39:A:300:TYR:HD1	39:A:318:MET:HE1	1.81	0.45
39:A:541:HIS:O	39:A:544:GLN:NE2	2.50	0.45
41:E:368:GLU:OE2	45:L:474:LYS:NZ	2.41	0.45
43:H:133:LEU:O	43:H:137:GLN:HB3	2.17	0.45
47:J:374:ILE:HD11	47:J:508:ILE:HB	1.98	0.45
47:J:492:LEU:O	47:J:497:ARG:NH2	2.49	0.45
48:N:491:LEU:HA	48:N:494:VAL:HG12	1.98	0.45
50:f:58:A:O2'	50:f:60:A:OP2	2.32	0.45
51:4:205:LYS:HG2	51:4:206:PRO:HD2	1.98	0.45
3:d:210:PRO:HD3	3:d:236:PHE:CE2	2.52	0.45
12:m:119:GLU:HA	12:m:122:ILE:HD12	1.98	0.45
16:R:34:ASP:HB3	16:R:82:LYS:HE2	1.98	0.45
18:2:617:G:OP1	35:j:89:GLY:N	2.49	0.45
18:2:1244:U:H2'	18:2:1245:G:H8	1.81	0.45
18:2:1513:C:H5''	31:l:10:HIS:H	1.81	0.45
33:V:220:ASP:OD1	33:V:221:LEU:N	2.50	0.45
35:j:54:LYS:HB3	35:j:91:LEU:HD11	1.98	0.45
39:A:78:CYS:SG	39:A:86:LEU:HB2	2.56	0.45
40:C:495:THR:H	40:C:498:GLU:HG2	1.80	0.45
42:F:282:ALA:O	42:F:285:THR:OG1	2.29	0.45
45:L:424:VAL:HG22	45:L:425:VAL:HG23	1.97	0.45
45:L:464:LEU:HD12	45:L:465:LYS:H	1.82	0.45
47:J:196:THR:O	47:J:198:ALA:N	2.49	0.45
48:N:179:LEU:HD22	48:N:490:ILE:HG13	1.99	0.45
51:4:201:LYS:HE2	51:4:287:PRO:HA	1.98	0.45
15:z:106:GLN:HA	15:z:109:GLU:HG2	1.98	0.45
18:2:697:G:O6	18:2:734:C:N4	2.49	0.45
18:2:1780:G:H2'	18:2:1781:A:H8	1.82	0.45
25:g:139:ALA:O	25:g:140:ARG:NE	2.49	0.45
29:P:50:PHE:HE2	29:P:58:LEU:HD22	1.81	0.45
29:P:51:ASP:OD1	29:P:52:LYS:N	2.49	0.45
33:V:104:HIS:NE2	33:V:122:SER:OG	2.40	0.45
39:A:496:ASP:O	39:A:516:SER:OG	2.35	0.45
39:A:597:ARG:HA	39:A:597:ARG:HD3	1.79	0.45
40:C:690:ALA:O	40:C:694:GLU:HG2	2.16	0.45
41:E:169:LEU:HD23	41:E:195:THR:HG21	1.99	0.45
44:K:171:LYS:O	44:K:175:SER:HB3	2.15	0.45
10:c:64:ASP:OD1	10:c:67:ASP:N	2.49	0.45
12:m:39:LYS:HE2	12:m:39:LYS:HB3	1.80	0.45
24:o:22:LEU:HA	24:o:25:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:212:LYS:HA	33:V:235:ILE:HG23	1.99	0.45
35:j:100:VAL:HG12	35:j:125:VAL:HG23	1.98	0.45
38:B:376:VAL:HA	38:B:392:SER:HA	1.99	0.45
40:C:753:HIS:CD2	40:C:780:VAL:HG22	2.51	0.45
47:J:166:ALA:HA	47:J:237:ILE:HB	1.99	0.45
48:N:285:ASP:HB3	48:N:288:LEU:HD22	1.99	0.45
2:p:47:THR:OG1	2:p:65:ARG:NH1	2.50	0.45
2:p:82:ARG:HH12	2:p:191:ASP:HB2	1.81	0.45
4:Q:95:ARG:O	18:2:1866:A:O2'	2.35	0.45
9:t:57:ALA:HB2	9:t:183:GLY:HA2	1.99	0.45
22:u:20:VAL:HA	22:u:69:TRP:O	2.16	0.45
27:x:39:LEU:HD23	27:x:39:LEU:HA	1.69	0.45
39:A:409:LYS:HE3	39:A:409:LYS:HB2	1.86	0.45
43:H:192:ILE:HG22	43:H:193:THR:H	1.81	0.45
44:K:103:LEU:HD23	44:K:103:LEU:HA	1.73	0.45
45:L:296:ASN:ND2	45:L:323:TYR:OH	2.50	0.45
2:p:42:ARG:NH2	2:p:232:HIS:O	2.30	0.45
3:d:117:ARG:NH1	18:2:1204:A:H5''	2.32	0.45
8:s:9:VAL:HG23	8:s:45:ILE:HG13	1.99	0.45
9:t:56:ARG:HD3	9:t:56:ARG:HA	1.81	0.45
33:V:59:LEU:HD13	33:V:90:TRP:CD1	2.52	0.45
39:A:299:LEU:O	39:A:303:SER:HB3	2.17	0.45
39:A:521:ASN:OD1	39:A:524:THR:OG1	2.31	0.45
40:C:358:VAL:HG22	40:C:374:ILE:HD12	1.98	0.45
41:E:91:ILE:HG21	41:E:131:LEU:HD13	1.99	0.45
41:E:162:ASP:OD1	41:E:163:ARG:N	2.50	0.45
47:J:349:LYS:NZ	47:J:350:TYR:O	2.49	0.45
47:J:425:ARG:HD2	47:J:455:ILE:HG12	1.99	0.45
7:r:159:ARG:HD3	7:r:173:ALA:HB2	1.99	0.45
19:w:37:GLU:OE1	33:V:106:LYS:NZ	2.49	0.45
21:e:22:LYS:HG3	21:e:23:TRP:CD1	2.51	0.45
39:A:180:GLN:HA	39:A:183:LYS:HE3	1.98	0.45
39:A:526:MET:O	39:A:530:LEU:HB2	2.17	0.45
40:C:818:VAL:HA	40:C:821:ILE:HG22	1.99	0.45
48:N:510:LYS:HD2	48:N:510:LYS:HA	1.73	0.45
2:p:83:LYS:NZ	2:p:105:LEU:O	2.49	0.44
18:2:1375:G:H2'	18:2:1376:A:C8	2.51	0.44
20:b:76:ARG:HH21	22:u:66:HIS:CD2	2.35	0.44
26:k:40:TYR:CZ	26:k:97:GLN:HG2	2.52	0.44
39:A:136:ASP:OD1	39:A:136:ASP:N	2.51	0.44
39:A:311:THR:HG23	39:A:315:MET:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:342:LEU:HB3	39:A:344:MET:HG2	1.98	0.44
39:A:526:MET:O	39:A:530:LEU:CB	2.65	0.44
41:E:364:PRO:HA	41:E:367:ALA:HB3	1.99	0.44
44:K:174:MET:HB3	44:K:179:TRP:HB2	1.99	0.44
45:L:336:PHE:HA	45:L:339:ILE:HG22	1.98	0.44
46:M:147:VAL:O	46:M:151:ILE:HG12	2.17	0.44
48:N:369:ILE:HD12	48:N:492:ARG:HH22	1.83	0.44
54:Z:91:LYS:HE2	54:Z:91:LYS:HB2	1.74	0.44
1:a:19:LEU:HD21	19:w:106:LEU:HD11	2.00	0.44
8:s:127:ASP:O	8:s:131:GLU:HG2	2.17	0.44
9:t:10:LYS:NZ	18:2:387:C:OP2	2.50	0.44
10:c:127:ARG:NE	18:2:523:A:OP1	2.45	0.44
18:2:699:C:H2'	18:2:700:G:C8	2.52	0.44
18:2:902:G:H2'	18:2:903:A:C8	2.52	0.44
18:2:1539:U:OP1	27:x:45:LEU:N	2.34	0.44
18:2:1620:A:H2'	24:o:40:ARG:HD3	1.99	0.44
20:b:194:PRO:HA	20:b:201:LYS:HA	1.99	0.44
27:x:129:ARG:HE	27:x:133:ARG:NH2	2.14	0.44
40:C:777:THR:O	40:C:781:ARG:HG3	2.17	0.44
42:F:95:HIS:HE1	42:F:132:THR:HG22	1.82	0.44
42:F:195:PRO:HG2	42:F:197:PRO:HB3	1.99	0.44
42:F:246:ARG:O	42:F:250:ASP:CB	2.65	0.44
44:K:165:LEU:HB3	44:K:169:GLN:HG3	2.00	0.44
47:J:412:LYS:HE3	47:J:488:PRO:HA	1.99	0.44
7:r:185:LEU:HD23	7:r:188:LYS:HE3	1.99	0.44
18:2:189:U:H2'	18:2:190:G:O4'	2.17	0.44
24:o:77:LYS:HA	24:o:95:GLY:O	2.17	0.44
26:k:24:ARG:HB2	26:k:29:ALA:HB2	1.99	0.44
42:F:334:LEU:HA	42:F:337:VAL:HG22	2.00	0.44
47:J:139:ASP:OD1	47:J:140:TRP:N	2.44	0.44
51:4:215:LYS:H	51:4:261:ARG:CZ	2.30	0.44
52:O:108:TYR:CZ	52:O:112:ARG:HD2	2.53	0.44
7:r:45:TRP:HA	7:r:48:TYR:HD2	1.83	0.44
36:G:39:ILE:O	36:G:73:THR:OG1	2.36	0.44
39:A:311:THR:HG21	39:A:314:GLU:HB2	2.00	0.44
40:C:694:GLU:HG3	40:C:714:PHE:CE2	2.53	0.44
40:C:874:PHE:HB2	42:F:354:LEU:HD23	2.00	0.44
43:H:120:TYR:HB3	43:H:150:LEU:HB2	2.00	0.44
43:H:193:THR:HG23	43:H:195:GLU:H	1.81	0.44
44:K:96:GLU:HB3	44:K:99:ILE:HG12	1.99	0.44
47:J:454:ILE:HB	47:J:462:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N:168:TRP:HE3	48:N:520:TYR:HB3	1.82	0.44
2:p:209:ASP:OD1	2:p:209:ASP:N	2.47	0.44
7:r:64:LYS:HG2	7:r:65:GLN:H	1.82	0.44
7:r:142:ARG:HG2	7:r:147:LEU:HD22	2.00	0.44
18:2:1115:U:O2	18:2:1118:C:N4	2.50	0.44
18:2:1599:U:OP1	29:P:80:ARG:NH1	2.50	0.44
18:2:1629:C:H2'	18:2:1630:A:O4'	2.18	0.44
22:u:26:ASP:OD2	22:u:28:HIS:N	2.50	0.44
33:V:24:THR:HG21	33:V:27:PHE:HD2	1.81	0.44
33:V:31:ILE:HD11	33:V:45:LEU:HD22	2.00	0.44
42:F:161:LYS:HB2	42:F:161:LYS:HE3	1.87	0.44
46:M:138:GLN:HB2	46:M:177:LYS:HE3	2.00	0.44
53:Y:195:VAL:O	53:Y:198:SER:N	2.31	0.44
6:W:9:ARG:NH2	18:2:1707:U:H5'	2.33	0.44
10:c:2:PRO:HG2	18:2:95:G:OP1	2.18	0.44
18:2:1673:U:O2'	21:e:84:GLY:O	2.22	0.44
25:g:130:LYS:NZ	25:g:134:GLY:O	2.36	0.44
26:k:6:PRO:HG2	26:k:58:GLU:HG2	1.99	0.44
27:x:9:VAL:HG21	27:x:139:ALA:HB2	1.98	0.44
33:V:110:SER:HB2	33:V:153:CYS:HA	1.98	0.44
39:A:550:HIS:CD2	43:H:216:TRP:HB3	2.52	0.44
40:C:868:GLU:OE1	40:C:872:ARG:NH1	2.50	0.44
41:E:16:ARG:HD3	41:E:44:LEU:HD13	1.99	0.44
43:H:133:LEU:HD11	43:H:149:VAL:HG21	1.99	0.44
45:L:237:LYS:O	45:L:240:ILE:HG22	2.16	0.44
46:M:290:LYS:HA	46:M:334:VAL:HG22	1.99	0.44
47:J:112:ASN:HD21	47:J:492:LEU:HA	1.82	0.44
47:J:168:ILE:HG22	47:J:239:MET:HB2	1.99	0.44
48:N:195:CYS:HA	48:N:358:TYR:O	2.18	0.44
9:t:80:ASP:OD1	9:t:81:VAL:N	2.50	0.44
32:U:135:HIS:HE1	32:U:140:TYR:HB3	1.82	0.44
40:C:753:HIS:O	40:C:757:ILE:HG22	2.18	0.44
45:L:310:GLU:HA	45:L:313:VAL:HG22	1.99	0.44
45:L:323:TYR:HA	45:L:326:MET:HB2	1.99	0.44
46:M:214:ASP:O	46:M:272:GLN:NE2	2.51	0.44
18:2:60:A:N3	18:2:316:G:O2'	2.46	0.44
18:2:702:G:H2'	18:2:703:C:C6	2.53	0.44
18:2:1496:U:H5'	31:l:26:ASN:OD1	2.18	0.44
26:k:62:ASP:N	26:k:62:ASP:OD1	2.50	0.44
40:C:757:ILE:O	40:C:762:ASN:ND2	2.45	0.44
43:H:172:LYS:HD2	43:H:192:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Y:403:VAL:HA	53:Y:415:GLY:H	1.83	0.44
2:p:166:LYS:HB3	2:p:166:LYS:HE2	1.66	0.44
8:s:43:LEU:HD13	8:s:72:PHE:HA	1.99	0.44
18:2:722:C:H1'	18:2:724:A:H62	1.81	0.44
18:2:1179:G:OP1	40:C:55:LYS:NZ	2.42	0.44
18:2:1273:C:N4	18:2:1508:A:N6	2.45	0.44
27:x:107:LEU:HD23	27:x:110:LEU:HD21	2.00	0.44
47:J:174:ASP:HB2	47:J:415:LYS:HD3	1.99	0.44
50:f:55:U:H4'	52:O:181:ARG:HD2	2.00	0.44
51:4:272:ARG:HE	51:4:275:ILE:HD11	1.83	0.44
8:s:76:GLN:HE21	8:s:94:PHE:HD2	1.66	0.43
26:k:43:VAL:HA	26:k:46:ARG:HE	1.83	0.43
35:j:111:ALA:HB2	35:j:119:ARG:HG3	2.00	0.43
40:C:814:ASP:HB2	40:C:816:PRO:HD2	2.00	0.43
41:E:404:VAL:HG11	42:F:336:MET:HE3	1.99	0.43
42:F:214:LYS:HD2	42:F:216:TYR:OH	2.18	0.43
43:H:241:LYS:O	43:H:245:LEU:HG	2.18	0.43
45:L:474:LYS:HA	45:L:474:LYS:HD2	1.73	0.43
48:N:28:MET:SD	48:N:69:TYR:OH	2.76	0.43
11:n:35:ARG:NH1	11:n:55:TYR:O	2.51	0.43
14:D:32:LYS:NZ	18:2:687:C:OP2	2.36	0.43
18:2:1557:C:H1'	18:2:1661:A:H5'	2.00	0.43
33:V:207:CYS:O	33:V:218:LEU:HA	2.18	0.43
40:C:320:LYS:HG2	40:C:360:ILE:HD11	2.00	0.43
45:L:379:PRO:HB2	45:L:381:ARG:H	1.83	0.43
48:N:245:VAL:HA	48:N:276:LEU:HB3	1.99	0.43
50:f:55:U:O3'	52:O:181:ARG:NH1	2.51	0.43
9:t:130:THR:OG1	9:t:132:GLU:OE1	2.30	0.43
18:2:747:U:C2	18:2:796:G:O6	2.71	0.43
18:2:848:U:H2'	18:2:849:A:C8	2.54	0.43
18:2:1292:C:O2	32:U:138:ARG:NH1	2.50	0.43
18:2:1566:G:O6	27:x:101:ARG:NH1	2.51	0.43
19:w:11:LYS:HB2	19:w:11:LYS:HE3	1.84	0.43
20:b:137:VAL:HA	20:b:150:MET:O	2.18	0.43
38:B:521:LYS:H	38:B:521:LYS:HD2	1.83	0.43
38:B:638:VAL:HA	38:B:644:THR:O	2.18	0.43
40:C:100:GLU:N	40:C:100:GLU:OE1	2.52	0.43
40:C:762:ASN:HB3	40:C:776:ARG:HH21	1.83	0.43
46:M:156:LEU:HD23	46:M:160:LYS:HD3	2.00	0.43
46:M:159:GLU:HA	46:M:162:HIS:ND1	2.34	0.43
47:J:213:ASN:HB2	47:J:216:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N:227:VAL:HG11	48:N:343:PHE:CE2	2.54	0.43
48:N:507:LEU:HB2	48:N:522:LEU:HD21	2.00	0.43
51:4:272:ARG:HA	51:4:275:ILE:HG12	1.99	0.43
52:O:12:PHE:HD2	52:O:77:LYS:HE2	1.84	0.43
1:a:57:LYS:HA	1:a:57:LYS:HD2	1.72	0.43
3:d:187:ARG:HE	3:d:192:LEU:HD12	1.82	0.43
18:2:1275:G:H4'	18:2:1322:G:H22	1.83	0.43
26:k:111:LEU:HD11	26:k:125:HIS:CG	2.54	0.43
37:I:149:ILE:HA	37:I:165:HIS:HA	2.00	0.43
39:A:298:ARG:HD3	39:A:298:ARG:HA	1.71	0.43
40:C:586:ARG:HA	40:C:589:MET:HE2	2.01	0.43
44:K:83:THR:HA	44:K:86:LYS:HE3	2.01	0.43
54:Z:34:ARG:HG2	54:Z:111:HIS:HB2	2.01	0.43
3:d:251:LEU:HD13	13:y:23:ILE:HD11	2.01	0.43
5:q:127:ARG:HH21	5:q:142:HIS:HB2	1.83	0.43
9:t:44:HIS:O	9:t:56:ARG:HB3	2.19	0.43
13:y:64:GLU:OE1	13:y:64:GLU:N	2.51	0.43
18:2:1511:U:H2'	18:2:1512:C:C6	2.53	0.43
20:b:76:ARG:HH21	22:u:66:HIS:CE1	2.35	0.43
40:C:514:PHE:CG	40:C:770:PRO:HB3	2.53	0.43
46:M:237:ILE:H	46:M:237:ILE:HD12	1.83	0.43
48:N:436:THR:HG23	48:N:482:LEU:HD13	1.99	0.43
4:Q:98:PRO:O	18:2:1868:U:N3	2.48	0.43
10:c:29:LEU:HD23	17:T:42:PHE:HE2	1.83	0.43
18:2:1575:G:H2'	18:2:1576:G:C8	2.52	0.43
25:g:57:LEU:HD11	25:g:115:TYR:CD2	2.54	0.43
33:V:251:ALA:HB2	33:V:289:LEU:HG	2.01	0.43
36:G:41:MET:HE3	36:G:41:MET:HB3	1.79	0.43
40:C:497:GLU:OE2	40:C:561:THR:OG1	2.31	0.43
40:C:672:PRO:HD2	40:C:675:LEU:HD12	1.99	0.43
41:E:232:ILE:O	41:E:236:PHE:HB2	2.18	0.43
45:L:541:ASP:OD1	45:L:542:PHE:N	2.52	0.43
47:J:206:LEU:O	47:J:207:THR:HG22	2.17	0.43
9:t:2:GLY:N	18:2:1798:C:HO2'	2.17	0.43
18:2:692:G:H2'	18:2:693:A:C8	2.54	0.43
18:2:1588:A:H2'	18:2:1589:A:C8	2.53	0.43
23:v:41:ALA:O	23:v:112:LYS:NZ	2.51	0.43
29:P:91:LEU:HD22	29:P:96:LEU:HD12	2.01	0.43
33:V:230:LEU:HD21	33:V:259:TRP:CD2	2.54	0.43
35:j:25:LYS:HE3	35:j:25:LYS:HB3	1.78	0.43
39:A:26:PRO:HA	39:A:29:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:129:LEU:HA	39:A:132:VAL:HG12	2.00	0.43
39:A:310:LEU:HD23	39:A:311:THR:HG22	2.00	0.43
39:A:397:GLU:OE1	39:A:399:ASN:HB2	2.19	0.43
40:C:120:LEU:HD23	40:C:120:LEU:HA	1.84	0.43
40:C:347:ARG:HH12	40:C:387:PRO:HD3	1.84	0.43
41:E:270:ARG:HD2	41:E:339:PHE:CE2	2.54	0.43
43:H:170:THR:HG23	43:H:173:LEU:H	1.83	0.43
46:M:172:LEU:HD12	46:M:184:VAL:HG21	2.00	0.43
47:J:223:GLN:HB3	47:J:247:LEU:HD21	1.99	0.43
47:J:239:MET:HG2	47:J:270:ILE:HG12	2.00	0.43
50:f:33:C:N4	50:f:36:U:OP2	2.46	0.43
9:t:81:VAL:HG12	9:t:102:VAL:HG12	1.99	0.43
10:c:139:LYS:HE2	38:B:553:GLN:HE22	1.82	0.43
13:y:68:SER:O	13:y:72:LEU:HG	2.19	0.43
23:v:79:VAL:HG11	23:v:85:LEU:HB2	2.01	0.43
24:o:21:ASP:H	24:o:24:GLN:NE2	2.17	0.43
38:B:549:MET:HA	38:B:554:VAL:HG22	2.00	0.43
39:A:84:LYS:HD3	39:A:84:LYS:HA	1.77	0.43
41:E:36:GLU:HB3	48:N:4:PHE:HB3	2.01	0.43
51:4:231:ARG:HE	51:4:279:VAL:HG21	1.84	0.43
53:Y:44:ILE:HA	53:Y:154:ALA:HB3	2.00	0.43
2:p:227:LYS:O	2:p:230:GLU:HG2	2.19	0.43
7:r:147:LEU:HD23	7:r:151:ASP:HB2	2.00	0.43
10:c:39:ASN:OD1	10:c:42:GLU:HG3	2.19	0.43
18:2:15:U:H2'	18:2:16:G:O4'	2.19	0.43
18:2:1220:A:P	21:e:127:ARG:HH21	2.42	0.43
18:2:1309:C:H2'	18:2:1310:U:O4'	2.19	0.43
23:v:23:LYS:HD2	23:v:23:LYS:HA	1.79	0.43
45:L:449:ASP:OD1	45:L:450:GLU:N	2.51	0.43
46:M:117:THR:OG1	46:M:120:ARG:N	2.47	0.43
47:J:95:HIS:HB2	47:J:298:VAL:HG22	1.99	0.43
47:J:436:TYR:CE2	47:J:438:HIS:HB3	2.54	0.43
47:J:536:ASP:OD2	47:J:546:ASN:ND2	2.38	0.43
48:N:176:PHE:CE2	48:N:259:THR:HA	2.54	0.43
48:N:252:LEU:HA	48:N:255:LEU:HD12	2.01	0.43
18:2:115:U:O2'	18:2:381:C:O2	2.30	0.43
18:2:1244:U:H2'	18:2:1245:G:C8	2.54	0.43
18:2:1424:G:H3'	18:2:1425:G:C8	2.54	0.43
18:2:1524:G:O2'	50:f:30:G:OP1	2.36	0.43
18:2:1620:A:O2'	18:2:1624:U:OP2	2.32	0.43
18:2:1669:G:H5''	25:g:130:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:1683:C:H2'	18:2:1684:C:C6	2.54	0.43
18:2:1713:C:H2'	18:2:1714:U:C6	2.54	0.43
21:e:16:ASP:N	21:e:16:ASP:OD1	2.51	0.43
33:V:107:ASP:HB2	33:V:125:ARG:HH11	1.83	0.43
38:B:327:VAL:HA	38:B:328:SER:HA	1.63	0.43
40:C:810:MET:HG3	40:C:811:PHE:CD1	2.54	0.43
42:F:102:ILE:HD13	42:F:202:VAL:HG21	2.01	0.43
44:K:52:LYS:HD2	44:K:55:GLN:HE21	1.84	0.43
44:K:145:VAL:HA	44:K:148:ILE:HG22	2.00	0.43
44:K:176:LYS:HD2	44:K:177:TYR:CZ	2.54	0.43
54:Z:97:LEU:HD22	54:Z:102:LEU:HD22	2.01	0.43
9:t:118:ALA:HB3	9:t:153:LYS:HE3	2.00	0.42
20:b:146:ARG:HD2	20:b:146:ARG:HA	1.85	0.42
23:v:43:ASP:O	23:v:45:ARG:NH1	2.52	0.42
24:o:21:ASP:OD1	24:o:22:LEU:N	2.51	0.42
27:x:21:PHE:HE1	27:x:112:MET:HE1	1.82	0.42
39:A:572:ARG:NH2	43:H:111:ASN:OD1	2.51	0.42
41:E:351:ILE:HG13	41:E:393:MET:HE2	2.01	0.42
44:K:36:GLN:HB3	44:K:72:LYS:HE3	2.01	0.42
46:M:13:ASP:OD1	46:M:13:ASP:N	2.52	0.42
47:J:383:THR:HG22	47:J:385:LYS:HZ2	1.84	0.42
47:J:507:PHE:HB3	47:J:508:ILE:HG13	2.00	0.42
18:2:705:G:H2'	18:2:706:U:C6	2.55	0.42
18:2:1261:C:O2	31:l:10:HIS:NE2	2.47	0.42
18:2:1320:G:H2'	18:2:1321:G:O4'	2.19	0.42
20:b:20:GLU:OE2	20:b:76:ARG:NH2	2.52	0.42
29:P:66:LYS:HE3	29:P:66:LYS:HB3	1.87	0.42
39:A:7:ARG:HH12	39:A:44:GLN:HE22	1.67	0.42
39:A:311:THR:OG1	39:A:312:GLN:N	2.52	0.42
41:E:92:VAL:HA	41:E:95:PHE:HB2	2.02	0.42
42:F:103:VAL:HG13	43:H:210:LEU:HD23	2.00	0.42
43:H:276:GLN:O	43:H:280:ARG:HG2	2.19	0.42
44:K:133:GLY:O	44:K:137:SER:CB	2.66	0.42
47:J:9:ALA:HA	47:J:71:SER:O	2.19	0.42
47:J:112:ASN:HD22	47:J:496:GLN:NE2	2.17	0.42
48:N:477:ALA:HB1	48:N:482:LEU:HD22	2.01	0.42
51:4:271:LEU:HD23	51:4:271:LEU:HA	1.86	0.42
5:q:225:ILE:HA	5:q:225:ILE:HD13	1.84	0.42
16:R:24:LEU:HD12	16:R:24:LEU:HA	1.86	0.42
18:2:573:U:H2'	18:2:574:A:H5''	2.01	0.42
18:2:1395:C:H1'	18:2:1474:A:C4	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:v:31:LEU:HG	23:v:33:ARG:H	1.85	0.42
26:k:34:LYS:HE2	26:k:103:LEU:HD22	2.01	0.42
33:V:259:TRP:CZ3	33:V:266:ILE:HG13	2.54	0.42
40:C:332:LYS:HA	40:C:332:LYS:HD2	1.82	0.42
40:C:862:LYS:HD2	43:H:247:MET:HG2	2.02	0.42
46:M:252:TYR:CE2	46:M:274:MET:HG2	2.54	0.42
48:N:265:TRP:CE2	48:N:510:LYS:HB2	2.53	0.42
5:q:23:LEU:HD21	10:c:6:SER:HB3	2.01	0.42
5:q:126:VAL:HG13	5:q:139:LEU:HG	2.02	0.42
9:t:135:GLU:O	9:t:139:LYS:HB2	2.19	0.42
18:2:184:G:H2'	18:2:185:G:H8	1.84	0.42
19:w:60:ARG:HE	19:w:66:VAL:HG22	1.85	0.42
33:V:46:THR:HG23	33:V:53:GLY:HA2	2.01	0.42
38:B:341:ARG:H	38:B:350:ALA:HB3	1.85	0.42
40:C:835:LEU:HB3	40:C:842:VAL:HG22	2.00	0.42
41:E:131:LEU:HA	41:E:131:LEU:HD12	1.74	0.42
47:J:485:ILE:HG22	47:J:488:PRO:HB3	1.99	0.42
48:N:178:GLN:O	48:N:182:MET:HG3	2.20	0.42
54:Z:89:GLN:HB2	54:Z:92:ASN:HB2	2.01	0.42
8:s:58:LYS:HE3	8:s:58:LYS:HB3	1.75	0.42
18:2:902:G:H2'	18:2:903:A:H8	1.85	0.42
18:2:1280:G:H2'	18:2:1281:G:H8	1.83	0.42
18:2:1479:G:H5''	25:g:138:ARG:HH21	1.84	0.42
35:j:49:GLY:O	35:j:99:GLU:HA	2.20	0.42
40:C:576:HIS:ND1	40:C:581:ARG:HD2	2.35	0.42
40:C:598:ILE:O	40:C:606:GLN:NE2	2.31	0.42
40:C:694:GLU:HG3	40:C:714:PHE:CD2	2.53	0.42
41:E:212:THR:HG22	41:E:245:ALA:HB1	2.02	0.42
42:F:146:VAL:HG21	42:F:182:HIS:CG	2.54	0.42
42:F:260:ASN:O	42:F:262:VAL:HG23	2.20	0.42
44:K:70:LEU:HD22	44:K:103:LEU:HD21	2.01	0.42
44:K:197:LYS:HE2	44:K:197:LYS:HB3	1.83	0.42
47:J:223:GLN:NE2	47:J:245:SER:O	2.31	0.42
47:J:313:LEU:HA	47:J:313:LEU:HD23	1.80	0.42
47:J:351:PRO:HG2	47:J:402:GLY:N	2.35	0.42
47:J:526:THR:HG21	47:J:595:PHE:HE2	1.83	0.42
4:Q:22:ARG:NH1	4:Q:29:CYS:SG	2.93	0.42
9:t:84:ASN:ND2	9:t:90:LEU:HD12	2.35	0.42
14:D:112:ASP:OD1	14:D:112:ASP:N	2.44	0.42
18:2:1734:G:O2'	18:2:1800:A:N6	2.49	0.42
20:b:175:VAL:N	20:b:182:LEU:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:o:108:LYS:H	24:o:111:MET:CE	2.33	0.42
26:k:34:LYS:HB3	26:k:100:ALA:HA	2.01	0.42
33:V:40:ILE:HD11	33:V:66:VAL:HG11	2.02	0.42
33:V:164:ILE:HB	33:V:177:TRP:O	2.19	0.42
39:A:286:SER:HA	40:C:728:GLY:HA2	2.02	0.42
39:A:383:VAL:HB	39:A:388:LYS:HD2	2.02	0.42
39:A:442:GLN:HE21	39:A:509:PRO:HG2	1.84	0.42
42:F:283:LEU:HA	42:F:286:VAL:HB	2.02	0.42
44:K:90:ASP:HB3	45:L:442:GLN:HG2	2.01	0.42
44:K:167:ASP:HA	44:K:170:LEU:HD12	2.02	0.42
45:L:364:ASN:HA	45:L:367:MET:HG2	2.02	0.42
46:M:263:ILE:O	46:M:268:LEU:HB2	2.19	0.42
47:J:183:THR:HA	47:J:213:ASN:HA	2.01	0.42
2:p:172:MET:HG3	2:p:197:ILE:HD11	2.02	0.42
7:r:148:SER:OG	7:r:149:LYS:N	2.51	0.42
18:2:595:U:H2'	18:2:596:U:C6	2.55	0.42
18:2:1215:C:O2'	18:2:1645:C:OP2	2.27	0.42
18:2:1755:C:H5'	18:2:1756:C:H5''	2.02	0.42
32:U:100:LEU:HA	32:U:100:LEU:HD23	1.82	0.42
33:V:17:TRP:HB2	33:V:36:ARG:HG3	2.01	0.42
40:C:873:VAL:HG13	43:H:264:MET:HE1	2.01	0.42
41:E:25:PHE:HA	41:E:28:VAL:HG12	2.01	0.42
42:F:251:LEU:HD12	42:F:251:LEU:HA	1.77	0.42
50:f:72:U:O4	50:f:73:A:N6	2.52	0.42
15:z:55:ILE:HD13	15:z:55:ILE:HG21	1.86	0.42
18:2:1033:G:H1	18:2:1080:A:HO2'	1.62	0.42
21:e:153:LEU:HD23	21:e:153:LEU:HA	1.90	0.42
33:V:155:ARG:HA	33:V:155:ARG:HD3	1.79	0.42
34:i:93:LEU:HD23	34:i:93:LEU:HA	1.85	0.42
36:G:81:LEU:HD23	36:G:81:LEU:HA	1.83	0.42
39:A:44:GLN:HE21	39:A:44:GLN:HB3	1.65	0.42
39:A:55:LEU:HD12	39:A:93:TYR:CD1	2.55	0.42
40:C:581:ARG:HB2	40:C:584:GLN:OE1	2.20	0.42
40:C:648:GLN:NE2	40:C:677:ILE:H	2.13	0.42
44:K:58:PRO:HB3	44:K:93:HIS:NE2	2.34	0.42
45:L:445:LYS:HD2	45:L:445:LYS:HA	1.79	0.42
46:M:250:ALA:HA	46:M:253:VAL:HG12	2.01	0.42
47:J:349:LYS:HD2	47:J:349:LYS:HA	1.90	0.42
48:N:439:ALA:HB2	48:N:447:LEU:HD13	2.02	0.42
1:a:209:GLU:HA	1:a:212:LYS:HB3	2.01	0.42
3:d:198:ALA:HB1	3:d:202:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:168:LYS:HE2	18:2:74:G:O6	2.20	0.42
18:2:1118:C:H6	18:2:1118:C:H2'	1.71	0.42
18:2:1727:G:H22	18:2:1808:U:H1'	1.85	0.42
39:A:551:GLN:O	39:A:555:THR:OG1	2.31	0.42
41:E:132:TYR:O	41:E:132:TYR:CD1	2.70	0.42
42:F:221:MET:O	46:M:62:SER:OG	2.35	0.42
44:K:66:THR:HA	44:K:69:ILE:HG22	2.01	0.42
45:L:367:MET:HE1	45:L:419:LYS:HB3	2.01	0.42
48:N:184:TYR:CG	48:N:492:ARG:HG3	2.55	0.42
48:N:232:ASP:O	48:N:235:ILE:HG22	2.20	0.42
48:N:361:ARG:O	48:N:372:ILE:HA	2.19	0.42
53:Y:296:VAL:O	53:Y:313:PRO:HA	2.20	0.42
4:Q:32:LYS:NZ	18:2:987:A:OP1	2.53	0.42
6:W:13:LEU:HD11	6:W:17:ARG:HH21	1.85	0.42
12:m:16:LEU:O	14:D:57:ARG:NH2	2.45	0.42
18:2:1134:G:H2'	18:2:1135:C:C6	2.55	0.42
21:e:97:PHE:HZ	21:e:112:LEU:HD22	1.85	0.42
22:u:47:LYS:HA	22:u:47:LYS:HD3	1.89	0.42
25:g:131:LYS:HB2	25:g:140:ARG:HH22	1.84	0.42
33:V:241:PHE:HA	33:V:248:LEU:HD23	2.02	0.42
35:j:35:ALA:O	35:j:39:ASN:HB2	2.19	0.42
38:B:612:ASN:N	38:B:626:ALA:O	2.47	0.42
39:A:198:CYS:HB3	39:A:202:ARG:HH22	1.85	0.42
40:C:493:LYS:HE2	40:C:493:LYS:HB2	1.90	0.42
43:H:315:ASP:N	43:H:315:ASP:OD1	2.49	0.42
45:L:376:THR:HA	45:L:377:MET:HA	1.71	0.42
45:L:401:MET:HA	45:L:408:VAL:HG11	2.02	0.42
46:M:248:LYS:HE3	46:M:248:LYS:HB2	1.76	0.42
48:N:323:PHE:HE2	48:N:465:ILE:HG12	1.84	0.42
7:r:46:LYS:HA	7:r:46:LYS:HD2	1.85	0.41
11:n:118:ARG:HG3	11:n:119:ASP:OD1	2.20	0.41
15:z:10:ARG:HB3	15:z:11:LYS:H	1.67	0.41
16:R:48:SER:HG	16:R:49:HIS:CE1	2.36	0.41
18:2:1527:C:H5''	25:g:142:GLN:HG2	2.02	0.41
28:h:26:SER:OG	28:h:28:ASN:O	2.36	0.41
40:C:602:ASP:OD1	48:N:73:HIS:ND1	2.53	0.41
40:C:828:ASN:HB3	40:C:830:GLU:HG2	2.02	0.41
47:J:390:ARG:HE	47:J:396:LEU:HD22	1.85	0.41
7:r:42:GLY:HA3	7:r:45:TRP:HD1	1.85	0.41
18:2:537:C:H2'	18:2:539:C:N4	2.34	0.41
18:2:1424:G:H3'	18:2:1425:G:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:1653:U:H2'	18:2:1654:G:C8	2.56	0.41
19:w:57:LEU:HD23	19:w:57:LEU:HA	1.84	0.41
22:u:32:HIS:CD2	22:u:45:VAL:HG21	2.55	0.41
23:v:63:LYS:HD3	23:v:63:LYS:HA	1.82	0.41
27:x:56:ARG:O	27:x:59:SER:OG	2.36	0.41
32:U:141:CYS:SG	32:U:145:CYS:N	2.93	0.41
35:j:58:GLU:HG2	36:G:60:HIS:CD2	2.55	0.41
39:A:331:ILE:HB	39:A:437:LEU:HD23	2.02	0.41
45:L:316:TYR:HD1	45:L:335:VAL:HG22	1.84	0.41
45:L:499:ASN:HD22	45:L:499:ASN:C	2.27	0.41
46:M:62:SER:HA	46:M:65:ASN:HB2	2.02	0.41
47:J:52:GLU:HG3	47:J:53:THR:HG23	2.01	0.41
47:J:493:ASP:OD1	47:J:496:GLN:HG2	2.20	0.41
57:J:603:ADP:H8	57:J:603:ADP:H2'	1.50	0.41
52:O:25:SER:N	52:O:32:TYR:O	2.43	0.41
2:p:28:LYS:HD3	2:p:28:LYS:HA	1.86	0.41
2:p:46:LYS:HB3	2:p:46:LYS:HE3	1.88	0.41
2:p:139:CYS:SG	2:p:140:VAL:N	2.92	0.41
18:2:74:G:H2'	18:2:75:G:C8	2.55	0.41
18:2:1234:C:H41	26:k:137:LYS:HD2	1.84	0.41
18:2:1616:U:H2'	18:2:1617:G:O4'	2.20	0.41
19:w:10:LYS:HB3	19:w:10:LYS:HE2	1.77	0.41
20:b:193:ASP:OD1	20:b:195:THR:OG1	2.30	0.41
28:h:35:VAL:HG13	28:h:105:SER:HB3	2.01	0.41
32:U:121:CYS:HA	32:U:122:PRO:HD3	1.91	0.41
33:V:292:SER:HB3	33:V:297:THR:HB	2.02	0.41
36:G:56:LYS:HE2	36:G:56:LYS:HB2	1.85	0.41
40:C:445:LEU:HD13	40:C:502:ILE:HB	2.02	0.41
40:C:827:ILE:HD12	41:E:343:THR:HG23	2.02	0.41
41:E:91:ILE:HG12	41:E:127:TYR:CD1	2.55	0.41
47:J:397:LYS:HE3	47:J:402:GLY:HA3	2.03	0.41
48:N:266:ASP:HA	48:N:508:ILE:O	2.20	0.41
14:D:14:ILE:HG13	14:D:27:ILE:HD11	2.01	0.41
18:2:1541:G:H21	27:x:12:GLN:HE22	1.68	0.41
19:w:32:LYS:HE3	19:w:33:ARG:NH1	2.35	0.41
21:e:195:GLU:O	21:e:198:ARG:HG2	2.20	0.41
25:g:37:ARG:HG3	27:x:7:LYS:O	2.20	0.41
27:x:64:LEU:HD23	27:x:64:LEU:HA	1.79	0.41
39:A:288:ASN:ND2	39:A:355:LEU:HD13	2.35	0.41
39:A:446:ILE:HB	39:A:511:LEU:HD23	2.01	0.41
39:A:582:LEU:HA	39:A:585:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:C:392:TYR:HB2	40:C:458:ILE:HG12	2.02	0.41
42:F:91:VAL:O	42:F:128:SER:HA	2.19	0.41
47:J:184:VAL:O	47:J:188:LEU:CB	2.69	0.41
51:4:231:ARG:HH11	51:4:231:ARG:HD2	1.70	0.41
2:p:123:ALA:HB2	2:p:165:ARG:HG3	2.02	0.41
3:d:156:ILE:HD13	3:d:156:ILE:HA	1.90	0.41
8:s:60:ILE:HB	8:s:92:VAL:HG12	2.02	0.41
12:m:37:ILE:HD11	12:m:63:VAL:HG11	2.03	0.41
14:D:75:ILE:HD13	14:D:75:ILE:HA	1.87	0.41
20:b:6:SER:O	20:b:10:LYS:HB2	2.21	0.41
24:o:34:MET:HB2	24:o:42:ARG:HA	2.02	0.41
27:x:107:LEU:HD22	27:x:112:MET:HB2	2.02	0.41
28:h:95:SER:O	28:h:99:LYS:HG2	2.21	0.41
32:U:135:HIS:CE1	32:U:140:TYR:HB3	2.55	0.41
33:V:114:SER:HA	33:V:156:PHE:CD2	2.53	0.41
40:C:370:VAL:HB	40:C:431:LEU:HD12	2.02	0.41
40:C:490:LEU:HD13	40:C:490:LEU:HA	1.95	0.41
44:K:88:MET:HA	45:L:291:ILE:HD13	2.01	0.41
45:L:191:ILE:O	45:L:195:GLN:HB2	2.20	0.41
46:M:239:ASP:OD1	46:M:240:LEU:N	2.52	0.41
48:N:267:ILE:HD11	48:N:278:PHE:HB3	2.02	0.41
52:O:228:LEU:HA	52:O:234:TYR:HA	2.02	0.41
3:d:192:LEU:HD21	18:2:1154:U:H2'	2.02	0.41
5:q:19:MET:HE2	5:q:108:ARG:HD2	2.02	0.41
5:q:108:ARG:NH2	18:2:846:G:OP2	2.53	0.41
18:2:659:G:H21	35:j:17:ARG:HH12	1.69	0.41
21:e:37:ASP:OD1	21:e:37:ASP:N	2.53	0.41
33:V:31:ILE:HB	33:V:43:TRP:CD1	2.55	0.41
33:V:157:SER:HB2	33:V:204:GLY:HA2	2.03	0.41
38:B:472:TRP:CE2	38:B:479:ILE:HD13	2.55	0.41
39:A:335:ARG:HH21	39:A:337:ASP:HB3	1.84	0.41
39:A:515:PRO:O	39:A:519:ILE:HG12	2.21	0.41
41:E:73:LYS:HD3	41:E:76:THR:HB	2.01	0.41
42:F:142:SER:OG	42:F:143:GLU:N	2.52	0.41
42:F:220:LEU:HB3	42:F:230:VAL:HG13	2.01	0.41
43:H:68:LEU:O	43:H:79:THR:N	2.40	0.41
46:M:243:ILE:HG23	46:M:247:ALA:HB3	2.03	0.41
48:N:245:VAL:HG21	48:N:495:ILE:HD11	2.01	0.41
48:N:455:TYR:O	48:N:456:HIS:ND1	2.51	0.41
14:D:61:ILE:HD13	14:D:61:ILE:HG21	1.86	0.41
19:w:21:TYR:CE2	19:w:76:GLU:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:o:92:SER:O	24:o:107:ILE:HG13	2.21	0.41
40:C:492:GLU:C	40:C:493:LYS:HD3	2.46	0.41
40:C:696:PRO:HG2	40:C:786:GLU:OE1	2.20	0.41
44:K:83:THR:HA	44:K:86:LYS:HG2	2.03	0.41
45:L:343:ILE:HD12	45:L:535:VAL:HG21	2.02	0.41
45:L:373:ILE:HG21	45:L:412:LEU:HD13	2.03	0.41
47:J:498:LEU:HB3	47:J:502:ARG:HH12	1.86	0.41
48:N:409:TRP:NE1	48:N:420:VAL:HG13	2.36	0.41
1:a:76:VAL:HG23	1:a:98:PRO:HA	2.02	0.41
3:d:117:ARG:HH11	3:d:117:ARG:HG3	1.83	0.41
5:q:127:ARG:HE	5:q:142:HIS:HA	1.85	0.41
5:q:151:ASP:HA	5:q:152:PRO:HD3	1.91	0.41
9:t:84:ASN:HD21	9:t:90:LEU:HD12	1.86	0.41
10:c:101:LYS:HE2	10:c:101:LYS:HB2	1.82	0.41
39:A:73:GLN:O	39:A:77:ILE:HG12	2.21	0.41
39:A:179:GLN:O	39:A:183:LYS:HG3	2.21	0.41
39:A:264:LYS:HB2	39:A:264:LYS:HE3	1.85	0.41
40:C:358:VAL:HA	40:C:374:ILE:HD12	2.02	0.41
41:E:73:LYS:HD3	41:E:73:LYS:HA	1.82	0.41
42:F:297:LYS:HA	42:F:297:LYS:HD3	1.85	0.41
43:H:85:PRO:HD3	43:H:99:TYR:CE1	2.56	0.41
47:J:384:GLY:O	47:J:387:THR:OG1	2.31	0.41
48:N:211:THR:OG1	48:N:212:ARG:N	2.54	0.41
48:N:431:LYS:HE2	48:N:431:LYS:HB2	1.81	0.41
2:p:39:PHE:HB3	2:p:74:LEU:HB3	2.03	0.41
8:s:101:LEU:HD23	8:s:101:LEU:HA	1.84	0.41
8:s:114:GLN:HE22	18:2:875:A:H1'	1.85	0.41
12:m:124:ARG:HH21	18:2:677:G:P	2.43	0.41
18:2:903:A:H2'	18:2:904:A:C8	2.56	0.41
18:2:1405:A:H2'	18:2:1406:G:O4'	2.21	0.41
18:2:1461:G:C6	18:2:1463:U:H1'	2.55	0.41
18:2:1551:U:P	20:b:9:ARG:HH22	2.43	0.41
18:2:1609:C:H2'	18:2:1610:G:C8	2.56	0.41
18:2:1778:C:H2'	18:2:1779:G:C8	2.56	0.41
22:u:11:ILE:HD13	22:u:11:ILE:HA	1.88	0.41
32:U:96:LYS:HD2	32:U:96:LYS:HA	1.84	0.41
33:V:200:VAL:HA	33:V:206:LEU:O	2.21	0.41
38:B:499:PRO:O	38:B:501:ARG:NE	2.54	0.41
39:A:7:ARG:HD2	39:A:7:ARG:HA	1.85	0.41
39:A:98:GLU:OE1	39:A:157:TYR:OH	2.39	0.41
39:A:380:LEU:C	39:A:388:LYS:HE3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A:575:ILE:HG23	43:H:115:LEU:HB2	2.02	0.41
40:C:588:LEU:HD12	40:C:588:LEU:HA	1.91	0.41
40:C:862:LYS:O	40:C:866:LEU:HD23	2.21	0.41
41:E:104:MET:HE1	41:E:153:PHE:HB3	2.03	0.41
41:E:132:TYR:CE1	41:E:136:LYS:CG	3.03	0.41
41:E:295:PHE:HB2	41:E:311:LYS:HB3	2.03	0.41
41:E:309:GLN:O	41:E:313:ARG:HG2	2.21	0.41
42:F:107:GLU:O	42:F:109:ARG:N	2.54	0.41
42:F:210:ARG:HB3	42:F:211:MET:H	1.80	0.41
42:F:348:ILE:HD13	43:H:253:MET:HE2	2.02	0.41
43:H:253:MET:HA	43:H:256:ASP:OD2	2.21	0.41
45:L:373:ILE:HA	45:L:398:MET:SD	2.60	0.41
48:N:391:ILE:HG12	48:N:446:TYR:HB2	2.02	0.41
48:N:413:LEU:HD23	48:N:420:VAL:HG21	2.03	0.41
50:f:62:C:H2'	50:f:63:A:H8	1.84	0.41
54:Z:53:ASP:N	54:Z:53:ASP:OD1	2.48	0.41
1:a:183:LEU:HD23	1:a:183:LEU:HA	1.89	0.41
2:p:31:TYR:HD2	2:p:62:LEU:HD11	1.84	0.41
18:2:481:C:P	47:J:7:ARG:HH22	2.44	0.41
18:2:528:A:H2'	18:2:529:A:H8	1.85	0.41
18:2:1402:A:H4'	28:h:51:LYS:HD2	2.03	0.41
22:u:93:THR:HG23	22:u:94:LEU:HD12	2.03	0.41
24:o:18:ARG:NH1	26:k:88:LYS:O	2.53	0.41
26:k:5:ILE:HD12	26:k:6:PRO:HD2	2.02	0.41
26:k:14:ARG:HD2	26:k:14:ARG:HA	1.89	0.41
27:x:65:TYR:HA	27:x:123:LEU:HD22	2.03	0.41
39:A:265:LYS:HD3	39:A:266:PRO:O	2.21	0.41
41:E:31:ILE:H	41:E:31:ILE:HD12	1.85	0.41
41:E:228:GLY:O	41:E:232:ILE:HG13	2.21	0.41
43:H:207:ASN:CB	43:H:212:ASN:HD21	2.34	0.41
46:M:103:LEU:HA	46:M:106:LEU:HD12	2.02	0.41
47:J:51:SER:OG	47:J:52:GLU:N	2.53	0.41
47:J:356:LYS:HB2	47:J:356:LYS:HE3	1.83	0.41
48:N:223:ILE:HD12	48:N:223:ILE:HA	1.92	0.41
48:N:260:ARG:HB2	48:N:430:TYR:HB2	2.02	0.41
3:d:70:VAL:C	3:d:72:ASP:H	2.29	0.40
3:d:200:ARG:O	10:c:54:ARG:NH2	2.52	0.40
15:z:20:ARG:HB3	15:z:76:TYR:CD1	2.56	0.40
18:2:115:U:H2'	18:2:116:U:C6	2.56	0.40
18:2:1354:G:N2	18:2:1357:A:OP2	2.55	0.40
22:u:1:MET:HG2	22:u:2:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:h:48:LEU:HD22	28:h:93:SER:HB2	2.03	0.40
33:V:133:ASN:ND2	33:V:135:LEU:HB2	2.35	0.40
33:V:140:TYR:HE2	33:V:144:ASP:HB3	1.86	0.40
39:A:296:LEU:HD23	39:A:299:LEU:HD23	2.04	0.40
41:E:16:ARG:O	41:E:19:VAL:HG22	2.21	0.40
41:E:26:LEU:HG	41:E:31:ILE:HD13	2.01	0.40
44:K:22:ASN:HA	44:K:23:PRO:HD3	1.79	0.40
44:K:70:LEU:HD23	44:K:70:LEU:HA	1.85	0.40
48:N:493:CYS:O	48:N:497:ILE:HG13	2.21	0.40
1:a:18:PHE:HD2	1:a:51:LEU:HD22	1.86	0.40
3:d:213:LEU:HD23	3:d:213:LEU:HA	1.93	0.40
4:Q:58:VAL:HG13	34:i:125:LYS:HB3	2.03	0.40
12:m:41:ALA:HB2	12:m:50:ILE:HD11	2.03	0.40
18:2:1277:C:H2'	18:2:1278:A:H8	1.85	0.40
18:2:1344:A:N6	18:2:1386:A:H5'	2.36	0.40
27:x:114:GLU:HB3	27:x:124:THR:HG22	2.02	0.40
33:V:164:ILE:HG13	33:V:221:LEU:HD13	2.03	0.40
33:V:298:LEU:HB3	33:V:310:TRP:HB2	2.04	0.40
45:L:298:GLU:O	45:L:302:LYS:HG2	2.21	0.40
46:M:19:ARG:NH1	46:M:44:GLN:HE22	2.19	0.40
47:J:86:ARG:NH1	47:J:91:ALA:O	2.53	0.40
52:O:100:LYS:HE3	52:O:100:LYS:HB3	1.84	0.40
3:d:76:LYS:HB2	3:d:76:LYS:HE2	1.90	0.40
3:d:125:LYS:NZ	18:2:1357:A:OP1	2.52	0.40
3:d:214:LEU:HD23	3:d:214:LEU:HA	1.86	0.40
5:q:155:LYS:HA	5:q:155:LYS:HD3	1.92	0.40
8:s:101:LEU:O	8:s:116:ARG:NH1	2.54	0.40
8:s:116:ARG:HA	8:s:117:PRO:HD3	1.96	0.40
8:s:126:HIS:CE1	8:s:181:THR:HG23	2.57	0.40
10:c:93:LYS:HA	10:c:93:LYS:HD2	1.83	0.40
12:m:2:GLY:N	18:2:923:G:OP1	2.54	0.40
18:2:883:U:H3	18:2:884:C:N4	2.20	0.40
24:o:95:GLY:HA2	24:o:103:ASN:O	2.21	0.40
38:B:509:LEU:HD22	38:B:512:VAL:HG22	2.02	0.40
38:B:521:LYS:HD3	38:B:572:PRO:HA	2.03	0.40
39:A:71:LEU:HD21	39:A:90:VAL:HG22	2.03	0.40
40:C:110:LEU:CA	40:C:149:ASN:HD21	2.35	0.40
40:C:678:ASN:HB3	40:C:681:LEU:HB3	2.03	0.40
42:F:89:GLY:N	42:F:126:LYS:O	2.54	0.40
45:L:316:TYR:CD1	45:L:335:VAL:HG22	2.56	0.40
45:L:362:LYS:HA	45:L:365:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:M:61:GLU:HG3	46:M:65:ASN:OD1	2.22	0.40
47:J:106:LEU:O	47:J:270:ILE:HA	2.22	0.40
48:N:179:LEU:HD23	48:N:182:MET:SD	2.60	0.40
51:4:326:ALA:HB1	51:4:328:LEU:HG	2.03	0.40
2:p:119:THR:HG23	2:p:155:TYR:HD1	1.85	0.40
11:n:133:PRO:O	18:2:383:G:O2'	2.39	0.40
18:2:526:A:H2'	18:2:527:C:C6	2.57	0.40
18:2:530:U:H2'	18:2:531:A:H8	1.85	0.40
23:v:42:LEU:HD21	23:v:50:CYS:SG	2.61	0.40
24:o:81:ARG:NH2	24:o:117:GLY:O	2.54	0.40
24:o:84:ILE:HD12	24:o:84:ILE:HA	1.89	0.40
33:V:144:ASP:N	33:V:144:ASP:OD1	2.54	0.40
39:A:364:PRO:HA	39:A:365:PRO:HD2	1.98	0.40
40:C:110:LEU:CD1	40:C:149:ASN:OD1	2.61	0.40
40:C:113:LEU:HD23	40:C:113:LEU:HA	1.90	0.40
40:C:136:LYS:O	40:C:140:THR:HG23	2.21	0.40
40:C:354:LEU:HB3	40:C:378:ILE:HG13	2.03	0.40
40:C:495:THR:OG1	40:C:496:THR:N	2.54	0.40
40:C:689:SER:O	40:C:693:LEU:HG	2.22	0.40
40:C:714:PHE:CE2	40:C:718:LEU:HD11	2.57	0.40
42:F:94:LEU:O	42:F:239:TYR:HA	2.20	0.40
42:F:293:VAL:HA	42:F:297:LYS:HB3	2.04	0.40
47:J:419:LYS:HA	47:J:419:LYS:HD2	1.91	0.40
50:f:65:C:H2'	50:f:66:C:H6	1.87	0.40
51:4:239:PHE:CE2	51:4:274:TYR:HB2	2.57	0.40
53:Y:51:ALA:HB2	61:Y:501:GTP:O1B	2.21	0.40
54:Z:104:LYS:HD2	54:Z:104:LYS:HA	1.92	0.40
1:a:59:LEU:HD23	1:a:59:LEU:HA	1.83	0.40
8:s:70:LYS:HD2	8:s:70:LYS:HA	1.67	0.40
12:m:29:THR:H	12:m:32:ASP:HB2	1.85	0.40
18:2:652:U:H2'	18:2:653:A:H8	1.86	0.40
18:2:669:A:N3	18:2:1164:G:O2'	2.46	0.40
18:2:1157:G:C8	35:j:5:ARG:HD3	2.54	0.40
18:2:1241:A:O2'	18:2:1266:C:O2'	2.39	0.40
18:2:1740:C:H2'	18:2:1741:U:C6	2.57	0.40
18:2:1823:A:H62	18:2:1824:A:N6	2.20	0.40
33:V:89:LEU:HG	33:V:101:PHE:HE2	1.86	0.40
39:A:536:VAL:HG21	42:F:307:PHE:CE2	2.57	0.40
41:E:300:TYR:HA	41:E:303:PHE:CE1	2.55	0.40
42:F:115:ARG:O	42:F:139:HIS:NE2	2.55	0.40
44:K:139:ARG:HA	44:K:142:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L:383:ASP:OD1	45:L:383:ASP:N	2.52	0.40
46:M:240:LEU:HD21	46:M:255:PHE:CG	2.57	0.40
48:N:265:TRP:HZ3	48:N:508:ILE:HG22	1.87	0.40
48:N:383:GLY:N	48:N:387:GLU:O	2.54	0.40
51:4:239:PHE:CE2	51:4:243:GLU:HG3	2.57	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	214/295 (72%)	205 (96%)	9 (4%)	0	100	100
2	p	209/264 (79%)	194 (93%)	15 (7%)	0	100	100
3	d	214/293 (73%)	196 (92%)	18 (8%)	0	100	100
4	Q	99/115 (86%)	95 (96%)	4 (4%)	0	100	100
5	q	253/263 (96%)	231 (91%)	22 (9%)	0	100	100
6	W	22/25 (88%)	22 (100%)	0	0	100	100
7	r	220/249 (88%)	203 (92%)	17 (8%)	0	100	100
8	s	165/194 (85%)	151 (92%)	14 (8%)	0	100	100
9	t	195/208 (94%)	177 (91%)	18 (9%)	0	100	100
10	c	178/194 (92%)	165 (93%)	13 (7%)	0	100	100
11	n	131/158 (83%)	119 (91%)	12 (9%)	0	100	100
12	m	147/151 (97%)	140 (95%)	7 (5%)	0	100	100
13	y	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
14	D	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
15	z	120/131 (92%)	111 (92%)	9 (8%)	0	100	100
16	R	80/84 (95%)	76 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	40/59 (68%)	37 (92%)	3 (8%)	0	100	100
19	w	124/135 (92%)	109 (88%)	15 (12%)	0	100	100
20	b	222/243 (91%)	203 (91%)	19 (9%)	0	100	100
21	e	187/204 (92%)	172 (92%)	15 (8%)	0	100	100
22	u	93/165 (56%)	84 (90%)	9 (10%)	0	100	100
23	v	107/132 (81%)	99 (92%)	8 (8%)	0	100	100
24	o	117/145 (81%)	113 (97%)	4 (3%)	0	100	100
25	g	136/146 (93%)	129 (95%)	7 (5%)	0	100	100
26	k	138/152 (91%)	129 (94%)	9 (6%)	0	100	100
27	x	139/145 (96%)	132 (95%)	7 (5%)	0	100	100
28	h	96/119 (81%)	88 (92%)	8 (8%)	0	100	100
29	P	68/125 (54%)	61 (90%)	7 (10%)	0	100	100
30	S	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
31	l	52/56 (93%)	48 (92%)	4 (8%)	0	100	100
32	U	53/156 (34%)	46 (87%)	7 (13%)	0	100	100
33	V	290/317 (92%)	248 (86%)	40 (14%)	2 (1%)	18	51
34	i	123/151 (82%)	108 (88%)	15 (12%)	0	100	100
35	j	137/143 (96%)	128 (93%)	8 (6%)	1 (1%)	18	51
36	G	86/112 (77%)	81 (94%)	5 (6%)	0	100	100
37	I	301/325 (93%)	292 (97%)	9 (3%)	0	100	100
38	B	528/814 (65%)	468 (89%)	60 (11%)	0	100	100
39	A	682/1382 (49%)	646 (95%)	36 (5%)	0	100	100
40	C	615/921 (67%)	571 (93%)	44 (7%)	0	100	100
41	E	406/445 (91%)	386 (95%)	20 (5%)	0	100	100
42	F	267/357 (75%)	237 (89%)	30 (11%)	0	100	100
43	H	289/352 (82%)	262 (91%)	27 (9%)	0	100	100
44	K	215/218 (99%)	195 (91%)	20 (9%)	0	100	100
45	L	370/564 (66%)	325 (88%)	45 (12%)	0	100	100
46	M	328/374 (88%)	302 (92%)	26 (8%)	0	100	100
47	J	572/599 (96%)	506 (88%)	65 (11%)	1 (0%)	43	74
48	N	441/548 (80%)	385 (87%)	56 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	X	76/78 (97%)	72 (95%)	4 (5%)	0	100	100
51	4	140/333 (42%)	119 (85%)	21 (15%)	0	100	100
52	O	294/315 (93%)	264 (90%)	30 (10%)	0	100	100
53	Y	408/472 (86%)	312 (76%)	94 (23%)	2 (0%)	24	57
54	Z	108/113 (96%)	94 (87%)	14 (13%)	0	100	100
All	All	10761/13821 (78%)	9789 (91%)	966 (9%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	V	175	LYS
53	Y	224	ILE
35	j	86	PRO
53	Y	51	ALA
47	J	193	GLU
33	V	174	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	180/243 (74%)	180 (100%)	0	100	100
2	p	192/231 (83%)	192 (100%)	0	100	100
3	d	182/225 (81%)	182 (100%)	0	100	100
4	Q	88/98 (90%)	88 (100%)	0	100	100
5	q	220/225 (98%)	220 (100%)	0	100	100
6	W	23/24 (96%)	23 (100%)	0	100	100
7	r	193/218 (88%)	193 (100%)	0	100	100
8	s	155/174 (89%)	155 (100%)	0	100	100
9	t	174/180 (97%)	173 (99%)	1 (1%)	78	79
10	c	160/168 (95%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	n	125/142 (88%)	125 (100%)	0	100	100
12	m	130/131 (99%)	130 (100%)	0	100	100
13	y	66/67 (98%)	66 (100%)	0	100	100
14	D	112/113 (99%)	112 (100%)	0	100	100
15	z	106/113 (94%)	106 (100%)	0	100	100
16	R	74/76 (97%)	74 (100%)	0	100	100
17	T	35/48 (73%)	35 (100%)	0	100	100
19	w	111/122 (91%)	111 (100%)	0	100	100
20	b	188/202 (93%)	188 (100%)	0	100	100
21	e	159/170 (94%)	159 (100%)	0	100	100
22	u	86/136 (63%)	86 (100%)	0	100	100
23	v	94/108 (87%)	94 (100%)	0	100	100
24	o	107/130 (82%)	107 (100%)	0	100	100
25	g	114/121 (94%)	114 (100%)	0	100	100
26	k	122/132 (92%)	122 (100%)	0	100	100
27	x	111/115 (96%)	111 (100%)	0	100	100
28	h	91/107 (85%)	91 (100%)	0	100	100
29	P	62/103 (60%)	62 (100%)	0	100	100
30	S	54/62 (87%)	54 (100%)	0	100	100
31	l	47/49 (96%)	47 (100%)	0	100	100
32	U	51/140 (36%)	51 (100%)	0	100	100
33	V	256/275 (93%)	256 (100%)	0	100	100
34	i	98/119 (82%)	98 (100%)	0	100	100
35	j	111/115 (96%)	111 (100%)	0	100	100
36	G	75/95 (79%)	75 (100%)	0	100	100
38	B	90/702 (13%)	90 (100%)	0	100	100
39	A	546/1259 (43%)	546 (100%)	0	100	100
40	C	554/811 (68%)	554 (100%)	0	100	100
41	E	380/406 (94%)	379 (100%)	1 (0%)	86	83
42	F	237/289 (82%)	237 (100%)	0	100	100
43	H	269/310 (87%)	269 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	K	192/193 (100%)	192 (100%)	0	100	100
45	L	342/515 (66%)	342 (100%)	0	100	100
46	M	305/335 (91%)	305 (100%)	0	100	100
47	J	506/526 (96%)	506 (100%)	0	100	100
48	N	398/494 (81%)	398 (100%)	0	100	100
51	4	109/304 (36%)	109 (100%)	0	100	100
52	O	190/280 (68%)	190 (100%)	0	100	100
53	Y	33/397 (8%)	33 (100%)	0	100	100
54	Z	79/96 (82%)	79 (100%)	0	100	100
All	All	8382/11694 (72%)	8380 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	t	155	ASN
41	E	132	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	50	ASN
2	p	43	ASN
2	p	158	HIS
3	d	136	HIS
4	Q	8	ASN
4	Q	17	HIS
5	q	232	ASN
8	s	25	GLN
8	s	39	GLN
8	s	44	ASN
8	s	126	HIS
8	s	168	HIS
9	t	84	ASN
10	c	124	HIS
10	c	156	HIS
11	n	13	GLN
11	n	19	ASN
15	z	22	GLN

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Mol	Chain	Res	Type
19	w	48	ASN
21	e	148	ASN
21	e	203	ASN
22	u	84	HIS
23	v	55	ASN
23	v	82	ASN
24	o	103	ASN
26	k	73	ASN
26	k	101	ASN
26	k	134	GLN
27	x	11	GLN
27	x	63	HIS
28	h	47	ASN
29	P	64	ASN
33	V	64	HIS
33	V	117	ASN
34	i	83	GLN
35	j	97	ASN
36	G	60	HIS
38	B	502	GLN
39	A	44	GLN
39	A	109	GLN
39	A	270	GLN
39	A	274	ASN
39	A	288	ASN
39	A	445	GLN
39	A	512	GLN
39	A	586	ASN
40	C	350	GLN
40	C	610	ASN
40	C	615	GLN
40	C	637	GLN
40	C	678	ASN
40	C	876	HIS
41	E	60	ASN
41	E	83	GLN
41	E	199	ASN
41	E	241	GLN
41	E	247	GLN
42	F	288	GLN
42	F	345	GLN
43	H	58	GLN

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Mol	Chain	Res	Type
43	H	207	ASN
43	H	212	ASN
43	H	242	ASN
43	H	324	ASN
43	H	328	GLN
43	H	336	GLN
44	K	6	GLN
44	K	10	ASN
44	K	47	ASN
44	K	55	GLN
44	K	115	GLN
44	K	151	GLN
45	L	199	GLN
45	L	218	ASN
45	L	241	ASN
45	L	243	GLN
45	L	364	ASN
45	L	443	GLN
45	L	499	ASN
46	M	270	HIS
46	M	273	ASN
47	J	12	ASN
47	J	74	ASN
47	J	429	HIS
47	J	468	GLN
47	J	496	GLN
48	N	73	HIS
48	N	242	GLN
48	N	322	ASN
48	N	486	ASN
48	N	513	ASN
54	Z	89	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	2	1710/1721 (99%)	514 (30%)	7 (0%)
50	f	74/75 (98%)	24 (32%)	0
All	All	1784/1796 (99%)	538 (30%)	7 (0%)

All (538) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	2	2	A
18	2	4	C
18	2	5	U
18	2	11	A
18	2	25	A
18	2	33	G
18	2	41	G
18	2	44	U
18	2	45	A
18	2	46	A
18	2	56	G
18	2	64	A
18	2	65	C
18	2	67	C
18	2	68	A
18	2	71	G
18	2	73	C
18	2	74	G
18	2	75	G
18	2	76	U
18	2	77	A
18	2	79	A
18	2	92	A
18	2	100	U
18	2	103	A
18	2	113	G
18	2	115	U
18	2	126	G
18	2	129	C
18	2	130	G
18	2	143	U
18	2	147	A
18	2	149	A
18	2	155	G
18	2	163	U
18	2	165	G
18	2	175	A
18	2	178	C
18	2	182	C
18	2	184	G
18	2	193	C
18	2	195	C
18	2	196	C

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Mol	Chain	Res	Type
18	2	197	U
18	2	198	U
18	2	199	C
18	2	201	C
18	2	202	G
18	2	204	G
18	2	205	G
18	2	210	U
18	2	214	U
18	2	220	U
18	2	224	A
18	2	291	G
18	2	292	A
18	2	293	C
18	2	297	A
18	2	308	G
18	2	309	G
18	2	312	G
18	2	315	C
18	2	319	C
18	2	320	G
18	2	331	C
18	2	332	G
18	2	333	G
18	2	335	G
18	2	344	U
18	2	345	U
18	2	346	C
18	2	347	G
18	2	362	C
18	2	364	A
18	2	367	U
18	2	368	U
18	2	369	C
18	2	381	C
18	2	382	C
18	2	385	G
18	2	386	C
18	2	391	C
18	2	400	C
18	2	402	C
18	2	407	G

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Mol	Chain	Res	Type
18	2	409	C
18	2	418	A
18	2	421	G
18	2	426	A
18	2	435	A
18	2	448	A
18	2	449	A
18	2	450	C
18	2	455	A
18	2	464	A
18	2	465	A
18	2	466	G
18	2	472	C
18	2	473	A
18	2	474	G
18	2	476	A
18	2	485	A
18	2	487	U
18	2	489	A
18	2	492	C
18	2	493	A
18	2	517	C
18	2	523	A
18	2	525	A
18	2	532	C
18	2	536	A
18	2	538	U
18	2	539	C
18	2	540	U
18	2	541	U
18	2	543	C
18	2	544	G
18	2	545	A
18	2	547	G
18	2	548	C
18	2	549	C
18	2	552	G
18	2	553	U
18	2	554	A
18	2	555	A
18	2	556	U
18	2	559	G

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Mol	Chain	Res	Type
18	2	563	G
18	2	564	A
18	2	568	C
18	2	570	C
18	2	574	A
18	2	575	A
18	2	576	A
18	2	587	A
18	2	588	G
18	2	591	U
18	2	593	C
18	2	594	A
18	2	600	G
18	2	604	A
18	2	606	G
18	2	607	U
18	2	608	C
18	2	614	C
18	2	617	G
18	2	621	C
18	2	623	G
18	2	627	U
18	2	628	A
18	2	629	A
18	2	639	C
18	2	640	A
18	2	642	U
18	2	643	A
18	2	644	G
18	2	646	G
18	2	655	A
18	2	658	U
18	2	659	G
18	2	660	C
18	2	662	G
18	2	664	A
18	2	668	A
18	2	669	A
18	2	671	A
18	2	672	A
18	2	673	G
18	2	691	G

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Mol	Chain	Res	Type
18	2	692	G
18	2	694	G
18	2	699	C
18	2	707	C
18	2	709	G
18	2	713	C
18	2	721	G
18	2	722	C
18	2	723	C
18	2	727	G
18	2	732	U
18	2	733	C
18	2	739	C
18	2	747	U
18	2	748	C
18	2	749	U
18	2	750	C
18	2	751	G
18	2	752	G
18	2	792	C
18	2	793	G
18	2	794	A
18	2	795	A
18	2	796	G
18	2	798	G
18	2	799	U
18	2	811	A
18	2	821	G
18	2	822	U
18	2	823	U
18	2	824	C
18	2	827	A
18	2	830	A
18	2	834	C
18	2	845	G
18	2	847	A
18	2	862	A
18	2	869	A
18	2	870	A
18	2	872	A
18	2	873	G
18	2	874	G

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Mol	Chain	Res	Type
18	2	875	A
18	2	881	G
18	2	882	U
18	2	883	U
18	2	884	C
18	2	886	A
18	2	887	U
18	2	888	U
18	2	889	U
18	2	890	U
18	2	891	G
18	2	893	U
18	2	894	G
18	2	897	U
18	2	898	U
18	2	899	U
18	2	900	C
18	2	901	G
18	2	902	G
18	2	904	A
18	2	912	C
18	2	913	A
18	2	914	U
18	2	919	A
18	2	920	A
18	2	921	G
18	2	922	A
18	2	933	G
18	2	938	A
18	2	943	U
18	2	952	G
18	2	954	U
18	2	963	A
18	2	969	U
18	2	970	G
18	2	971	G
18	2	983	A
18	2	989	C
18	2	990	A
18	2	992	A
18	2	997	A
18	2	1001	A

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Mol	Chain	Res	Type
18	2	1002	U
18	2	1006	C
18	2	1008	A
18	2	1017	U
18	2	1019	C
18	2	1021	U
18	2	1023	A
18	2	1026	C
18	2	1045	U
18	2	1047	C
18	2	1049	A
18	2	1050	A
18	2	1053	C
18	2	1056	U
18	2	1058	A
18	2	1059	G
18	2	1060	A
18	2	1061	U
18	2	1062	A
18	2	1081	U
18	2	1083	A
18	2	1085	C
18	2	1087	A
18	2	1088	U
18	2	1089	G
18	2	1096	G
18	2	1100	A
18	2	1109	C
18	2	1113	A
18	2	1114	U
18	2	1115	U
18	2	1116	C
18	2	1117	C
18	2	1118	C
18	2	1120	U
18	2	1138	C
18	2	1143	A
18	2	1148	A
18	2	1153	C
18	2	1154	U
18	2	1157	G
18	2	1168	G

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Mol	Chain	Res	Type
18	2	1170	A
18	2	1171	G
18	2	1180	C
18	2	1183	A
18	2	1188	A
18	2	1195	A
18	2	1197	G
18	2	1207	G
18	2	1210	G
18	2	1215	C
18	2	1216	C
18	2	1218	C
18	2	1224	G
18	2	1240	A
18	2	1242	U
18	2	1243	U
18	2	1250	A
18	2	1251	A
18	2	1253	A
18	2	1256	G
18	2	1257	G
18	2	1258	A
18	2	1259	A
18	2	1263	U
18	2	1265	A
18	2	1269	G
18	2	1271	C
18	2	1273	C
18	2	1274	G
18	2	1275	G
18	2	1282	A
18	2	1283	C
18	2	1285	G
18	2	1286	G
18	2	1287	A
18	2	1293	A
18	2	1295	A
18	2	1298	G
18	2	1300	U
18	2	1301	A
18	2	1302	G
18	2	1303	C

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Mol	Chain	Res	Type
18	2	1304	U
18	2	1305	C
18	2	1308	U
18	2	1312	G
18	2	1313	A
18	2	1315	U
18	2	1316	C
18	2	1323	U
18	2	1330	G
18	2	1333	U
18	2	1341	C
18	2	1342	U
18	2	1344	A
18	2	1352	G
18	2	1358	U
18	2	1362	U
18	2	1371	U
18	2	1372	U
18	2	1375	G
18	2	1376	A
18	2	1378	A
18	2	1381	G
18	2	1382	A
18	2	1387	G
18	2	1389	C
18	2	1397	U
18	2	1398	G
18	2	1403	C
18	2	1405	A
18	2	1406	G
18	2	1407	U
18	2	1415	C
18	2	1425	G
18	2	1428	G
18	2	1429	G
18	2	1430	C
18	2	1431	G
18	2	1442	U
18	2	1444	U
18	2	1449	G
18	2	1452	A
18	2	1455	A

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Mol	Chain	Res	Type
18	2	1462	U
18	2	1463	U
18	2	1464	C
18	2	1475	G
18	2	1477	U
18	2	1478	U
18	2	1480	A
18	2	1483	A
18	2	1484	A
18	2	1485	U
18	2	1487	A
18	2	1489	A
18	2	1493	C
18	2	1494	U
18	2	1495	G
18	2	1497	G
18	2	1498	A
18	2	1500	G
18	2	1502	C
18	2	1504	U
18	2	1508	A
18	2	1520	G
18	2	1521	C
18	2	1522	A
18	2	1523	C
18	2	1531	A
18	2	1532	C
18	2	1533	A
18	2	1536	G
18	2	1541	G
18	2	1543	U
18	2	1548	G
18	2	1552	G
18	2	1553	C
18	2	1555	U
18	2	1556	A
18	2	1557	C
18	2	1558	C
18	2	1559	C
18	2	1561	A
18	2	1573	G
18	2	1575	G

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Mol	Chain	Res	Type
18	2	1577	G
18	2	1580	A
18	2	1581	C
18	2	1585	U
18	2	1586	U
18	2	1587	G
18	2	1588	A
18	2	1591	C
18	2	1592	C
18	2	1599	U
18	2	1601	A
18	2	1602	U
18	2	1603	G
18	2	1604	G
18	2	1606	G
18	2	1613	G
18	2	1617	G
18	2	1620	A
18	2	1621	U
18	2	1622	U
18	2	1623	A
18	2	1624	U
18	2	1637	A
18	2	1639	G
18	2	1641	A
18	2	1642	U
18	2	1646	C
18	2	1648	G
18	2	1651	A
18	2	1654	G
18	2	1664	A
18	2	1665	G
18	2	1669	G
18	2	1671	G
18	2	1682	C
18	2	1683	C
18	2	1686	G
18	2	1687	C
18	2	1695	A
18	2	1698	C
18	2	1699	A
18	2	1703	C

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Mol	Chain	Res	Type
18	2	1718	G
18	2	1720	U
18	2	1721	U
18	2	1726	G
18	2	1729	U
18	2	1733	U
18	2	1737	G
18	2	1742	C
18	2	1744	G
18	2	1746	U
18	2	1751	C
18	2	1752	C
18	2	1753	C
18	2	1755	C
18	2	1756	C
18	2	1758	G
18	2	1759	G
18	2	1760	G
18	2	1761	U
18	2	1772	C
18	2	1773	C
18	2	1774	C
18	2	1776	G
18	2	1777	G
18	2	1781	A
18	2	1783	C
18	2	1784	G
18	2	1785	C
18	2	1787	G
18	2	1800	A
18	2	1805	G
18	2	1806	A
18	2	1814	G
18	2	1821	U
18	2	1824	A
18	2	1825	A
18	2	1831	A
18	2	1834	A
18	2	1835	A
18	2	1838	U
18	2	1839	U
18	2	1840	U

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Mol	Chain	Res	Type
18	2	1849	A
18	2	1851	A
18	2	1854	U
18	2	1861	G
18	2	1862	G
18	2	1863	A
18	2	1865	C
18	2	1866	A
18	2	1869	A
50	f	2	G
50	f	6	A
50	f	9	A
50	f	12	G
50	f	16	C
50	f	18	G
50	f	19	G
50	f	20	A
50	f	21	A
50	f	22	G
50	f	24	G
50	f	35	A
50	f	48	C
50	f	49	G
50	f	52	G
50	f	56	C
50	f	58	A
50	f	59	A
50	f	69	U
50	f	70	G
50	f	72	U
50	f	74	C
50	f	75	C
50	f	76	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	2	332	G
18	2	1058	A
18	2	1060	A
18	2	1292	C
18	2	1474	A

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Mol	Chain	Res	Type
18	2	1621	U
18	2	1698	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	ADP	J	603	58	27,29,29	3.34	10 (37%)	42,45,45	3.02	15 (35%)
56	SF4	J	601	47	0,12,12	-	-	-		
60	MET	f	701	-	6,7,8	0.55	0	2,7,9	0.79	0
56	SF4	J	602	47	0,12,12	-	-	-		
59	ATP	J	605	58	29,33,33	3.27	9 (31%)	44,52,52	2.41	16 (36%)
61	GTP	Y	501	58	30,34,34	0.85	1 (3%)	46,54,54	1.95	10 (21%)

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	ADP	J	603	58	-	7/16/32/32	0/3/3/3
56	SF4	J	601	47	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	MET	f	701	-	-	0/5/6/8	-
56	SF4	J	602	47	-	-	0/6/5/5
59	ATP	J	605	58	-	7/22/38/38	0/3/3/3
61	GTP	Y	501	58	-	5/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	J	603	ADP	C2'-C3'	-10.56	1.24	1.53
59	J	605	ATP	C3'-C4'	-9.80	1.28	1.53
59	J	605	ATP	C2'-C1'	-8.28	1.27	1.53
57	J	603	ADP	O4'-C4'	-6.52	1.30	1.45
59	J	605	ATP	O4'-C1'	6.26	1.56	1.42
57	J	603	ADP	C3'-C4'	5.50	1.67	1.53
59	J	605	ATP	C6-N6	4.65	1.45	1.34
59	J	605	ATP	C2'-C3'	4.60	1.65	1.53
57	J	603	ADP	C1'-N9	-4.44	1.33	1.46
57	J	603	ADP	C6-N6	4.41	1.45	1.34
59	J	605	ATP	O4'-C4'	4.22	1.54	1.45
57	J	603	ADP	O4'-C1'	4.13	1.51	1.42
57	J	603	ADP	O2'-C2'	3.82	1.52	1.43
57	J	603	ADP	C5-C4	-3.79	1.31	1.39
59	J	605	ATP	C5-C4	-3.02	1.33	1.39
59	J	605	ATP	C5-N7	-2.72	1.33	1.39
57	J	603	ADP	C2'-C1'	2.61	1.61	1.53
59	J	605	ATP	C8-N9	-2.43	1.33	1.37
57	J	603	ADP	C5-N7	-2.21	1.34	1.39
61	Y	501	GTP	C5-N7	-2.14	1.34	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	J	603	ADP	C1'-N9-C8	-10.16	104.20	127.14
57	J	603	ADP	C4-N9-C1'	9.81	149.97	126.59
61	Y	501	GTP	C5-C4-N3	-6.00	118.72	128.46
57	J	603	ADP	N3-C2-N1	-5.66	119.75	128.60
59	J	605	ATP	C1'-N9-C8	-5.50	114.72	127.14
61	Y	501	GTP	C2-N3-C4	5.30	121.74	112.30
57	J	603	ADP	C5-C4-N3	-5.23	119.93	126.75
59	J	605	ATP	C5-C4-N3	-5.18	119.99	126.75
59	J	605	ATP	N3-C2-N1	-5.11	120.61	128.60
59	J	605	ATP	N6-C6-N1	-4.76	107.92	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	J	605	ATP	PA-O3A-PB	-4.55	117.21	132.83
61	Y	501	GTP	N9-C4-N3	4.45	134.87	125.94
59	J	605	ATP	C4-N9-C1'	4.41	137.10	126.59
57	J	603	ADP	N6-C6-N1	-4.39	108.73	118.35
59	J	605	ATP	N9-C8-N7	-3.95	108.50	113.91
61	Y	501	GTP	PA-O3A-PB	-3.80	119.78	132.83
59	J	605	ATP	C5-C6-N6	3.79	131.69	123.43
57	J	603	ADP	PA-O3A-PB	-3.69	120.18	132.83
57	J	603	ADP	C5-C6-N6	3.60	131.26	123.43
57	J	603	ADP	C2-N3-C4	3.52	120.06	111.75
59	J	605	ATP	N3-C4-N9	3.46	132.79	127.08
59	J	605	ATP	C2-N3-C4	3.31	119.57	111.75
61	Y	501	GTP	C2-N1-C6	-3.08	119.49	125.10
57	J	603	ADP	N9-C8-N7	-2.99	109.83	113.91
59	J	605	ATP	PB-O3B-PG	-2.92	122.81	132.83
57	J	603	ADP	C5-C4-N9	2.73	108.96	105.78
57	J	603	ADP	C2'-C1'-N9	2.72	120.20	113.30
59	J	605	ATP	C3'-C2'-C1'	2.68	106.52	101.43
61	Y	501	GTP	C5-C6-N1	2.65	119.92	113.19
59	J	605	ATP	C5-N7-C8	2.62	107.23	103.51
61	Y	501	GTP	O6-C6-C5	-2.59	119.74	126.60
61	Y	501	GTP	PB-O3B-PG	-2.54	124.10	132.83
57	J	603	ADP	C5-N7-C8	2.47	107.02	103.51
57	J	603	ADP	N3-C4-N9	2.44	131.10	127.08
61	Y	501	GTP	C3'-C2'-C1'	2.31	105.82	101.43
59	J	605	ATP	C4-N9-C8	2.23	108.15	105.73
59	J	605	ATP	C2'-C3'-C4'	2.22	106.96	102.64
61	Y	501	GTP	O2G-PG-O3B	2.15	111.85	104.64
57	J	603	ADP	C6-C5-C4	2.13	120.05	117.18
59	J	605	ATP	C6-C5-C4	2.04	119.93	117.18
57	J	603	ADP	C2'-C3'-C4'	2.03	106.58	102.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	J	603	ADP	C5'-O5'-PA-O2A
59	J	605	ATP	C5'-O5'-PA-O3A
61	Y	501	GTP	C5'-O5'-PA-O1A
57	J	603	ADP	O4'-C4'-C5'-O5'
59	J	605	ATP	O4'-C4'-C5'-O5'
61	Y	501	GTP	C2'-C1'-N9-C4

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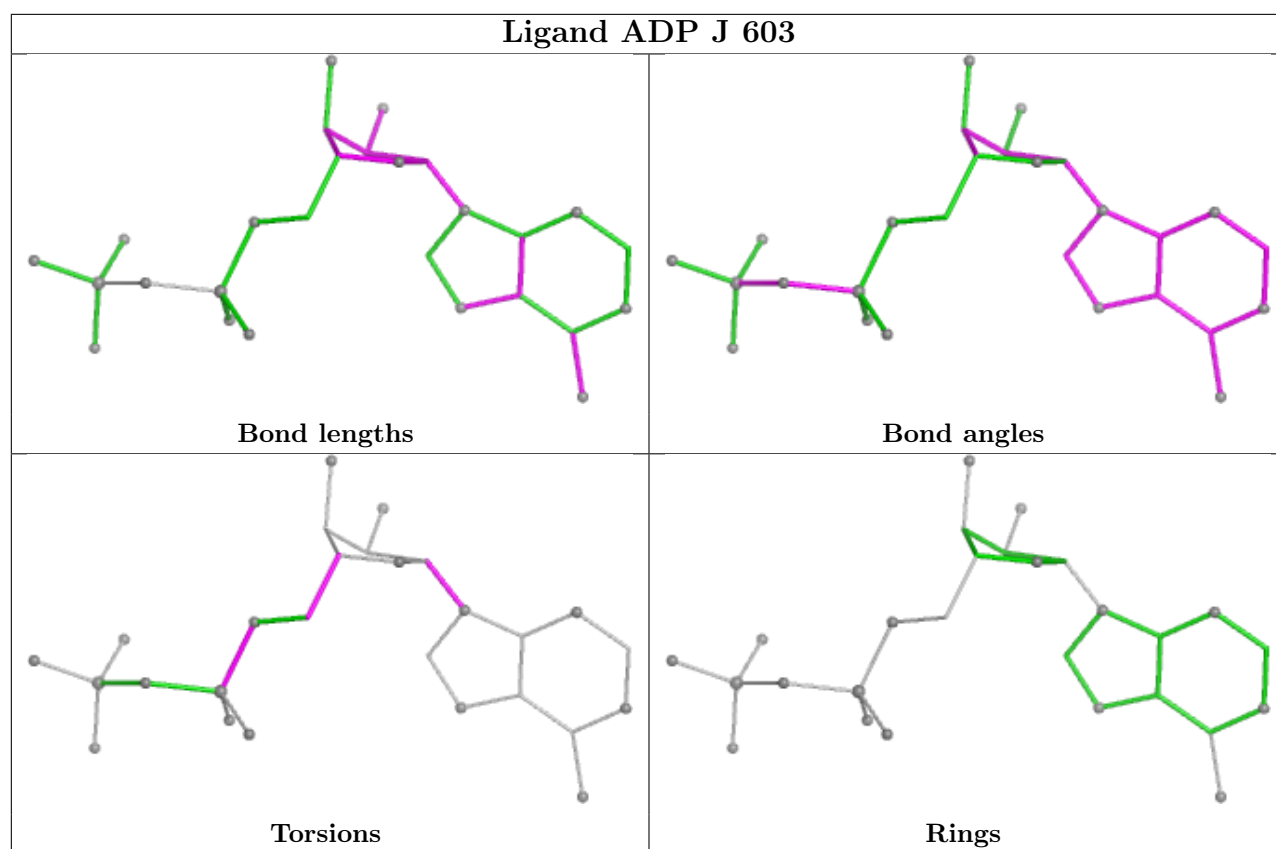
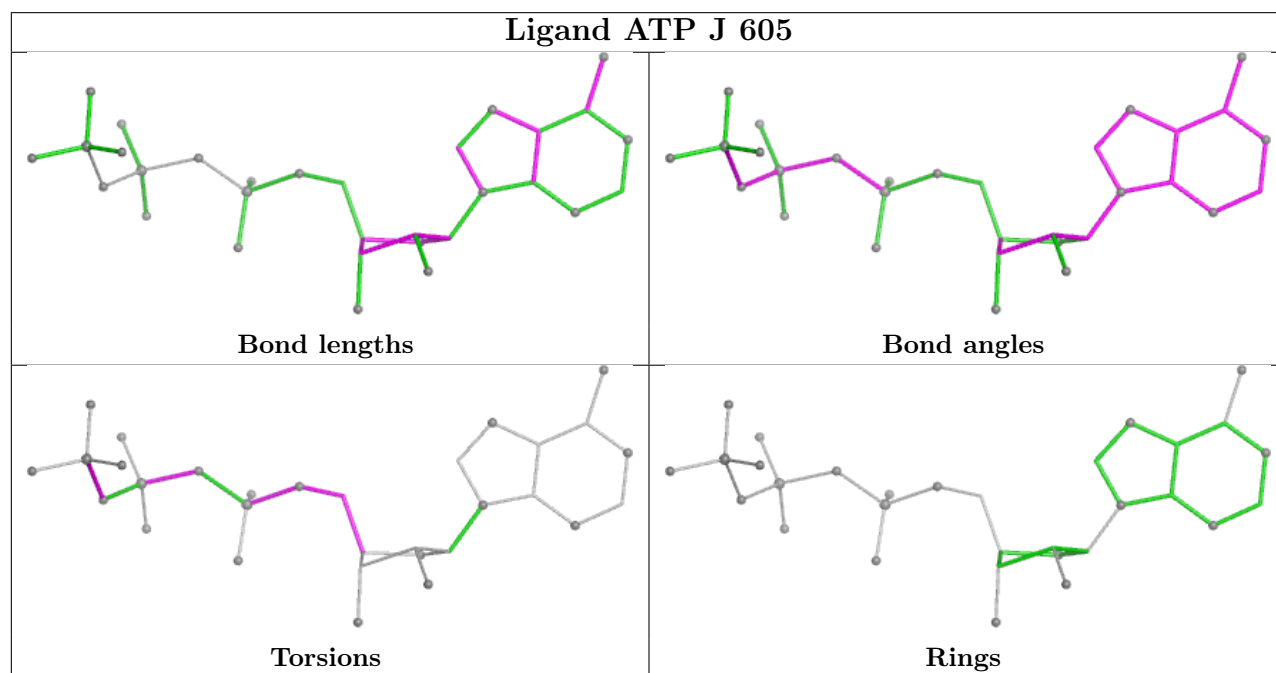
Mol	Chain	Res	Type	Atoms
59	J	605	ATP	C4'-C5'-O5'-PA
61	Y	501	GTP	C2'-C1'-N9-C8
59	J	605	ATP	PB-O3B-PG-O1G
57	J	603	ADP	C5'-O5'-PA-O3A
61	Y	501	GTP	C5'-O5'-PA-O3A
57	J	603	ADP	C2'-C1'-N9-C8
57	J	603	ADP	C5'-O5'-PA-O1A
59	J	605	ATP	C5'-O5'-PA-O2A
57	J	603	ADP	C3'-C4'-C5'-O5'
59	J	605	ATP	PA-O3A-PB-O1B
57	J	603	ADP	O4'-C1'-N9-C8
61	Y	501	GTP	O4'-C4'-C5'-O5'
59	J	605	ATP	PA-O3A-PB-O2B

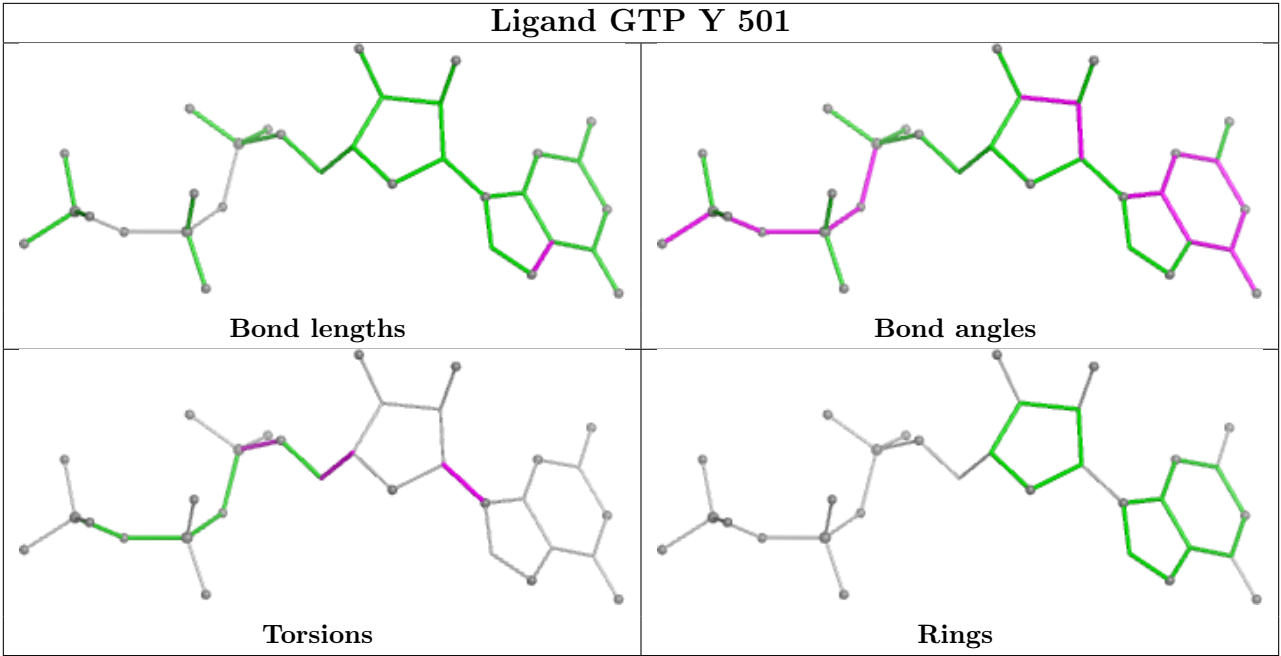
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	J	603	ADP	1	0
56	J	601	SF4	1	0
59	J	605	ATP	4	0
61	Y	501	GTP	2	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	2	3
46	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	96:GLY	C	97:GLU	N	10.75
1	2	1207:G	O3'	1208:A	P	4.50
1	2	368:U	O3'	369:C	P	3.24
1	2	1682:C	O3'	1683:C	P	3.13

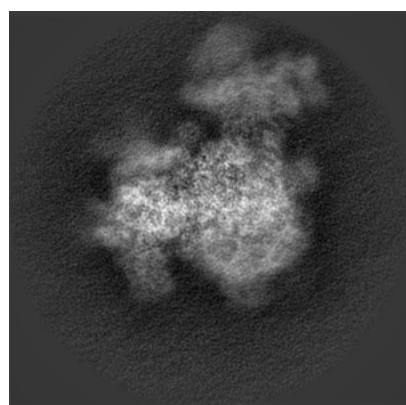
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11602. These allow visual inspection of the internal detail of the map and identification of artifacts.

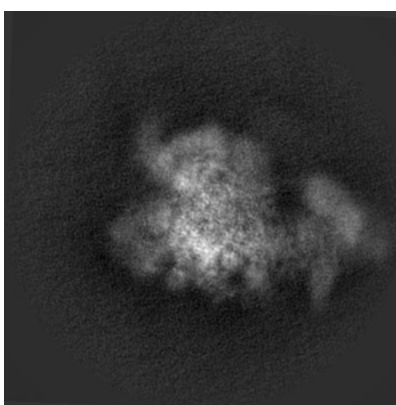
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

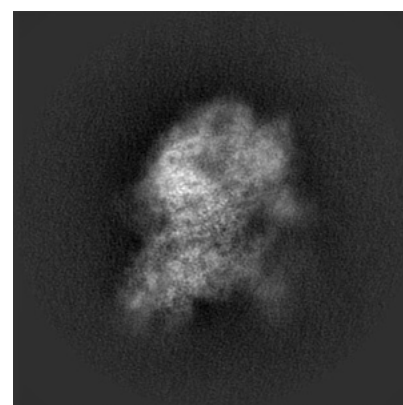
6.1.1 Primary map



X



Y

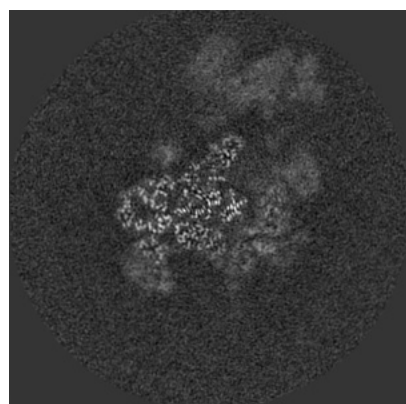


Z

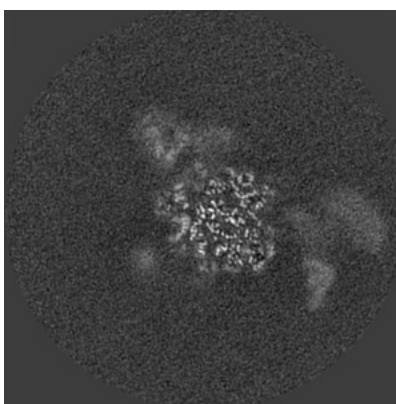
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

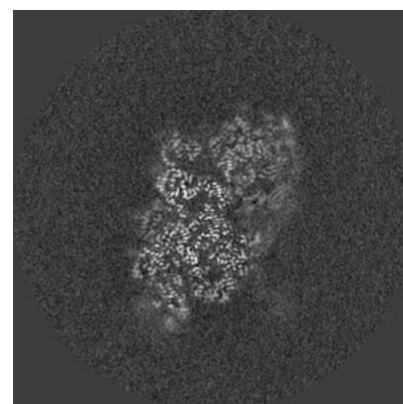
6.2.1 Primary map



X Index: 200



Y Index: 200

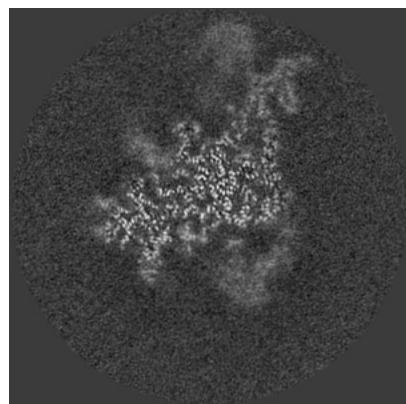


Z Index: 200

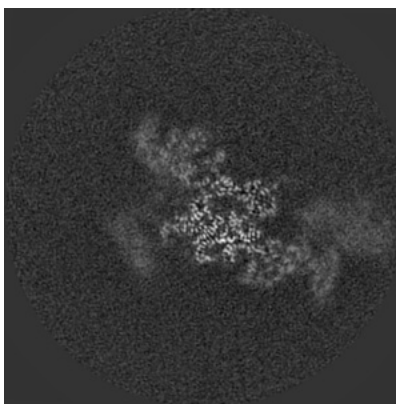
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

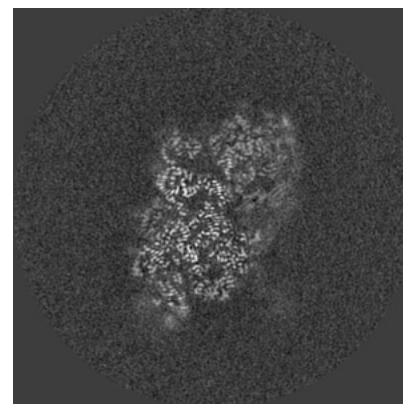
6.3.1 Primary map



X Index: 165



Y Index: 218

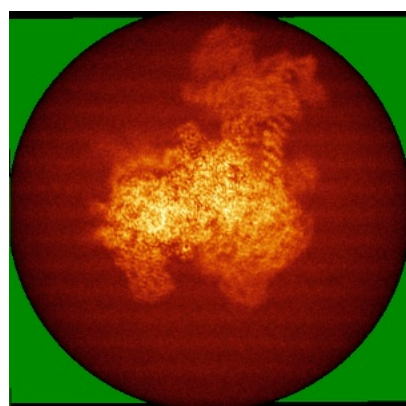


Z Index: 200

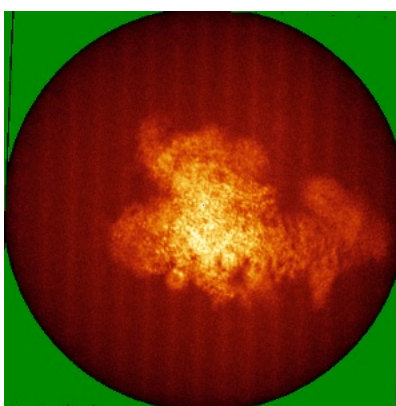
The images above show the largest variance slices of the map in three orthogonal directions.

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

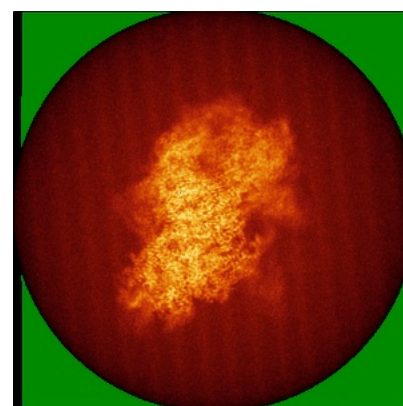
6.4.1 Primary map



X



Y

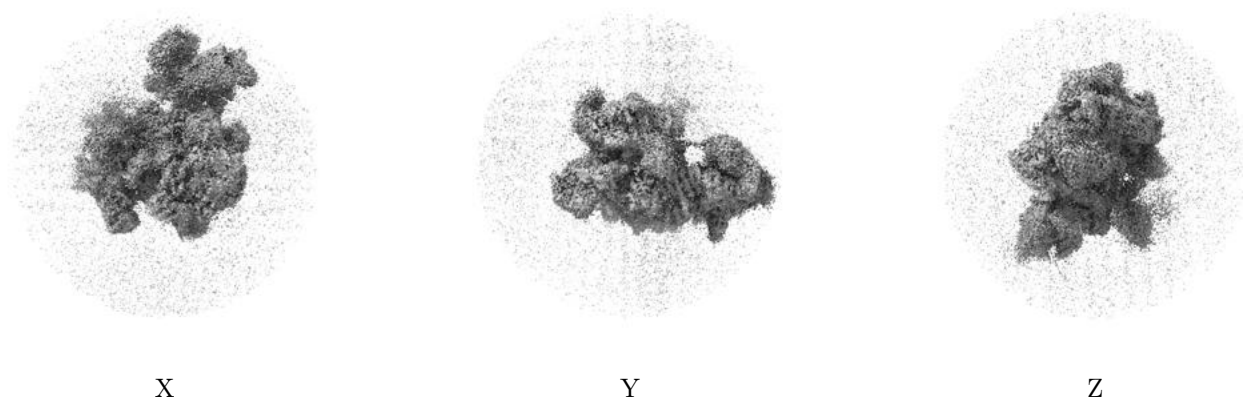


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

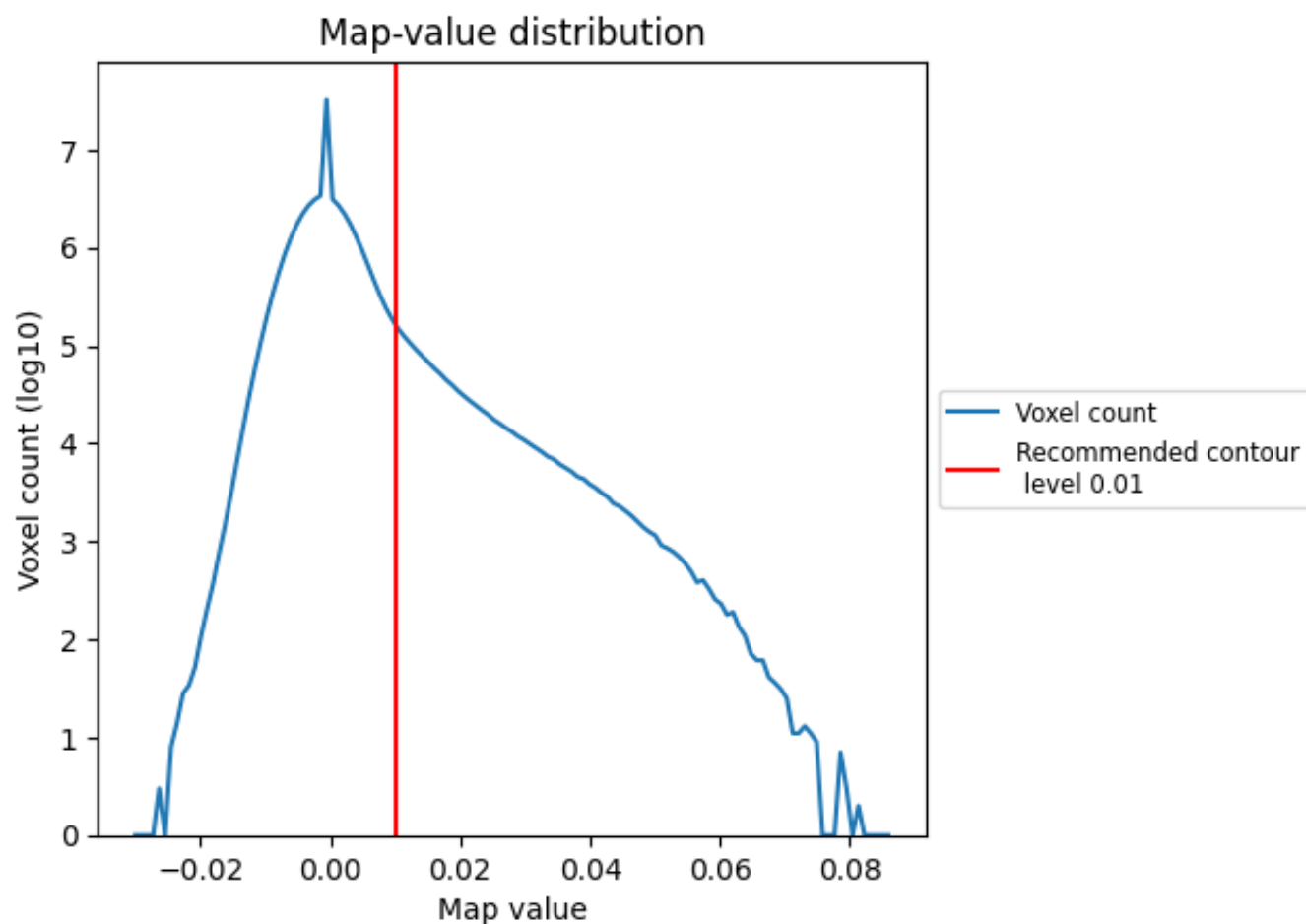
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

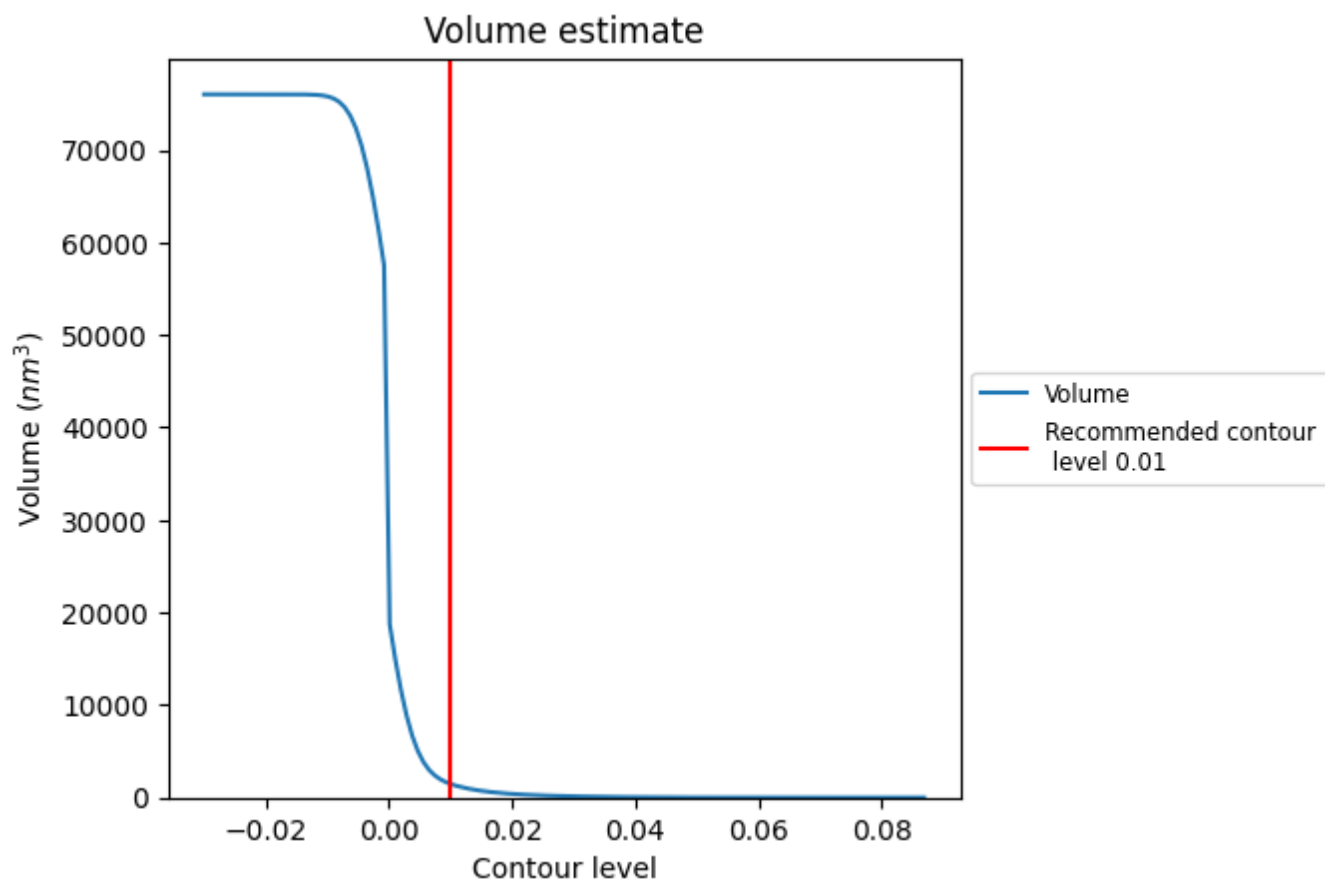
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

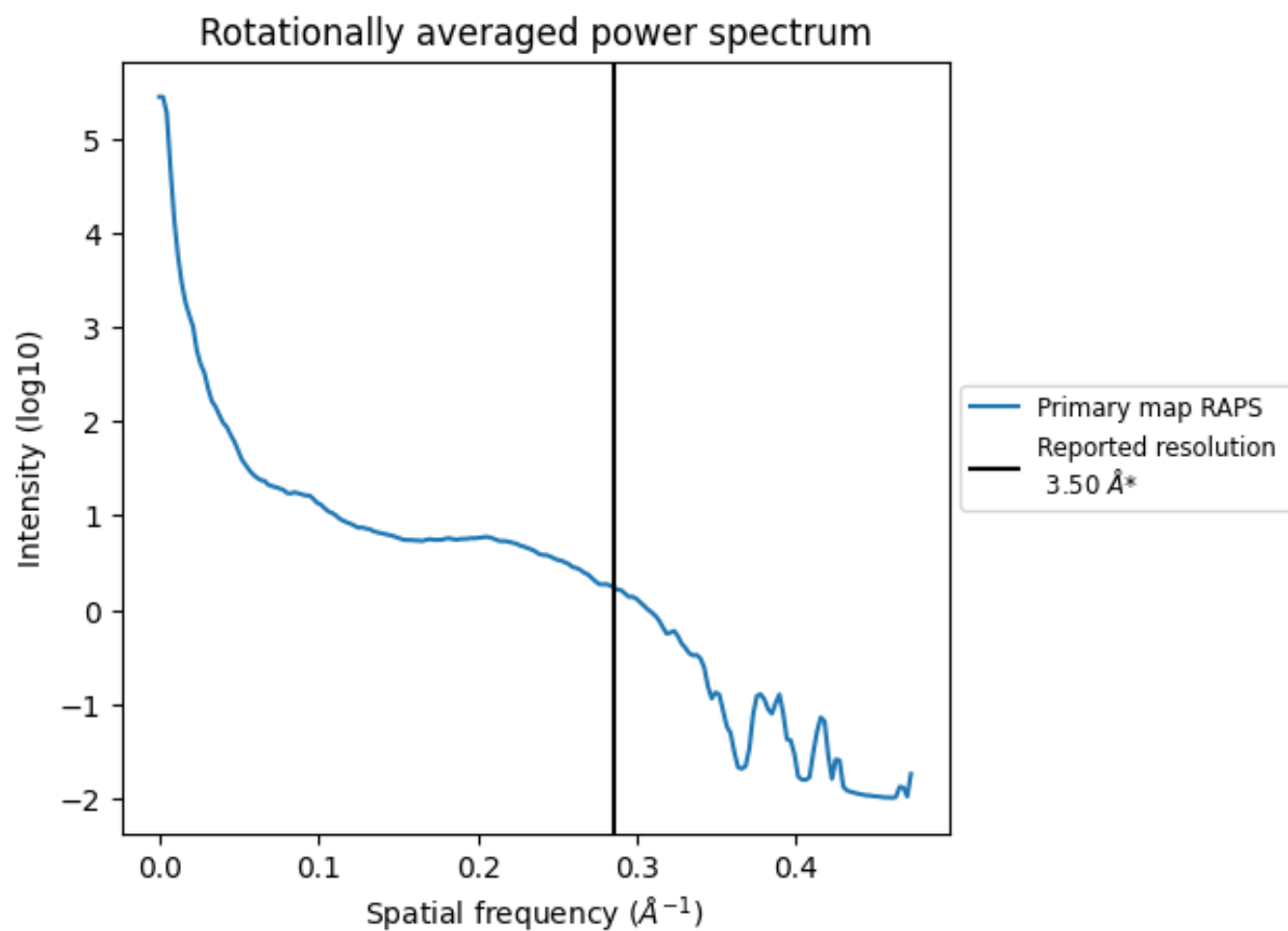
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1473 nm^3 ; this corresponds to an approximate mass of 1330 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

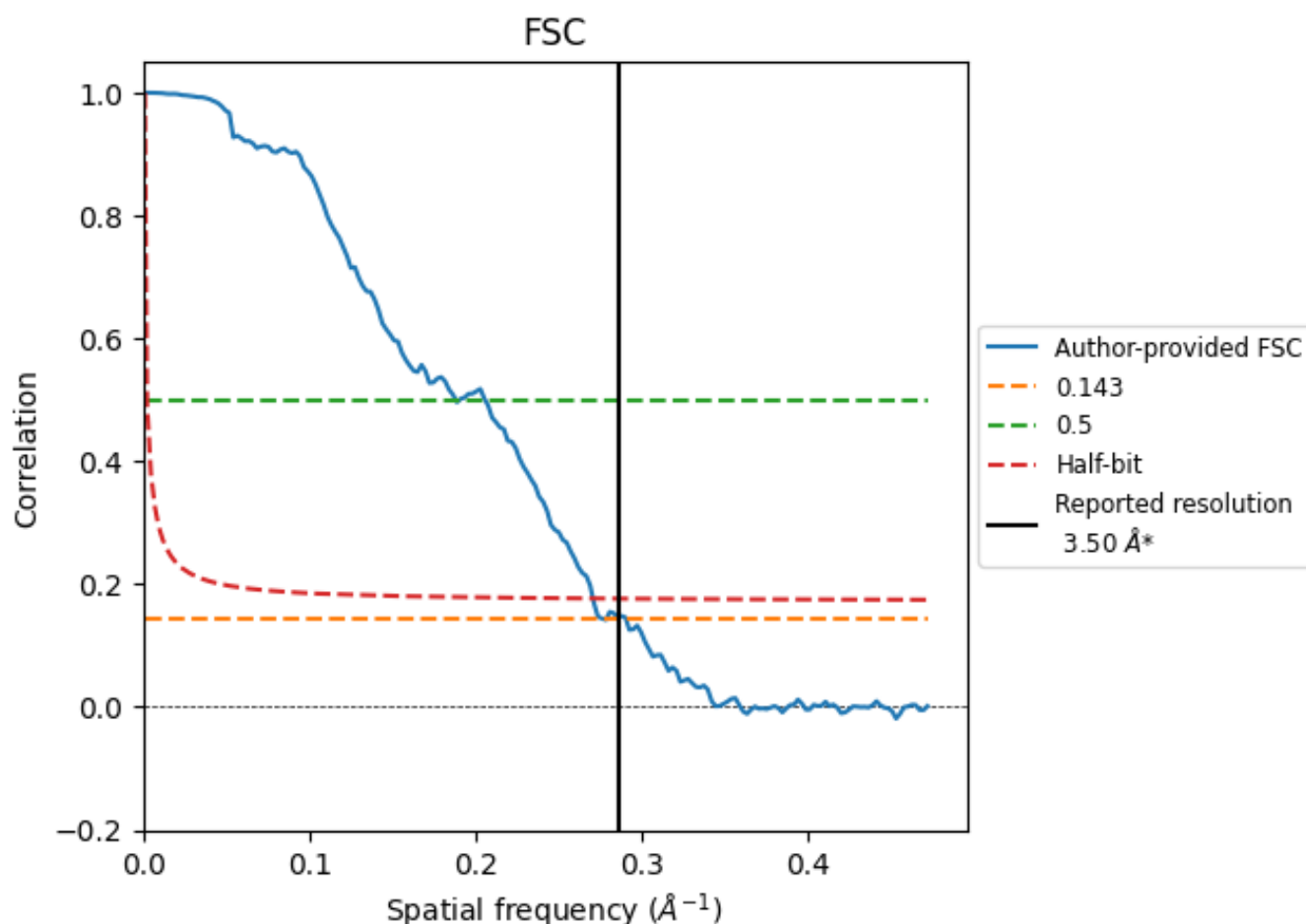


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

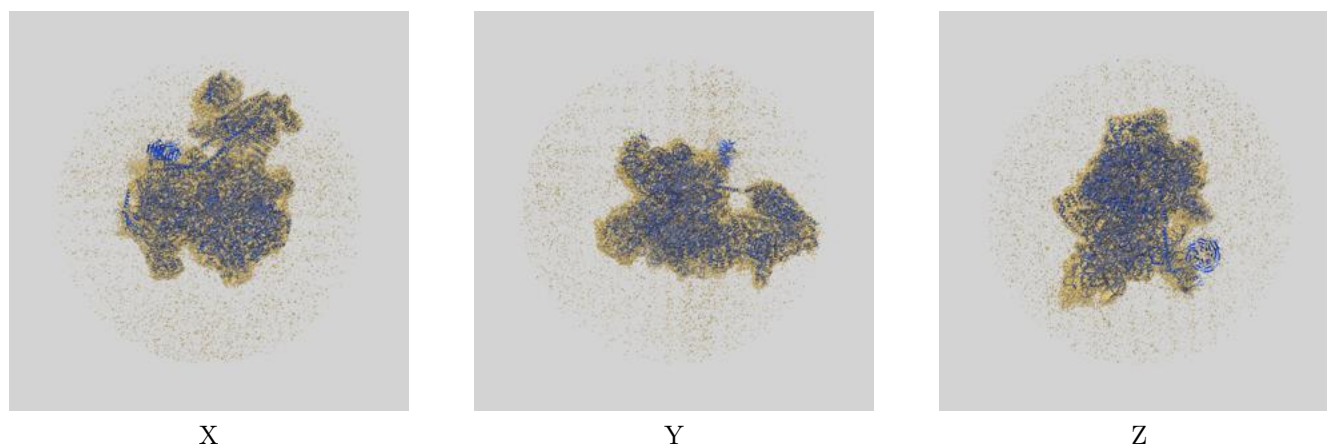
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.60	5.32	3.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

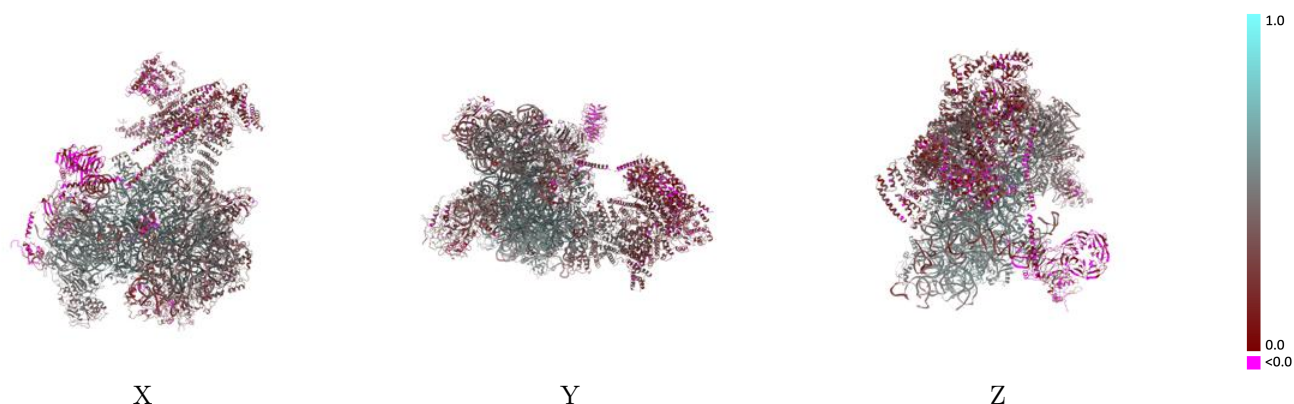
This section contains information regarding the fit between EMDB map EMD-11602 and PDB model 7A09. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



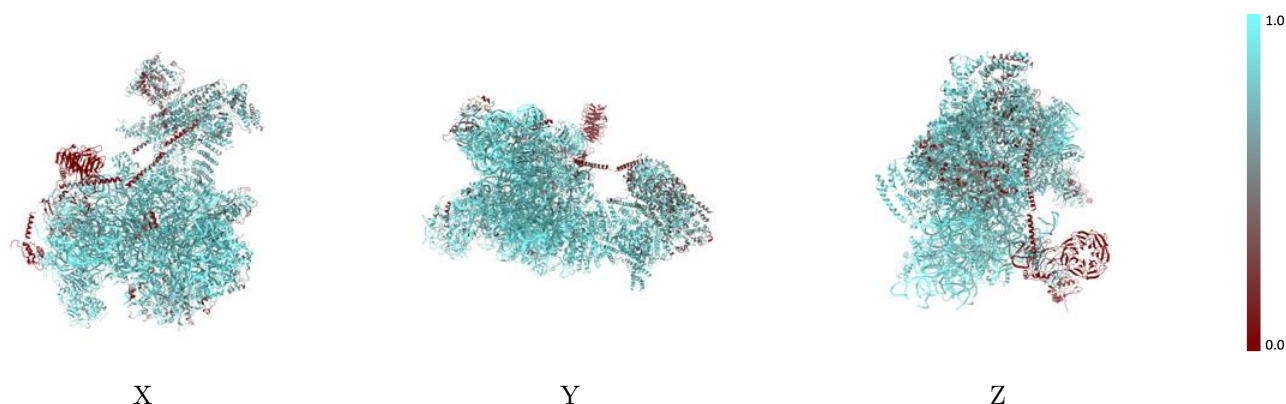
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



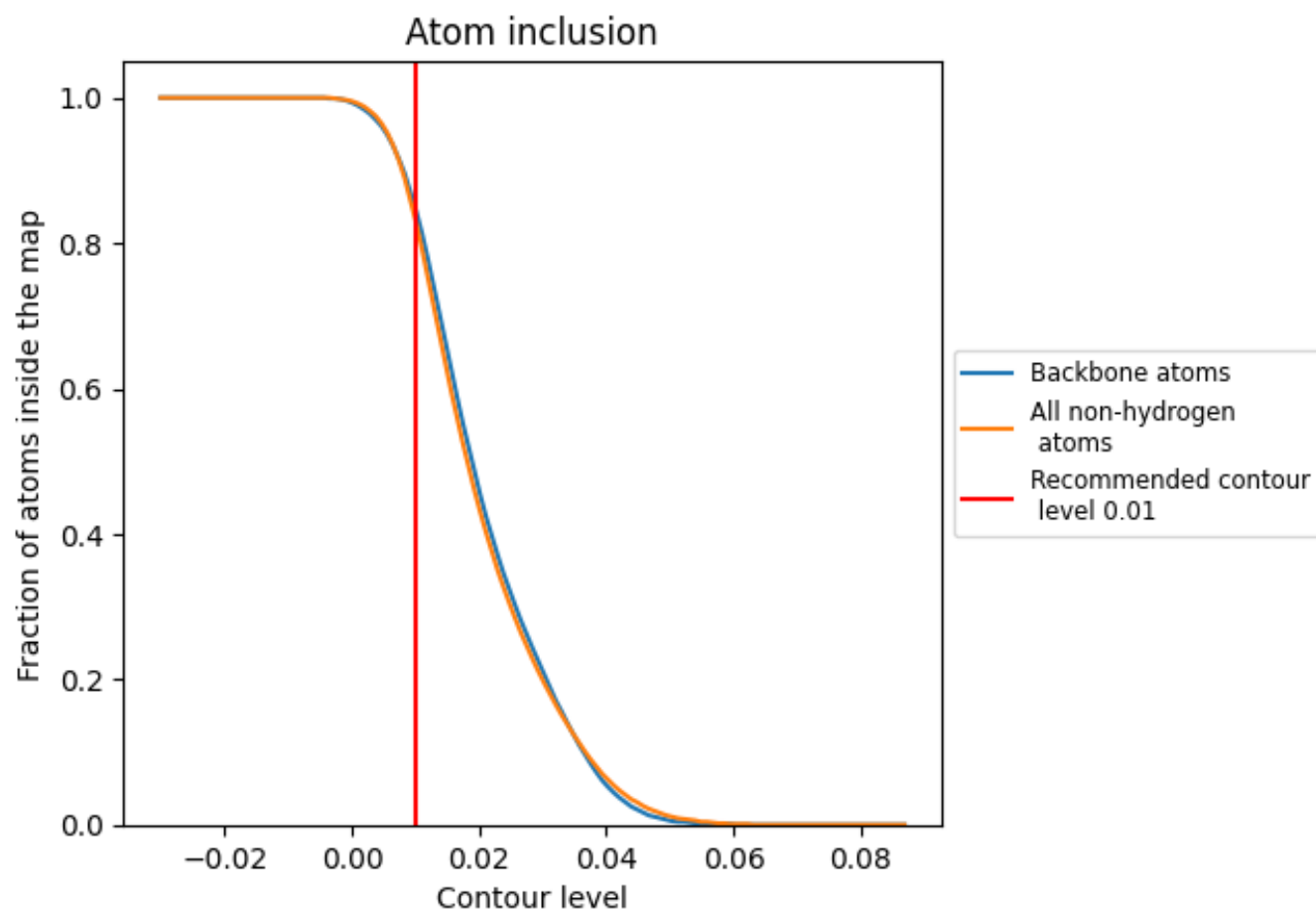
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.3990
2	 0.9680	 0.4800
4	 0.7780	 0.3780
A	 0.7280	 0.3030
B	 0.3860	 0.1700
C	 0.8430	 0.3840
D	 0.9370	 0.5480
E	 0.7770	 0.2550
F	 0.6330	 0.2030
G	 0.8460	 0.4710
H	 0.6510	 0.2120
I	 0.0130	 0.0160
J	 0.8730	 0.4370
K	 0.5400	 0.1930
L	 0.4400	 0.1530
M	 0.6990	 0.2230
N	 0.7120	 0.2910
O	 0.7870	 0.3250
P	 0.8490	 0.3750
Q	 0.9260	 0.5360
R	 0.9250	 0.5260
S	 0.8440	 0.4400
T	 0.9410	 0.5160
U	 0.6040	 0.2410
V	 0.8270	 0.3880
W	 0.9380	 0.5250
X	 0.4280	 0.1410
Y	 0.7720	 0.2760
Z	 0.7590	 0.4040
a	 0.9260	 0.5140
b	 0.8100	 0.4000
c	 0.9320	 0.5300
d	 0.9370	 0.5420
e	 0.8760	 0.4380
f	 0.9320	 0.3740



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Chain	Atom inclusion	Q-score
g	 0.8530	 0.4370
h	 0.7900	 0.4100
i	 0.9340	 0.5180
j	 0.9300	 0.5520
k	 0.8000	 0.3770
l	 0.8480	 0.4420
m	 0.9410	 0.5280
n	 0.9460	 0.5440
o	 0.6790	 0.3310
p	 0.9440	 0.5270
q	 0.9510	 0.5420
r	 0.9350	 0.4860
s	 0.9040	 0.4810
t	 0.9420	 0.5080
u	 0.7620	 0.3280
v	 0.5050	 0.2240
w	 0.8710	 0.4640
x	 0.8940	 0.4100
y	 0.9380	 0.5280
z	 0.9270	 0.5150