



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:11 PM UTC

PDB ID : 6ZON / pdb_00006zon
EMDB ID : EMD-11325
Title : SARS-CoV-2 Nsp1 bound to a human 43S preinitiation ribosome complex - state 1
Authors : Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-07-07
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

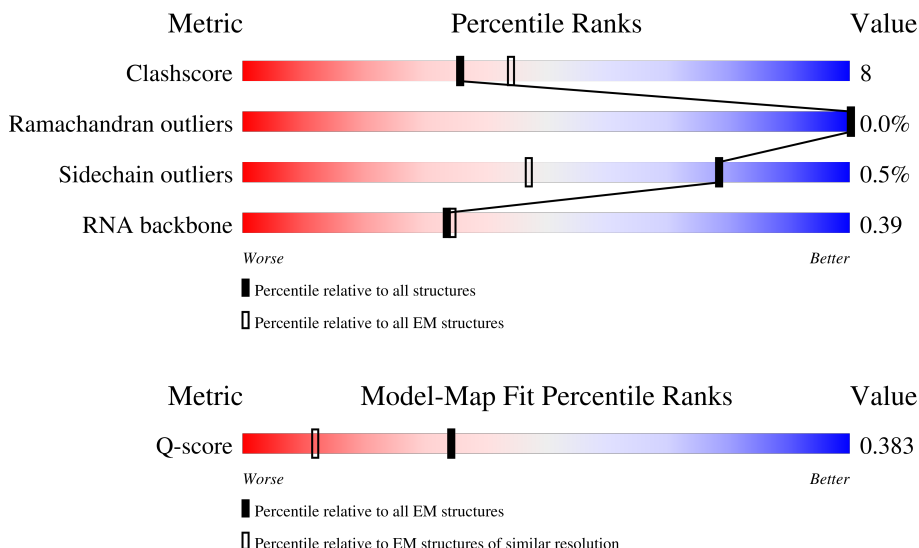
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



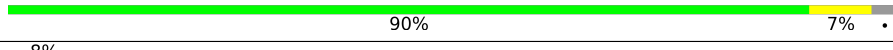
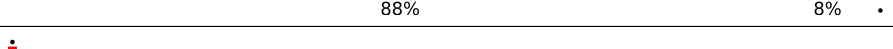
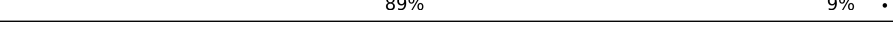
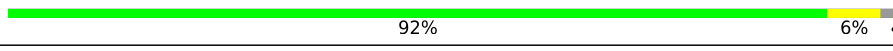
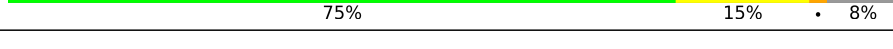
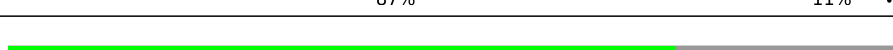
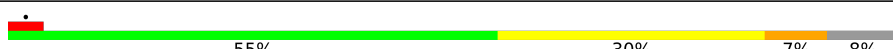
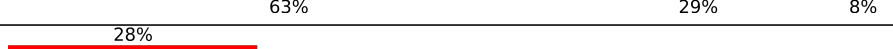
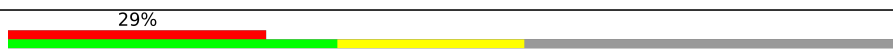
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	

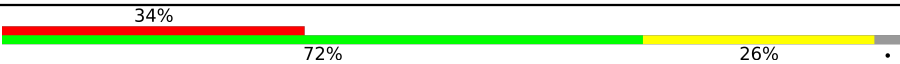
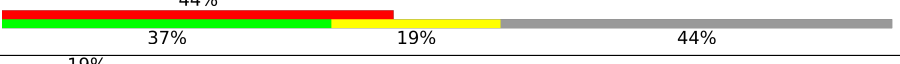
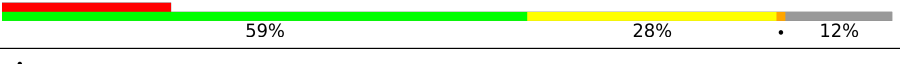
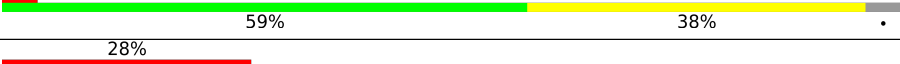
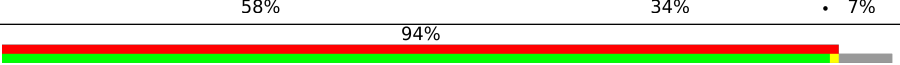
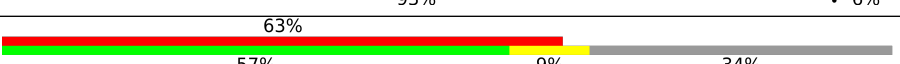
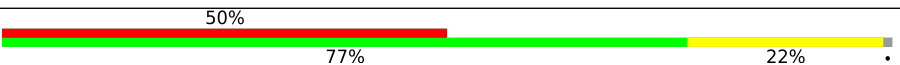
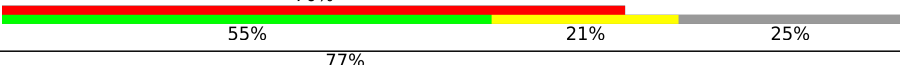
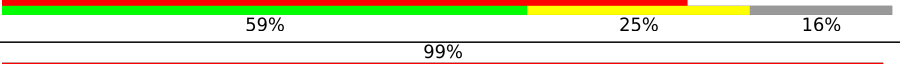
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Mol	Chain	Length	Quality of chain
4	Q	115	
5	q	263	
6	W	25	
7	r	249	
8	s	194	
9	t	208	
10	c	194	
11	n	158	
12	m	151	
13	i	151	
14	y	83	
15	f	130	
16	j	143	
17	z	133	
18	R	84	
19	T	59	
20	2	1868	
21	w	135	
22	g	146	
23	b	243	
24	e	204	
25	u	165	
26	v	132	
27	o	145	
28	k	152	

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Mol	Chain	Length	Quality of chain
29	x	145	
30	h	119	
31	P	125	
32	S	69	
33	l	56	
34	U	156	
35	V	317	
36	I	325	
37	B	814	
38	A	703	
39	C	913	
40	E	445	
41	F	357	
42	H	352	
43	K	218	
44	L	564	
45	M	374	
46	D	548	
47	Y	78	
48	J	180	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 109201 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 S14.

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

- Molecule 14 is a protein called 40S ribosomal protein S21.

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

- Molecule 15 is a protein called 40S ribosomal protein S15a.

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

- Molecule 16 is a protein called 40S ribosomal protein S23.

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

- Molecule 17 is a protein called 40S ribosomal protein S24.

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

- Molecule 18 is a protein called 40S ribosomal protein S27.

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

- Molecule 19 is a protein called 40S ribosomal protein S30.

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

- Molecule 20 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	1721	Total	C	N	O	P	0	0
			36718	16400	6603	12004	1711		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

- Molecule 21 is a protein called 40S ribosomal protein S17.

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

- Molecule 22 is a protein called 40S ribosomal protein S16.

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

- Molecule 23 is a protein called 40S ribosomal protein S3.

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

- Molecule 24 is a protein called 40S ribosomal protein S5.

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

- Molecule 25 is a protein called 40S ribosomal protein S10.

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

- Molecule 26 is a protein called 40S ribosomal protein S12.

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

- Molecule 27 is a protein called 40S ribosomal protein S15.

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

- Molecule 28 is a protein called 40S ribosomal protein S18.

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

- Molecule 29 is a protein called 40S ribosomal protein S19.

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

- Molecule 30 is a protein called 40S ribosomal protein S20.

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

- Molecule 31 is a protein called 40S ribosomal protein S25.

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

- Molecule 32 is a protein called 40S ribosomal protein S28.

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

- Molecule 33 is a protein called 40S ribosomal protein S29.

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

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

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

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

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit I.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A	694	Total	C	N	O	S	0	0
			5394	3385	982	1005	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C	625	Total	C	N	O	S	0	0
			5070	3204	898	933	35		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called Unknown factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Y	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 48 is a protein called Host translation inhibitor Nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	J	30	Total	C	N	O	S	0	0
			244	148	44	51	1		

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

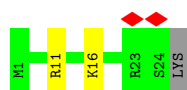
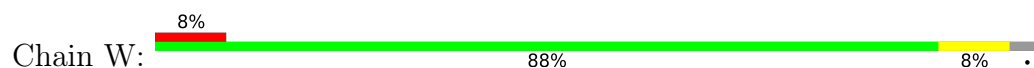
Mol	Chain	Residues	Atoms		AltConf
49	Q	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	U	1	Total	Zn	0
			1	1	



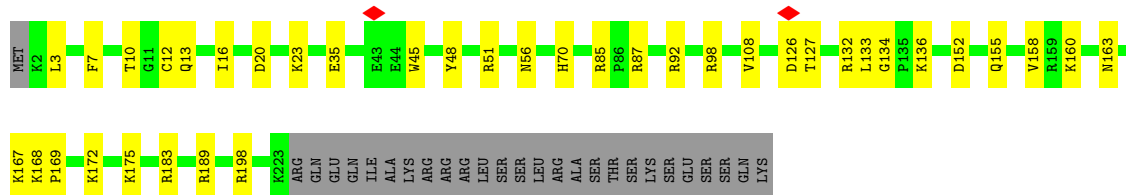
- Molecule 5: 40S ribosomal protein S4, X isoform



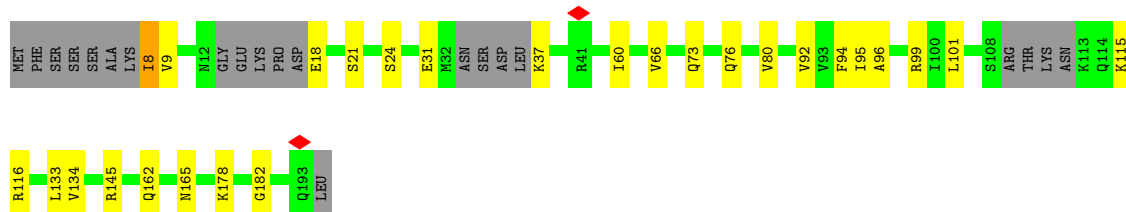
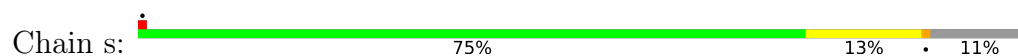
- Molecule 6: 60S ribosomal protein L41



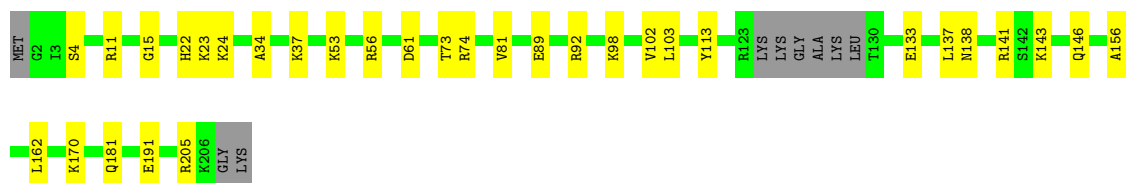
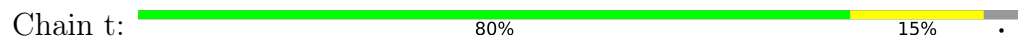
- Molecule 7: 40S ribosomal protein S6

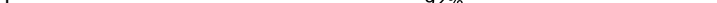


- Molecule 8: 40S ribosomal protein S7



- Molecule 9: 40S ribosomal protein S8

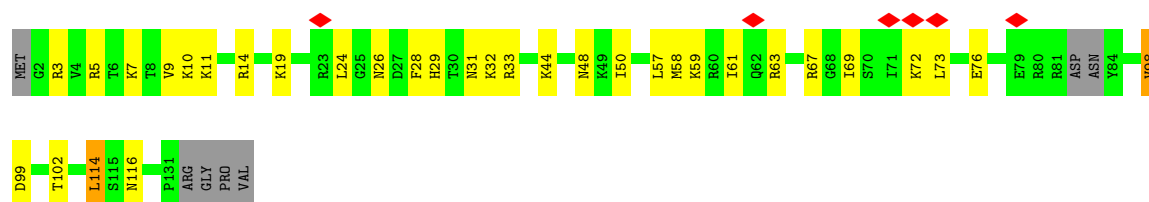


- Chain j:  92% 6%



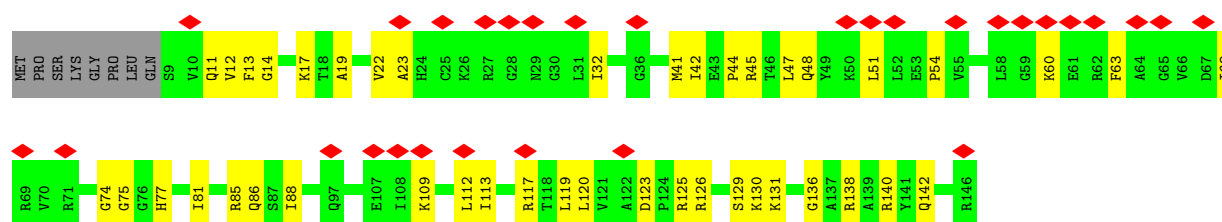
- Molecule 21: 40S ribosomal protein S17

Chain w:  70% 23% 5%



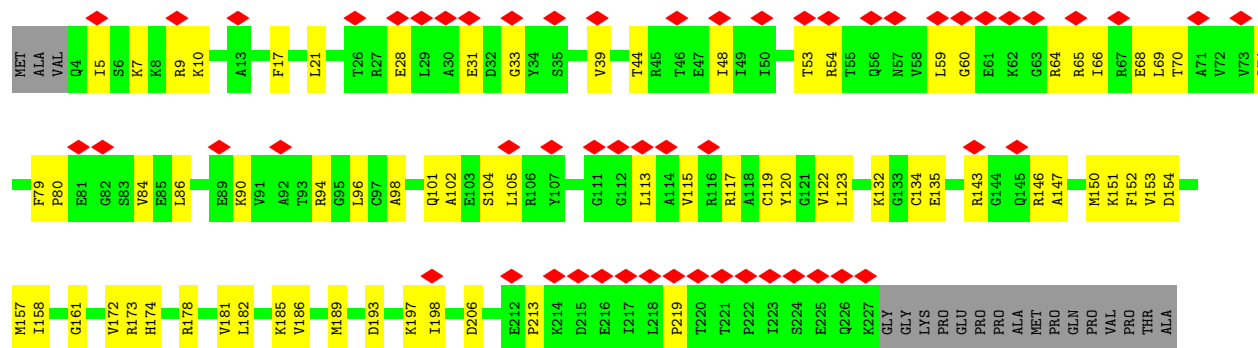
- Molecule 22: 40S ribosomal protein S16

Chain g:  21% 65% 29% 5%



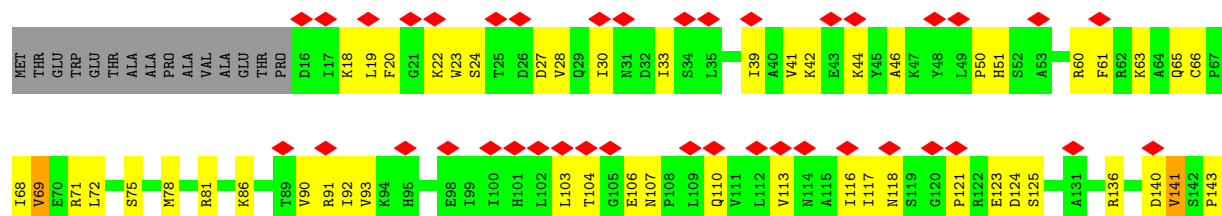
- Molecule 23: 40S ribosomal protein S3

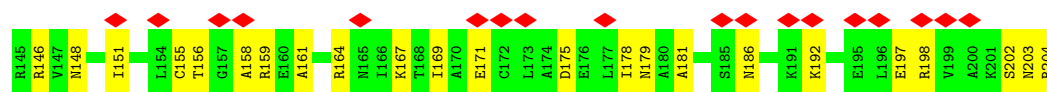
Chain b:  23% 63% 29% 8%



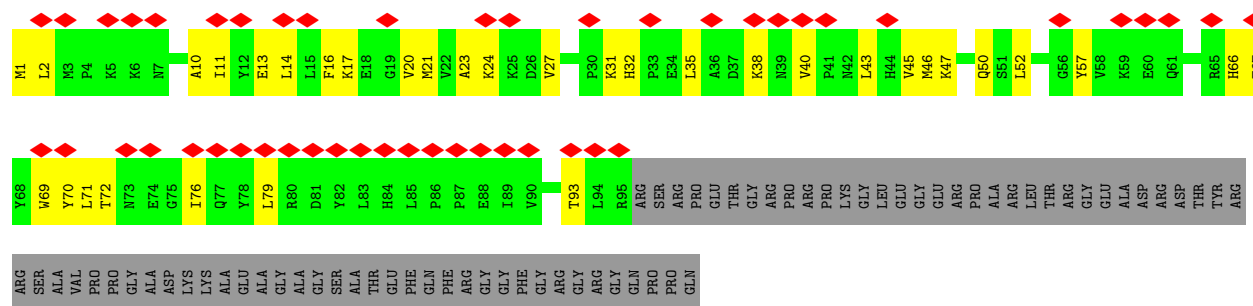
- Molecule 24: 40S ribosomal protein S5

Chain e:  28% 56% 36% 7%

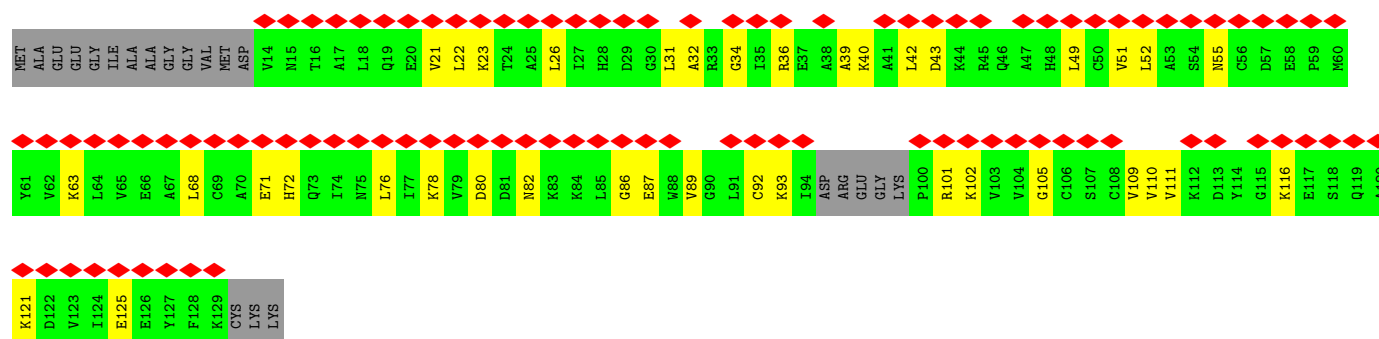
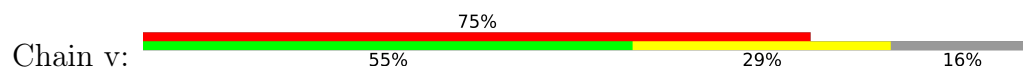




• Molecule 25: 40S ribosomal protein S10



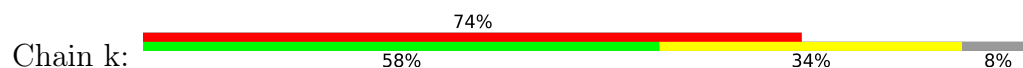
• Molecule 26: 40S ribosomal protein S12

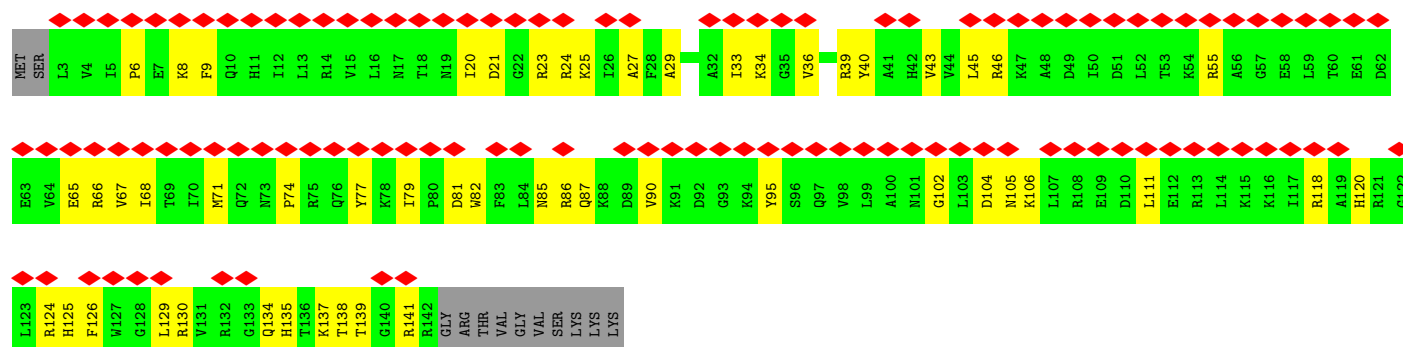


• Molecule 27: 40S ribosomal protein S15

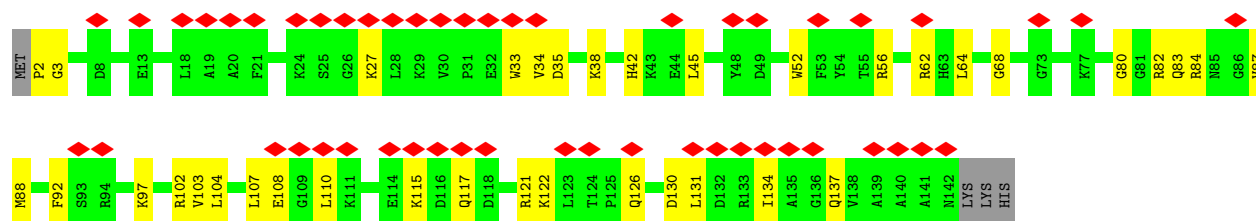


• Molecule 28: 40S ribosomal protein S18

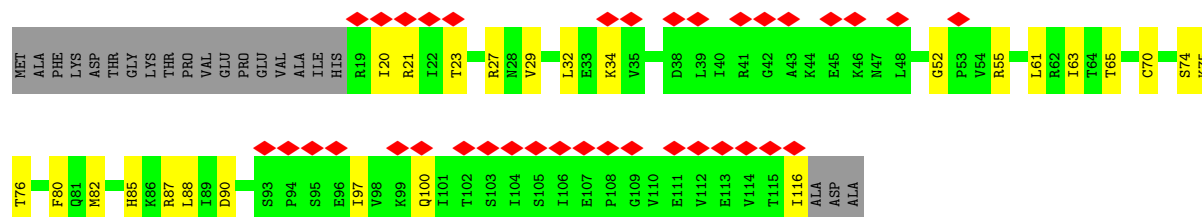




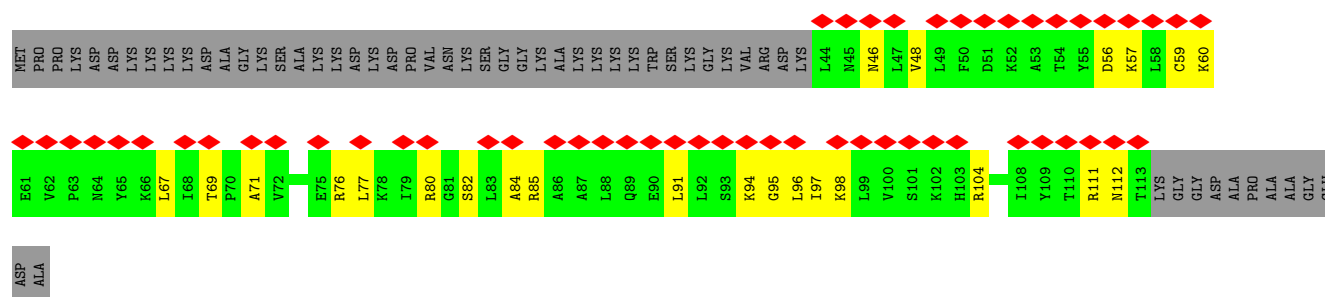
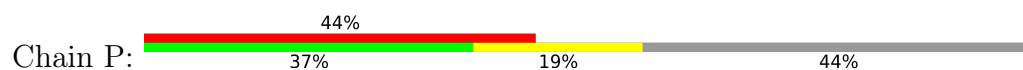
• Molecule 29: 40S ribosomal protein S19



• Molecule 30: 40S ribosomal protein S20



• Molecule 31: 40S ribosomal protein S25



• Molecule 32: 40S ribosomal protein S28

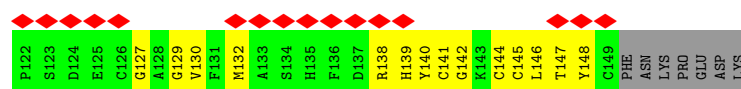
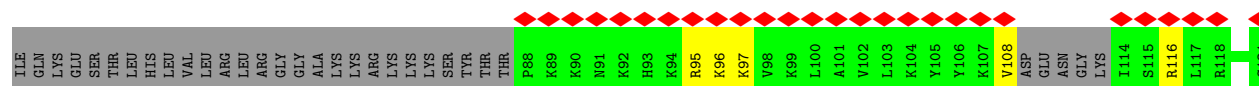
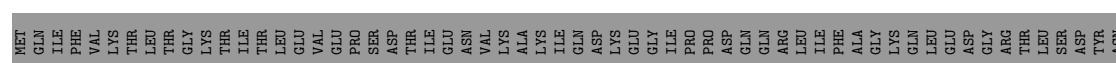




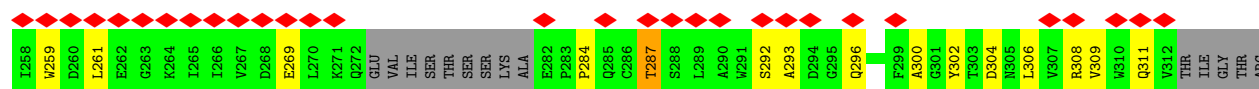
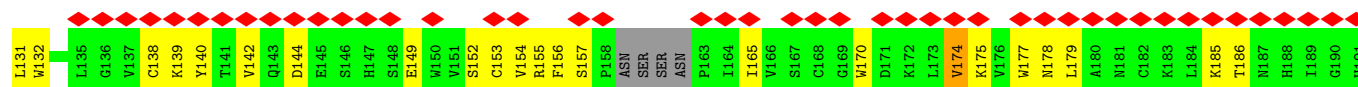
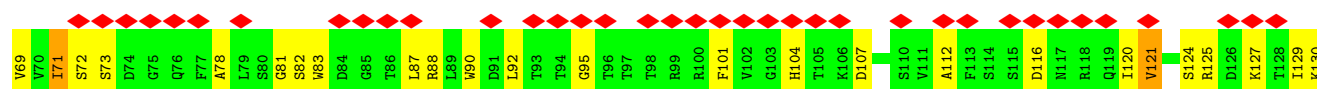
• Molecule 33: 40S ribosomal protein S29



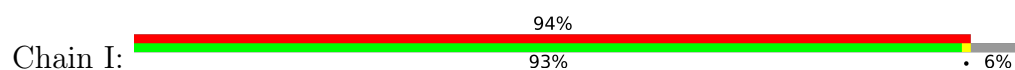
• Molecule 34: Ubiquitin-40S ribosomal protein S27a

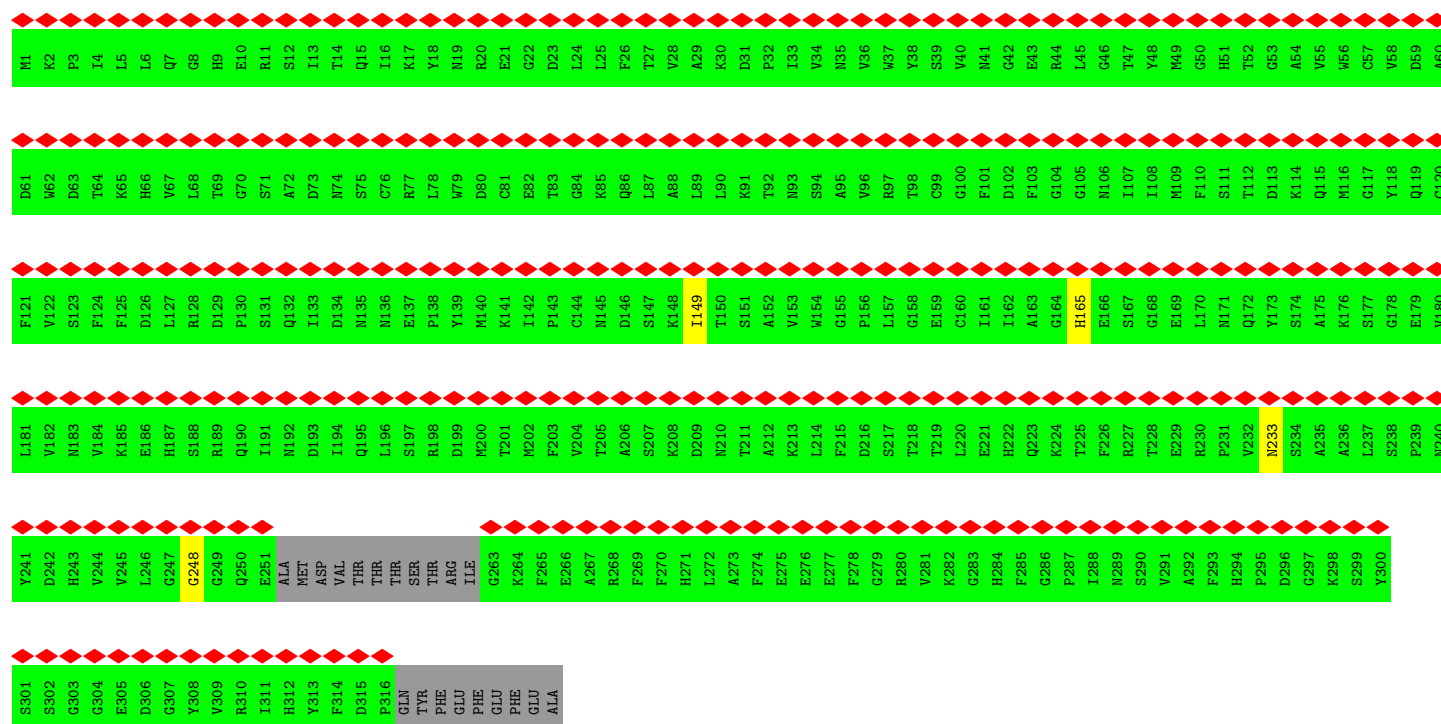


• Molecule 35: Receptor of activated protein C kinase 1

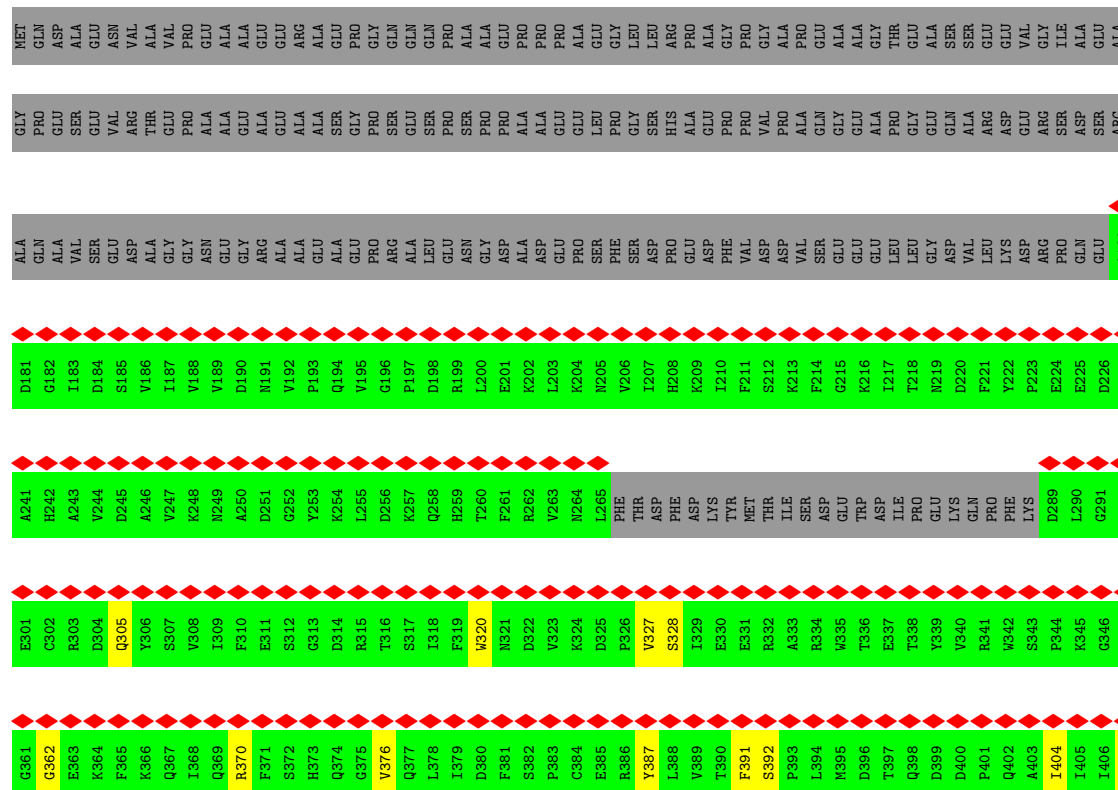


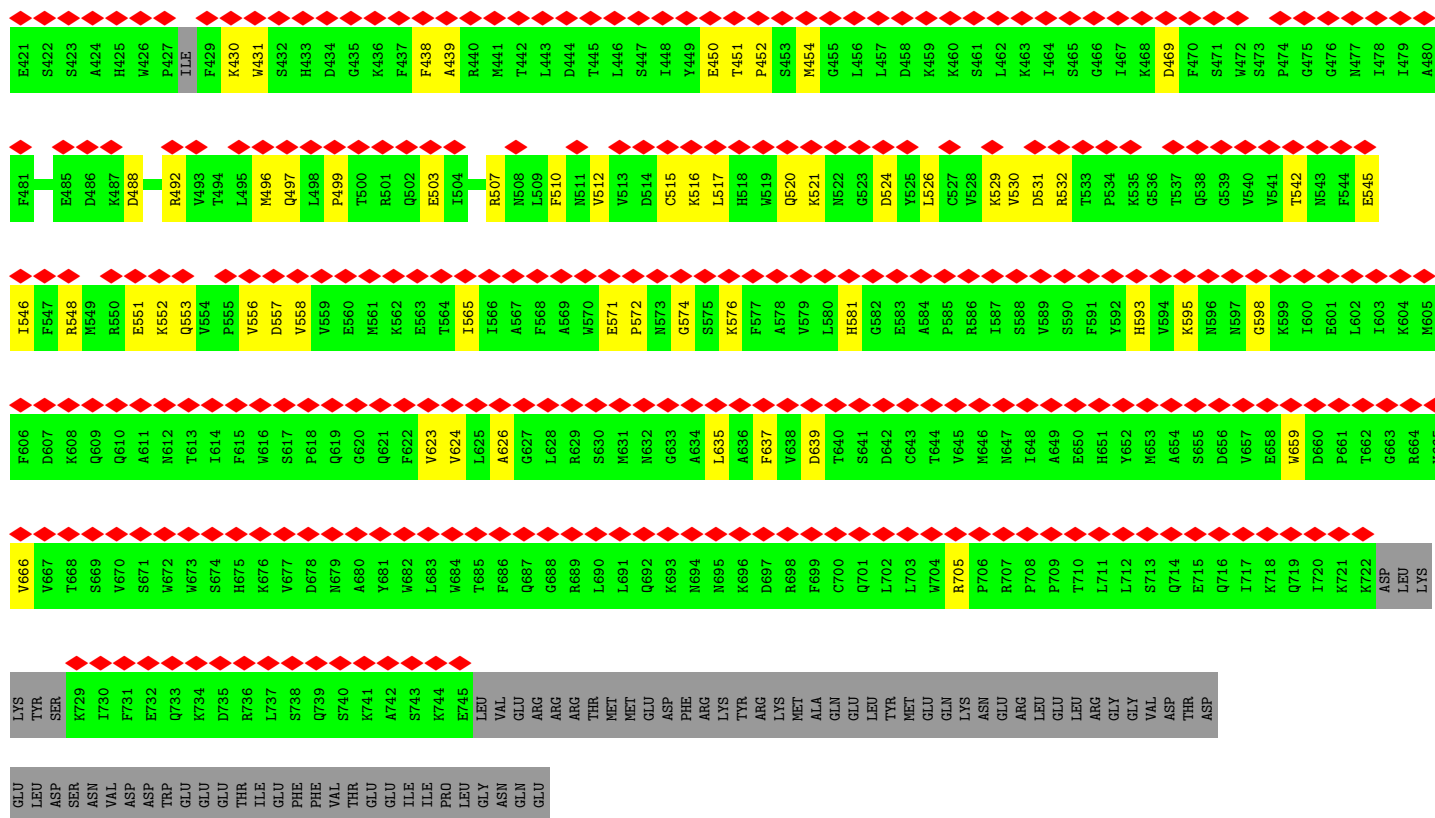
• Molecule 36: Eukaryotic translation initiation factor 3 subunit I



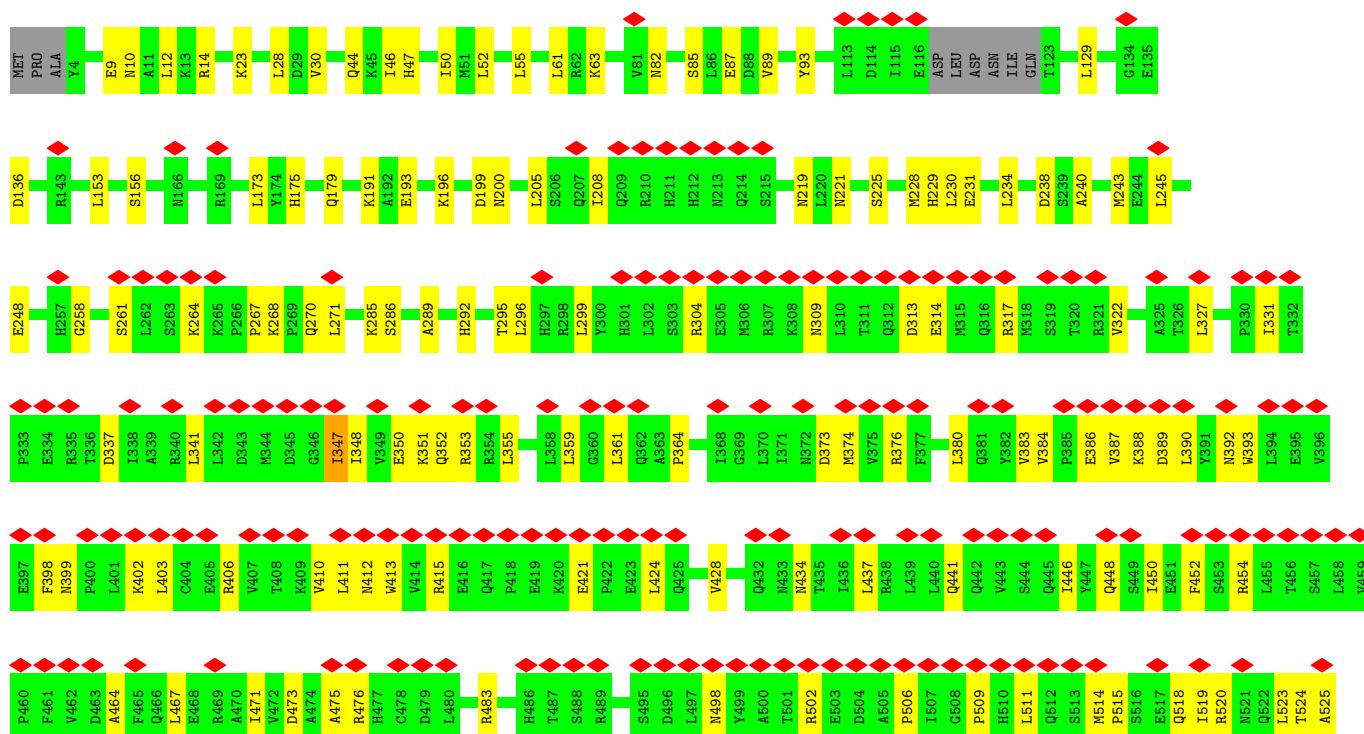
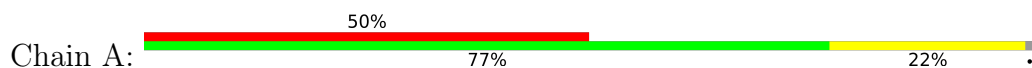


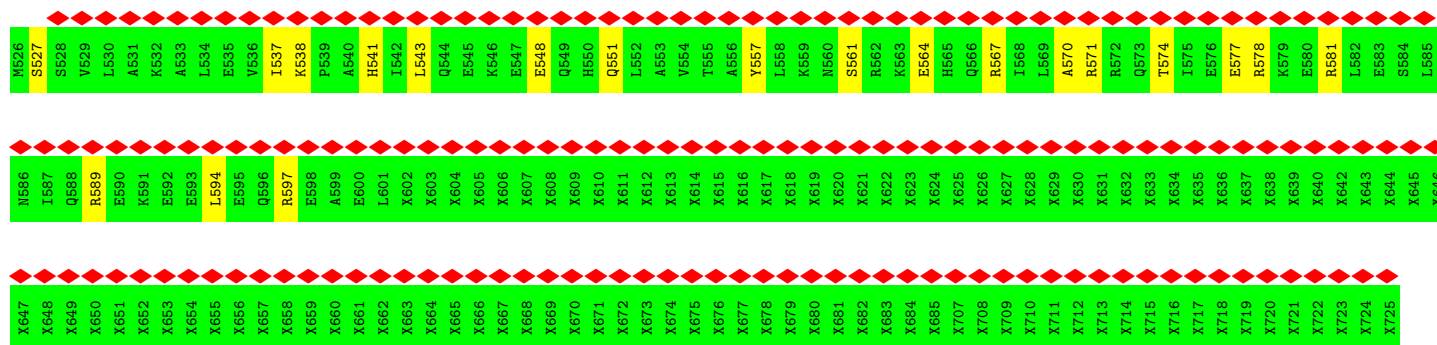
• Molecule 37: Eukaryotic translation initiation factor 3 subunit B



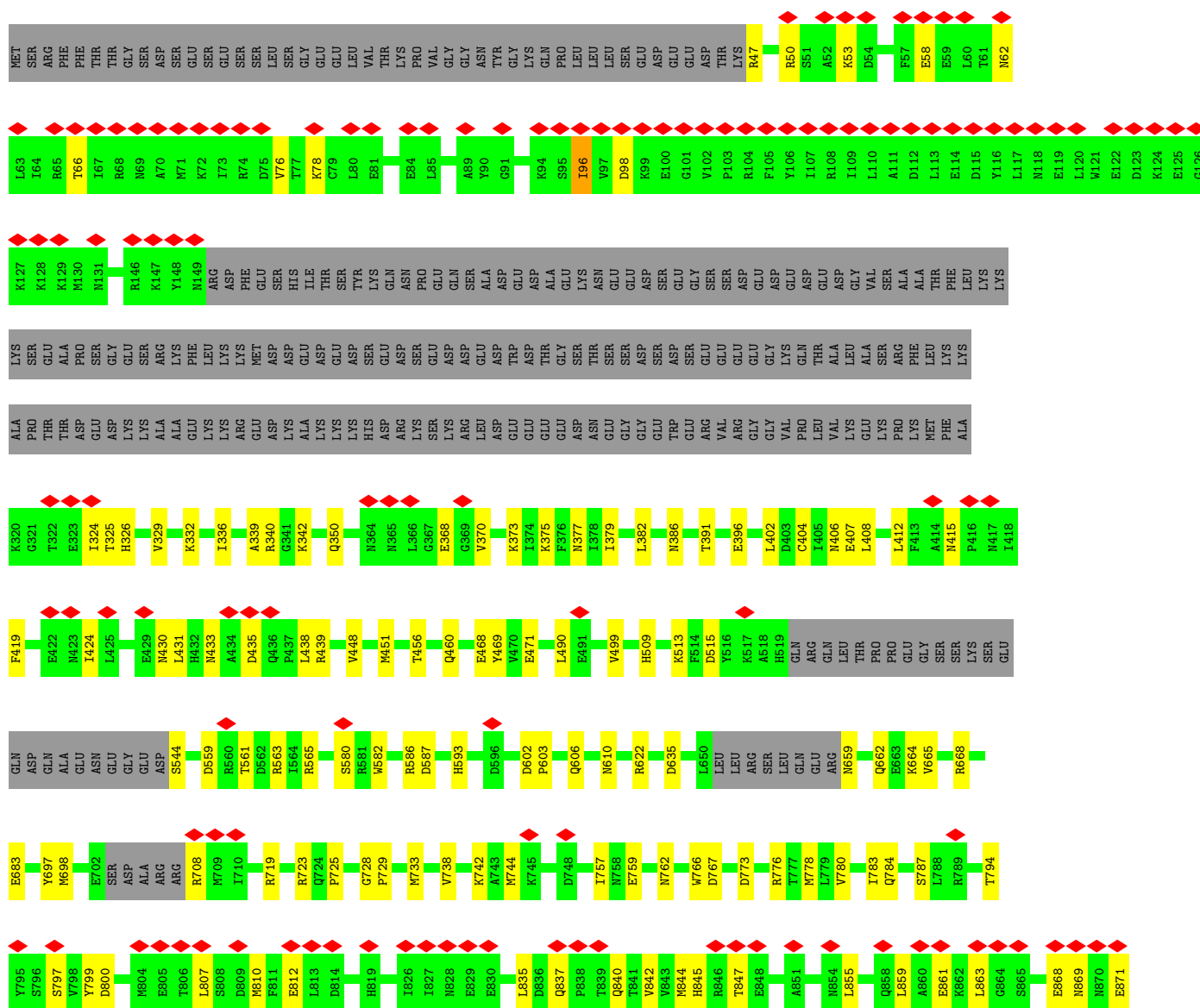


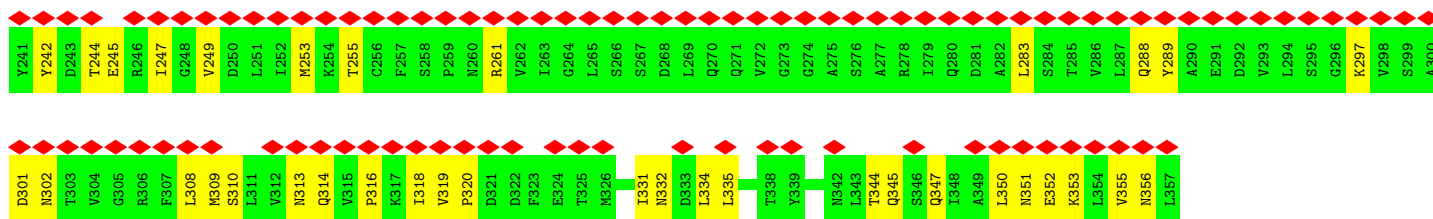
- Molecule 38: Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A



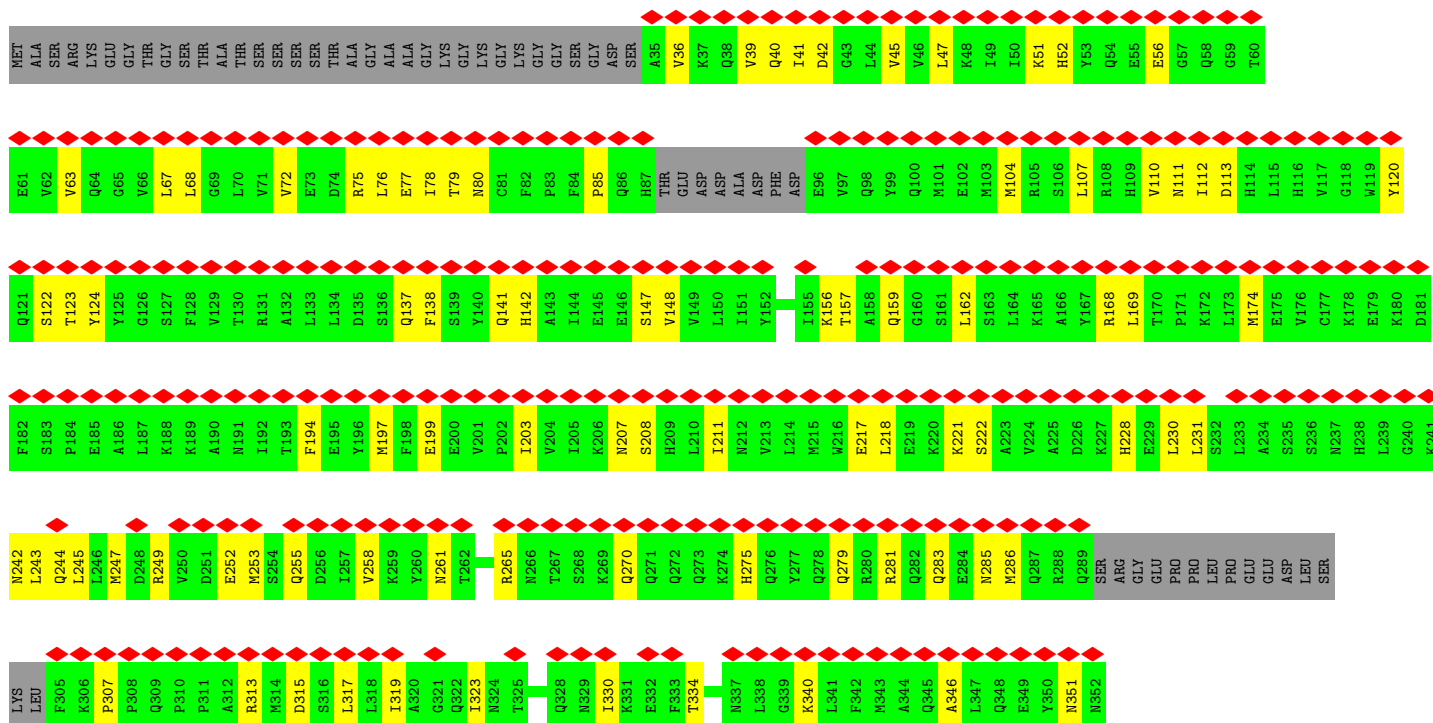
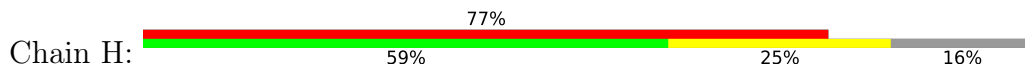


• Molecule 39: Eukaryotic translation initiation factor 3 subunit C

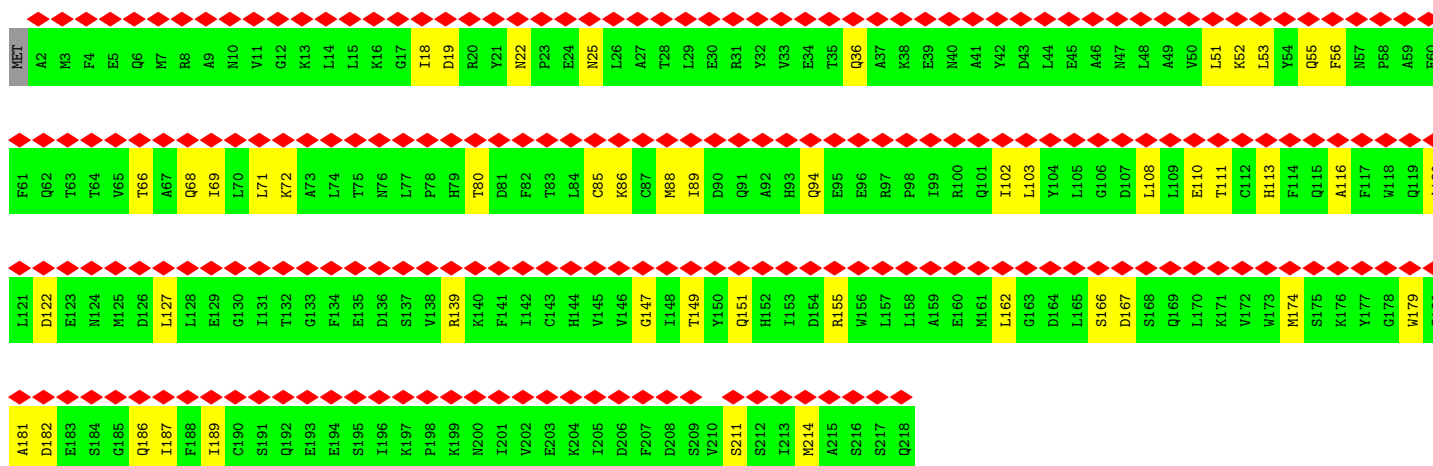
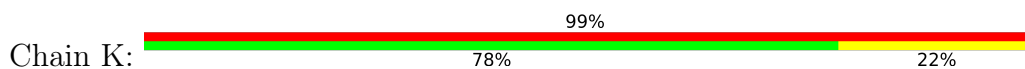




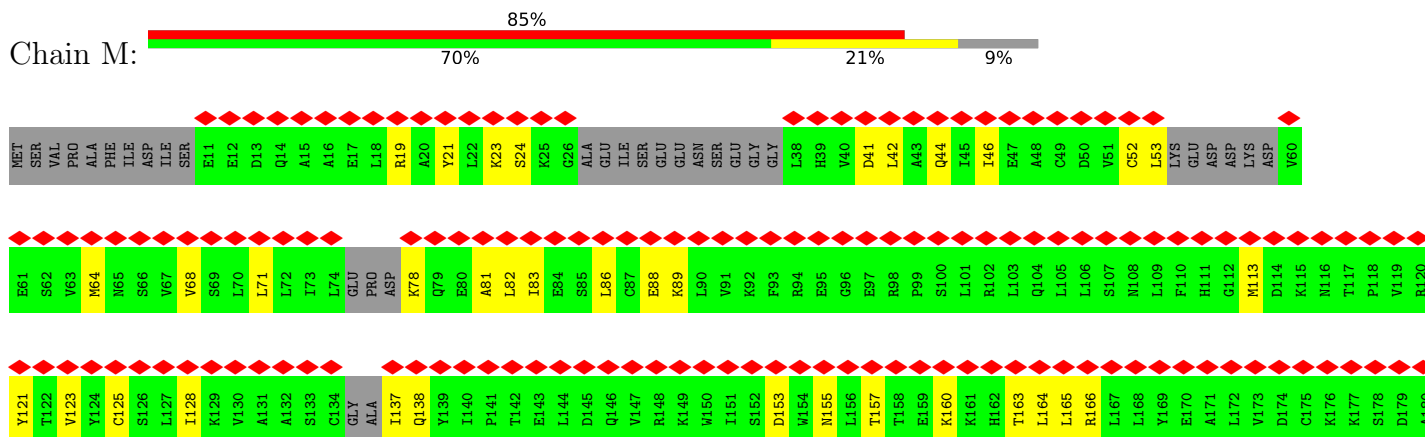
• Molecule 42: Eukaryotic translation initiation factor 3 subunit H

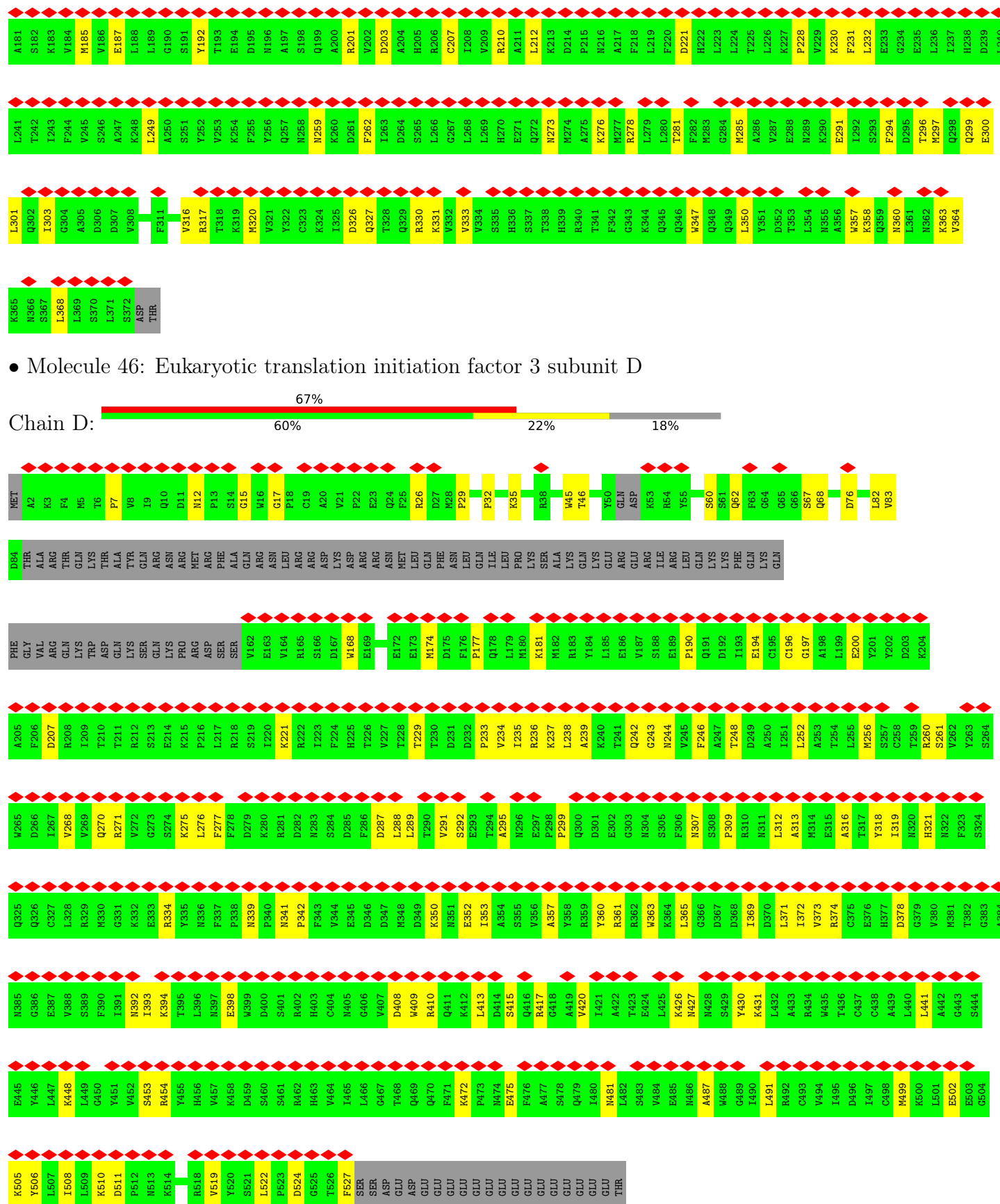


• Molecule 43: Eukaryotic translation initiation factor 3 subunit K



Chain L:

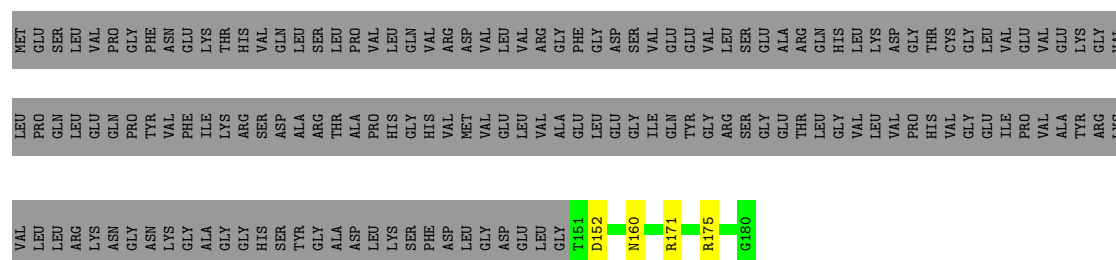




Chain Y: 87% 88% 12%



Chain J: 14% 83%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13928	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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:
ZN

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	0.60	0/1742	0.57	0/2367
2	p	0.55	0/1742	0.58	2/2330 (0.1%)
3	d	0.67	0/1710	0.64	0/2310
4	Q	0.67	0/828	0.68	0/1109
5	q	0.64	0/2073	0.64	2/2791 (0.1%)
6	W	0.45	0/231	0.68	0/294
7	r	0.48	0/1817	0.53	0/2421
8	s	0.48	0/1418	0.57	0/1895
9	t	0.60	0/1666	0.57	0/2223
10	c	0.67	0/1524	0.63	0/2035
11	n	0.67	0/1139	0.59	0/1524
12	m	0.60	0/1226	0.54	0/1649
13	i	0.57	0/951	0.64	0/1275
14	y	0.59	0/631	0.56	0/844
15	f	0.72	0/1051	0.71	1/1406 (0.1%)
16	j	0.64	0/1097	0.63	0/1464
17	z	0.62	0/1016	0.68	2/1349 (0.1%)
18	R	0.60	0/653	0.59	0/876
19	T	0.56	0/356	0.62	0/466
20	2	0.63	0/41057	0.52	2/63985 (0.0%)
21	w	0.34	0/1024	0.65	0/1377
22	g	0.27	0/1117	0.64	0/1494
23	b	0.30	0/1773	0.70	2/2387 (0.1%)
24	e	0.26	0/1516	0.64	0/2037
25	u	0.22	0/823	0.56	0/1111
26	v	0.22	0/870	0.57	0/1168
27	o	0.22	0/999	0.55	0/1336
28	k	0.25	0/1180	0.62	0/1581
29	x	0.19	0/1113	0.50	0/1493
30	h	0.24	0/789	0.56	0/1059
31	P	0.26	0/563	0.60	0/758
32	S	0.32	0/481	0.69	0/643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.30	0/461	0.79	0/612
34	U	0.23	0/474	0.62	0/626
35	V	0.24	0/2369	0.62	2/3221 (0.1%)
36	I	0.12	0/1495	0.34	0/2073
37	B	0.18	0/2981	0.46	0/4115
38	A	0.25	0/4971	0.54	0/6711
39	C	0.27	0/5154	0.56	1/6942 (0.0%)
40	E	0.18	0/3503	0.49	0/4728
41	F	0.20	0/2126	0.54	0/2890
42	H	0.20	0/2458	0.52	0/3313
43	K	0.22	0/1785	0.57	0/2414
44	L	0.24	0/3187	0.64	6/4299 (0.1%)
45	M	0.19	0/2756	0.53	0/3714
46	D	0.23	0/3699	0.55	0/5001
48	J	0.64	0/249	0.65	0/335
All	All	0.49	0/113844	0.56	20/162051 (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
1	a	0	1
8	s	0	1
32	S	0	3
33	I	0	1
35	V	0	1
44	L	0	1
All	All	0	8

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	C	665	VAL	N-CA-C	-7.67	106.42	113.71
44	L	379	PRO	CA-C-N	6.43	133.27	121.70
44	L	379	PRO	C-N-CA	6.43	133.27	121.70
44	L	348	SER	CA-C-N	6.40	133.23	121.70
44	L	348	SER	C-N-CA	6.40	133.23	121.70
17	z	103	SER	CA-C-N	-6.10	111.93	122.79
17	z	103	SER	C-N-CA	-6.10	111.93	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	L	353	THR	CA-C-N	5.92	132.36	121.70
44	L	353	THR	C-N-CA	5.92	132.36	121.70
35	V	174	VAL	CA-C-N	5.72	132.47	121.54
35	V	174	VAL	C-N-CA	5.72	132.47	121.54
5	q	86	PHE	CA-C-N	5.35	131.76	121.54
5	q	86	PHE	C-N-CA	5.35	131.76	121.54
23	b	219	PRO	CA-C-N	5.19	131.46	121.54
23	b	219	PRO	C-N-CA	5.19	131.46	121.54
20	2	1119	A	N9-C1'-C2'	5.17	119.76	112.00
20	2	501	C	C2-N1-C1'	5.12	134.16	118.80
15	f	66	THR	N-CA-C	-5.08	102.26	110.14
2	p	62	LEU	CA-CB-CG	5.04	133.94	116.30
2	p	176	VAL	N-CA-C	-5.04	107.92	112.96

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	L	432	HIS	Peptide
32	S	34	PHE	Peptide
32	S	35	MET	Peptide
32	S	46	VAL	Peptide
35	V	174	VAL	Peptide
1	a	73	ASP	Peptide
33	l	28	HIS	Peptide
8	s	134	VAL	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	18	0
2	p	1715	0	1785	17	0
3	d	1674	0	1764	10	0
4	Q	814	0	863	9	0
5	q	2031	0	2133	11	0
6	W	230	0	276	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	r	1794	0	1942	26	0
8	s	1399	0	1492	17	0
9	t	1638	0	1710	21	0
10	c	1499	0	1618	21	0
11	n	1119	0	1186	8	0
12	m	1202	0	1289	11	0
13	i	939	0	965	13	0
14	y	625	0	628	2	0
15	f	1034	0	1080	12	0
16	j	1080	0	1147	6	0
17	z	999	0	1071	13	0
18	R	640	0	665	7	0
19	T	354	0	388	0	0
20	2	36718	0	18573	317	0
21	w	1011	0	1053	24	0
22	g	1100	0	1166	27	0
23	b	1745	0	1839	47	0
24	e	1495	0	1549	57	0
25	u	799	0	823	26	0
26	v	861	0	895	31	0
27	o	980	0	1025	38	0
28	k	1162	0	1221	36	0
29	x	1094	0	1120	31	0
30	h	780	0	850	18	0
31	P	557	0	610	19	0
32	S	479	0	507	13	0
33	l	450	0	448	20	0
34	U	465	0	483	18	0
35	V	2314	0	2273	73	0
36	I	1497	0	676	2	0
37	B	2966	0	1764	43	0
38	A	5394	0	5062	113	0
39	C	5070	0	5110	85	0
40	E	3437	0	3433	80	0
41	F	2090	0	2092	59	0
42	H	2413	0	2411	70	0
43	K	1750	0	1717	31	0
44	L	3111	0	3085	71	0
45	M	2718	0	2768	51	0
46	D	3617	0	3495	75	0
47	Y	390	0	84	5	0
48	J	244	0	213	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Q	1	0	0	0	0
49	U	1	0	0	0	0
49	l	1	0	0	0	0
All	All	109201	0	90053	1472	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 8.

All (1472) 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)
8:s:8:ILE:N	8:s:24:SER:HG	1.63	0.96
20:2:1652:G:H1	20:2:1672:U:H3	1.15	0.94
20:2:1657:G:H1	20:2:1667:U:H3	1.15	0.93
20:2:536:A:H61	20:2:546:G:H1	1.09	0.91
20:2:536:A:N6	20:2:546:G:H1	1.71	0.89
15:f:2:VAL:N	20:2:1091:C:HO2'	1.76	0.84
20:2:1452:A:C2	20:2:1473:G:N2	2.49	0.79
35:V:87:LEU:HB2	35:V:101:PHE:HB2	1.67	0.76
20:2:1669:G:H5''	22:g:130:LYS:HB3	1.70	0.71
44:L:472:VAL:HB	44:L:511:GLY:HA3	1.72	0.71
20:2:925:G:H1	20:2:1017:U:H3	1.39	0.69
23:b:33:GLY:HA3	23:b:53:THR:HG22	1.74	0.68
20:2:1452:A:H61	20:2:1473:G:H1'	1.58	0.67
24:e:19:LEU:HB3	24:e:23:TRP:HB2	1.77	0.67
20:2:949:G:H1	20:2:977:C:H5	1.41	0.67
20:2:698:G:H1	20:2:732:U:H3	1.43	0.67
24:e:175:ASP:O	24:e:179:ASN:HB2	1.95	0.67
40:E:14:LEU:HA	40:E:217:TRP:HE1	1.59	0.67
20:2:1760:G:N3	20:2:1773:C:N4	2.42	0.66
46:D:200:GLU:OE2	46:D:334:ARG:NH1	2.28	0.66
2:p:173:THR:O	2:p:177:GLN:HB2	1.96	0.66
8:s:76:GLN:HE21	8:s:94:PHE:HB2	1.60	0.66
40:E:129:ASP:O	40:E:132:TYR:CD2	2.48	0.66
20:2:1608:U:O4	20:2:1632:G:N2	2.29	0.65
24:e:50:PRO:HG2	24:e:90:VAL:HG23	1.79	0.65
35:V:131:LEU:HB3	35:V:139:LYS:HE2	1.79	0.65
39:C:869:ASN:HD21	42:H:258:VAL:HB	1.61	0.65
41:F:242:TYR:H	41:F:245:GLU:HB2	1.62	0.65
20:2:1412:C:H2'	20:2:1413:G:H8	1.61	0.65
20:2:1330:G:H8	20:2:1492:U:H5''	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:u:21:MET:HB3	25:u:69:TRP:HB2	1.79	0.65
39:C:697:TYR:HH	39:C:708:ARG:N	1.95	0.65
46:D:233:PRO:HG2	46:D:342:PRO:HB2	1.76	0.65
40:E:8:THR:HA	46:D:7:PRO:HB3	1.79	0.64
43:K:149:THR:HA	44:L:503:THR:HA	1.78	0.64
20:2:1272:C:HO2'	33:l:2:GLY:N	1.94	0.64
35:V:61:GLY:O	35:V:88:ARG:NH2	2.31	0.64
40:E:298:CYS:HA	40:E:302:ASN:HD22	1.63	0.64
41:F:210:ARG:HG3	42:H:217:GLU:HG3	1.78	0.64
35:V:205:SER:HG	35:V:246:TYR:HH	1.46	0.64
15:f:102:ILE:H	15:f:113:HIS:HD2	1.43	0.64
21:w:29:HIS:HD2	21:w:33:ARG:HH21	1.45	0.64
27:o:98:ASN:HB3	27:o:120:SER:HB2	1.80	0.63
35:V:234:ASP:HB2	35:V:252:THR:HB	1.80	0.63
27:o:105:VAL:HA	28:k:118:ARG:HH22	1.64	0.63
28:k:20:ILE:HD11	28:k:33:ILE:HG13	1.81	0.63
22:g:109:LYS:HD2	22:g:113:ILE:HD11	1.81	0.63
35:V:217:MET:HE3	35:V:229:THR:HG23	1.80	0.63
20:2:1256:G:H5'	33:l:29:GLY:HA3	1.80	0.62
23:b:134:CYS:SG	23:b:135:GLU:N	2.73	0.62
9:t:133:GLU:O	9:t:137:LEU:HB2	1.99	0.62
38:A:268:LYS:HG3	38:A:270:GLN:H	1.62	0.62
39:C:430:ASN:HB2	39:C:438:LEU:HA	1.81	0.62
10:c:80:ARG:NH2	20:2:818:A:OP1	2.31	0.62
23:b:120:TYR:HA	23:b:123:LEU:HB2	1.80	0.62
15:f:71:LYS:NZ	20:2:1156:U:OP1	2.33	0.62
20:2:1302:G:N1	20:2:1307:U:N3	2.45	0.62
39:C:563:ARG:NH2	39:C:602:ASP:OD2	2.32	0.62
20:2:1374:C:H1'	20:2:1465:A:H8	1.65	0.62
32:S:40:ARG:HH21	32:S:42:ILE:HG21	1.64	0.61
42:H:249:ARG:HH11	42:H:319:ILE:HG22	1.65	0.61
38:A:286:SER:HA	39:C:728:GLY:HA2	1.82	0.61
40:E:144:TYR:H	40:E:179:MET:HE2	1.65	0.61
46:D:378:ASP:HB2	46:D:393:ILE:H	1.64	0.61
20:2:1661:A:OP1	33:l:19:ARG:NH2	2.33	0.61
22:g:112:LEU:HB3	22:g:120:LEU:HD11	1.83	0.61
17:z:29:HIS:NE2	17:z:69:THR:OG1	2.28	0.61
20:2:1719:A:N6	20:2:1814:G:O2'	2.34	0.61
28:k:21:ASP:H	28:k:24:ARG:HH21	1.49	0.60
46:D:233:PRO:HA	46:D:236:ARG:HD2	1.82	0.60
20:2:1286:G:N2	20:2:1312:G:O2'	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1373:C:HO2'	20:2:1465:A:HO2'	1.50	0.60
37:B:565:ILE:HA	37:B:581:HIS:HA	1.82	0.60
42:H:346:ALA:HB1	45:M:360:ASN:HB3	1.83	0.60
46:D:243:GLY:HA3	46:D:372:ILE:HD11	1.83	0.60
4:Q:77:CYS:O	4:Q:81:SER:HB3	2.02	0.60
20:2:1491:G:H21	30:h:70:CYS:HB3	1.67	0.60
24:e:63:LYS:O	24:e:71:ARG:NH1	2.35	0.60
35:V:230:LEU:HD11	35:V:261:LEU:HD21	1.83	0.60
7:r:13:GLN:HE22	20:2:153:G:H21	1.50	0.60
26:v:55:ASN:HD21	26:v:82:ASN:HB2	1.67	0.60
45:M:297:MET:HA	45:M:300:GLU:HB2	1.82	0.60
13:i:67:ASP:OD1	13:i:67:ASP:N	2.35	0.59
20:2:928:G:H1	20:2:1013:U:H3	1.49	0.59
24:e:24:SER:O	24:e:107:ASN:ND2	2.35	0.59
24:e:125:SER:HB2	24:e:136:ARG:HB3	1.84	0.59
45:M:166:ARG:NH1	45:M:192:TYR:OH	2.35	0.59
1:a:205:ARG:HE	1:a:210:ILE:HD13	1.67	0.59
44:L:187:ILE:HG13	44:L:191:ILE:HD12	1.84	0.59
24:e:63:LYS:HB2	24:e:71:ARG:HH22	1.68	0.59
30:h:80:PHE:HB3	33:l:52:PHE:HB3	1.83	0.59
40:E:29:LYS:NZ	40:E:320:VAL:O	2.35	0.59
10:c:39:ASN:ND2	20:2:643:A:OP1	2.36	0.59
21:w:99:ASP:OD1	21:w:99:ASP:N	2.33	0.59
20:2:1520:G:H21	27:o:126:VAL:HG11	1.68	0.59
38:A:355:LEU:HD12	39:C:725:PRO:HB2	1.85	0.59
23:b:59:LEU:HA	23:b:66:ILE:HB	1.83	0.59
1:a:85:ARG:NH1	1:a:203:PHE:O	2.36	0.59
45:M:113:MET:HE1	45:M:123:VAL:HG21	1.84	0.59
24:e:75:SER:O	24:e:159:ARG:NH2	2.35	0.59
41:F:97:VAL:HG11	42:H:51:LYS:HB2	1.85	0.59
20:2:1756:C:N4	20:2:1775:U:OP2	2.36	0.59
24:e:104:THR:HG23	24:e:106:GLU:H	1.68	0.59
45:M:125:CYS:HA	45:M:128:ILE:HD12	1.84	0.59
45:M:165:LEU:HD21	45:M:187:GLU:HG3	1.84	0.59
20:2:952:G:O2'	20:2:953:C:O2	2.20	0.58
20:2:1398:G:H1'	35:V:88:ARG:HH12	1.68	0.58
38:A:515:PRO:HA	38:A:518:GLN:HB2	1.84	0.58
40:E:376:ARG:HH22	44:L:482:THR:HG22	1.67	0.58
8:s:73:GLN:HA	8:s:76:GLN:HB2	1.84	0.58
28:k:65:GLU:HA	28:k:68:ILE:HD12	1.86	0.58
35:V:59:LEU:HD21	35:V:92:LEU:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:14:ARG:HB2	38:A:30:VAL:HG11	1.85	0.58
41:F:106:TYR:O	41:F:109:ARG:NH1	2.35	0.58
20:2:1269:G:H1	20:2:1513:C:H42	1.51	0.58
44:L:534:LYS:HZ1	44:L:538:ARG:HH22	1.51	0.58
20:2:1338:G:OP1	30:h:76:THR:OG1	2.21	0.58
42:H:252:GLU:HG2	42:H:255:GLN:HE21	1.68	0.58
46:D:392:ASN:HD21	46:D:394:LYS:HE2	1.68	0.58
23:b:31:GLU:O	23:b:54:ARG:NH1	2.37	0.58
26:v:21:VAL:HG13	26:v:22:LEU:HG	1.86	0.58
26:v:36:ARG:NH1	34:U:129:GLY:O	2.31	0.58
37:B:520:GLN:HB3	37:B:524:ASP:H	1.68	0.58
38:A:230:LEU:HG	38:A:271:LEU:HD13	1.85	0.58
39:C:373:LYS:O	39:C:377:ASN:ND2	2.37	0.58
46:D:288:LEU:HB3	46:D:313:ALA:HB1	1.85	0.58
20:2:1231:C:H42	20:2:1527:C:H42	1.50	0.58
20:2:1455:A:OP1	21:w:5:ARG:NH2	2.36	0.58
38:A:87:GLU:HG2	38:A:173:LEU:HD22	1.84	0.58
44:L:465:LYS:HE2	44:L:516:ALA:HB3	1.86	0.58
20:2:1302:G:N2	20:2:1307:U:O4	2.36	0.58
30:h:97:ILE:O	30:h:100:GLN:NE2	2.35	0.58
46:D:234:VAL:HG13	46:D:237:LYS:HE3	1.86	0.58
46:D:363:TRP:HB2	46:D:371:LEU:HB3	1.86	0.58
7:r:183:ARG:NH2	20:2:317:C:OP2	2.35	0.58
20:2:952:G:H1	20:2:974:C:H5	1.52	0.58
23:b:154:ASP:OD1	23:b:154:ASP:N	2.36	0.58
35:V:44:LYS:HB2	35:V:56:GLN:HB2	1.84	0.58
7:r:198:ARG:NH1	20:2:126:G:OP2	2.36	0.58
20:2:1612:G:H5'	27:o:18:ARG:HH22	1.67	0.58
23:b:172:VAL:HG22	23:b:185:LYS:HG3	1.86	0.58
38:A:476:ARG:NH2	39:C:794:THR:O	2.37	0.58
7:r:172:LYS:NZ	20:2:67:C:OP2	2.35	0.57
17:z:103:SER:HB3	17:z:107:ARG:HH21	1.68	0.57
20:2:1243:U:O2	20:2:1517:G:N2	2.37	0.57
20:2:1270:G:O6	20:2:1512:C:N4	2.37	0.57
20:2:1292:C:N3	34:U:138:ARG:NH2	2.45	0.57
20:2:1647:A:OP1	22:g:138:ARG:NH1	2.35	0.57
35:V:154:VAL:O	35:V:155:ARG:NH1	2.36	0.57
45:M:357:TRP:HA	45:M:360:ASN:HB2	1.85	0.57
20:2:1552:G:H1	20:2:1558:C:H5''	1.69	0.57
28:k:34:LYS:NZ	28:k:104:ASP:OD1	2.38	0.57
42:H:141:GLN:NE2	42:H:174:MET:SD	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1452:A:H2	20:2:1473:G:N2	2.02	0.57
20:2:1679:A:H2'	24:e:60:ARG:HG3	1.86	0.57
41:F:193:GLU:HG2	41:F:195:PRO:HD3	1.85	0.57
4:Q:2:THR:N	20:2:1199:A:OP1	2.37	0.57
20:2:601:G:OP1	48:J:171:ARG:NH1	2.36	0.57
46:D:316:ALA:HA	46:D:319:ILE:HD12	1.86	0.57
20:2:1234:C:H4'	20:2:1246:A:H61	1.69	0.57
20:2:1589:A:N3	20:2:1653:U:O2'	2.38	0.57
31:P:56:ASP:O	31:P:60:LYS:HB3	2.05	0.57
31:P:67:LEU:O	31:P:76:ARG:NH2	2.38	0.57
35:V:15:ASN:ND2	35:V:37:ASP:OD2	2.38	0.57
38:A:589:ARG:NH1	42:H:142:HIS:O	2.38	0.57
2:p:78:GLU:OE1	38:A:10:ASN:ND2	2.38	0.57
20:2:1038:U:O2'	39:C:47:ARG:NH2	2.37	0.57
20:2:1242:U:H4'	20:2:1243:U:H5'	1.86	0.57
39:C:593:HIS:NE2	46:D:32:PRO:O	2.36	0.57
43:K:116:ALA:HA	43:K:120:ALA:HB3	1.86	0.57
23:b:197:LYS:HG3	23:b:198:ILE:HG23	1.87	0.57
35:V:129:ILE:O	35:V:140:TYR:OH	2.23	0.57
38:A:196:LYS:O	38:A:200:ASN:ND2	2.38	0.57
17:z:102:THR:O	17:z:106:GLN:NE2	2.38	0.57
20:2:537:C:N4	20:2:540:U:O2	2.38	0.57
20:2:1782:G:H2'	20:2:1784:G:H1'	1.87	0.57
25:u:23:ALA:HB3	25:u:67:PHE:HB2	1.85	0.57
16:j:68:LYS:NZ	20:2:617:G:OP2	2.34	0.57
22:g:123:ASP:OD2	22:g:125:ARG:NH1	2.36	0.57
33:l:21:CYS:HA	33:l:30:LEU:HD11	1.84	0.57
38:A:351:LYS:HG2	39:C:725:PRO:HB3	1.85	0.57
43:K:89:ILE:HD13	43:K:94:GLN:HE21	1.69	0.57
20:2:198:U:O2'	20:2:203:G:N2	2.38	0.57
38:A:314:GLU:HA	38:A:317:ARG:HB2	1.87	0.57
46:D:256:MET:HB3	46:D:487:ALA:HB1	1.87	0.57
33:l:10:HIS:HD2	33:l:12:ARG:HG2	1.69	0.56
7:r:132:ARG:O	20:2:168:C:O2'	2.24	0.56
8:s:145:ARG:NH1	15:f:49:GLU:OE2	2.37	0.56
38:A:359:LEU:HD22	38:A:361:LEU:HD22	1.86	0.56
1:a:128:ARG:NH2	1:a:151:ASP:O	2.38	0.56
5:q:240:ARG:NH2	20:2:844:U:OP1	2.36	0.56
12:m:99:ARG:NH2	12:m:119:GLU:OE2	2.37	0.56
20:2:1314:U:OP2	26:v:102:LYS:NZ	2.38	0.56
20:2:1316:C:H5'	25:u:2:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1569:A:OP1	29:x:97:LYS:NZ	2.36	0.56
20:2:1593:C:OP2	31:P:104:ARG:NH2	2.36	0.56
20:2:1614:A:OP2	27:o:42:ARG:NH1	2.38	0.56
25:u:27:VAL:HG13	25:u:43:LEU:HD13	1.87	0.56
38:A:44:GLN:H	38:A:47:HIS:HD2	1.51	0.56
40:E:49:ASN:HA	40:E:73:LYS:HZ1	1.70	0.56
41:F:283:LEU:HD13	45:M:358:LYS:HA	1.87	0.56
45:M:78:LYS:HZ1	45:M:81:ALA:HB3	1.70	0.56
4:Q:52:ASP:OD2	13:i:121:ARG:NH1	2.39	0.56
7:r:85:ARG:O	7:r:87:ARG:NH1	2.39	0.56
9:t:89:GLU:OE1	9:t:92:ARG:NH1	2.37	0.56
20:2:536:A:N1	20:2:546:G:N2	2.53	0.56
20:2:1256:G:N2	33:l:30:LEU:O	2.38	0.56
20:2:1259:A:H62	20:2:1518:C:H2'	1.70	0.56
20:2:1542:C:OP1	29:x:62:ARG:NE	2.39	0.56
21:w:28:PHE:O	21:w:32:LYS:HB2	2.04	0.56
40:E:80:GLN:HA	40:E:83:GLN:HE21	1.71	0.56
7:r:136:LYS:NZ	7:r:175:LYS:O	2.38	0.56
9:t:141:ARG:HH11	9:t:146:GLN:HE22	1.52	0.56
20:2:587:A:H5'	20:2:592:C:H41	1.71	0.56
20:2:1275:G:O2'	20:2:1321:G:N2	2.37	0.56
28:k:82:TRP:O	28:k:87:GLN:NE2	2.39	0.56
35:V:37:ASP:OD1	35:V:37:ASP:N	2.37	0.56
41:F:93:ARG:HB2	41:F:130:GLU:HA	1.88	0.56
46:D:408:ASP:OD1	46:D:410:ARG:NH1	2.35	0.56
23:b:157:MET:HG2	23:b:189:MET:HB2	1.86	0.56
27:o:18:ARG:HD2	28:k:90:VAL:HA	1.88	0.56
28:k:25:LYS:O	28:k:29:ALA:N	2.34	0.56
30:h:55:ARG:HB3	30:h:87:ARG:HG2	1.85	0.56
35:V:20:GLN:NE2	35:V:153:CYS:SG	2.78	0.56
37:B:576:LYS:HA	37:B:593:HIS:HA	1.88	0.56
39:C:606:GLN:O	39:C:610:ASN:ND2	2.39	0.56
41:F:221:MET:SD	41:F:221:MET:N	2.78	0.56
28:k:25:LYS:HA	28:k:55:ARG:HA	1.87	0.56
30:h:20:ILE:HG13	30:h:116:ILE:HD12	1.87	0.56
38:A:231:GLU:HA	38:A:234:LEU:HB2	1.87	0.56
38:A:412:ASN:HA	38:A:415:ARG:HB2	1.88	0.56
44:L:527:MET:HA	44:L:530:ILE:HD12	1.87	0.56
20:2:1532:C:O2'	20:2:1601:A:N1	2.39	0.56
20:2:1597:C:OP2	31:P:85:ARG:NH2	2.38	0.56
38:A:12:LEU:HG	38:A:50:ILE:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:72:C:OP2	20:2:74:G:N2	2.39	0.56
20:2:1512:C:H5''	33:l:12:ARG:HH11	1.71	0.56
24:e:123:GLU:HA	24:e:140:ASP:HA	1.86	0.56
25:u:13:GLU:O	25:u:17:LYS:HB2	2.06	0.56
38:A:537:ILE:HD12	41:F:289:TYR:HB2	1.88	0.56
42:H:40:GLN:HB3	42:H:77:GLU:HA	1.88	0.56
46:D:76:ASP:OD1	46:D:76:ASP:N	2.38	0.56
7:r:152:ASP:OD2	7:r:155:GLN:NE2	2.39	0.55
10:c:113:GLN:OE1	10:c:154:GLN:NE2	2.39	0.55
20:2:1416:C:H1'	29:x:3:GLY:HA2	1.88	0.55
20:2:1454:A:OP2	21:w:3:ARG:NH1	2.39	0.55
28:k:27:ALA:HB2	28:k:45:LEU:HD13	1.87	0.55
30:h:21:ARG:HD2	30:h:88:LEU:HD13	1.87	0.55
37:B:407:TRP:HA	37:B:415:LYS:H	1.71	0.55
39:C:759:GLU:HA	39:C:762:ASN:HB2	1.87	0.55
43:K:211:SER:HA	43:K:214:MET:HG2	1.88	0.55
37:B:548:ARG:NH2	37:B:595:LYS:O	2.39	0.55
41:F:318:ILE:O	42:H:351:ASN:ND2	2.39	0.55
32:S:31:ARG:NH2	32:S:41:SER:O	2.39	0.55
37:B:520:GLN:HG2	37:B:524:ASP:HB2	1.88	0.55
38:A:205:LEU:HA	38:A:208:ILE:HD12	1.88	0.55
38:A:538:LYS:HB3	38:A:543:LEU:HD11	1.89	0.55
7:r:12:CYS:SG	7:r:127:THR:OG1	2.64	0.55
11:n:114:SER:OG	11:n:116:CYS:SG	2.64	0.55
20:2:627:U:H4'	20:2:628:A:H5'	1.87	0.55
20:2:1546:G:N2	20:2:1670:C:O2	2.39	0.55
21:w:69:ILE:HG21	21:w:73:LEU:HD12	1.87	0.55
28:k:137:LYS:HG2	28:k:138:THR:HG23	1.88	0.55
40:E:317:SER:O	40:E:321:ASN:ND2	2.40	0.55
42:H:80:ASN:ND2	42:H:113:ASP:O	2.30	0.55
42:H:217:GLU:HG2	42:H:221:LYS:HD3	1.89	0.55
42:H:270:GLN:HG2	42:H:307:PRO:HA	1.87	0.55
20:2:1338:G:N3	20:2:1490:G:N2	2.54	0.55
34:U:127:GLY:H	34:U:130:VAL:HB	1.71	0.55
37:B:431:TRP:HA	37:B:438:PHE:HA	1.89	0.55
20:2:1657:G:N2	20:2:1667:U:O2	2.32	0.55
21:w:114:LEU:HD22	21:w:116:ASN:HB2	1.89	0.55
35:V:35:SER:OG	35:V:36:ARG:N	2.39	0.55
44:L:461:ARG:HH21	44:L:501:VAL:HG21	1.72	0.55
46:D:373:VAL:HG11	46:D:441:LEU:HD22	1.89	0.55
8:s:60:ILE:HB	8:s:92:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:o:62:LYS:HA	27:o:65:LYS:HE2	1.88	0.55
39:C:431:LEU:O	39:C:433:ASN:ND2	2.40	0.55
39:C:561:THR:HG22	39:C:563:ARG:H	1.71	0.55
42:H:194:PHE:HA	42:H:197:MET:HE2	1.88	0.55
46:D:190:PRO:O	46:D:361:ARG:NH2	2.39	0.55
24:e:61:PHE:HB2	32:S:51:ARG:HH21	1.71	0.55
42:H:80:ASN:HD22	42:H:112:ILE:HG22	1.70	0.55
3:d:196:ILE:HB	3:d:223:TYR:HB2	1.88	0.55
20:2:1295:A:OP1	27:o:62:LYS:NZ	2.37	0.55
9:t:11:ARG:NH1	9:t:15:GLY:O	2.38	0.55
20:2:1292:C:O2	34:U:138:ARG:NE	2.37	0.55
26:v:31:LEU:HD13	26:v:89:VAL:HG13	1.88	0.55
26:v:92:CYS:HB2	26:v:101:ARG:HH12	1.72	0.55
27:o:50:ARG:HG3	27:o:52:LYS:H	1.72	0.55
27:o:101:THR:OG1	27:o:103:ASN:ND2	2.40	0.55
39:C:837:GLN:O	39:C:840:GLN:NE2	2.40	0.55
39:C:871:GLU:OE1	40:E:414:ARG:NH1	2.40	0.55
41:F:198:ILE:HD11	41:F:215:ALA:HB1	1.89	0.55
9:t:22:HIS:HB3	20:2:433:A:H5''	1.89	0.54
23:b:68:GLU:HG3	25:u:93:THR:HG21	1.89	0.54
24:e:179:ASN:HD21	24:e:186:ASN:HB3	1.72	0.54
38:A:564:GLU:OE2	41:F:261:ARG:NH2	2.40	0.54
9:t:73:THR:O	9:t:74:ARG:NH1	2.40	0.54
22:g:60:LYS:HD2	22:g:63:PHE:HD2	1.72	0.54
23:b:158:ILE:HG12	23:b:189:MET:HE3	1.90	0.54
39:C:869:ASN:OD1	42:H:261:ASN:ND2	2.40	0.54
45:M:19:ARG:NH1	45:M:44:GLN:OE1	2.41	0.54
5:q:153:LEU:O	5:q:174:LYS:NZ	2.37	0.54
20:2:1399:C:H42	20:2:1447:G:H1	1.55	0.54
20:2:1592:C:H5''	24:e:91:ARG:HH21	1.73	0.54
20:2:1608:U:OP1	28:k:134:GLN:NE2	2.39	0.54
11:n:20:LYS:NZ	20:2:223:C:OP1	2.40	0.54
20:2:1585:U:O2'	20:2:1587:G:OP2	2.25	0.54
21:w:7:LYS:O	21:w:11:LYS:HB3	2.07	0.54
26:v:51:VAL:HB	26:v:109:VAL:HB	1.90	0.54
38:A:384:VAL:HG12	38:A:386:GLU:H	1.72	0.54
41:F:355:VAL:HG13	42:H:313:ARG:HH21	1.72	0.54
44:L:494:LYS:HZ1	44:L:498:LYS:HG3	1.73	0.54
38:A:373:ASP:HA	38:A:376:ARG:HE	1.72	0.54
41:F:92:VAL:HB	41:F:237:VAL:HG23	1.90	0.54
42:H:253:MET:HE3	42:H:323:ILE:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:K:68:GLN:HG2	43:K:127:LEU:HD11	1.89	0.54
10:c:107:GLU:O	10:c:113:GLN:NE2	2.40	0.54
28:k:23:ARG:NH1	31:P:46:ASN:O	2.41	0.54
28:k:86:ARG:HD2	28:k:106:LYS:HD3	1.87	0.54
30:h:61:LEU:HB2	30:h:82:MET:HB3	1.90	0.54
39:C:664:LYS:O	39:C:668:ARG:NH1	2.40	0.54
15:f:6:VAL:HG12	15:f:34:ILE:HD11	1.90	0.54
20:2:1533:A:O3'	24:e:81:ARG:NH1	2.41	0.54
20:2:1617:G:O6	27:o:40:ARG:NH2	2.37	0.54
20:2:1648:G:N2	20:2:1675:A:O5'	2.40	0.54
27:o:98:ASN:HD21	27:o:100:LYS:HG2	1.73	0.54
38:A:347:ILE:HA	38:A:350:GLU:HB3	1.90	0.54
40:E:135:ALA:HA	40:E:138:GLN:HB2	1.90	0.54
42:H:230:LEU:O	42:H:340:LYS:NZ	2.37	0.54
8:s:101:LEU:O	8:s:116:ARG:NH1	2.41	0.54
13:i:36:SER:OG	13:i:37:PHE:N	2.40	0.54
24:e:50:PRO:HB3	24:e:69:VAL:HG22	1.89	0.54
27:o:98:ASN:HD22	27:o:122:THR:HA	1.73	0.54
41:F:211:MET:N	41:F:211:MET:SD	2.79	0.54
45:M:327:GLN:O	45:M:330:ARG:NH2	2.40	0.54
46:D:197:GLY:HA3	46:D:357:ALA:HA	1.89	0.54
8:s:99:ARG:NH1	20:2:913:A:OP1	2.41	0.54
12:m:14:SER:HB3	20:2:1016:U:H5''	1.89	0.54
20:2:1748:G:H1	20:2:1786:U:H3	1.56	0.54
39:C:325:THR:OG1	39:C:326:HIS:N	2.41	0.54
40:E:331:ASP:N	40:E:331:ASP:OD1	2.41	0.54
40:E:372:VAL:HA	40:E:375:ILE:HG22	1.89	0.54
37:B:358:ALA:HA	37:B:370:ARG:HA	1.90	0.53
38:A:225:SER:O	38:A:229:HIS:ND1	2.41	0.53
39:C:784:GLN:NE2	39:C:812:GLU:OE2	2.41	0.53
45:M:121:TYR:HE1	45:M:164:LEU:HB2	1.73	0.53
12:m:83:ASP:OD1	12:m:83:ASP:N	2.38	0.53
18:R:34:ASP:OD1	18:R:34:ASP:N	2.40	0.53
20:2:1496:U:O2'	20:2:1498:A:OP1	2.26	0.53
27:o:61:ARG:HA	27:o:64:LYS:HD2	1.90	0.53
35:V:125:ARG:O	35:V:127:LYS:NZ	2.36	0.53
39:C:490:LEU:HD12	39:C:499:VAL:HG22	1.89	0.53
46:D:410:ARG:NH2	46:D:454:ARG:O	2.41	0.53
28:k:74:PRO:HB2	28:k:79:ILE:HB	1.89	0.53
35:V:302:TYR:HB2	35:V:306:LEU:HB2	1.88	0.53
38:A:243:MET:HG3	38:A:245:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:525:ALA:O	41:F:314:GLN:NE2	2.42	0.53
42:H:137:GLN:HE21	42:H:169:LEU:H	1.57	0.53
3:d:200:ARG:O	10:c:54:ARG:NH2	2.40	0.53
20:2:560:A:O2'	37:B:488:ASP:OD2	2.21	0.53
21:w:10:LYS:O	21:w:14:ARG:NH1	2.41	0.53
23:b:96:LEU:HD11	23:b:198:ILE:HG22	1.90	0.53
24:e:197:GLU:OE1	24:e:198:ARG:NH1	2.42	0.53
40:E:4:TYR:HB3	40:E:255:ARG:HH12	1.72	0.53
40:E:426:LEU:HB2	44:L:547:ILE:HD13	1.91	0.53
42:H:258:VAL:HA	42:H:261:ASN:HB2	1.91	0.53
45:M:364:VAL:HG22	45:M:368:LEU:HD23	1.90	0.53
9:t:205:ARG:O	9:t:205:ARG:NH1	2.36	0.53
20:2:938:A:H62	20:2:1004:U:H3	1.55	0.53
26:v:121:LYS:O	26:v:125:GLU:HB3	2.09	0.53
32:S:43:ILE:HB	32:S:64:GLU:HB3	1.91	0.53
39:C:861:GLU:OE1	40:E:407:LYS:NZ	2.35	0.53
40:E:229:ARG:NH2	40:E:328:CYS:SG	2.81	0.53
42:H:67:LEU:HD21	42:H:120:TYR:HB3	1.91	0.53
44:L:394:TYR:HA	44:L:397:LYS:HD2	1.90	0.53
45:M:249:LEU:HD11	45:M:278:ARG:HA	1.90	0.53
9:t:53:LYS:NZ	20:2:309:G:OP2	2.42	0.53
20:2:196:C:O2'	20:2:204:G:N2	2.42	0.53
20:2:1658:G:OP1	20:2:1660:C:N4	2.41	0.53
26:v:23:LYS:NZ	26:v:87:GLU:O	2.41	0.53
26:v:86:GLY:HA3	26:v:105:GLY:HA2	1.89	0.53
31:P:95:GLY:O	31:P:112:ASN:ND2	2.42	0.53
44:L:275:VAL:HA	44:L:278:LEU:HB3	1.90	0.53
9:t:98:LYS:HB3	20:2:377:G:H5'	1.91	0.53
20:2:1221:G:O2'	20:2:1676:U:O2	2.26	0.53
23:b:174:HIS:ND1	23:b:182:LEU:O	2.41	0.53
27:o:98:ASN:ND2	27:o:121:ILE:O	2.42	0.53
3:d:104:ASP:OD1	3:d:104:ASP:N	2.38	0.53
20:2:940:U:H3	20:2:1002:U:H3	1.55	0.53
41:F:345:GLN:O	44:L:537:ARG:NH1	2.42	0.53
43:K:85:CYS:HA	43:K:88:MET:HG2	1.89	0.53
10:c:166:GLY:O	37:B:492:ARG:NH1	2.42	0.53
11:n:136:LYS:NZ	20:2:372:U:OP1	2.41	0.53
21:w:33:ARG:NH1	35:V:107:ASP:OD2	2.41	0.53
37:B:516:LYS:NZ	37:B:517:LEU:O	2.42	0.53
39:C:424:ILE:HG12	39:C:439:ARG:HB3	1.91	0.53
20:2:160:U:O2'	20:2:162:C:OP2	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:573:U:H1'	20:2:576:A:H2	1.73	0.53
20:2:1252:C:OP2	30:h:75:LYS:NZ	2.42	0.53
37:B:293:LEU:HA	37:B:362:GLY:HA2	1.90	0.53
37:B:548:ARG:NH2	37:B:598:GLY:O	2.42	0.53
39:C:580:SER:OG	39:C:622:ARG:NH2	2.41	0.53
1:a:41:ARG:HE	1:a:45:GLY:HA2	1.75	0.52
20:2:1643:U:O2'	22:g:142:GLN:O	2.22	0.52
22:g:136:GLY:O	22:g:140:ARG:NH2	2.42	0.52
39:C:370:VAL:HG22	39:C:431:LEU:HD12	1.91	0.52
41:F:109:ARG:O	42:H:111:ASN:ND2	2.42	0.52
46:D:260:ARG:NH2	46:D:481:ASN:O	2.37	0.52
23:b:21:LEU:HD21	23:b:39:VAL:HG21	1.91	0.52
27:o:108:LYS:HD2	27:o:111:MET:HE3	1.90	0.52
41:F:161:LYS:HD3	41:F:165:PRO:HA	1.91	0.52
44:L:530:ILE:O	44:L:534:LYS:N	2.39	0.52
1:a:108:PHE:HB2	1:a:136:GLU:HG2	1.92	0.52
3:d:199:PRO:HG2	10:c:58:ARG:HD2	1.91	0.52
20:2:1271:C:H4'	20:2:1303:C:H4'	1.91	0.52
20:2:1452:A:N1	20:2:1473:G:C2	2.77	0.52
23:b:5:ILE:HG13	23:b:9:ARG:HE	1.73	0.52
46:D:256:MET:HE2	46:D:491:LEU:HD22	1.91	0.52
46:D:271:ARG:NH1	46:D:502:GLU:O	2.43	0.52
8:s:8:ILE:N	8:s:24:SER:OG	2.37	0.52
8:s:95:ILE:HD11	8:s:133:LEU:HD13	1.91	0.52
35:V:186:THR:HG21	35:V:224:GLY:HA3	1.91	0.52
45:M:185:MET:HG2	45:M:207:CYS:HB3	1.90	0.52
3:d:116:THR:OG1	3:d:119:GLY:O	2.23	0.52
20:2:874:G:H2'	20:2:875:A:H8	1.74	0.52
20:2:1677:U:OP1	24:e:71:ARG:NH2	2.40	0.52
25:u:72:THR:O	25:u:76:ILE:N	2.43	0.52
28:k:66:ARG:HH21	28:k:77:TYR:HE2	1.58	0.52
30:h:32:LEU:HG	30:h:87:ARG:HD2	1.91	0.52
31:P:96:LEU:HD12	31:P:97:ILE:HG23	1.92	0.52
37:B:546:ILE:N	37:B:557:ASP:O	2.40	0.52
37:B:659:TRP:HA	37:B:666:VAL:HA	1.90	0.52
5:q:171:ASP:OD1	5:q:171:ASP:N	2.39	0.52
20:2:195:C:H2'	20:2:196:C:H4'	1.90	0.52
22:g:47:LEU:HD12	22:g:81:ILE:HG13	1.91	0.52
35:V:107:ASP:HB2	35:V:125:ARG:HG3	1.90	0.52
42:H:281:ARG:O	42:H:285:ASN:ND2	2.43	0.52
46:D:369:ILE:HG12	46:D:499:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1500:G:O2'	23:b:178:ARG:O	2.28	0.52
34:U:139:HIS:HB2	34:U:148:TYR:HB2	1.91	0.52
43:K:110:GLU:OE2	44:L:327:ARG:NH1	2.43	0.52
44:L:327:ARG:HH21	44:L:457:LEU:HD22	1.73	0.52
23:b:150:MET:HB3	23:b:152:PHE:HE1	1.75	0.52
31:P:59:CYS:SG	31:P:94:LYS:NZ	2.83	0.52
31:P:91:LEU:HD12	31:P:94:LYS:HD2	1.92	0.52
35:V:239:LEU:HD23	35:V:250:ALA:HA	1.92	0.52
38:A:403:LEU:HA	38:A:406:ARG:HB2	1.92	0.52
46:D:248:THR:HA	46:D:374:ARG:H	1.75	0.52
10:c:121:LYS:NZ	20:2:527:C:O2'	2.41	0.52
29:x:104:LEU:HD13	29:x:121:ARG:HD3	1.92	0.52
35:V:52:TYR:OH	35:V:311:GLN:NE2	2.43	0.52
35:V:130:LYS:HE3	35:V:142:VAL:HG21	1.90	0.52
46:D:12:ASN:ND2	46:D:17:GLY:O	2.43	0.52
46:D:238:LEU:HB3	46:D:242:GLN:HE21	1.74	0.52
15:f:31:SER:H	15:f:34:ILE:HD12	1.75	0.52
20:2:880:G:N2	20:2:906:U:O2	2.40	0.52
20:2:1215:C:O2	20:2:1218:C:N4	2.41	0.52
23:b:193:ASP:OD2	23:b:197:LYS:N	2.36	0.52
24:e:65:GLN:NE2	46:D:415:SER:OG	2.43	0.52
39:C:515:ASP:OD2	39:C:544:SER:OG	2.29	0.52
41:F:129:VAL:HG13	41:F:170:LEU:HD22	1.91	0.52
20:2:1308:U:O4	34:U:96:LYS:NZ	2.43	0.51
20:2:1514:G:H2'	20:2:1515:G:H8	1.76	0.51
28:k:67:VAL:O	28:k:71:MET:HB2	2.10	0.51
32:S:45:ASN:HD22	32:S:65:ALA:HB2	1.75	0.51
40:E:99:GLU:O	40:E:116:TYR:OH	2.28	0.51
46:D:318:TYR:HA	46:D:321:HIS:HB2	1.93	0.51
20:2:1600:G:OP2	24:e:164:ARG:NH2	2.43	0.51
45:M:273:ASN:HA	45:M:276:LYS:HB3	1.92	0.51
46:D:510:LYS:NZ	46:D:511:ASP:O	2.43	0.51
4:Q:45:VAL:HA	13:i:113:GLN:HE22	1.73	0.51
11:n:48:LYS:NZ	11:n:52:GLU:OE1	2.40	0.51
16:j:48:LYS:HG3	20:2:483:C:H5'	1.92	0.51
20:2:1473:G:N7	22:g:117:ARG:NH2	2.59	0.51
20:2:1610:G:N2	28:k:85:ASN:OD1	2.44	0.51
37:B:320:TRP:H	37:B:328:SER:H	1.58	0.51
5:q:21:ASP:OD1	5:q:21:ASP:N	2.35	0.51
15:f:102:ILE:H	15:f:113:HIS:CD2	2.26	0.51
20:2:1681:U:O2	20:2:1683:C:N4	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:v:71:GLU:OE1	34:U:116:ARG:NH1	2.44	0.51
40:E:129:ASP:CA	40:E:132:TYR:HD2	2.23	0.51
45:M:228:PRO:HA	45:M:231:PHE:HB3	1.92	0.51
46:D:29:PRO:HB3	46:D:68:GLN:HE21	1.74	0.51
24:e:167:LYS:HD3	24:e:171:GLU:HG3	1.92	0.51
38:A:289:ALA:HA	38:A:292:HIS:HB3	1.92	0.51
43:K:155:ARG:HB3	43:K:187:ILE:HD11	1.93	0.51
20:2:1562:C:H2'	20:2:1563:G:C8	2.46	0.51
27:o:21:ASP:O	27:o:24:GLN:NE2	2.37	0.51
29:x:27:LYS:HE3	29:x:110:LEU:HB2	1.93	0.51
29:x:56:ARG:HG3	29:x:103:VAL:HG21	1.92	0.51
35:V:78:ALA:HB3	35:V:90:TRP:HB2	1.92	0.51
7:r:168:LYS:NZ	7:r:169:PRO:O	2.41	0.51
22:g:129:SER:OG	22:g:130:LYS:N	2.44	0.51
23:b:74:GLN:HG3	23:b:79:PHE:HB2	1.92	0.51
41:F:308:LEU:HB2	45:M:350:LEU:HD11	1.93	0.51
25:u:14:LEU:HD22	25:u:35:LEU:HD13	1.93	0.51
37:B:545:GLU:HG3	37:B:558:VAL:HG22	1.92	0.51
40:E:387:LYS:NZ	44:L:469:THR:OG1	2.43	0.51
41:F:154:LYS:HZ3	41:F:157:TYR:HB3	1.74	0.51
46:D:229:THR:HG22	46:D:235:ILE:HG21	1.93	0.51
30:h:90:ASP:OD1	30:h:90:ASP:N	2.44	0.51
38:A:483:ARG:NH2	39:C:797:SER:O	2.44	0.51
39:C:559:ASP:O	39:C:565:ARG:NH2	2.44	0.51
40:E:255:ARG:HB2	40:E:292:ILE:HD11	1.93	0.51
42:H:207:ASN:HB3	42:H:211:ILE:HD12	1.92	0.51
44:L:428:TYR:O	44:L:436:HIS:NE2	2.39	0.51
16:j:68:LYS:HB3	16:j:91:LEU:HD22	1.91	0.51
16:j:95:GLU:OE1	16:j:140:ARG:NH2	2.43	0.51
20:2:1301:A:O2'	33:l:3:HIS:ND1	2.44	0.51
20:2:1403:C:O2'	20:2:1405:A:OP2	2.28	0.51
35:V:237:ASN:ND2	35:V:287:THR:O	2.44	0.51
45:M:326:ASP:HB2	45:M:331:LYS:HB3	1.92	0.51
5:q:174:LYS:O	5:q:179:ASN:ND2	2.44	0.50
9:t:143:LYS:NZ	20:2:203:G:OP2	2.44	0.50
23:b:115:VAL:O	23:b:119:CYS:HB2	2.11	0.50
28:k:40:TYR:HA	28:k:43:VAL:HG12	1.93	0.50
35:V:213:ASP:OD1	35:V:213:ASP:N	2.43	0.50
38:A:313:ASP:O	38:A:317:ARG:N	2.42	0.50
38:A:523:LEU:HD13	42:H:231:LEU:HB2	1.92	0.50
46:D:60:SER:O	46:D:62:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:35:ARG:NH2	11:n:55:TYR:O	2.34	0.50
37:B:520:GLN:NE2	37:B:571:GLU:O	2.44	0.50
38:A:245:LEU:HB3	38:A:248:GLU:HB2	1.93	0.50
39:C:509:HIS:O	39:C:513:LYS:NZ	2.36	0.50
42:H:45:VAL:HG11	42:H:78:ILE:HG22	1.92	0.50
44:L:431:VAL:HA	44:L:434:ASN:HA	1.92	0.50
46:D:413:LEU:O	46:D:417:ARG:NH1	2.44	0.50
20:2:1334:G:H2'	20:2:1335:G:H8	1.77	0.50
22:g:44:PRO:HG3	22:g:77:HIS:HB3	1.93	0.50
25:u:24:LYS:HA	25:u:66:HIS:HA	1.93	0.50
37:B:376:VAL:HA	37:B:392:SER:HA	1.94	0.50
38:A:476:ARG:O	38:A:502:ARG:NH2	2.45	0.50
44:L:296:ASN:HD22	44:L:323:TYR:HE1	1.58	0.50
46:D:244:ASN:O	46:D:276:LEU:N	2.40	0.50
2:p:107:ARG:NH2	13:i:133:THR:O	2.45	0.50
4:Q:22:ARG:NH2	13:i:145:GLY:O	2.45	0.50
20:2:1601:A:OP2	20:2:1636:G:N1	2.44	0.50
28:k:36:VAL:HG12	28:k:40:TYR:HB3	1.94	0.50
40:E:212:THR:HA	40:E:215:ILE:HB	1.92	0.50
41:F:103:VAL:HG11	42:H:211:ILE:HG23	1.93	0.50
41:F:310:SER:HA	41:F:313:ASN:HB2	1.92	0.50
46:D:207:ASP:OD2	46:D:448:LYS:NZ	2.44	0.50
2:p:209:ASP:N	2:p:209:ASP:OD1	2.45	0.50
12:m:5:HIS:HB3	12:m:117:LEU:HD13	1.93	0.50
17:z:18:LEU:O	17:z:85:ASN:ND2	2.44	0.50
20:2:1059:G:N1	20:2:1830:U:OP1	2.36	0.50
20:2:1662:U:O4	20:2:1663:A:N6	2.45	0.50
24:e:167:LYS:HA	31:P:71:ALA:HB1	1.92	0.50
35:V:244:ASN:HD21	35:V:296:GLN:H	1.59	0.50
37:B:520:GLN:NE2	37:B:574:GLY:O	2.45	0.50
41:F:353:LYS:HA	41:F:356:ASN:HD22	1.77	0.50
42:H:42:ASP:HB2	42:H:79:THR:HA	1.94	0.50
44:L:489:GLN:HE22	44:L:496:LYS:HE2	1.77	0.50
46:D:270:GLN:HB3	46:D:277:PHE:HB2	1.94	0.50
5:q:91:SER:OG	5:q:98:ASN:ND2	2.44	0.50
7:r:92:ARG:O	20:2:453:C:O2'	2.26	0.50
9:t:61:ASP:OD1	9:t:61:ASP:N	2.43	0.50
20:2:1656:G:N2	20:2:1668:U:O2	2.39	0.50
25:u:46:MET:HG3	25:u:47:LYS:HE2	1.93	0.50
29:x:134:ILE:HG23	29:x:137:GLN:HE21	1.74	0.50
40:E:136:LYS:NZ	46:D:15:GLY:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:60:SER:O	39:C:340:ARG:NH2	2.44	0.50
20:2:1539:U:H2'	20:2:1540:G:H8	1.76	0.50
38:A:175:HIS:O	38:A:179:GLN:NE2	2.45	0.50
39:C:386:ASN:ND2	39:C:391:THR:OG1	2.42	0.50
40:E:283:GLN:HE21	46:D:35:LYS:HG3	1.77	0.50
20:2:1400:U:H2'	20:2:1401:A:C5	2.47	0.50
20:2:1563:G:OP1	29:x:121:ARG:NH1	2.43	0.50
23:b:105:LEU:HD22	23:b:122:VAL:HG21	1.93	0.50
24:e:144:LEU:O	24:e:148:ASN:ND2	2.44	0.50
26:v:43:ASP:OD1	34:U:116:ARG:NH1	2.43	0.50
38:A:387:VAL:HA	38:A:390:LEU:HD23	1.93	0.50
41:F:93:ARG:N	41:F:129:VAL:O	2.44	0.50
42:H:63:VAL:H	42:H:122:SER:HG	1.57	0.50
26:v:80:ASP:OD1	26:v:80:ASP:N	2.44	0.50
33:l:22:ARG:HD2	33:l:37:ASN:HB3	1.92	0.50
38:A:594:LEU:HD22	38:A:597:ARG:HH21	1.77	0.50
39:C:419:PHE:HB2	39:C:439:ARG:HA	1.94	0.50
39:C:799:TYR:HB3	39:C:844:MET:HE3	1.94	0.50
46:D:168:TRP:HE1	46:D:522:LEU:HD13	1.75	0.50
20:2:1464:C:O2'	20:2:1465:A:O4'	2.28	0.49
25:u:52:LEU:HB3	25:u:57:TYR:HB2	1.94	0.49
38:A:331:ILE:HB	38:A:437:LEU:HD11	1.93	0.49
39:C:50:ARG:NH1	39:C:58:GLU:OE2	2.44	0.49
44:L:528:ILE:O	44:L:532:ASP:N	2.38	0.49
41:F:140:ASN:ND2	41:F:147:ALA:O	2.43	0.49
12:m:70:LYS:NZ	20:2:1020:A:N7	2.60	0.49
20:2:1628:C:OP1	29:x:38:LYS:NZ	2.38	0.49
24:e:124:ASP:HB2	24:e:141:VAL:HG22	1.93	0.49
35:V:24:THR:HG22	35:V:26:GLN:H	1.77	0.49
39:C:683:GLU:HB3	39:C:733:MET:HE1	1.94	0.49
41:F:96:PRO:HB2	42:H:47:LEU:HD21	1.94	0.49
42:H:39:VAL:HA	42:H:76:LEU:HB3	1.94	0.49
47:Y:6:UNK:N	47:Y:46:UNK:O	2.45	0.49
10:c:136:ARG:HD3	10:c:160:SER:HA	1.94	0.49
35:V:24:THR:HG23	35:V:71:ILE:HG21	1.93	0.49
37:B:517:LEU:HB2	37:B:526:LEU:HD11	1.94	0.49
44:L:489:GLN:HE21	44:L:492:VAL:HG13	1.76	0.49
10:c:134:HIS:ND1	10:c:163:SER:OG	2.44	0.49
33:l:11:PRO:HB3	33:l:13:LYS:HE2	1.95	0.49
38:A:136:ASP:N	38:A:136:ASP:OD1	2.42	0.49
38:A:341:LEU:HD22	39:C:698:MET:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:399:ASN:HB3	38:A:402:LYS:HB2	1.94	0.49
38:A:446:ILE:HD11	45:M:316:VAL:HG11	1.95	0.49
39:C:379:ILE:HA	39:C:382:LEU:HD12	1.94	0.49
44:L:407:GLN:NE2	44:L:410:GLU:OE1	2.45	0.49
20:2:551:U:H2'	20:2:552:G:C8	2.48	0.49
25:u:1:MET:HG2	25:u:47:LYS:HG3	1.94	0.49
35:V:300:ALA:O	35:V:308:ARG:N	2.39	0.49
40:E:306:ASP:N	40:E:306:ASP:OD1	2.43	0.49
42:H:36:VAL:HG11	42:H:76:LEU:HB2	1.93	0.49
43:K:36:GLN:HB3	43:K:72:LYS:HE2	1.93	0.49
13:i:134:PRO:HB3	20:2:944:A:H5''	1.95	0.49
20:2:1660:C:H4'	20:2:1663:A:H62	1.77	0.49
38:A:541:HIS:NE2	41:F:288:GLN:OE1	2.46	0.49
40:E:402:GLN:OE1	40:E:403:GLN:NE2	2.46	0.49
40:E:418:LEU:HG	41:F:350:LEU:HD22	1.94	0.49
42:H:315:ASP:OD1	42:H:315:ASP:N	2.46	0.49
44:L:396:ASP:OD1	44:L:396:ASP:N	2.45	0.49
44:L:526:ASP:HA	44:L:529:HIS:HB2	1.94	0.49
20:2:72:C:H2'	20:2:74:G:H1'	1.95	0.49
20:2:1590:C:OP1	29:x:82:ARG:NE	2.36	0.49
21:w:59:LYS:O	21:w:63:ARG:NH1	2.40	0.49
27:o:81:ARG:NH1	27:o:120:SER:OG	2.45	0.49
38:A:295:THR:O	38:A:299:LEU:N	2.43	0.49
41:F:109:ARG:NE	41:F:113:ALA:O	2.45	0.49
45:M:296:THR:O	45:M:299:GLN:NE2	2.46	0.49
45:M:360:ASN:HA	45:M:363:LYS:HD2	1.95	0.49
7:r:189:ARG:NH2	20:2:332:G:O6	2.46	0.49
9:t:103:LEU:HD22	9:t:170:LYS:HB3	1.94	0.49
20:2:1463:U:H4'	20:2:1464:C:H5'	1.94	0.49
20:2:1560:U:O2	20:2:1575:G:O6	2.30	0.49
20:2:1657:G:H2'	20:2:1658:G:H8	1.78	0.49
37:B:496:MET:HG2	37:B:503:GLU:HA	1.95	0.49
37:B:516:LYS:O	37:B:529:LYS:N	2.46	0.49
39:C:762:ASN:HA	39:C:766:TRP:HB2	1.93	0.49
40:E:112:MET:SD	40:E:112:MET:N	2.83	0.49
46:D:252:LEU:HD22	46:D:491:LEU:HD11	1.94	0.49
20:2:1784:G:H5''	20:2:1785:C:H2'	1.94	0.49
29:x:117:GLN:OE1	29:x:122:LYS:NZ	2.45	0.49
38:A:193:GLU:HA	38:A:196:LYS:HB2	1.95	0.49
38:A:199:ASP:N	38:A:199:ASP:OD1	2.46	0.49
38:A:389:ASP:HA	38:A:392:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:E:298:CYS:O	40:E:303:PHE:N	2.46	0.49
15:f:112:ASP:OD1	15:f:112:ASP:N	2.46	0.48
20:2:1610:G:OP1	28:k:125:HIS:NE2	2.46	0.48
25:u:21:MET:O	25:u:69:TRP:N	2.43	0.48
29:x:80:GLY:HA3	29:x:92:PHE:HE1	1.78	0.48
39:C:744:MET:HE2	39:C:787:SER:HB3	1.95	0.48
43:K:86:LYS:HG3	43:K:103:LEU:HD11	1.95	0.48
44:L:265:LEU:HB3	44:L:279:ARG:HB2	1.95	0.48
44:L:489:GLN:O	44:L:493:PHE:N	2.43	0.48
46:D:350:LYS:NZ	46:D:352:GLU:OE2	2.42	0.48
7:r:70:HIS:O	7:r:98:ARG:NH2	2.46	0.48
26:v:36:ARG:O	26:v:40:LYS:HB2	2.13	0.48
29:x:126:GLN:NE2	29:x:130:ASP:OD2	2.46	0.48
39:C:780:VAL:HA	39:C:783:ILE:HG22	1.94	0.48
10:c:144:ILE:HG22	10:c:146:SER:H	1.78	0.48
20:2:1676:U:H1'	24:e:78:MET:HE1	1.94	0.48
26:v:71:GLU:OE1	26:v:72:HIS:NE2	2.46	0.48
7:r:20:ASP:HB3	7:r:23:LYS:HD2	1.94	0.48
20:2:1144:A:H2'	20:2:1145:A:C8	2.48	0.48
20:2:1656:G:H1	20:2:1668:U:H3	1.61	0.48
35:V:112:ALA:HB3	35:V:121:VAL:HG13	1.95	0.48
38:A:498:ASN:HA	38:A:520:ARG:HH12	1.79	0.48
39:C:402:LEU:O	39:C:406:ASN:ND2	2.46	0.48
40:E:23:LEU:HD12	40:E:41:LYS:HZ2	1.77	0.48
20:2:1525:C:H2'	20:2:1526:G:H8	1.78	0.48
35:V:72:SER:OG	35:V:73:SER:N	2.46	0.48
38:A:383:VAL:O	38:A:388:LYS:NZ	2.41	0.48
40:E:85:GLN:O	40:E:89:GLU:N	2.47	0.48
40:E:181:ASN:HD21	40:E:184:ALA:H	1.61	0.48
43:K:122:ASP:OD1	43:K:122:ASP:N	2.46	0.48
17:z:44:LEU:HD23	17:z:55:ILE:HD12	1.94	0.48
28:k:130:ARG:HA	28:k:130:ARG:HD3	1.65	0.48
29:x:134:ILE:HA	29:x:137:GLN:HG2	1.95	0.48
31:P:98:LYS:NZ	31:P:111:ARG:O	2.46	0.48
39:C:336:ILE:O	39:C:350:GLN:NE2	2.41	0.48
44:L:237:LYS:NZ	44:L:421:LEU:O	2.37	0.48
7:r:45:TRP:HA	7:r:48:TYR:HD2	1.77	0.48
38:A:523:LEU:HD22	42:H:231:LEU:HD12	1.95	0.48
42:H:72:VAL:HB	42:H:75:ARG:HG3	1.96	0.48
44:L:229:ASN:HD21	44:L:278:LEU:HD11	1.77	0.48
44:L:244:LEU:HD22	44:L:439:PRO:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:D:196:CYS:HB3	46:D:339:ASN:HD22	1.78	0.48
20:2:1452:A:N6	20:2:1473:G:H1'	2.28	0.48
35:V:165:ILE:HD11	35:V:179:LEU:HD13	1.94	0.48
42:H:141:GLN:HG2	42:H:147:SER:HB3	1.96	0.48
7:r:3:LEU:HD12	7:r:16:ILE:HD11	1.94	0.48
21:w:26:ASN:HA	21:w:58:MET:HG2	1.96	0.48
24:e:118:ASN:ND2	24:e:181:ALA:O	2.47	0.48
24:e:155:CYS:SG	24:e:159:ARG:NH2	2.86	0.48
27:o:72:LYS:HD2	27:o:73:PRO:HD2	1.95	0.48
28:k:39:ARG:HD2	29:x:45:LEU:HD23	1.96	0.48
39:C:368:GLU:HG2	39:C:415:ASN:HD21	1.78	0.48
43:K:66:THR:HA	43:K:69:ILE:HG22	1.96	0.48
20:2:1531:A:H4'	20:2:1605:G:H4'	1.96	0.48
20:2:1598:G:N7	31:P:82:SER:OG	2.45	0.48
26:v:92:CYS:HA	26:v:102:LYS:HD3	1.96	0.48
38:A:331:ILE:HD12	38:A:437:LEU:HD21	1.95	0.48
38:A:483:ARG:NH1	39:C:799:TYR:O	2.45	0.48
44:L:434:ASN:O	44:L:436:HIS:ND1	2.47	0.48
45:M:259:ASN:HB2	45:M:262:PHE:HB3	1.96	0.48
2:p:52:THR:HG23	2:p:57:ILE:HA	1.95	0.47
2:p:68:GLU:HG2	2:p:85:LYS:HG2	1.96	0.47
20:2:640:A:H2'	20:2:641:A:C8	2.49	0.47
22:g:54:PRO:HG2	22:g:88:ILE:HD11	1.96	0.47
26:v:93:LYS:O	26:v:101:ARG:NH1	2.47	0.47
27:o:27:ASP:OD1	27:o:27:ASP:N	2.42	0.47
35:V:120:ILE:O	35:V:132:TRP:N	2.46	0.47
38:A:471:ILE:O	38:A:475:ALA:N	2.47	0.47
39:C:324:ILE:HG22	39:C:325:THR:H	1.80	0.47
40:E:15:ASP:HB3	40:E:18:LEU:HG	1.94	0.47
44:L:531:ALA:HA	44:L:534:LYS:HB2	1.95	0.47
46:D:505:LYS:HB2	46:D:524:ASP:HA	1.95	0.47
47:Y:30:UNK:O	47:Y:49:UNK:N	2.47	0.47
18:R:75:GLU:HA	46:D:83:VAL:HG23	1.95	0.47
20:2:1289:U:OP2	34:U:95:ARG:NE	2.47	0.47
38:A:267:PRO:HB2	38:A:271:LEU:HD11	1.95	0.47
38:A:393:TRP:HB3	38:A:403:LEU:HD11	1.96	0.47
39:C:419:PHE:HD2	39:C:439:ARG:HG2	1.79	0.47
39:C:807:LEU:HA	39:C:810:MET:HB2	1.96	0.47
44:L:227:VAL:HB	44:L:352:ARG:HH12	1.79	0.47
1:a:3:GLY:N	14:y:78:ILE:O	2.45	0.47
11:n:104:LYS:HA	11:n:104:LYS:HD2	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:g:32:ILE:HG12	22:g:68:ILE:HB	1.97	0.47
24:e:155:CYS:SG	24:e:156:THR:N	2.87	0.47
35:V:40:ILE:HG13	35:V:59:LEU:HD13	1.96	0.47
39:C:339:ALA:HA	39:C:342:LYS:HE3	1.94	0.47
44:L:366:GLN:OE1	44:L:419:LYS:NZ	2.47	0.47
9:t:162:LEU:HD11	9:t:191:GLU:HG2	1.96	0.47
20:2:436:G:OP2	20:2:471:G:O2'	2.30	0.47
20:2:1289:U:H5'	25:u:2:LEU:HD13	1.95	0.47
34:U:132:MET:HE3	34:U:141:CYS:HB2	1.95	0.47
40:E:316:GLU:HA	40:E:319:LEU:HB2	1.95	0.47
41:F:334:LEU:HD22	42:H:334:THR:HG23	1.97	0.47
5:q:136:ILE:HG21	5:q:148:ARG:HD2	1.97	0.47
8:s:162:GLN:NE2	8:s:165:ASN:OD1	2.47	0.47
20:2:1010:G:H2'	20:2:1011:A:C8	2.50	0.47
20:2:1224:G:N2	20:2:1643:U:O4	2.48	0.47
20:2:1401:A:H4'	30:h:52:GLY:HA3	1.96	0.47
23:b:7:LYS:HD3	23:b:10:LYS:HZ1	1.79	0.47
24:e:90:VAL:HA	24:e:93:VAL:HG12	1.96	0.47
25:u:10:ALA:HB1	25:u:38:LYS:HD3	1.97	0.47
26:v:87:GLU:OE1	26:v:101:ARG:NH2	2.47	0.47
39:C:868:GLU:OE2	40:E:414:ARG:NH1	2.47	0.47
40:E:144:TYR:HB2	40:E:179:MET:HG2	1.97	0.47
45:M:68:VAL:HA	45:M:71:LEU:HD12	1.95	0.47
4:Q:11:ALA:HB3	4:Q:33:ASP:HB2	1.96	0.47
20:2:1375:G:H5''	21:w:67:ARG:HH22	1.80	0.47
21:w:57:LEU:O	21:w:61:ILE:HB	2.14	0.47
21:w:72:LYS:NZ	21:w:76:GLU:OE2	2.47	0.47
23:b:172:VAL:HG13	23:b:185:LYS:HE3	1.96	0.47
25:u:46:MET:O	25:u:50:GLN:HB2	2.15	0.47
27:o:108:LYS:HB2	27:o:111:MET:HG3	1.97	0.47
28:k:102:GLY:HA2	28:k:105:ASN:HD22	1.79	0.47
37:B:469:ASP:OD1	37:B:469:ASP:N	2.47	0.47
38:A:55:LEU:HD13	38:A:93:TYR:HB2	1.96	0.47
38:A:261:SER:O	38:A:264:LYS:NZ	2.47	0.47
38:A:446:ILE:HD13	38:A:511:LEU:HD21	1.96	0.47
39:C:326:HIS:HA	39:C:329:VAL:HG12	1.96	0.47
39:C:668:ARG:HH12	46:D:82:LEU:HD21	1.80	0.47
41:F:144:ASP:H	41:F:182:HIS:HE1	1.62	0.47
41:F:163:VAL:HA	42:H:85:PRO:HB3	1.97	0.47
42:H:218:LEU:O	42:H:222:SER:OG	2.30	0.47
43:K:52:LYS:HG2	44:L:292:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:D:177:PRO:O	46:D:181:LYS:NZ	2.45	0.47
20:2:546:G:H4'	20:2:548:C:H5'	1.97	0.47
20:2:1233:G:O2'	20:2:1254:C:N4	2.48	0.47
20:2:1665:G:N2	29:x:87:VAL:O	2.48	0.47
20:2:1678:A:OP2	24:e:63:LYS:NZ	2.43	0.47
28:k:135:HIS:O	28:k:139:THR:N	2.45	0.47
35:V:178:ASN:HD21	35:V:185:LYS:HD3	1.80	0.47
38:A:519:ILE:HG22	41:F:316:PRO:HG3	1.96	0.47
45:M:281:THR:O	45:M:285:MET:N	2.46	0.47
9:t:113:TYR:OH	9:t:156:ALA:O	2.32	0.47
17:z:76:TYR:OH	17:z:86:GLU:OE2	2.21	0.47
20:2:1139:C:H5	20:2:1149:A:H62	1.62	0.47
37:B:327:VAL:HA	37:B:328:SER:HA	1.60	0.47
39:C:456:THR:HG22	39:C:460:GLN:HE21	1.80	0.47
39:C:859:LEU:HD13	42:H:247:MET:HG2	1.96	0.47
40:E:68:HIS:HA	40:E:71:ARG:HB2	1.96	0.47
42:H:157:THR:HG22	42:H:162:LEU:HA	1.96	0.47
45:M:291:GLU:HG3	45:M:333:VAL:HG13	1.97	0.47
17:z:20:ARG:HE	17:z:22:GLN:HE21	1.63	0.47
17:z:116:LYS:HB3	20:2:161:U:H5'	1.96	0.47
20:2:878:G:H1	20:2:908:A:H61	1.62	0.47
20:2:1455:A:H2'	20:2:1456:G:H8	1.79	0.47
24:e:19:LEU:HD23	24:e:23:TRP:HD1	1.80	0.47
35:V:31:ILE:HB	35:V:43:TRP:HB2	1.96	0.47
2:p:35:ALA:HB3	2:p:42:ARG:HA	1.97	0.46
10:c:138:ARG:NH2	10:c:153:SER:OG	2.48	0.46
13:i:98:ARG:HD3	13:i:99:ALA:O	2.15	0.46
16:j:93:PHE:O	16:j:140:ARG:NH1	2.48	0.46
20:2:1231:C:H5''	28:k:135:HIS:HE1	1.80	0.46
20:2:1556:A:C6	33:l:13:LYS:HA	2.51	0.46
21:w:19:LYS:HD2	23:b:213:PRO:HG3	1.97	0.46
22:g:17:LYS:HA	22:g:126:ARG:HH12	1.81	0.46
24:e:27:ASP:OD1	24:e:27:ASP:N	2.46	0.46
37:B:552:LYS:HG3	37:B:553:GLN:HG3	1.97	0.46
39:C:697:TYR:OH	39:C:708:ARG:N	2.47	0.46
40:E:205:LEU:HD13	46:D:26:ARG:HH11	1.80	0.46
40:E:352:SER:HA	40:E:390:HIS:HA	1.97	0.46
41:F:301:ASP:OD2	45:M:347:TRP:NE1	2.47	0.46
44:L:441:LEU:HA	44:L:445:LYS:HG2	1.96	0.46
45:M:153:ASP:O	45:M:155:ASN:ND2	2.48	0.46
46:D:341:ASN:HB2	46:D:353:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1401:A:H2'	20:2:1402:A:C8	2.50	0.46
20:2:1616:U:O4	27:o:40:ARG:NH1	2.47	0.46
23:b:132:LYS:HB3	23:b:189:MET:HB3	1.96	0.46
25:u:52:LEU:HD22	25:u:57:TYR:HD2	1.81	0.46
26:v:63:LYS:HD2	34:U:108:VAL:HB	1.97	0.46
35:V:32:LEU:HD11	35:V:71:ILE:HD12	1.98	0.46
20:2:1613:G:OP1	27:o:42:ARG:NH2	2.48	0.46
23:b:65:ARG:NH1	23:b:68:GLU:OE1	2.49	0.46
35:V:67:SER:HB3	35:V:83:TRP:CD1	2.50	0.46
35:V:132:TRP:HA	35:V:138:CYS:HA	1.96	0.46
41:F:352:GLU:O	41:F:356:ASN:ND2	2.48	0.46
46:D:270:GLN:HG3	46:D:505:LYS:HE3	1.98	0.46
20:2:190:G:O2'	20:2:209:A:N6	2.49	0.46
23:b:70:THR:HG23	23:b:84:VAL:HG12	1.96	0.46
23:b:206:ASP:N	23:b:206:ASP:OD1	2.46	0.46
35:V:155:ARG:HG3	35:V:199:THR:HA	1.97	0.46
39:C:62:ASN:O	39:C:66:THR:OG1	2.33	0.46
45:M:46:ILE:HD11	45:M:71:LEU:HD21	1.98	0.46
46:D:410:ARG:NH2	46:D:453:SER:OG	2.48	0.46
46:D:413:LEU:HD23	46:D:420:VAL:HG21	1.98	0.46
2:p:157:GLN:H	2:p:160:GLN:HE21	1.64	0.46
20:2:857:U:H2'	20:2:858:A:C8	2.50	0.46
20:2:1232:U:H3	20:2:1526:G:H1	1.62	0.46
20:2:1284:A:O2'	26:v:34:GLY:N	2.48	0.46
20:2:1298:G:H5'	27:o:77:LYS:HG3	1.98	0.46
32:S:16:LYS:HD2	32:S:31:ARG:HB2	1.96	0.46
40:E:309:GLN:OE1	40:E:313:ARG:NH1	2.45	0.46
40:E:331:ASP:O	40:E:335:ASN:ND2	2.49	0.46
42:H:261:ASN:O	42:H:265:ARG:N	2.39	0.46
43:K:186:GLN:HE22	44:L:508:ALA:H	1.63	0.46
7:r:132:ARG:HG3	7:r:133:LEU:HG	1.98	0.46
10:c:57:ALA:O	10:c:61:LEU:HB2	2.16	0.46
20:2:1238:U:O2'	27:o:125:PRO:O	2.34	0.46
38:A:548:GLU:HA	38:A:551:GLN:HB2	1.97	0.46
39:C:847:THR:HG21	40:E:397:ALA:HB1	1.97	0.46
40:E:129:ASP:O	40:E:132:TYR:HD2	1.97	0.46
40:E:129:ASP:HA	40:E:132:TYR:HB3	1.98	0.46
44:L:304:MET:SD	44:L:304:MET:N	2.88	0.46
45:M:53:LEU:HD22	45:M:64:MET:HE1	1.96	0.46
1:a:80:ARG:NH2	1:a:165:ASN:O	2.35	0.46
20:2:1513:C:H5''	33:l:10:HIS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:33:ILE:HG21	32:S:35:MET:HE1	1.97	0.46
24:e:72:LEU:O	24:e:75:SER:OG	2.30	0.46
29:x:88:MET:HE2	29:x:88:MET:HB3	1.83	0.46
34:U:140:TYR:CZ	34:U:142:GLY:HA2	2.51	0.46
39:C:96:ILE:HG22	39:C:98:ASP:H	1.81	0.46
41:F:302:ASN:HD21	45:M:221:ASP:HB3	1.81	0.46
41:F:309:MET:O	41:F:313:ASN:N	2.49	0.46
42:H:123:THR:OG1	42:H:124:TYR:N	2.48	0.46
1:a:6:ASP:OD1	1:a:6:ASP:N	2.49	0.46
6:W:11:ARG:NH2	20:2:1844:U:OP1	2.43	0.46
8:s:31:GLU:O	8:s:37:LYS:N	2.48	0.46
10:c:121:LYS:HG3	37:B:510:PHE:HD2	1.80	0.46
20:2:722:C:H5''	20:2:723:C:H5'	1.98	0.46
31:P:80:ARG:O	31:P:84:ALA:N	2.39	0.46
40:E:91:ILE:HA	40:E:94:MET:HB2	1.98	0.46
48:J:171:ARG:HD3	48:J:175:ARG:HH21	1.80	0.46
11:n:75:GLY:HA3	11:n:88:ILE:HD12	1.97	0.46
12:m:69:ASN:OD1	12:m:69:ASN:N	2.49	0.46
20:2:1535:U:H3'	20:2:1536:G:H8	1.81	0.46
37:B:497:GLN:HG3	37:B:499:PRO:HD2	1.98	0.46
38:A:82:ASN:O	38:A:85:SER:OG	2.34	0.46
39:C:430:ASN:ND2	39:C:435:ASP:OD2	2.49	0.46
40:E:313:ARG:HH22	40:E:359:LYS:HA	1.81	0.46
40:E:314:GLU:O	40:E:317:SER:OG	2.32	0.46
46:D:261:SER:HB3	46:D:430:TYR:HB2	1.98	0.46
1:a:81:ASN:HA	1:a:84:GLN:HG3	1.98	0.46
2:p:179:ASN:HB3	2:p:183:GLU:HB3	1.98	0.46
20:2:1249:C:OP1	20:2:1252:C:N4	2.48	0.46
20:2:1579:A:O2'	20:2:1581:C:OP2	2.32	0.46
24:e:204:ARG:NH1	32:S:60:GLU:OE2	2.48	0.46
39:C:757:ILE:HD12	39:C:776:ARG:HG2	1.97	0.46
40:E:87:GLU:OE2	40:E:133:ARG:NH2	2.48	0.46
41:F:297:LYS:HE2	41:F:297:LYS:HB3	1.72	0.46
44:L:395:GLY:HA2	44:L:398:MET:HG2	1.97	0.46
2:p:139:CYS:SG	2:p:140:VAL:N	2.89	0.45
20:2:1538:C:H2'	20:2:1539:U:C6	2.51	0.45
20:2:1754:G:OP2	20:2:1779:G:N2	2.37	0.45
25:u:24:LYS:HG3	25:u:66:HIS:CE1	2.51	0.45
35:V:66:VAL:HA	35:V:82:SER:HA	1.98	0.45
35:V:257:LYS:NZ	35:V:269:GLU:OE2	2.48	0.45
39:C:78:LYS:HA	39:C:78:LYS:HD2	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:F:121:LEU:HB2	41:F:133:ASN:HB3	1.96	0.45
20:2:1613:G:OP2	27:o:39:ALA:N	2.49	0.45
25:u:11:ILE:HG12	25:u:40:VAL:HG11	1.97	0.45
25:u:16:PHE:HB2	25:u:79:LEU:HD23	1.99	0.45
35:V:124:SER:OG	35:V:125:ARG:N	2.49	0.45
37:B:512:VAL:HG22	37:B:532:ARG:HD3	1.99	0.45
46:D:292:SER:HA	46:D:427:ASN:HB3	1.97	0.45
20:2:726:C:H2'	20:2:727:G:H8	1.81	0.45
40:E:278:VAL:HA	40:E:281:ILE:HG12	1.99	0.45
42:H:41:ILE:HD13	42:H:203:ILE:HG23	1.97	0.45
43:K:166:SER:OG	43:K:167:ASP:N	2.49	0.45
8:s:18:GLU:O	8:s:21:SER:OG	2.29	0.45
20:2:1447:G:OP2	30:h:85:HIS:NE2	2.48	0.45
22:g:48:GLN:HA	22:g:51:LEU:HD12	1.97	0.45
23:b:94:ARG:NE	23:b:101:GLN:HE21	2.15	0.45
35:V:116:ASP:OD1	35:V:116:ASP:N	2.48	0.45
39:C:635:ASP:OD1	39:C:635:ASP:N	2.45	0.45
44:L:438:GLU:HG3	44:L:439:PRO:HD3	1.97	0.45
45:M:121:TYR:OH	45:M:163:THR:OG1	2.31	0.45
7:r:163:ASN:HA	20:2:67:C:H41	1.79	0.45
17:z:55:ILE:HG22	17:z:75:ILE:HG23	1.98	0.45
20:2:1301:A:C4	33:l:6:LEU:HD21	2.51	0.45
26:v:32:ALA:HB3	26:v:110:VAL:HB	1.99	0.45
37:B:391:PHE:HA	37:B:404:ILE:HA	1.98	0.45
38:A:296:LEU:HB3	38:A:322:VAL:HG12	1.99	0.45
40:E:132:TYR:CD1	40:E:132:TYR:C	2.93	0.45
42:H:68:LEU:HD11	42:H:104:MET:HE1	1.98	0.45
42:H:330:ILE:O	42:H:334:THR:N	2.48	0.45
43:K:174:MET:HA	43:K:179:TRP:HB2	1.98	0.45
46:D:67:SER:O	46:D:67:SER:OG	2.30	0.45
2:p:117:TRP:HB3	2:p:153:THR:HG22	1.99	0.45
20:2:880:G:H1	20:2:906:U:H3	1.65	0.45
20:2:1238:U:H1'	27:o:126:VAL:HG22	1.99	0.45
22:g:19:ALA:HB2	22:g:75:GLY:HA3	1.99	0.45
23:b:53:THR:O	23:b:90:LYS:NZ	2.45	0.45
23:b:64:ARG:NH2	25:u:71:LEU:O	2.49	0.45
24:e:92:ILE:HD13	24:e:169:ILE:HD13	1.98	0.45
29:x:2:PRO:HB2	29:x:3:GLY:H	1.61	0.45
35:V:152:SER:OG	35:V:196:ASN:O	2.35	0.45
35:V:157:SER:HA	35:V:200:VAL:HG11	1.98	0.45
38:A:348:ILE:O	38:A:352:GLN:NE2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:441:GLN:NE2	38:A:506:PRO:O	2.47	0.45
44:L:281:HIS:O	44:L:285:GLY:N	2.49	0.45
45:M:46:ILE:HG23	45:M:86:LEU:HD13	1.99	0.45
45:M:88:GLU:OE1	45:M:89:LYS:NZ	2.46	0.45
45:M:203:ASP:OD1	45:M:203:ASP:N	2.49	0.45
20:2:1452:A:N1	20:2:1473:G:N3	2.65	0.45
20:2:1550:G:O2'	20:2:1558:C:O2	2.34	0.45
27:o:123:TYR:OH	28:k:124:ARG:NH1	2.49	0.45
35:V:149:GLU:HB3	35:V:170:TRP:HB2	1.98	0.45
10:c:143:ASN:HB3	20:2:823:U:H5	1.81	0.45
10:c:174:LYS:HE3	20:2:560:A:H5'	1.98	0.45
18:R:67:THR:OG1	18:R:70:LYS:O	2.35	0.45
20:2:145:G:H2'	20:2:146:G:C8	2.52	0.45
20:2:1501:C:H2'	20:2:1502:C:H6	1.81	0.45
20:2:1521:C:H5''	28:k:129:LEU:HD22	1.99	0.45
34:U:144:CYS:HB2	34:U:146:LEU:HB2	1.99	0.45
35:V:304:ASP:OD1	35:V:304:ASP:N	2.47	0.45
38:A:153:LEU:O	38:A:156:SER:OG	2.33	0.45
38:A:353:ARG:HH21	38:A:364:PRO:HD3	1.82	0.45
38:A:398:PHE:HD2	38:A:509:PRO:HB2	1.82	0.45
43:K:151:GLN:HG3	44:L:505:GLY:HA3	1.99	0.45
45:M:210:ARG:HE	45:M:210:ARG:HB2	1.63	0.45
46:D:398:GLU:HB2	46:D:409:TRP:CE2	2.51	0.45
47:Y:3:UNK:O	47:Y:78:UNK:N	2.49	0.45
2:p:73:ASP:OD1	13:i:128:ARG:NH2	2.46	0.45
7:r:56:ASN:HB2	7:r:108:VAL:HG12	1.98	0.45
8:s:115:LYS:HD3	20:2:868:G:C5	2.52	0.45
20:2:1498:A:H1'	23:b:181:VAL:HG11	1.99	0.45
20:2:1622:U:OP2	20:2:1623:A:O2'	2.34	0.45
24:e:30:ILE:HA	24:e:117:ILE:HD11	1.99	0.45
42:H:283:GLN:HA	42:H:286:MET:HE3	1.98	0.45
45:M:82:LEU:HD12	45:M:83:ILE:HG23	1.98	0.45
46:D:378:ASP:OD2	46:D:392:ASN:ND2	2.50	0.45
20:2:1778:C:H2'	20:2:1779:G:C4	2.52	0.45
22:g:14:GLY:HA3	22:g:86:GLN:HG2	1.98	0.45
38:A:285:LYS:HD3	38:A:285:LYS:HA	1.79	0.45
38:A:448:GLN:HE21	38:A:514:MET:HE1	1.82	0.45
43:K:182:ASP:OD1	43:K:182:ASP:N	2.48	0.45
44:L:538:ARG:HE	44:L:538:ARG:HB3	1.62	0.45
45:M:157:THR:HG23	45:M:160:LYS:H	1.82	0.45
46:D:268:VAL:HG11	46:D:527:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:16:LYS:HB3	6:W:16:LYS:HE3	1.70	0.44
7:r:134:GLY:HA3	7:r:158:VAL:HG21	1.99	0.44
10:c:152:ASP:OD1	10:c:152:ASP:N	2.44	0.44
18:R:33:MET:HE3	18:R:33:MET:HB2	1.87	0.44
29:x:131:LEU:HD13	29:x:134:ILE:HD12	1.98	0.44
38:A:570:ALA:O	38:A:574:THR:N	2.51	0.44
40:E:351:ILE:HB	40:E:391:VAL:HG23	1.99	0.44
42:H:147:SER:OG	42:H:148:VAL:N	2.50	0.44
20:2:1388:A:H61	23:b:161:GLY:HA3	1.81	0.44
20:2:1432:U:H2'	20:2:1438:A:C4	2.52	0.44
23:b:143:ARG:NH1	48:J:160:ASN:OD1	2.48	0.44
35:V:249:CYS:HA	35:V:259:TRP:HB2	1.98	0.44
38:A:44:GLN:H	38:A:47:HIS:CD2	2.33	0.44
40:E:26:LEU:HA	40:E:29:LYS:HB3	1.98	0.44
40:E:129:ASP:HA	40:E:132:TYR:HD2	1.82	0.44
40:E:364:PRO:HA	40:E:367:ALA:HB3	1.99	0.44
45:M:52:CYS:SG	45:M:53:LEU:N	2.90	0.44
20:2:1821:U:O2'	20:2:1822:A:O4'	2.34	0.44
23:b:117:ARG:HA	48:J:152:ASP:HB2	2.00	0.44
25:u:32:HIS:CE1	25:u:45:VAL:HG11	2.51	0.44
34:U:95:ARG:O	34:U:97:LYS:NZ	2.50	0.44
38:A:230:LEU:O	38:A:234:LEU:N	2.47	0.44
38:A:386:GLU:HG2	38:A:413:TRP:CD2	2.52	0.44
38:A:524:THR:HA	42:H:228:HIS:HB2	1.99	0.44
40:E:262:ILE:HG12	40:E:335:ASN:HB3	1.99	0.44
1:a:200:ASP:N	1:a:200:ASP:OD1	2.49	0.44
5:q:133:THR:H	20:2:297:A:H5''	1.82	0.44
8:s:178:LYS:NZ	8:s:182:GLY:O	2.43	0.44
13:i:54:CYS:HB3	13:i:81:VAL:HG23	1.99	0.44
20:2:698:G:O6	20:2:732:U:O4	2.36	0.44
20:2:1226:G:N1	20:2:1639:G:OP2	2.39	0.44
20:2:1537:A:H5''	29:x:84:ARG:HH12	1.82	0.44
38:A:191:LYS:NZ	38:A:243:MET:O	2.51	0.44
39:C:587:ASP:OD1	39:C:587:ASP:N	2.50	0.44
40:E:222:PHE:HB3	40:E:232:ILE:HD11	1.98	0.44
40:E:237:LEU:HD21	40:E:257:LEU:HD21	2.00	0.44
40:E:416:GLN:O	40:E:420:MET:N	2.48	0.44
43:K:108:LEU:HB2	43:K:113:HIS:HB2	1.98	0.44
44:L:359:MET:HE3	44:L:359:MET:HB3	1.84	0.44
46:D:295:ALA:HB2	46:D:426:LYS:HG3	1.98	0.44
46:D:307:ASN:HA	46:D:312:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1317:C:H2'	20:2:1318:G:C8	2.52	0.44
37:B:626:ALA:HA	37:B:635:LEU:HA	1.98	0.44
38:A:327:LEU:O	38:A:434:ASN:ND2	2.51	0.44
38:A:450:ILE:HD11	38:A:454:ARG:HG2	1.99	0.44
46:D:365:LEU:HD11	46:D:371:LEU:HD13	1.98	0.44
20:2:1317:C:H2'	20:2:1318:G:H8	1.83	0.44
20:2:1578:U:OP1	20:2:1581:C:N4	2.50	0.44
35:V:67:SER:N	35:V:81:GLY:O	2.44	0.44
39:C:800:ASP:OD1	39:C:800:ASP:N	2.50	0.44
40:E:5:ASP:OD1	40:E:5:ASP:N	2.42	0.44
44:L:206:LYS:HA	44:L:206:LYS:HD3	1.68	0.44
47:Y:5:UNK:HA	47:Y:47:UNK:HA	2.00	0.44
47:Y:5:UNK:N	47:Y:76:UNK:O	2.51	0.44
9:t:81:VAL:HG12	9:t:102:VAL:HG12	2.00	0.44
11:n:83:GLN:NE2	20:2:373:G:H21	2.16	0.44
15:f:4:MET:SD	20:2:682:U:O2'	2.75	0.44
20:2:1119:A:H3'	20:2:1120:U:C6	2.53	0.44
20:2:1545:A:H4'	22:g:74:GLY:HA2	2.00	0.44
29:x:42:HIS:ND1	29:x:82:ARG:O	2.49	0.44
39:C:855:LEU:HB3	42:H:243:LEU:HD22	1.99	0.44
40:E:90:PRO:HA	40:E:93:LYS:HG2	1.99	0.44
41:F:175:THR:HA	41:F:202:VAL:HG13	1.99	0.44
42:H:137:GLN:O	42:H:141:GLN:N	2.50	0.44
43:K:19:ASP:O	43:K:25:ASN:ND2	2.51	0.44
20:2:1714:U:H2'	20:2:1715:A:C8	2.53	0.44
25:u:31:LYS:HD3	25:u:31:LYS:HA	1.81	0.44
38:A:63:LYS:HD3	38:A:63:LYS:HA	1.71	0.44
40:E:294:GLU:HA	40:E:297:GLU:HB3	2.00	0.44
1:a:57:LYS:HD3	14:y:70:LEU:HD13	2.00	0.44
7:r:167:LYS:NZ	20:2:70:G:OP2	2.50	0.44
20:2:1274:G:H5'	25:u:47:LYS:HZ2	1.83	0.44
20:2:1612:G:OP1	27:o:18:ARG:NH2	2.50	0.44
20:2:1652:G:O6	20:2:1672:U:O4	2.36	0.44
37:B:507:ARG:HD3	37:B:556:VAL:HG11	2.00	0.44
39:C:719:ARG:O	39:C:723:ARG:NE	2.37	0.44
40:E:338:LEU:HB2	40:E:374:LEU:HD11	1.98	0.44
3:d:72:ASP:HB3	3:d:74:LYS:HG2	2.00	0.43
20:2:368:U:H5''	20:2:369:C:H3'	1.99	0.43
20:2:528:A:H2'	20:2:529:A:C8	2.52	0.43
27:o:82:ASP:OD1	27:o:82:ASP:N	2.51	0.43
32:S:42:ILE:HB	32:S:64:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:E:319:LEU:HD13	40:E:329:LEU:HA	1.98	0.43
41:F:331:ILE:O	41:F:335:LEU:N	2.41	0.43
44:L:403:LYS:HA	44:L:403:LYS:HD3	1.79	0.43
1:a:144:THR:N	1:a:158:ASP:OD2	2.50	0.43
4:Q:4:LYS:NZ	20:2:1864:U:OP2	2.51	0.43
20:2:1301:A:O2'	20:2:1303:C:OP1	2.36	0.43
22:g:42:ILE:HG23	22:g:44:PRO:HD2	2.00	0.43
23:b:113:LEU:HD21	23:b:117:ARG:HB3	2.00	0.43
24:e:68:ILE:HG13	24:e:151:ILE:HD11	2.00	0.43
24:e:103:LEU:HD21	31:P:67:LEU:HB2	2.00	0.43
31:P:57:LYS:HE3	31:P:77:LEU:HD22	1.98	0.43
37:B:305:GLN:O	37:B:705:ARG:N	2.50	0.43
37:B:548:ARG:HD3	37:B:551:GLU:HG3	2.00	0.43
38:A:238:ASP:OD1	38:A:238:ASP:N	2.44	0.43
40:E:280:VAL:HA	40:E:283:GLN:HG2	2.00	0.43
46:D:291:VAL:HG11	46:D:312:LEU:HG	2.00	0.43
20:2:1277:C:H2'	20:2:1278:A:C8	2.53	0.43
20:2:1308:U:H5	34:U:96:LYS:HD2	1.83	0.43
26:v:26:LEU:HD13	26:v:31:LEU:HD12	2.01	0.43
26:v:52:LEU:HD11	26:v:76:LEU:HD12	2.00	0.43
37:B:623:VAL:H	37:B:639:ASP:HA	1.83	0.43
38:A:219:ASN:HD21	38:A:221:ASN:HD22	1.67	0.43
38:A:464:ALA:HA	38:A:467:LEU:HD12	2.00	0.43
39:C:468:GLU:HA	39:C:471:GLU:HG2	1.99	0.43
39:C:767:ASP:OD1	39:C:776:ARG:NH2	2.49	0.43
41:F:124:VAL:HG23	41:F:129:VAL:HA	2.00	0.43
43:K:71:LEU:HD21	43:K:102:ILE:HD12	2.01	0.43
43:K:80:THR:HG21	44:L:327:ARG:HB2	1.98	0.43
44:L:525:LYS:O	44:L:529:HIS:ND1	2.40	0.43
7:r:160:LYS:NZ	20:2:67:C:OP1	2.38	0.43
17:z:50:THR:OG1	17:z:51:THR:N	2.51	0.43
20:2:1552:G:O2'	20:2:1556:A:OP2	2.31	0.43
25:u:20:VAL:HG12	25:u:70:TYR:HA	1.99	0.43
30:h:23:THR:HA	30:h:88:LEU:HB3	2.00	0.43
35:V:140:TYR:OH	35:V:144:ASP:OD2	2.35	0.43
35:V:155:ARG:HA	35:V:155:ARG:HD3	1.86	0.43
37:B:515:CYS:HA	37:B:530:VAL:HG12	2.00	0.43
39:C:582:TRP:O	39:C:586:ARG:N	2.52	0.43
40:E:334:GLU:HA	40:E:337:ARG:HB2	2.00	0.43
42:H:52:HIS:ND1	42:H:56:GLU:OE2	2.51	0.43
42:H:107:LEU:HA	42:H:110:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L:314:THR:OG1	44:L:356:LYS:NZ	2.49	0.43
20:2:981:A:H2'	20:2:982:G:C8	2.53	0.43
20:2:1779:G:O2'	20:2:1780:G:O4'	2.32	0.43
28:k:6:PRO:HD2	28:k:9:PHE:HB2	2.00	0.43
37:B:521:LYS:HB2	37:B:572:PRO:HA	2.00	0.43
38:A:52:LEU:HD22	38:A:89:VAL:HG23	2.01	0.43
38:A:390:LEU:HD21	38:A:410:VAL:HG11	1.99	0.43
39:C:404:CYS:HA	39:C:407:GLU:HG2	1.99	0.43
44:L:227:VAL:HG22	44:L:231:LEU:HB2	1.99	0.43
46:D:239:ALA:O	46:D:275:LYS:NZ	2.49	0.43
2:p:28:LYS:HE2	2:p:50:THR:HG22	2.00	0.43
4:Q:52:ASP:OD1	4:Q:52:ASP:N	2.39	0.43
17:z:10:ARG:HB3	17:z:11:LYS:H	1.56	0.43
20:2:1112:U:H2'	20:2:1113:A:C8	2.54	0.43
20:2:1748:G:H2'	20:2:1749:G:C8	2.54	0.43
21:w:24:LEU:HB2	21:w:31:ASN:HD22	1.84	0.43
24:e:18:LYS:HD2	24:e:24:SER:HA	2.00	0.43
38:A:191:LYS:HG2	38:A:243:MET:HE2	2.01	0.43
38:A:337:ASP:OD1	38:A:337:ASP:N	2.51	0.43
38:A:473:ASP:OD1	38:A:473:ASP:N	2.51	0.43
17:z:84:LYS:HE3	17:z:84:LYS:HB2	1.83	0.43
18:R:11:SER:HB2	18:R:14:GLU:HG2	2.01	0.43
20:2:1139:C:H2'	20:2:1140:G:O4'	2.19	0.43
20:2:1256:G:H5''	33:l:40:ARG:HH21	1.83	0.43
23:b:60:GLY:HA3	23:b:65:ARG:HB2	2.00	0.43
23:b:74:GLN:NE2	23:b:80:PRO:O	2.52	0.43
28:k:81:ASP:HB2	28:k:95:TYR:CD2	2.54	0.43
35:V:104:HIS:HE2	35:V:130:LYS:HD3	1.84	0.43
40:E:356:LEU:HA	40:E:359:LYS:HB2	1.99	0.43
45:M:42:LEU:HD21	45:M:71:LEU:HD23	2.00	0.43
3:d:108:LYS:HE3	3:d:110:MET:HB3	2.01	0.43
20:2:700:G:H2'	20:2:701:G:H8	1.84	0.43
20:2:752:G:O6	20:2:791:C:O5'	2.36	0.43
20:2:1326:U:OP1	33:l:25:SER:OG	2.31	0.43
27:o:127:LYS:HD3	27:o:127:LYS:HA	1.78	0.43
35:V:165:ILE:HB	35:V:177:TRP:HB2	2.01	0.43
37:B:387:TYR:HA	37:B:408:ASP:HA	2.01	0.43
38:A:28:LEU:HD12	38:A:61:LEU:HD12	2.01	0.43
38:A:175:HIS:CD2	38:A:228:MET:HB3	2.53	0.43
38:A:411:LEU:O	38:A:415:ARG:N	2.51	0.43
39:C:375:LYS:HB3	39:C:408:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:738:VAL:O	39:C:742:LYS:NZ	2.44	0.43
39:C:773:ASP:HA	39:C:776:ARG:HD2	2.01	0.43
42:H:242:ASN:HA	42:H:245:LEU:HD12	2.00	0.43
44:L:376:THR:HA	44:L:377:MET:HA	1.72	0.43
45:M:23:LYS:HA	45:M:23:LYS:HD3	1.75	0.43
20:2:699:C:H2'	20:2:700:G:C8	2.54	0.43
20:2:1557:C:H1'	20:2:1661:A:H5'	2.01	0.43
23:b:28:GLU:HG2	23:b:69:LEU:HD21	2.01	0.43
23:b:98:ALA:O	23:b:102:ALA:CB	2.67	0.43
29:x:108:GLU:OE2	29:x:115:LYS:NZ	2.41	0.43
35:V:225:LYS:HA	35:V:225:LYS:HD2	1.88	0.43
38:A:129:LEU:HD21	39:C:469:TYR:HE2	1.84	0.43
40:E:342:GLU:O	40:E:346:ARG:NE	2.46	0.43
42:H:275:HIS:O	42:H:279:GLN:NE2	2.42	0.43
46:D:287:ASP:OD2	46:D:321:HIS:NE2	2.52	0.43
46:D:508:ILE:HG23	46:D:519:VAL:HG12	2.01	0.43
12:m:91:LEU:HD12	12:m:125:LEU:HD12	2.00	0.43
13:i:104:ARG:NH1	20:2:959:G:OP1	2.51	0.43
22:g:13:PHE:HB3	22:g:22:VAL:HG12	2.00	0.43
29:x:33:TRP:HZ2	29:x:102:ARG:HG3	1.84	0.43
38:A:574:THR:HA	38:A:577:GLU:HG3	2.01	0.43
39:C:448:VAL:HG23	39:C:451:MET:HE3	2.01	0.43
40:E:409:LYS:O	44:L:387:HIS:NE2	2.52	0.43
44:L:284:LEU:HD12	44:L:287:TYR:HB3	2.00	0.43
45:M:41:ASP:O	45:M:44:GLN:NE2	2.52	0.43
5:q:141:THR:OG1	5:q:143:ASP:OD1	2.35	0.42
9:t:4:SER:HB2	9:t:24:LYS:HD3	2.00	0.42
20:2:1605:G:O6	20:2:1632:G:O2'	2.32	0.42
35:V:8:ARG:NH2	35:V:49:GLU:OE1	2.52	0.42
35:V:144:ASP:OD1	35:V:144:ASP:N	2.52	0.42
42:H:249:ARG:O	42:H:253:MET:N	2.50	0.42
7:r:7:PHE:HD2	7:r:10:THR:HG22	1.84	0.42
20:2:494:C:N4	20:2:509:G:H21	2.17	0.42
20:2:708:C:H2'	20:2:709:G:C8	2.54	0.42
20:2:1275:G:H4'	20:2:1276:A:C8	2.55	0.42
20:2:1297:U:N3	20:2:1300:U:OP1	2.38	0.42
23:b:146:ARG:NH1	23:b:147:ALA:O	2.52	0.42
24:e:20:PHE:HB2	24:e:22:LYS:HG2	2.00	0.42
26:v:36:ARG:HA	26:v:36:ARG:HD2	1.86	0.42
34:U:138:ARG:HB2	34:U:147:THR:HG23	2.00	0.42
35:V:209:SER:N	35:V:217:MET:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:398:PHE:O	45:M:317:ARG:NH2	2.52	0.42
39:C:53:LYS:H	39:C:53:LYS:HG2	1.69	0.42
39:C:603:PRO:HA	39:C:606:GLN:HB2	2.01	0.42
40:E:281:ILE:O	40:E:285:SER:OG	2.34	0.42
42:H:156:LYS:HA	42:H:159:GLN:HE21	1.84	0.42
43:K:174:MET:HE1	43:K:187:ILE:HG12	2.01	0.42
44:L:268:MET:SD	44:L:268:MET:N	2.80	0.42
45:M:230:LYS:HA	45:M:230:LYS:HD2	1.82	0.42
1:a:36:GLN:O	1:a:53:ARG:NH1	2.52	0.42
15:f:22:LYS:HD3	18:R:3:LEU:HD12	2.02	0.42
27:o:79:HIS:HA	27:o:97:TYR:HB3	2.00	0.42
29:x:38:LYS:HE3	29:x:38:LYS:HB2	1.81	0.42
29:x:107:LEU:HA	29:x:110:LEU:HD23	2.01	0.42
35:V:112:ALA:HB1	35:V:156:PHE:HB3	2.00	0.42
35:V:218:LEU:HG	35:V:228:TYR:HD2	1.84	0.42
1:a:33:GLN:HB3	1:a:154:LEU:HD12	2.02	0.42
8:s:80:VAL:HG22	8:s:92:VAL:HG23	2.01	0.42
13:i:150:ARG:HH11	20:2:1063:C:H5'	1.85	0.42
15:f:20:ARG:HA	15:f:20:ARG:HD2	1.81	0.42
20:2:726:C:H2'	20:2:727:G:C8	2.54	0.42
23:b:48:ILE:HG21	23:b:86:LEU:HG	2.01	0.42
24:e:192:LYS:HD3	24:e:192:LYS:HA	1.86	0.42
25:u:35:LEU:HD11	25:u:38:LYS:HD2	2.01	0.42
33:l:49:ASP:N	33:l:49:ASP:OD1	2.47	0.42
37:B:624:VAL:HA	37:B:637:PHE:HA	2.00	0.42
40:E:117:LEU:HD22	40:E:157:LEU:HD21	2.01	0.42
41:F:332:ASN:HA	41:F:335:LEU:HB3	2.01	0.42
17:z:66:GLY:HA2	20:2:581:U:H4'	2.00	0.42
21:w:7:LYS:O	21:w:11:LYS:CB	2.67	0.42
23:b:64:ARG:HH12	23:b:65:ARG:HH11	1.67	0.42
24:e:66:CYS:HB3	24:e:71:ARG:HH11	1.85	0.42
26:v:49:LEU:HB3	26:v:111:VAL:HB	2.01	0.42
38:A:523:LEU:HD23	38:A:523:LEU:HA	1.91	0.42
41:F:211:MET:HE2	41:F:211:MET:HB2	1.83	0.42
42:H:243:LEU:HD23	42:H:247:MET:HG3	2.02	0.42
43:K:53:LEU:HA	43:K:56:PHE:HB3	2.01	0.42
46:D:299:PRO:HB2	46:D:309:PRO:HG3	2.01	0.42
9:t:34:ALA:HB2	9:t:56:ARG:HD3	2.02	0.42
20:2:1455:A:H2'	20:2:1456:G:C8	2.55	0.42
20:2:1530:U:H1'	29:x:87:VAL:HG12	2.01	0.42
23:b:151:LYS:HG2	23:b:153:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:143:PRO:HA	24:e:146:ARG:HD3	2.02	0.42
27:o:96:VAL:O	27:o:103:ASN:N	2.51	0.42
28:k:23:ARG:HB3	31:P:80:ARG:HH21	1.85	0.42
32:S:10:LYS:HD3	32:S:38:THR:HG21	2.02	0.42
35:V:44:LYS:HD3	35:V:44:LYS:HA	1.90	0.42
38:A:258:GLY:O	38:A:261:SER:OG	2.31	0.42
39:C:863:LEU:HD11	41:F:344:THR:HG22	2.02	0.42
43:K:181:ALA:HA	43:K:187:ILE:HA	2.02	0.42
46:D:45:TRP:HD1	46:D:46:THR:HG23	1.83	0.42
2:p:34:LYS:O	2:p:98:THR:OG1	2.35	0.42
3:d:198:ALA:HB1	3:d:202:THR:HG21	2.02	0.42
12:m:94:LYS:HB2	12:m:94:LYS:HE3	1.92	0.42
20:2:535:G:H2'	20:2:536:A:C8	2.55	0.42
20:2:700:G:H2'	20:2:701:G:C8	2.55	0.42
20:2:1269:G:H22	20:2:1513:C:H42	1.67	0.42
21:w:98:VAL:HG13	21:w:102:THR:HB	2.02	0.42
24:e:178:ILE:HD12	24:e:181:ALA:HB3	2.02	0.42
26:v:116:LYS:HD3	26:v:116:LYS:HA	1.88	0.42
35:V:17:TRP:H	35:V:36:ARG:HG2	1.85	0.42
38:A:240:ALA:HA	38:A:243:MET:HG2	2.01	0.42
41:F:217:VAL:HG23	41:F:233:THR:HB	2.02	0.42
42:H:141:GLN:HE21	42:H:169:LEU:HB3	1.84	0.42
46:D:242:GLN:HE22	46:D:372:ILE:HG12	1.85	0.42
2:p:44:ILE:HD12	2:p:69:VAL:HG21	2.02	0.42
2:p:192:SER:HB2	38:A:23:LYS:HD2	2.01	0.42
20:2:1280:G:H2'	20:2:1281:G:C8	2.55	0.42
20:2:1627:C:OP1	29:x:83:GLN:NE2	2.52	0.42
39:C:778:MET:HE3	39:C:778:MET:HB3	1.94	0.42
39:C:845:HIS:CD2	40:E:395:ASN:HD21	2.37	0.42
40:E:319:LEU:HB3	40:E:329:LEU:HD22	2.02	0.42
44:L:487:ARG:HA	44:L:488:ILE:HA	1.67	0.42
13:i:124:MET:HE3	13:i:124:MET:HB3	1.85	0.42
15:f:15:ASN:HD21	15:f:71:LYS:HD2	1.84	0.42
20:2:639:C:HO2'	20:2:640:A:H8	1.65	0.42
20:2:1221:G:H2'	20:2:1222:G:C8	2.55	0.42
20:2:1292:C:O2'	34:U:147:THR:OG1	2.27	0.42
24:e:164:ARG:HD2	24:e:164:ARG:HA	1.77	0.42
32:S:14:VAL:HA	32:S:32:VAL:HG12	2.01	0.42
38:A:571:ARG:HH22	42:H:79:THR:HG21	1.85	0.42
38:A:578:ARG:HD3	38:A:581:ARG:HH21	1.85	0.42
44:L:324:LEU:HD12	44:L:371:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L:353:THR:H	44:L:354:THR:HA	1.84	0.42
7:r:126:ASP:OD1	7:r:126:ASP:N	2.52	0.42
20:2:1252:C:H5''	20:2:1254:C:C2	2.54	0.42
20:2:1259:A:H1'	20:2:1264:C:H42	1.84	0.42
20:2:1562:C:H2'	20:2:1563:G:H8	1.85	0.42
24:e:28:VAL:HG21	24:e:41:VAL:HG11	2.02	0.42
26:v:39:ALA:HA	26:v:42:LEU:HB2	2.02	0.42
26:v:40:LYS:HE2	26:v:40:LYS:HB3	1.89	0.42
30:h:74:SER:O	30:h:74:SER:OG	2.34	0.42
32:S:64:GLU:HB2	32:S:66:ARG:CZ	2.50	0.42
35:V:203:ASP:OD1	35:V:203:ASP:N	2.46	0.42
35:V:236:ILE:HD12	35:V:250:ALA:HB1	2.01	0.42
35:V:241:PHE:HA	35:V:248:LEU:HA	2.01	0.42
35:V:292:SER:OG	35:V:293:ALA:N	2.53	0.42
36:I:233:ASN:H	36:I:248:GLY:HA2	1.84	0.42
41:F:115:ARG:NH2	41:F:178:ASP:OD1	2.53	0.42
43:K:147:GLY:HA2	43:K:189:ILE:HG21	2.02	0.42
44:L:237:LYS:HD2	44:L:237:LYS:HA	1.84	0.42
44:L:504:SER:HA	44:L:514:GLN:HB2	2.02	0.42
46:D:194:GLU:HB3	46:D:360:TYR:HB2	2.01	0.42
12:m:55:ARG:NH1	12:m:56:ASP:OD1	2.53	0.41
20:2:1231:C:N4	20:2:1527:C:H42	2.16	0.41
20:2:1334:G:H2'	20:2:1335:G:C8	2.55	0.41
20:2:1539:U:H2'	20:2:1540:G:C8	2.54	0.41
20:2:1648:G:O2'	20:2:1674:G:O6	2.29	0.41
22:g:12:VAL:HG13	22:g:23:ALA:HB3	2.01	0.41
24:e:121:PRO:HG2	24:e:146:ARG:HG2	2.01	0.41
29:x:64:LEU:HD12	29:x:68:GLY:HA2	2.02	0.41
38:A:353:ARG:HD2	38:A:353:ARG:HA	1.84	0.41
38:A:452:PHE:HZ	38:A:464:ALA:HB1	1.84	0.41
41:F:347:GLN:O	41:F:351:ASN:N	2.50	0.41
46:D:291:VAL:HG21	46:D:312:LEU:HB3	2.01	0.41
8:s:66:VAL:HG12	8:s:96:ALA:HB1	2.01	0.41
20:2:391:C:H2'	20:2:392:A:H8	1.85	0.41
20:2:532:C:H2'	20:2:533:A:H8	1.85	0.41
20:2:1412:C:H2'	20:2:1413:G:C8	2.49	0.41
26:v:78:LYS:HA	26:v:78:LYS:HD3	1.88	0.41
26:v:93:LYS:H	26:v:102:LYS:HB3	1.85	0.41
42:H:168:ARG:HG3	42:H:199:GLU:HG3	2.01	0.41
43:K:19:ASP:HA	43:K:22:ASN:HD21	1.85	0.41
44:L:441:LEU:HD13	44:L:445:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M:137:ILE:HG13	45:M:138:GLN:HG2	2.01	0.41
45:M:201:ARG:HG2	45:M:232:LEU:HD11	2.02	0.41
20:2:551:U:H2'	20:2:552:G:H8	1.85	0.41
20:2:562:U:H2'	20:2:563:G:C8	2.54	0.41
20:2:1521:C:H5'	27:o:126:VAL:HB	2.01	0.41
23:b:173:ARG:HB3	23:b:174:HIS:H	1.79	0.41
24:e:39:ILE:HG13	24:e:116:ILE:HG21	2.01	0.41
28:k:6:PRO:HB2	28:k:8:LYS:HG2	2.03	0.41
29:x:34:VAL:O	29:x:52:TRP:NE1	2.41	0.41
30:h:63:ILE:HG22	30:h:65:THR:HG23	2.02	0.41
41:F:249:VAL:O	41:F:253:MET:N	2.48	0.41
42:H:110:VAL:HG13	42:H:112:ILE:HG12	2.01	0.41
42:H:244:GLN:HE21	42:H:247:MET:HE2	1.85	0.41
46:D:246:PHE:HE1	46:D:275:LYS:HD2	1.85	0.41
20:2:896:U:O2'	20:2:897:U:O4'	2.38	0.41
22:g:85:ARG:HH21	22:g:119:LEU:HD21	1.85	0.41
24:e:51:HIS:HB2	24:e:86:LYS:HD2	2.01	0.41
35:V:59:LEU:HG	35:V:95:GLY:HA2	2.00	0.41
37:B:430:LYS:O	37:B:439:ALA:N	2.52	0.41
37:B:451:THR:HA	37:B:452:PRO:HA	1.79	0.41
38:A:285:LYS:HG3	39:C:729:PRO:HD3	2.01	0.41
39:C:835:LEU:HA	39:C:842:VAL:HA	2.01	0.41
40:E:185:ALA:HA	40:E:188:ASP:HB2	2.02	0.41
43:K:51:LEU:HD21	43:K:69:ILE:HG21	2.02	0.41
44:L:405:ASP:HA	44:L:406:PRO:HD3	1.87	0.41
3:d:179:THR:HG21	3:d:198:ALA:H	1.84	0.41
20:2:696:G:H2'	20:2:697:G:H8	1.86	0.41
20:2:1524:G:OP2	28:k:141:ARG:NH1	2.47	0.41
20:2:1718:G:O2'	20:2:1815:A:N6	2.53	0.41
22:g:41:MET:SD	22:g:45:ARG:NH2	2.94	0.41
24:e:202:SER:OG	24:e:203:ASN:N	2.54	0.41
26:v:42:LEU:HD22	26:v:68:LEU:HB3	2.02	0.41
38:A:351:LYS:HE3	38:A:351:LYS:HB3	1.90	0.41
38:A:557:TYR:O	38:A:561:SER:N	2.54	0.41
38:A:564:GLU:HG2	38:A:567:ARG:HE	1.86	0.41
40:E:190:THR:OG1	40:E:191:ARG:NH1	2.53	0.41
40:E:312:LEU:HD11	40:E:333:ILE:HG23	2.02	0.41
45:M:294:PHE:HB2	45:M:330:ARG:HB3	2.01	0.41
45:M:301:LEU:HB2	45:M:303:ILE:HG12	2.02	0.41
20:2:851:C:H5''	20:2:852:G:H5'	2.03	0.41
20:2:1514:G:H2'	20:2:1515:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:w:44:LYS:O	21:w:48:ASN:N	2.44	0.41
24:e:158:ALA:HA	24:e:161:ALA:HB3	2.00	0.41
32:S:31:ARG:HD2	32:S:31:ARG:HA	1.79	0.41
34:U:140:TYR:HE1	34:U:145:CYS:HA	1.85	0.41
35:V:153:CYS:HB2	35:V:197:THR:HA	2.02	0.41
38:A:9:GLU:HG3	38:A:46:ILE:HG12	2.03	0.41
44:L:474:LYS:HD2	44:L:474:LYS:HA	1.85	0.41
46:D:221:LYS:HA	46:D:221:LYS:HD2	1.93	0.41
5:q:124:CYS:HB3	5:q:141:THR:HB	2.02	0.41
20:2:1610:G:H2'	20:2:1611:G:C8	2.55	0.41
27:o:22:LEU:HA	27:o:25:LEU:HB2	2.01	0.41
29:x:97:LYS:HE2	29:x:97:LYS:HB2	1.89	0.41
38:A:380:LEU:O	38:A:388:LYS:NZ	2.44	0.41
40:E:51:VAL:HG11	40:E:74:ARG:HB2	2.03	0.41
41:F:115:ARG:O	41:F:139:HIS:NE2	2.41	0.41
44:L:470:MET:HE2	44:L:513:PHE:HB2	2.02	0.41
44:L:544:ILE:HA	44:L:547:ILE:HD12	2.01	0.41
45:M:21:TYR:O	45:M:24:SER:OG	2.31	0.41
45:M:212:LEU:O	45:M:276:LYS:NZ	2.53	0.41
9:t:181:GLN:NE2	20:2:380:G:OP2	2.53	0.41
10:c:32:ILE:HD11	10:c:40:LYS:HD3	2.03	0.41
20:2:1280:G:H2'	20:2:1281:G:H8	1.85	0.41
24:e:42:LYS:HD2	24:e:44:LYS:H	1.86	0.41
28:k:46:ARG:HB3	29:x:35:ASP:HB2	2.01	0.41
28:k:111:LEU:HD13	28:k:126:PHE:HZ	1.84	0.41
39:C:332:LYS:HD2	39:C:332:LYS:HA	1.88	0.41
42:H:197:MET:HE3	42:H:317:LEU:HB3	2.03	0.41
43:K:18:ILE:HD13	43:K:18:ILE:HA	1.95	0.41
1:a:210:ILE:HD12	1:a:210:ILE:HA	1.92	0.41
9:t:23:LYS:HB2	9:t:23:LYS:HE3	1.87	0.41
10:c:94:LEU:HD23	10:c:97:ILE:HD12	2.03	0.41
20:2:797:C:O2'	20:2:798:G:N3	2.51	0.41
20:2:848:U:H2'	20:2:849:A:H8	1.86	0.41
20:2:1276:A:H61	20:2:1321:G:H2'	1.85	0.41
20:2:1335:G:H3'	20:2:1336:C:H6	1.86	0.41
21:w:5:ARG:HB2	21:w:10:LYS:HE3	2.02	0.41
21:w:9:VAL:HG12	21:w:50:ILE:HG13	2.02	0.41
22:g:85:ARG:HE	22:g:119:LEU:HD11	1.86	0.41
24:e:116:ILE:HD12	24:e:116:ILE:HA	1.89	0.41
31:P:69:THR:HG22	31:P:71:ALA:H	1.86	0.41
35:V:8:ARG:HB3	35:V:309:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:V:34:ALA:HB2	35:V:69:VAL:HG22	2.03	0.41
35:V:284:PRO:HB2	35:V:302:TYR:HD2	1.85	0.41
36:I:149:ILE:HA	36:I:165:HIS:HA	2.03	0.41
38:A:309:ASN:OD1	38:A:309:ASN:N	2.54	0.41
38:A:421:GLU:HB3	38:A:424:LEU:HB2	2.02	0.41
41:F:319:VAL:HA	41:F:320:PRO:HD3	1.90	0.41
42:H:208:SER:H	42:H:211:ILE:HD12	1.86	0.41
46:D:472:LYS:HB2	46:D:475:GLU:HG2	2.02	0.41
10:c:125:HIS:O	10:c:129:LEU:HB2	2.21	0.41
20:2:537:C:H42	20:2:544:G:H1	1.68	0.41
20:2:874:G:H2'	20:2:875:A:C8	2.56	0.41
20:2:887:U:C4	20:2:900:C:C4	3.09	0.41
20:2:1376:A:OP2	21:w:67:ARG:NH2	2.54	0.41
20:2:1610:G:H2'	20:2:1611:G:H8	1.86	0.41
20:2:1736:G:H2'	20:2:1737:G:C8	2.56	0.41
22:g:131:LYS:O	22:g:140:ARG:NH1	2.54	0.41
24:e:42:LYS:O	24:e:46:ALA:N	2.54	0.41
24:e:110:GLN:HA	24:e:113:VAL:HG12	2.02	0.41
40:E:291:PRO:O	40:E:295:PHE:N	2.54	0.41
43:K:52:LYS:O	43:K:55:GLN:NE2	2.47	0.41
43:K:139:ARG:NH2	43:K:162:LEU:O	2.54	0.41
44:L:224:VAL:HA	44:L:227:VAL:HG12	2.03	0.41
44:L:430:ASN:OD1	44:L:430:ASN:N	2.53	0.41
44:L:486:PHE:HA	44:L:489:GLN:HB2	2.01	0.41
44:L:541:ASP:HA	44:L:545:ARG:HH21	1.85	0.41
1:a:38:ILE:HD13	1:a:38:ILE:HA	1.89	0.40
7:r:35:GLU:HG2	7:r:51:ARG:HB2	2.03	0.40
9:t:205:ARG:HD2	9:t:205:ARG:HA	1.73	0.40
10:c:174:LYS:HB2	20:2:560:A:H5'	2.03	0.40
12:m:125:LEU:HA	12:m:125:LEU:HD23	1.86	0.40
20:2:1324:G:O2'	20:2:1510:G:O2'	2.33	0.40
21:w:73:LEU:HD23	21:w:76:GLU:HG3	2.03	0.40
23:b:101:GLN:HA	23:b:104:SER:HB3	2.02	0.40
27:o:118:GLU:HG2	28:k:120:HIS:H	1.85	0.40
30:h:27:ARG:NH2	33:l:50:ILE:O	2.54	0.40
30:h:34:LYS:HD2	30:h:34:LYS:HA	1.80	0.40
39:C:659:ASN:OD1	39:C:662:GLN:NE2	2.54	0.40
41:F:244:THR:HA	41:F:247:ILE:HG22	2.03	0.40
42:H:148:VAL:HA	42:H:168:ARG:HB3	2.02	0.40
44:L:460:ILE:HG13	44:L:499:ASN:HB2	2.01	0.40
46:D:289:LEU:HD22	46:D:431:LYS:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:D:506:TYR:HA	46:D:522:LEU:HB2	2.02	0.40
4:Q:7:ASN:ND2	4:Q:10:ARG:O	2.55	0.40
7:r:163:ASN:OD1	7:r:163:ASN:N	2.53	0.40
8:s:9:VAL:HG13	8:s:24:SER:HB2	2.03	0.40
20:2:942:G:H2'	20:2:943:U:C6	2.56	0.40
20:2:1643:U:H2'	20:2:1644:C:C6	2.57	0.40
20:2:1748:G:H2'	20:2:1749:G:H8	1.86	0.40
27:o:67:ALA:HB2	27:o:73:PRO:HB3	2.03	0.40
38:A:374:MET:HE2	38:A:374:MET:HB2	2.00	0.40
41:F:161:LYS:HB2	41:F:161:LYS:HE2	1.85	0.40
44:L:525:LYS:O	44:L:529:HIS:N	2.49	0.40
46:D:174:MET:SD	46:D:174:MET:N	2.94	0.40
1:a:52:LYS:HD2	1:a:52:LYS:HA	1.87	0.40
1:a:207:PRO:HA	1:a:210:ILE:HG22	2.03	0.40
2:p:222:LYS:HE3	2:p:222:LYS:HB3	1.95	0.40
5:q:250:GLU:H	5:q:250:GLU:HG3	1.73	0.40
12:m:40:LEU:HA	12:m:40:LEU:HD23	1.90	0.40
16:j:37:LYS:HE3	16:j:37:LYS:HB3	1.75	0.40
20:2:1214:A:H61	20:2:1685:U:H3	1.68	0.40
20:2:1256:G:H5''	33:l:40:ARG:HE	1.87	0.40
20:2:1443:C:C2	22:g:11:GLN:HG2	2.56	0.40
20:2:1758:G:OP1	20:2:1772:C:N4	2.53	0.40
24:e:103:LEU:HD11	31:P:67:LEU:HD22	2.03	0.40
27:o:17:TYR:HD2	27:o:36:LEU:HD13	1.86	0.40
37:B:450:GLU:O	37:B:454:MET:N	2.49	0.40
38:A:577:GLU:O	38:A:581:ARG:N	2.53	0.40
41:F:106:TYR:HB2	41:F:175:THR:HG21	2.01	0.40
41:F:140:ASN:HB2	41:F:147:ALA:HB3	2.02	0.40
41:F:261:ARG:HG3	42:H:207:ASN:H	1.86	0.40
45:M:320:MET:HE2	45:M:320:MET:HB3	1.96	0.40
9:t:37:LYS:HE2	9:t:37:LYS:HB2	1.90	0.40
20:2:115:U:H2'	20:2:116:U:C6	2.57	0.40
20:2:1118:C:H6	20:2:1118:C:H2'	1.72	0.40
20:2:1713:C:H2'	20:2:1714:U:C6	2.57	0.40
33:l:42:CYS:HA	33:l:45:GLN:HB2	2.02	0.40
38:A:304:ARG:HA	38:A:304:ARG:HD3	1.94	0.40
38:A:523:LEU:O	38:A:527:SER:OG	2.35	0.40
40:E:289:LYS:HA	40:E:289:LYS:HD2	1.93	0.40
41:F:97:VAL:HG21	42:H:51:LYS:HG2	2.03	0.40
42:H:138:PHE:HA	42:H:141:GLN:HB2	2.04	0.40
3:d:156:ILE:HD13	3:d:156:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:1515:G:H2'	20:2:1516:G:H8	1.86	0.40
20:2:1780:G:H2'	20:2:1781:A:H8	1.86	0.40
23:b:17:PHE:O	23:b:21:LEU:HB2	2.21	0.40
31:P:56:ASP:O	31:P:60:LYS:CB	2.68	0.40
37:B:531:ASP:HA	37:B:542:THR:HB	2.03	0.40
39:C:396:GLU:H	39:C:396:GLU:HG3	1.76	0.40
40:E:403:GLN:NE2	40:E:406:GLU:OE2	2.39	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%)	209 (98%)	5 (2%)	0	100	100
2	p	209/264 (79%)	196 (94%)	13 (6%)	0	100	100
3	d	214/293 (73%)	199 (93%)	15 (7%)	0	100	100
4	Q	99/115 (86%)	95 (96%)	4 (4%)	0	100	100
5	q	253/263 (96%)	241 (95%)	12 (5%)	0	100	100
6	W	22/25 (88%)	22 (100%)	0	0	100	100
7	r	220/249 (88%)	209 (95%)	11 (5%)	0	100	100
8	s	165/194 (85%)	160 (97%)	5 (3%)	0	100	100
9	t	195/208 (94%)	182 (93%)	13 (7%)	0	100	100
10	c	178/194 (92%)	172 (97%)	6 (3%)	0	100	100
11	n	131/158 (83%)	126 (96%)	5 (4%)	0	100	100
12	m	147/151 (97%)	147 (100%)	0	0	100	100
13	i	123/151 (82%)	114 (93%)	9 (7%)	0	100	100
14	y	80/83 (96%)	79 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	f	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
16	j	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
17	z	120/133 (90%)	115 (96%)	5 (4%)	0	100	100
18	R	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
19	T	40/59 (68%)	39 (98%)	1 (2%)	0	100	100
21	w	124/135 (92%)	112 (90%)	12 (10%)	0	100	100
22	g	136/146 (93%)	125 (92%)	11 (8%)	0	100	100
23	b	222/243 (91%)	196 (88%)	26 (12%)	0	100	100
24	e	187/204 (92%)	167 (89%)	20 (11%)	0	100	100
25	u	93/165 (56%)	83 (89%)	10 (11%)	0	100	100
26	v	107/132 (81%)	97 (91%)	10 (9%)	0	100	100
27	o	117/145 (81%)	112 (96%)	5 (4%)	0	100	100
28	k	138/152 (91%)	126 (91%)	12 (9%)	0	100	100
29	x	139/145 (96%)	131 (94%)	8 (6%)	0	100	100
30	h	96/119 (81%)	87 (91%)	9 (9%)	0	100	100
31	P	68/125 (54%)	61 (90%)	7 (10%)	0	100	100
32	S	59/69 (86%)	51 (86%)	8 (14%)	0	100	100
33	l	52/56 (93%)	45 (86%)	7 (14%)	0	100	100
34	U	53/156 (34%)	51 (96%)	2 (4%)	0	100	100
35	V	290/317 (92%)	258 (89%)	31 (11%)	1 (0%)	36	70
36	I	301/325 (93%)	293 (97%)	8 (3%)	0	100	100
37	B	528/814 (65%)	491 (93%)	37 (7%)	0	100	100
38	A	588/703 (84%)	562 (96%)	26 (4%)	0	100	100
39	C	615/913 (67%)	575 (94%)	40 (6%)	0	100	100
40	E	406/445 (91%)	394 (97%)	12 (3%)	0	100	100
41	F	267/357 (75%)	244 (91%)	23 (9%)	0	100	100
42	H	289/352 (82%)	270 (93%)	19 (7%)	0	100	100
43	K	215/218 (99%)	202 (94%)	13 (6%)	0	100	100
44	L	370/564 (66%)	332 (90%)	38 (10%)	0	100	100
45	M	328/374 (88%)	314 (96%)	14 (4%)	0	100	100
46	D	441/548 (80%)	402 (91%)	39 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	J	28/180 (16%)	25 (89%)	3 (11%)	0	100	100
All	All	9011/11294 (80%)	8443 (94%)	567 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	V	175	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	173/243 (71%)	171 (99%)	2 (1%)	63	82
2	p	192/231 (83%)	192 (100%)	0	100	100
3	d	182/225 (81%)	181 (100%)	1 (0%)	81	89
4	Q	88/98 (90%)	87 (99%)	1 (1%)	65	83
5	q	220/225 (98%)	218 (99%)	2 (1%)	70	85
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%)	154 (99%)	1 (1%)	78	88
9	t	174/180 (97%)	173 (99%)	1 (1%)	78	88
10	c	160/168 (95%)	160 (100%)	0	100	100
11	n	125/142 (88%)	123 (98%)	2 (2%)	55	79
12	m	130/131 (99%)	130 (100%)	0	100	100
13	i	98/119 (82%)	98 (100%)	0	100	100
14	y	66/67 (98%)	66 (100%)	0	100	100
15	f	112/113 (99%)	111 (99%)	1 (1%)	70	85
16	j	111/115 (96%)	110 (99%)	1 (1%)	70	85
17	z	106/115 (92%)	105 (99%)	1 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	74/76 (97%)	74 (100%)	0	100	100
19	T	35/48 (73%)	35 (100%)	0	100	100
21	w	111/122 (91%)	109 (98%)	2 (2%)	51	77
22	g	114/121 (94%)	114 (100%)	0	100	100
23	b	188/202 (93%)	186 (99%)	2 (1%)	65	83
24	e	159/170 (94%)	157 (99%)	2 (1%)	61	81
25	u	86/136 (63%)	86 (100%)	0	100	100
26	v	94/108 (87%)	94 (100%)	0	100	100
27	o	107/130 (82%)	107 (100%)	0	100	100
28	k	122/132 (92%)	122 (100%)	0	100	100
29	x	111/115 (96%)	111 (100%)	0	100	100
30	h	91/107 (85%)	90 (99%)	1 (1%)	65	83
31	P	62/103 (60%)	61 (98%)	1 (2%)	55	79
32	S	54/62 (87%)	53 (98%)	1 (2%)	50	76
33	l	47/49 (96%)	47 (100%)	0	100	100
34	U	51/140 (36%)	51 (100%)	0	100	100
35	V	256/275 (93%)	252 (98%)	4 (2%)	55	79
37	B	90/702 (13%)	90 (100%)	0	100	100
38	A	545/553 (99%)	543 (100%)	2 (0%)	84	90
39	C	553/811 (68%)	550 (100%)	3 (0%)	81	89
40	E	380/406 (94%)	377 (99%)	3 (1%)	73	86
41	F	237/289 (82%)	236 (100%)	1 (0%)	84	90
42	H	269/310 (87%)	269 (100%)	0	100	100
43	K	192/193 (100%)	191 (100%)	1 (0%)	81	89
44	L	342/515 (66%)	339 (99%)	3 (1%)	70	85
45	M	305/335 (91%)	305 (100%)	0	100	100
46	D	398/494 (81%)	398 (100%)	0	100	100
48	J	26/151 (17%)	26 (100%)	0	100	100
All	All	7407/9443 (78%)	7368 (100%)	39 (0%)	78	89

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	157	VAL
1	a	200	ASP
3	d	94	ILE
4	Q	18	VAL
5	q	12	VAL
5	q	126	VAL
8	s	8	ILE
9	t	138	ASN
11	n	56	ILE
11	n	120	VAL
15	f	80	ASP
16	j	112	VAL
17	z	102	THR
21	w	98	VAL
21	w	114	LEU
23	b	44	THR
23	b	186	VAL
24	e	69	VAL
24	e	141	VAL
30	h	29	VAL
31	P	48	VAL
32	S	55	VAL
35	V	6	THR
35	V	71	ILE
35	V	121	VAL
35	V	287	THR
38	A	347	ILE
38	A	428	VAL
39	C	76	VAL
39	C	96	ILE
39	C	412	LEU
40	E	51	VAL
40	E	132	TYR
40	E	385	ASP
41	F	255	THR
43	K	111	THR
44	L	408	VAL
44	L	468	THR
44	L	546	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	33	GLN
1	a	131	HIS
1	a	164	ASN
1	a	193	HIS
2	p	40	ASN
2	p	157	GLN
2	p	158	HIS
2	p	160	GLN
2	p	179	ASN
3	d	172	ASN
3	d	235	ASN
5	q	8	HIS
5	q	17	HIS
5	q	98	ASN
5	q	138	HIS
5	q	142	HIS
5	q	214	ASN
5	q	224	ASN
6	W	22	GLN
7	r	13	GLN
7	r	56	ASN
8	s	73	GLN
8	s	76	GLN
8	s	162	GLN
9	t	64	ASN
9	t	146	GLN
9	t	165	GLN
9	t	167	GLN
10	c	132	GLN
10	c	143	ASN
10	c	154	GLN
11	n	11	GLN
11	n	13	GLN
11	n	83	GLN
11	n	94	HIS
11	n	112	HIS
11	n	141	ASN
12	m	62	GLN
13	i	38	ASN
13	i	43	HIS
13	i	79	GLN
13	i	83	GLN
13	i	113	GLN

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Mol	Chain	Res	Type
15	f	113	HIS
16	j	61	GLN
16	j	73	GLN
16	j	97	ASN
17	z	22	GLN
17	z	106	GLN
18	R	26	GLN
19	T	44	ASN
19	T	58	ASN
21	w	31	ASN
21	w	116	ASN
21	w	121	GLN
22	g	97	GLN
23	b	4	GLN
23	b	101	GLN
23	b	145	GLN
24	e	65	GLN
24	e	74	ASN
24	e	82	ASN
24	e	137	GLN
24	e	148	ASN
24	e	179	ASN
25	u	73	ASN
26	v	55	ASN
26	v	119	GLN
27	o	98	ASN
27	o	104	GLN
28	k	19	ASN
28	k	101	ASN
28	k	105	ASN
28	k	135	HIS
29	x	10	ASN
29	x	11	GLN
29	x	51	ASN
29	x	63	HIS
29	x	128	GLN
29	x	137	GLN
30	h	47	ASN
31	P	46	ASN
33	l	10	HIS
34	U	91	ASN
35	V	20	GLN

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Mol	Chain	Res	Type
35	V	178	ASN
35	V	215	GLN
35	V	237	ASN
35	V	296	GLN
35	V	305	ASN
35	V	311	GLN
37	B	477	ASN
37	B	520	GLN
37	B	522	ASN
38	A	10	ASN
38	A	16	ASN
38	A	47	HIS
38	A	76	ASN
38	A	166	ASN
38	A	226	GLN
38	A	288	ASN
38	A	362	GLN
38	A	392	ASN
38	A	448	GLN
38	A	544	GLN
38	A	549	GLN
38	A	550	HIS
38	A	551	GLN
38	A	566	GLN
38	A	586	ASN
39	C	430	ASN
39	C	433	ASN
39	C	460	GLN
39	C	465	HIS
39	C	584	GLN
39	C	595	GLN
39	C	630	HIS
39	C	676	HIS
39	C	753	HIS
39	C	852	GLN
39	C	854	ASN
40	E	49	ASN
40	E	83	GLN
40	E	180	GLN
40	E	181	ASN
40	E	210	GLN
40	E	283	GLN

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Mol	Chain	Res	Type
40	E	302	ASN
40	E	373	ASN
40	E	395	ASN
41	F	155	ASN
41	F	160	HIS
41	F	182	HIS
41	F	260	ASN
41	F	347	GLN
41	F	356	ASN
42	H	38	GLN
42	H	141	GLN
42	H	159	GLN
42	H	244	GLN
42	H	255	GLN
42	H	266	ASN
42	H	285	ASN
42	H	324	ASN
42	H	336	GLN
42	H	345	GLN
42	H	348	GLN
42	H	351	ASN
43	K	10	ASN
43	K	22	ASN
43	K	25	ASN
43	K	91	GLN
43	K	144	HIS
43	K	186	GLN
44	L	181	GLN
44	L	239	ASN
44	L	312	GLN
44	L	363	GLN
44	L	489	GLN
45	M	65	ASN
45	M	155	ASN
45	M	205	HIS
45	M	258	ASN
45	M	355	ASN
46	D	57	ASN
46	D	68	GLN
46	D	191	GLN
46	D	242	GLN
46	D	270	GLN

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Mol	Chain	Res	Type
46	D	296	ASN
46	D	320	ASN
46	D	336	ASN
46	D	341	ASN
46	D	351	ASN
46	D	392	ASN
46	D	427	ASN
46	D	481	ASN
48	J	158	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	2	1709/1868 (91%)	459 (26%)	9 (0%)

All (459) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	2	2	A
20	2	17	C
20	2	23	G
20	2	33	G
20	2	41	G
20	2	44	U
20	2	45	A
20	2	46	A
20	2	49	C
20	2	56	G
20	2	62	G
20	2	67	C
20	2	68	A
20	2	71	G
20	2	73	C
20	2	74	G
20	2	75	G
20	2	76	U
20	2	79	A
20	2	92	A
20	2	103	A
20	2	113	G
20	2	114	G

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Mol	Chain	Res	Type
20	2	115	U
20	2	126	G
20	2	130	G
20	2	142	C
20	2	143	U
20	2	147	A
20	2	149	A
20	2	158	A
20	2	160	U
20	2	164	A
20	2	168	C
20	2	178	C
20	2	182	C
20	2	184	G
20	2	190	G
20	2	194	C
20	2	196	C
20	2	197	U
20	2	199	C
20	2	200	G
20	2	201	C
20	2	202	G
20	2	204	G
20	2	206	G
20	2	210	U
20	2	308	G
20	2	310	C
20	2	312	G
20	2	313	A
20	2	319	C
20	2	320	G
20	2	333	G
20	2	344	U
20	2	345	U
20	2	347	G
20	2	351	G
20	2	362	C
20	2	364	A
20	2	368	U
20	2	369	C
20	2	382	C
20	2	384	U

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Mol	Chain	Res	Type
20	2	385	G
20	2	386	C
20	2	400	C
20	2	409	C
20	2	418	A
20	2	429	C
20	2	436	G
20	2	438	G
20	2	448	A
20	2	449	A
20	2	450	C
20	2	455	A
20	2	464	A
20	2	465	A
20	2	470	G
20	2	471	G
20	2	472	C
20	2	474	G
20	2	482	G
20	2	483	C
20	2	487	U
20	2	492	C
20	2	509	G
20	2	516	A
20	2	517	C
20	2	523	A
20	2	525	A
20	2	537	C
20	2	538	U
20	2	539	C
20	2	541	U
20	2	542	U
20	2	545	A
20	2	546	G
20	2	547	G
20	2	548	C
20	2	549	C
20	2	551	U
20	2	559	G
20	2	560	A
20	2	563	G
20	2	568	C

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Mol	Chain	Res	Type
20	2	570	C
20	2	574	A
20	2	576	A
20	2	587	A
20	2	588	G
20	2	591	U
20	2	603	C
20	2	604	A
20	2	607	U
20	2	608	C
20	2	614	C
20	2	617	G
20	2	621	C
20	2	623	G
20	2	627	U
20	2	628	A
20	2	629	A
20	2	632	C
20	2	638	C
20	2	639	C
20	2	640	A
20	2	643	A
20	2	644	G
20	2	655	A
20	2	659	G
20	2	660	C
20	2	664	A
20	2	668	A
20	2	669	A
20	2	671	A
20	2	672	A
20	2	673	G
20	2	683	G
20	2	687	C
20	2	690	G
20	2	698	G
20	2	707	C
20	2	709	G
20	2	721	G
20	2	723	C
20	2	731	G
20	2	737	G

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Mol	Chain	Res	Type
20	2	748	C
20	2	750	C
20	2	751	G
20	2	792	C
20	2	793	G
20	2	794	A
20	2	795	A
20	2	796	G
20	2	798	G
20	2	799	U
20	2	800	U
20	2	801	U
20	2	810	A
20	2	821	G
20	2	822	U
20	2	827	A
20	2	830	A
20	2	847	A
20	2	853	C
20	2	869	A
20	2	870	A
20	2	872	A
20	2	873	G
20	2	874	G
20	2	878	G
20	2	880	G
20	2	883	U
20	2	884	C
20	2	886	A
20	2	887	U
20	2	888	U
20	2	889	U
20	2	890	U
20	2	891	G
20	2	893	U
20	2	895	G
20	2	896	U
20	2	897	U
20	2	898	U
20	2	899	U
20	2	901	G
20	2	902	G

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Mol	Chain	Res	Type
20	2	903	A
20	2	905	C
20	2	912	C
20	2	913	A
20	2	920	A
20	2	922	A
20	2	933	G
20	2	938	A
20	2	943	U
20	2	952	G
20	2	953	C
20	2	963	A
20	2	971	G
20	2	990	A
20	2	992	A
20	2	1002	U
20	2	1008	A
20	2	1017	U
20	2	1023	A
20	2	1026	C
20	2	1045	U
20	2	1049	A
20	2	1053	C
20	2	1056	U
20	2	1058	A
20	2	1060	A
20	2	1061	U
20	2	1062	A
20	2	1063	C
20	2	1074	C
20	2	1083	A
20	2	1085	C
20	2	1096	G
20	2	1109	C
20	2	1114	U
20	2	1115	U
20	2	1117	C
20	2	1118	C
20	2	1119	A
20	2	1120	U
20	2	1138	C
20	2	1140	G

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Mol	Chain	Res	Type
20	2	1144	A
20	2	1153	C
20	2	1154	U
20	2	1157	G
20	2	1168	G
20	2	1171	G
20	2	1188	A
20	2	1195	A
20	2	1203	G
20	2	1207	G
20	2	1215	C
20	2	1216	C
20	2	1218	C
20	2	1220	A
20	2	1227	G
20	2	1228	A
20	2	1230	C
20	2	1231	C
20	2	1232	U
20	2	1240	A
20	2	1242	U
20	2	1244	U
20	2	1245	G
20	2	1248	U
20	2	1250	A
20	2	1251	A
20	2	1252	C
20	2	1253	A
20	2	1256	G
20	2	1257	G
20	2	1258	A
20	2	1259	A
20	2	1261	C
20	2	1263	U
20	2	1264	C
20	2	1269	G
20	2	1272	C
20	2	1275	G
20	2	1276	A
20	2	1283	C
20	2	1284	A
20	2	1285	G

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Mol	Chain	Res	Type
20	2	1286	G
20	2	1287	A
20	2	1291	A
20	2	1293	A
20	2	1295	A
20	2	1303	C
20	2	1304	U
20	2	1308	U
20	2	1309	C
20	2	1312	G
20	2	1313	A
20	2	1315	U
20	2	1319	U
20	2	1322	G
20	2	1324	G
20	2	1327	G
20	2	1330	G
20	2	1331	C
20	2	1332	A
20	2	1333	U
20	2	1334	G
20	2	1336	C
20	2	1337	C
20	2	1340	U
20	2	1341	C
20	2	1343	U
20	2	1348	G
20	2	1364	U
20	2	1371	U
20	2	1372	U
20	2	1378	A
20	2	1381	G
20	2	1384	C
20	2	1397	U
20	2	1398	G
20	2	1400	U
20	2	1401	A
20	2	1402	A
20	2	1404	U
20	2	1405	A
20	2	1410	C
20	2	1416	C

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Mol	Chain	Res	Type
20	2	1428	G
20	2	1429	G
20	2	1430	C
20	2	1439	A
20	2	1440	C
20	2	1441	U
20	2	1442	U
20	2	1447	G
20	2	1448	A
20	2	1449	G
20	2	1450	G
20	2	1454	A
20	2	1456	G
20	2	1462	U
20	2	1463	U
20	2	1464	C
20	2	1475	G
20	2	1476	A
20	2	1477	U
20	2	1480	A
20	2	1486	A
20	2	1489	A
20	2	1490	G
20	2	1492	U
20	2	1493	C
20	2	1495	G
20	2	1497	G
20	2	1498	A
20	2	1499	U
20	2	1500	G
20	2	1501	C
20	2	1507	G
20	2	1508	A
20	2	1509	U
20	2	1513	C
20	2	1519	U
20	2	1520	G
20	2	1521	C
20	2	1522	A
20	2	1525	C
20	2	1532	C
20	2	1533	A

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Mol	Chain	Res	Type
20	2	1535	U
20	2	1536	G
20	2	1547	C
20	2	1548	G
20	2	1553	C
20	2	1554	C
20	2	1555	U
20	2	1557	C
20	2	1559	C
20	2	1566	G
20	2	1568	C
20	2	1570	G
20	2	1580	A
20	2	1585	U
20	2	1586	U
20	2	1587	G
20	2	1591	C
20	2	1592	C
20	2	1598	G
20	2	1599	U
20	2	1601	A
20	2	1603	G
20	2	1606	G
20	2	1612	G
20	2	1613	G
20	2	1621	U
20	2	1623	A
20	2	1624	U
20	2	1632	G
20	2	1633	A
20	2	1636	G
20	2	1638	G
20	2	1647	A
20	2	1648	G
20	2	1654	G
20	2	1661	A
20	2	1665	G
20	2	1669	G
20	2	1671	G
20	2	1673	U
20	2	1678	A
20	2	1681	U

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Mol	Chain	Res	Type
20	2	1686	G
20	2	1695	A
20	2	1698	C
20	2	1699	A
20	2	1718	G
20	2	1719	A
20	2	1720	U
20	2	1721	U
20	2	1725	U
20	2	1726	G
20	2	1730	U
20	2	1737	G
20	2	1742	C
20	2	1744	G
20	2	1751	C
20	2	1752	C
20	2	1755	C
20	2	1756	C
20	2	1757	G
20	2	1758	G
20	2	1759	G
20	2	1760	G
20	2	1761	U
20	2	1772	C
20	2	1773	C
20	2	1774	C
20	2	1776	G
20	2	1777	G
20	2	1779	G
20	2	1783	C
20	2	1784	G
20	2	1785	C
20	2	1786	U
20	2	1806	A
20	2	1808	U
20	2	1810	U
20	2	1821	U
20	2	1822	A
20	2	1823	A
20	2	1824	A
20	2	1825	A
20	2	1826	G

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Mol	Chain	Res	Type
20	2	1831	A
20	2	1834	A
20	2	1835	A
20	2	1836	G
20	2	1838	U
20	2	1849	G
20	2	1850	A
20	2	1851	A
20	2	1861	G
20	2	1862	G
20	2	1863	A
20	2	1864	U
20	2	1865	C
20	2	1866	A
20	2	1867	U
20	2	1869	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	2	332	G
20	2	550	C
20	2	868	G
20	2	912	C
20	2	1060	A
20	2	1292	C
20	2	1329	U
20	2	1474	A
20	2	1807	C

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	2	4
38	A	3
45	M	1
10	c	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	685:UNK	C	707:UNK	N	30.94
1	A	640:UNK	C	642:UNK	N	11.63
1	M	96:GLY	C	97:GLU	N	9.05
1	2	746:C	O3'	747:U	P	4.59
1	2	1207:G	O3'	1208:A	P	4.33
1	A	601:LEU	C	602:UNK	N	3.40
1	2	1682:C	O3'	1683:C	P	3.22
1	2	368:U	O3'	369:C	P	3.18
1	c	162:ARG	C	163:SER	N	1.18

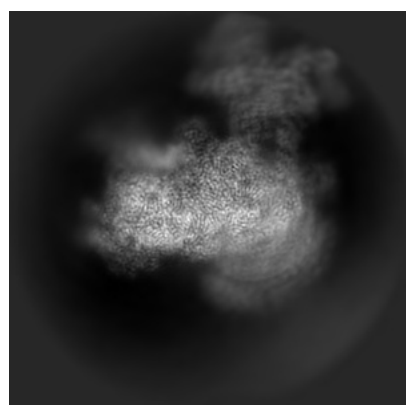
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11325. These allow visual inspection of the internal detail of the map and identification of artifacts.

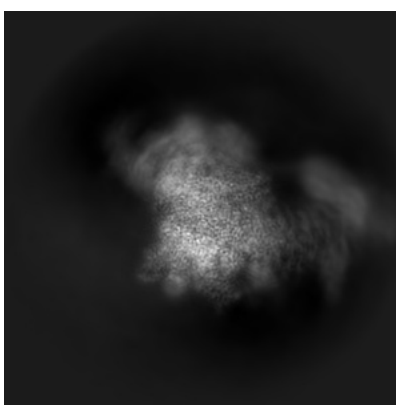
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

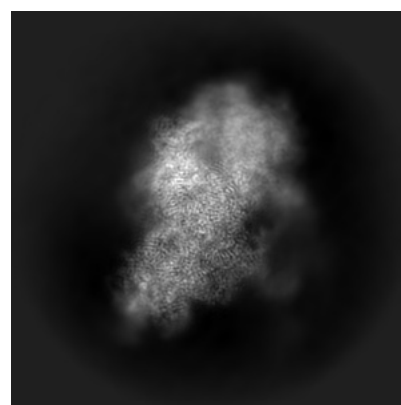
6.1.1 Primary map



X



Y

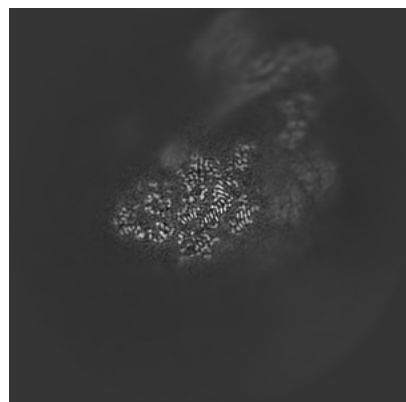


Z

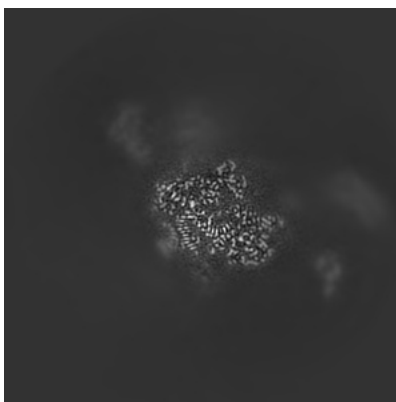
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

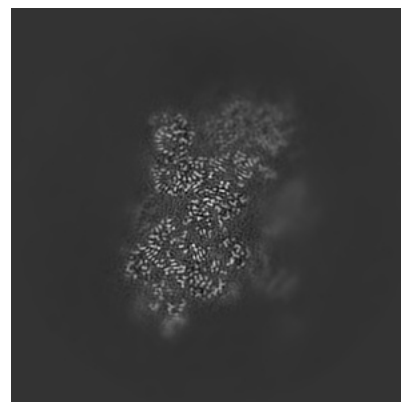
6.2.1 Primary map



X Index: 180



Y Index: 180

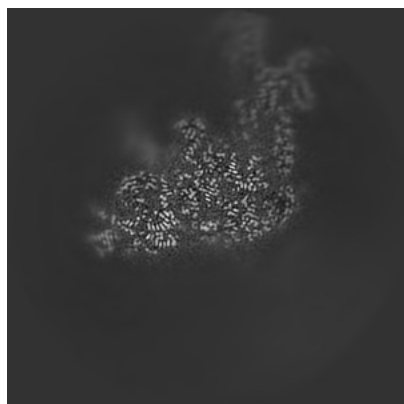


Z Index: 180

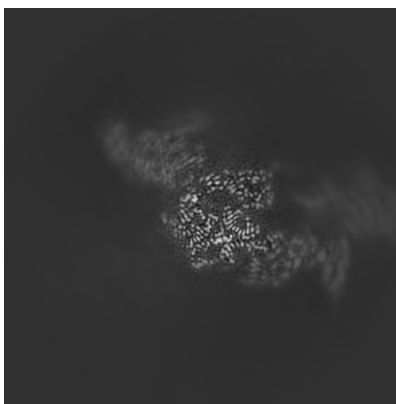
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

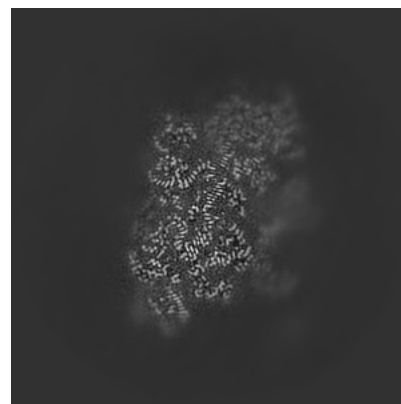
6.3.1 Primary map



X Index: 158



Y Index: 204

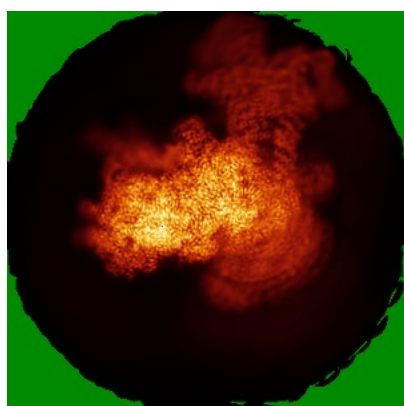


Z Index: 175

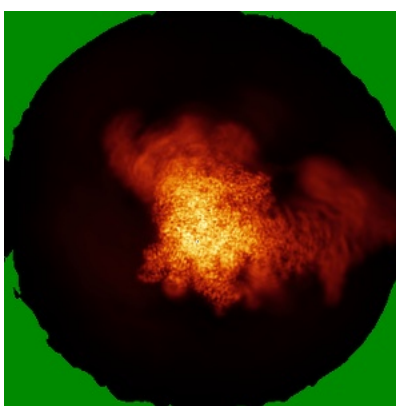
The images above show the largest variance slices of the map in three orthogonal directions.

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

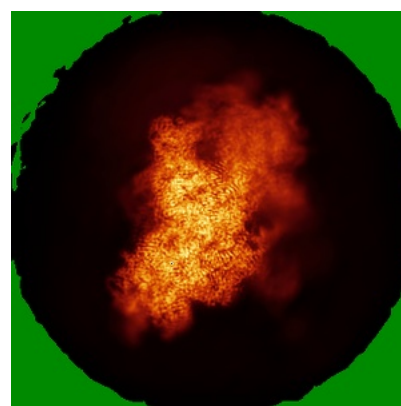
6.4.1 Primary map



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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

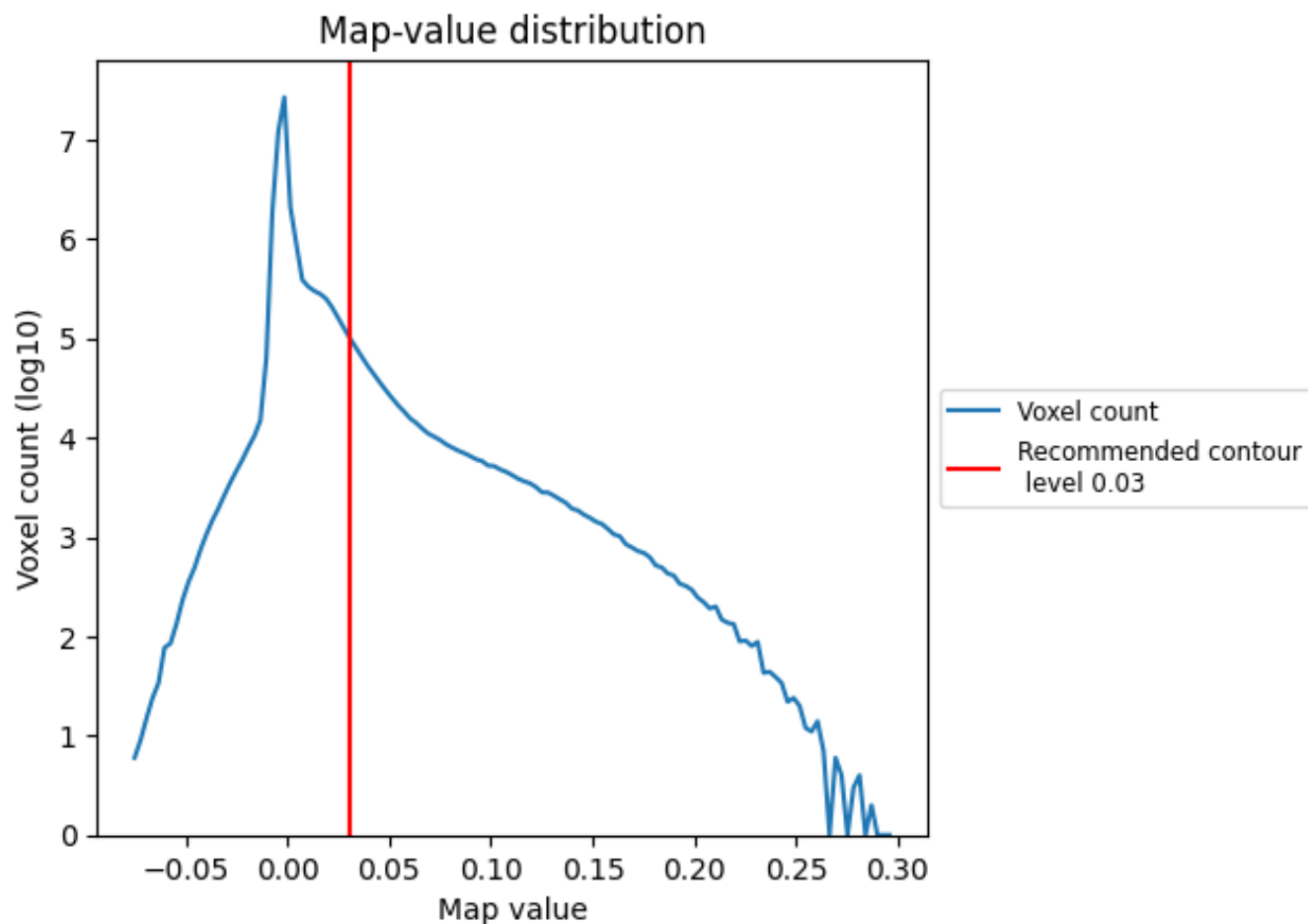
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

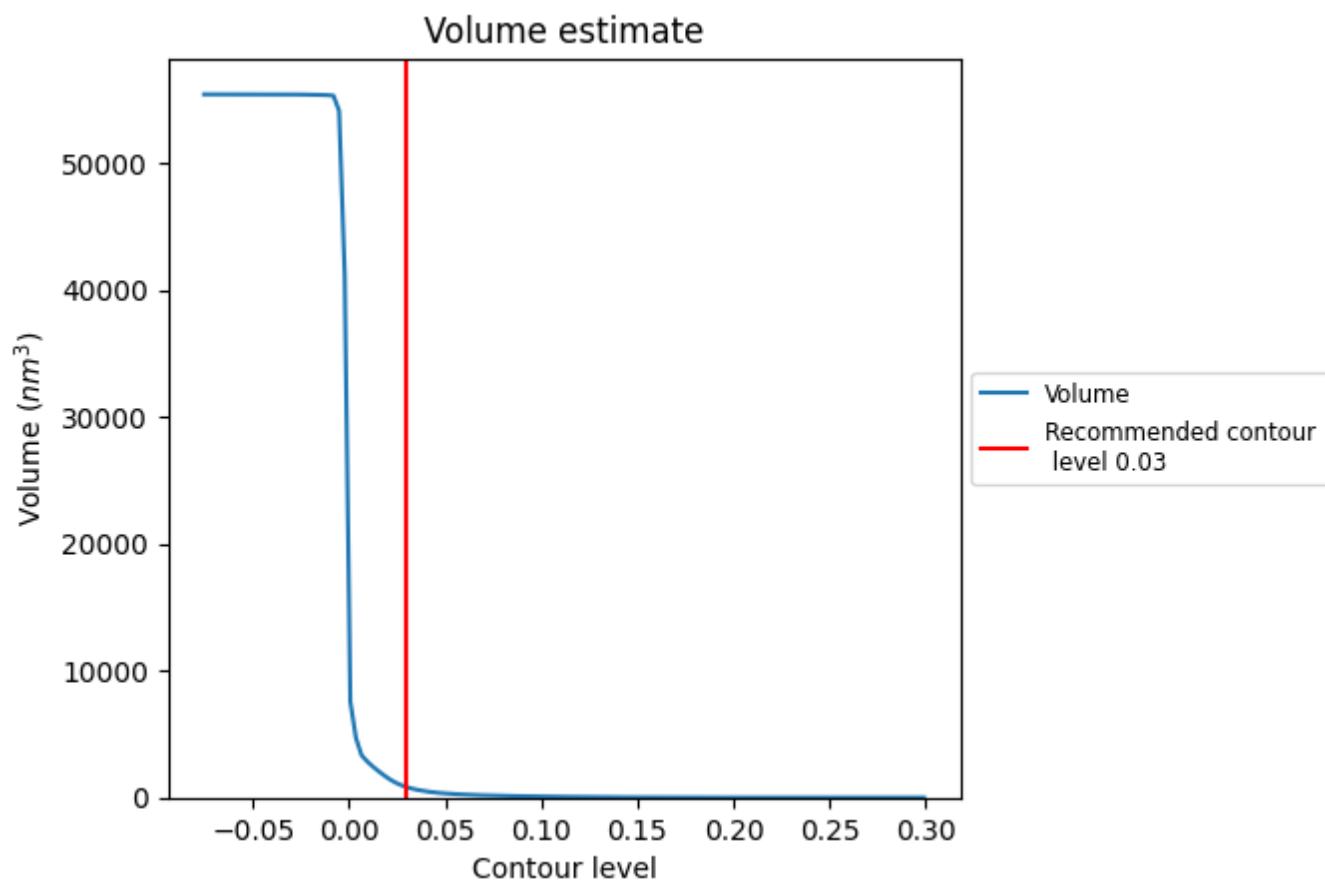
This section contains the results of statistical analysis of the map.

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.

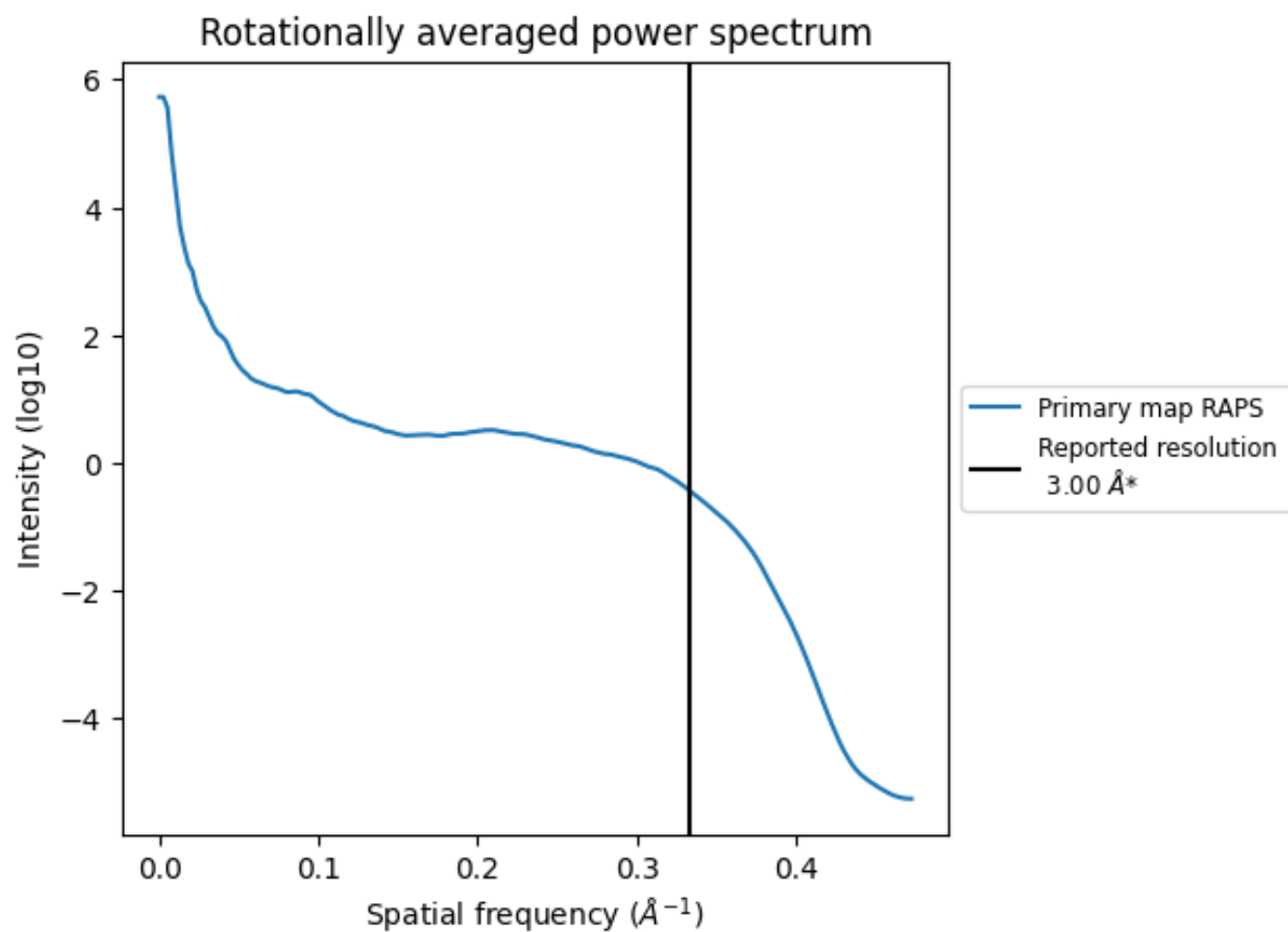
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 823 nm³; this corresponds to an approximate mass of 744 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 ⓘ

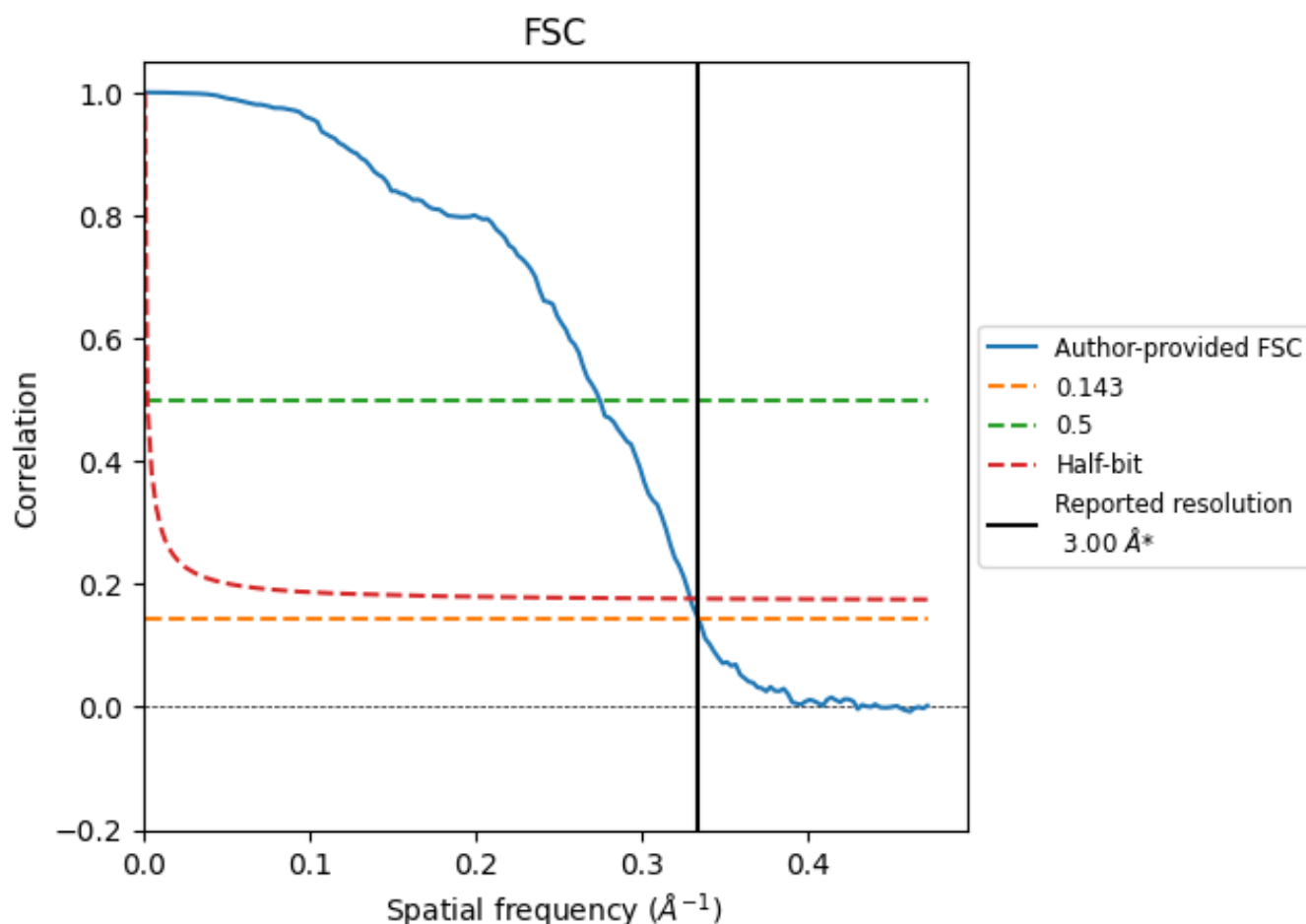


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.64	3.04
Unmasked-calculated*	-	-	-

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

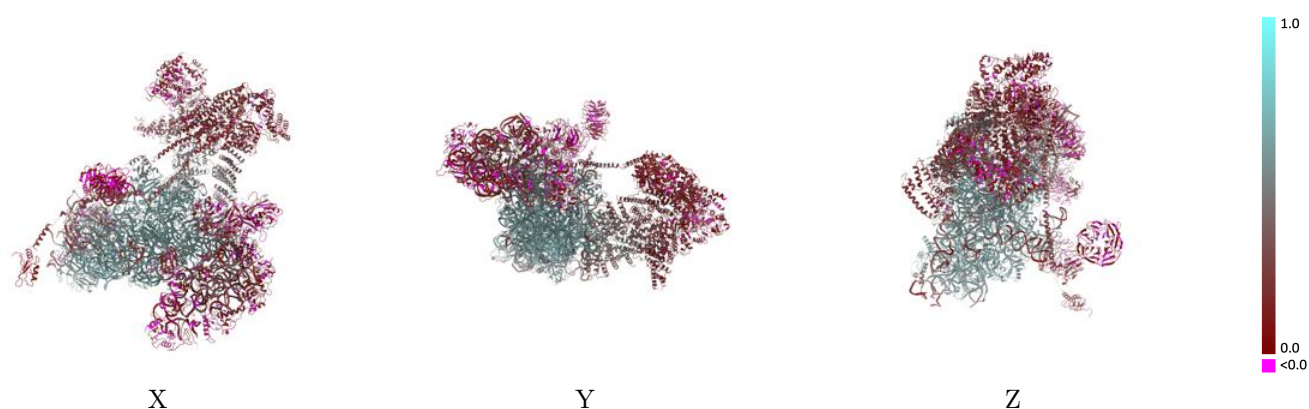
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11325 and PDB model 6ZON. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

This section was not generated.

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

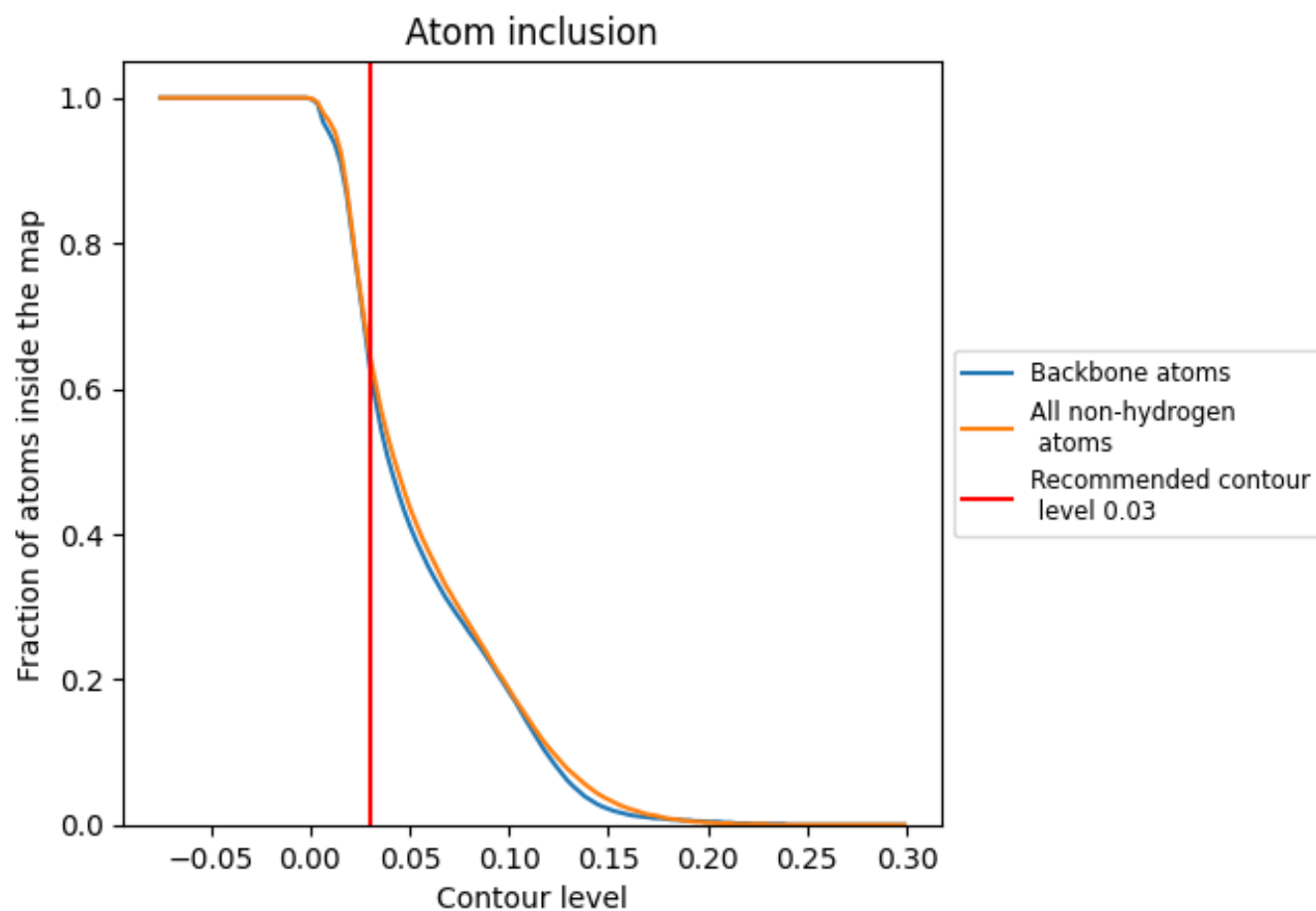


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 65% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6460	 0.3830
2	 0.9280	 0.4900
A	 0.4200	 0.3060
B	 0.0590	 0.2170
C	 0.6080	 0.3870
D	 0.1590	 0.1600
E	 0.2590	 0.1990
F	 0.0650	 0.1380
H	 0.0940	 0.1550
I	 0.0000	 0.0460
J	 0.9620	 0.6020
K	 0.0070	 0.1210
L	 0.0170	 0.1190
M	 0.0650	 0.1540
P	 0.1760	 0.1100
Q	 0.9510	 0.6040
R	 0.9630	 0.5890
S	 0.6750	 0.2810
T	 0.9760	 0.6080
U	 0.1950	 0.0920
V	 0.3440	 0.1140
W	 0.8660	 0.5620
Y	 0.1640	 0.1650
a	 0.9430	 0.5910
b	 0.6390	 0.2680
c	 0.9650	 0.6150
d	 0.9740	 0.6240
e	 0.5740	 0.2270
f	 0.9860	 0.6390
g	 0.6710	 0.2320
h	 0.5470	 0.2410
i	 0.9560	 0.5900
j	 0.9810	 0.6290
k	 0.1890	 0.1370
l	 0.8410	 0.2370



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Chain	Atom inclusion	Q-score
m	 0.9590	 0.5960
n	 0.9780	 0.6220
o	 0.1850	 0.0840
p	 0.9320	 0.5880
q	 0.9810	 0.6190
r	 0.9160	 0.5420
s	 0.9030	 0.5270
t	 0.9350	 0.5730
u	 0.4370	 0.1460
v	 0.1080	 0.0660
w	 0.8130	 0.4160
x	 0.5410	 0.2130
y	 0.9640	 0.6080
z	 0.9580	 0.5970