



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 10:50 PM UTC

PDB ID : 5YLZ / pdb_00005ylz
EMDB ID : EMD-6839
Title : Cryo-EM Structure of the Post-catalytic Spliceosome from *Saccharomyces cerevisiae* at 3.6 angstrom
Authors : Wan, R.; Yan, C.; Bai, R.; Lei, J.; Shi, Y.
Deposited on : 2017-10-20
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

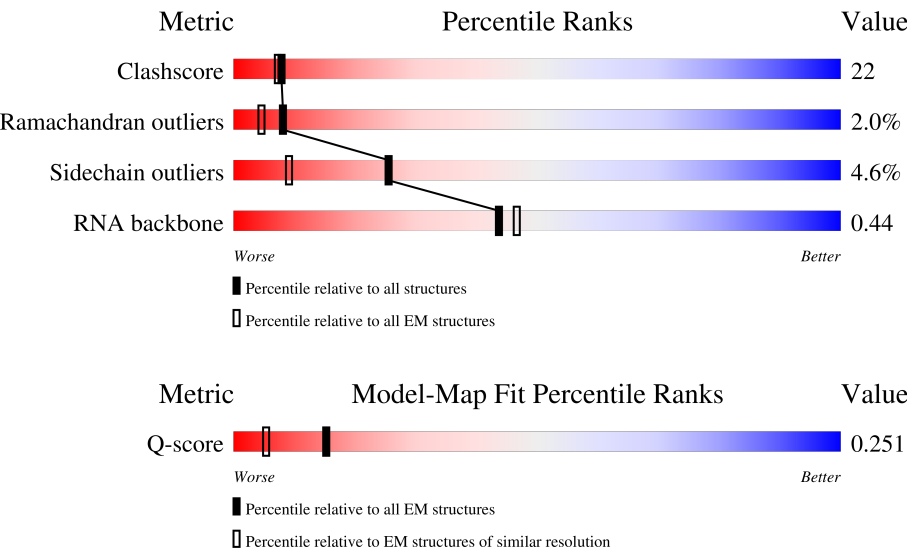
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	2413	11% 38% 38% 20%
2	B	214	13% 36% 11% 8% 45%
3	C	1008	9% 45% 40% 13%

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Mol	Chain	Length	Quality of chain
4	D	112	
5	E	369	
6	F	1175	
7	G	175	
8	H	859	
9	I	687	
10	J	590	
11	K	215	
12	L	157	
13	T	455	
14	M	364	
15	N	339	
16	O	451	
17	P	175	
18	Q	379	
19	R	135	
20	S	577	
21	U	251	
22	V	382	
23	W	1145	
24	a	196	
24	h	196	
25	b	94	
25	i	94	
26	c	86	

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Mol	Chain	Length	Quality of chain
26	j	86	
27	d	77	
27	k	77	
28	e	101	
28	l	101	
29	f	146	
29	m	146	
30	g	110	
30	n	110	
31	o	238	
32	p	111	
33	q	503	
33	r	503	
33	s	503	
33	t	503	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	IHP	A	3000	-	-	X	-
37	ZN	M	400	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 76247 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1931	Total	C	N	O	S	0	0
			15931	10239	2737	2897	58		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	117	Total	C	N	O	P	0	0
			2465	1104	414	830	117		

- Molecule 3 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	878	Total	C	N	O	S	0	0
			7019	4529	1166	1295	29		

- Molecule 4 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	103	Total	C	N	O	P	0	0
			2192	982	391	716	103		

- Molecule 5 is a RNA chain called mRNA/intron lariat.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	62	Total	C	N	O	P	0	0
			1310	590	224	434	62		

- Molecule 6 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	91	Total	C	N	O	P	0	0
			1909	854	309	655	91		

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	156	Total	C	N	O	S	0	0
			926	585	160	180	1		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	562	Total	C	N	O	S	0	0
			3012	1844	572	595	1		

- Molecule 9 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	517	Total	C	N	O	S	0	0
			3424	2130	643	643	8		

- Molecule 10 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	432	Total	C	N	O	S	0	0
			2949	1827	545	569	8		

- Molecule 11 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total	C	N	O	S	0	0
			777	476	143	157	1		

- Molecule 12 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	157	Total	C	N	O	S	0	0
			1291	808	240	232	11		

- Molecule 13 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	344	Total	C	N	O	S	0	0
			2357	1504	414	432	7		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	185	Total	C	N	O	S	0	0
			1472	930	256	271	15		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	261	Total	C	N	O	S	0	0
			2089	1320	369	388	12		

- Molecule 16 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	337	Total	C	N	O	S	0	0
			2646	1669	466	501	10		

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	69	Total	C	N	O	S	0	0
			560	351	112	96	1		

- Molecule 18 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	201	Total	C	N	O	S	0	0
			1583	988	290	298	7		

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	27	Total	C	N	O	0	0
			190	112	38	40		

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	207	Total	C	N	O	S	0	0
			1701	1096	275	323	7		

- Molecule 21 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	148	Total	C	N	O	S	0	0
			1202	780	204	214	4		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	88	Total	C	N	O		0	0
			554	350	100	104			

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	703	Total	C	N	O	S	0	0
			5553	3521	941	1060	31		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
24	h	78	Total	C	N	O	S	0	0
			610	389	110	108	3		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
25	i	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	70	Total	C	N	O	S	0	0
			554	355	98	100	1		
26	j	70	Total	C	N	O	S	0	0
			554	355	98	100	1		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
27	k	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
28	l	81	Total	C	N	O	S	0	0
			616	393	107	114	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
29	m	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
30	n	65	Total	C	N	O	S	0	0
			528	340	102	84	2		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	o	135	Total	C	N	O	0	0
			841	538	142	161		

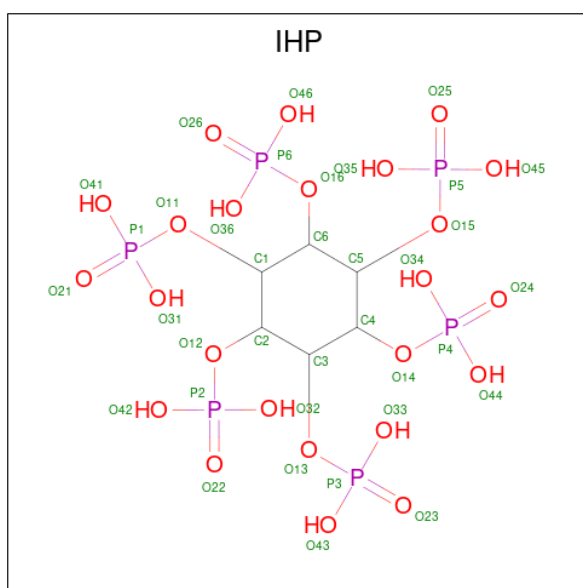
- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	p	81	Total	C	N	O	0	0
			513	332	89	92		

- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

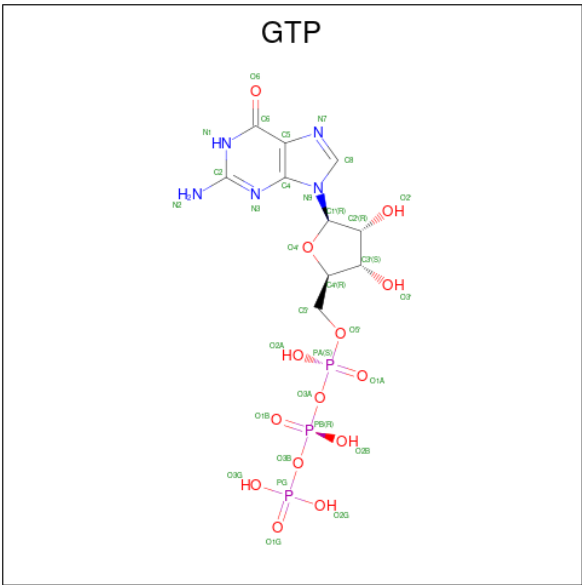
Mol	Chain	Residues	Atoms					AltConf	Trace
33	q	129	Total	C	N	O	S	0	0
			850	537	137	174	2		
33	r	125	Total	C	N	O	S	0	0
			823	521	133	167	2		
33	s	126	Total	C	N	O	S	0	0
			830	525	134	169	2		
33	t	128	Total	C	N	O	S	0	0
			843	532	136	173	2		

- Molecule 34 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 35 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

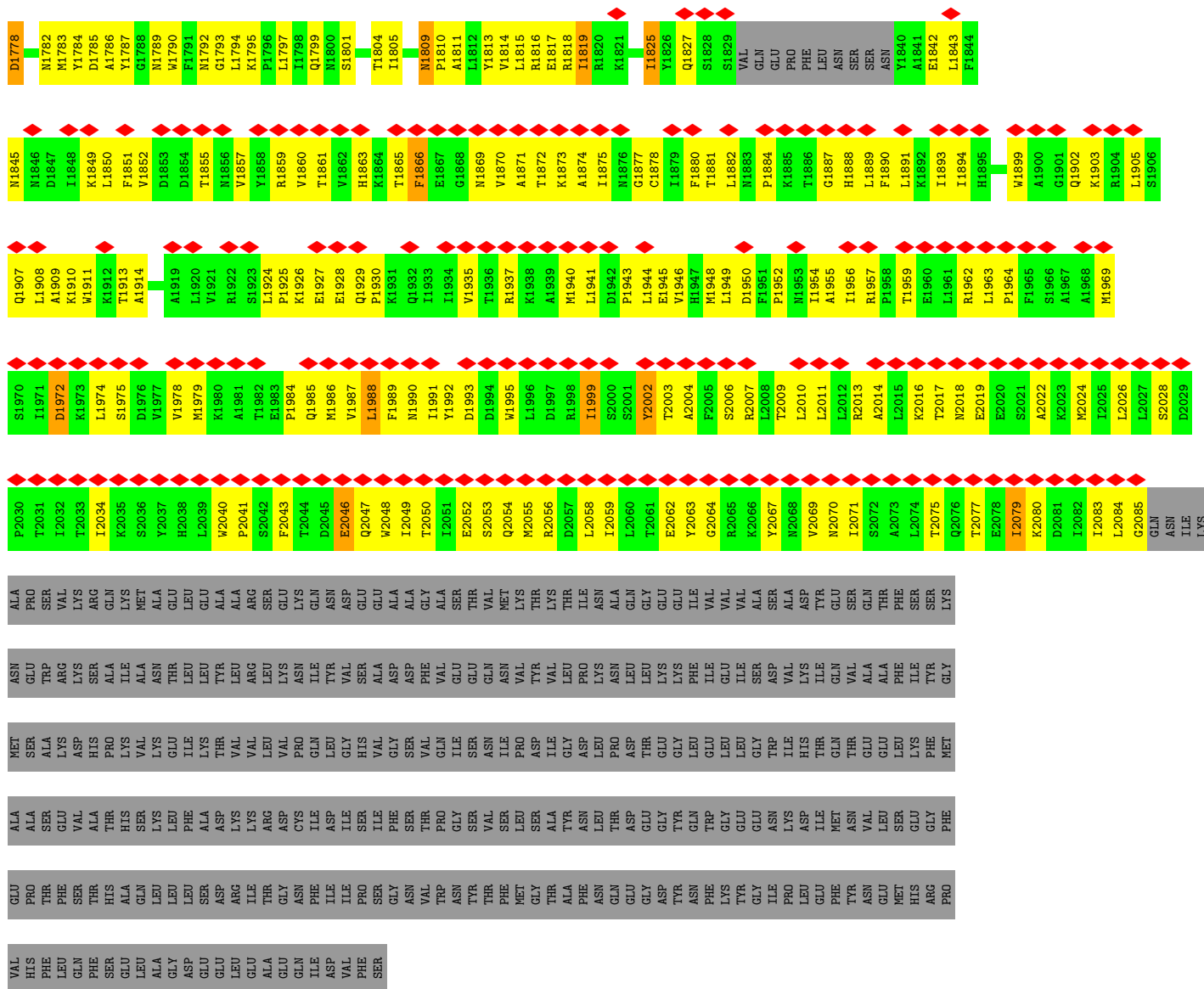
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	C	1	Total	Mg	0
			1	1	
36	D	5	Total	Mg	0
			5	5	

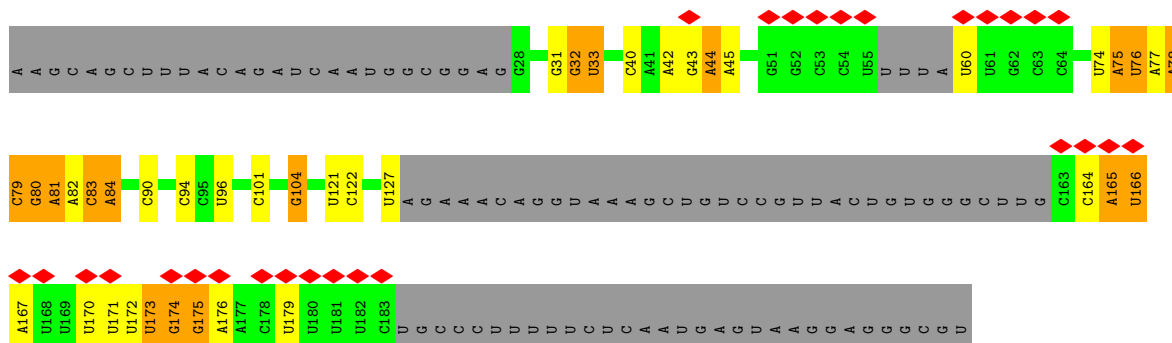
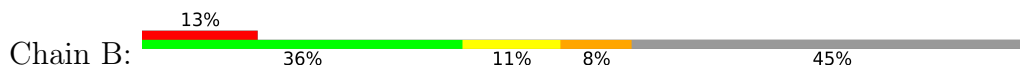
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	L	3	Total	Zn	0
			3	3	
37	M	2	Total	Zn	0
			2	2	
37	N	1	Total	Zn	0
			1	1	

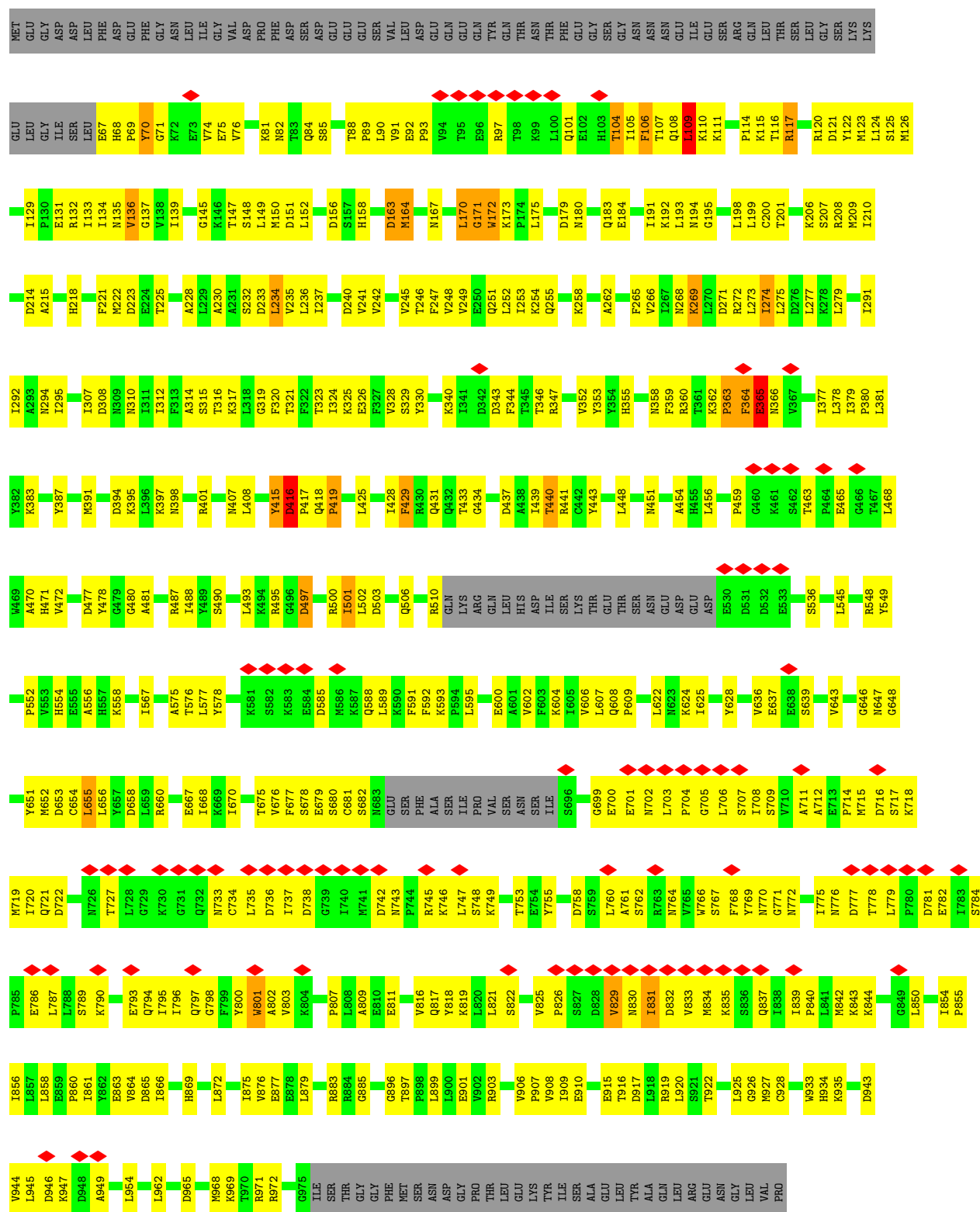
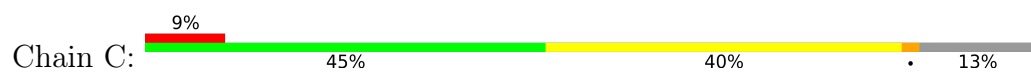




• Molecule 2: U5 snRNA

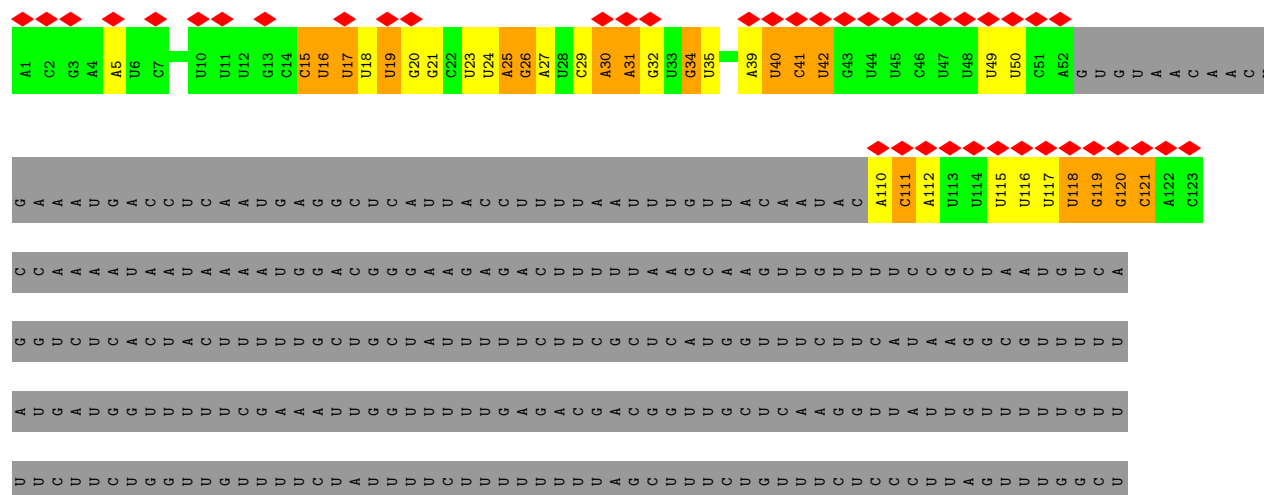


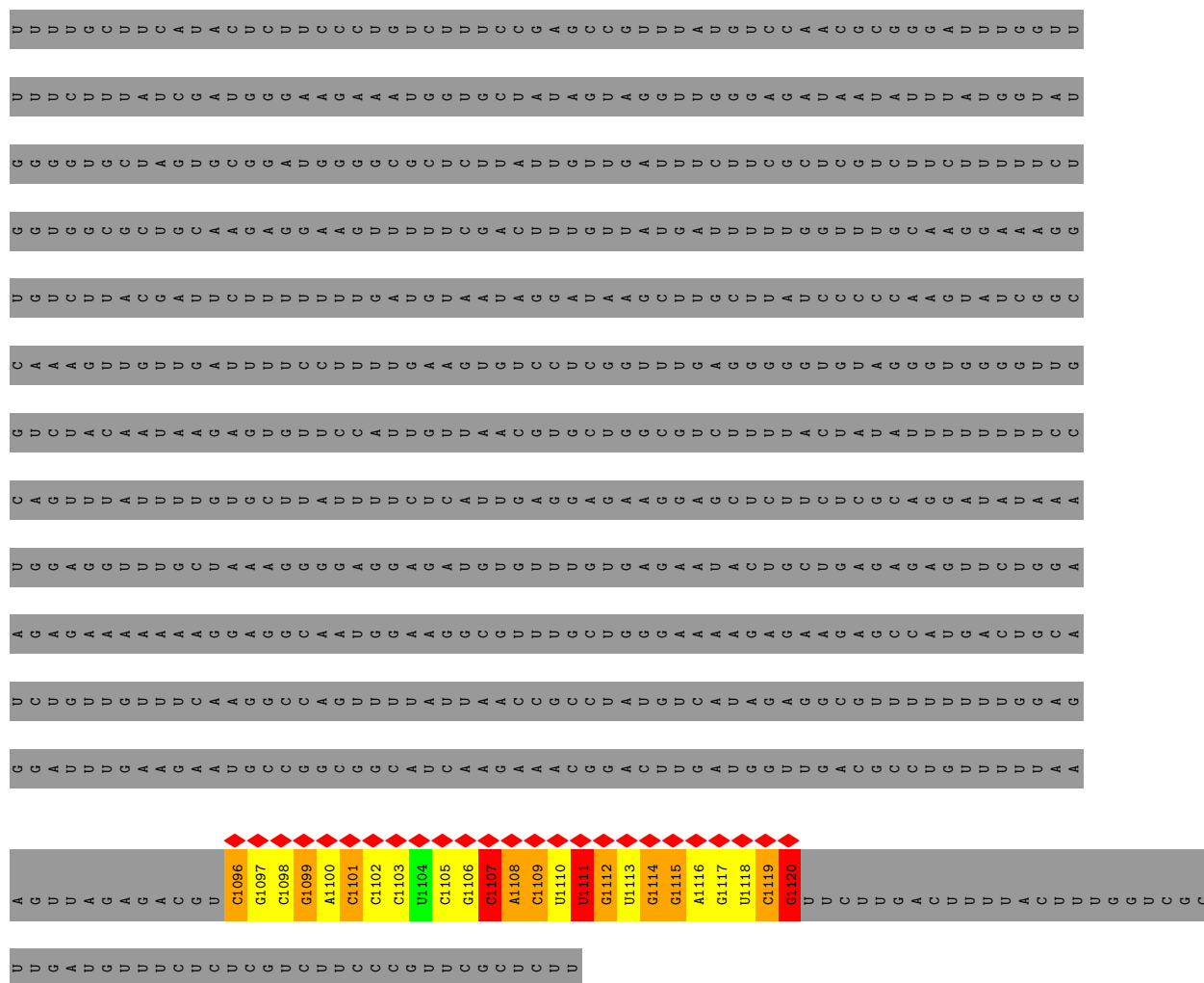
• Molecule 3: Pre-mRNA-splicing factor SNU114



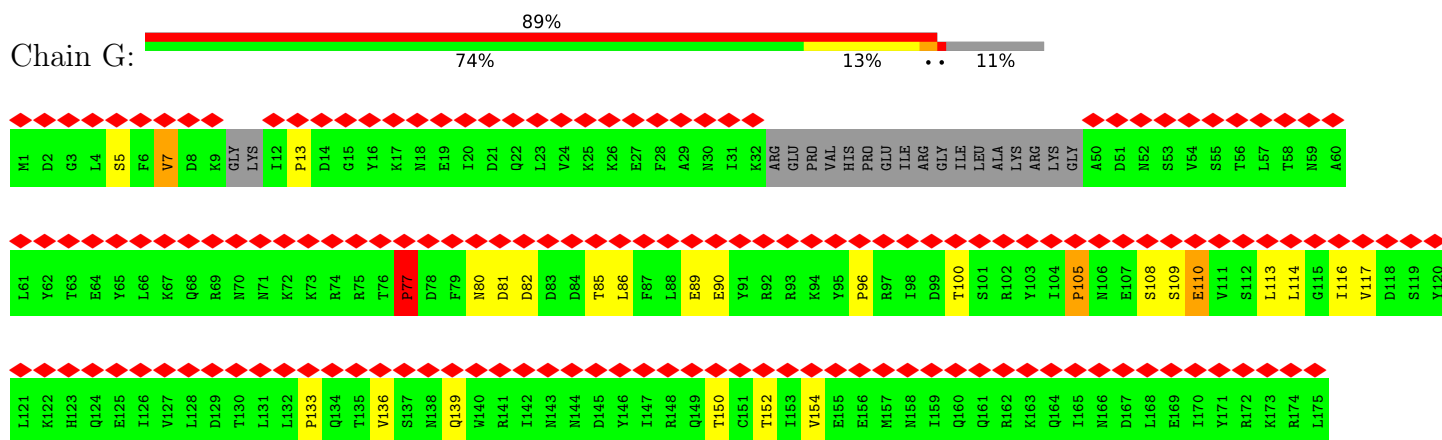
• Molecule 4: U6 snRNA



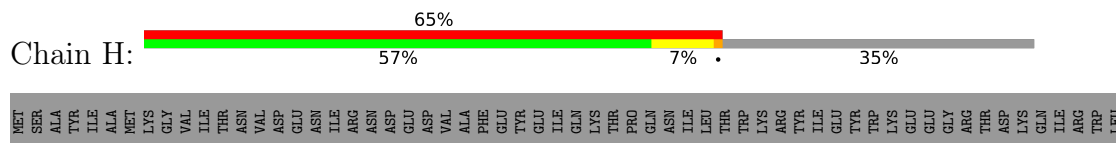




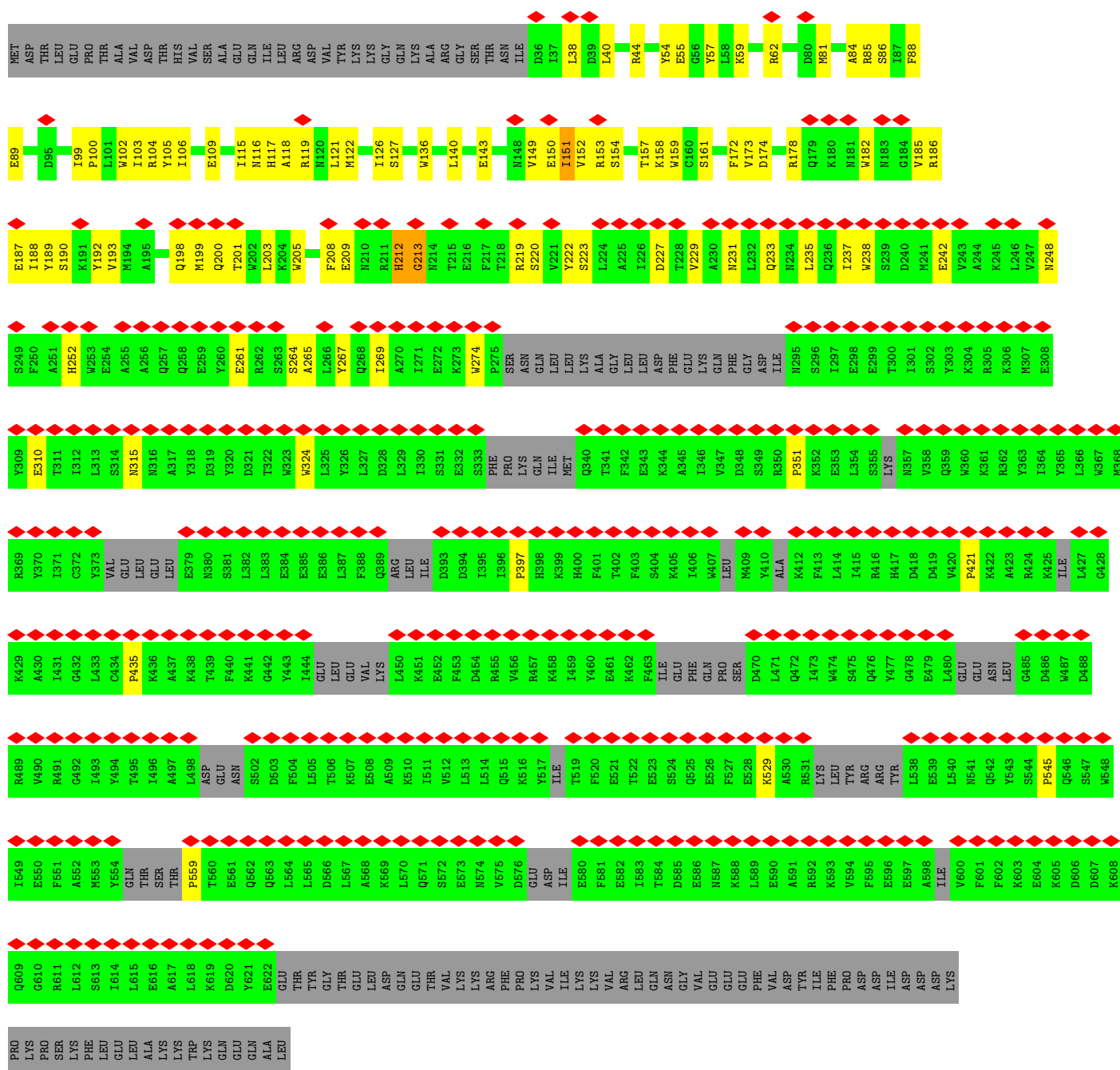
● Molecule 7: Pre-mRNA-splicing factor SNT309



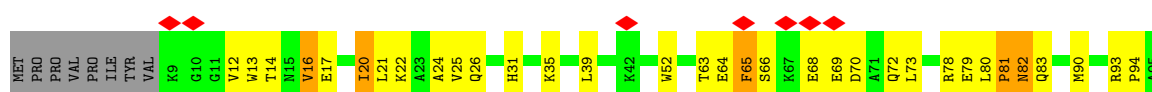
● Molecule 8: Pre-mRNA-splicing factor SYF1



- Molecule 9: Pre-mRNA-splicing factor CLF1

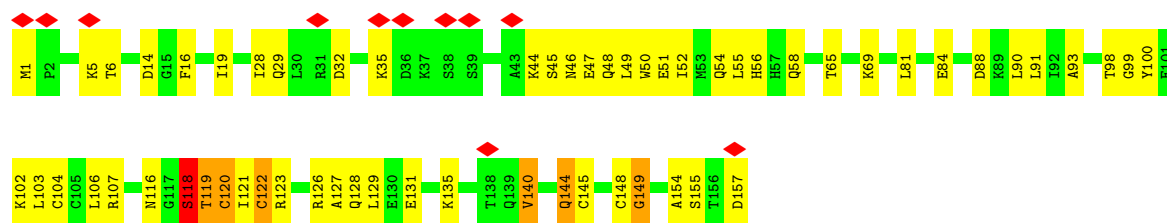


• Molecule 10: Pre-mRNA-splicing factor CEF1

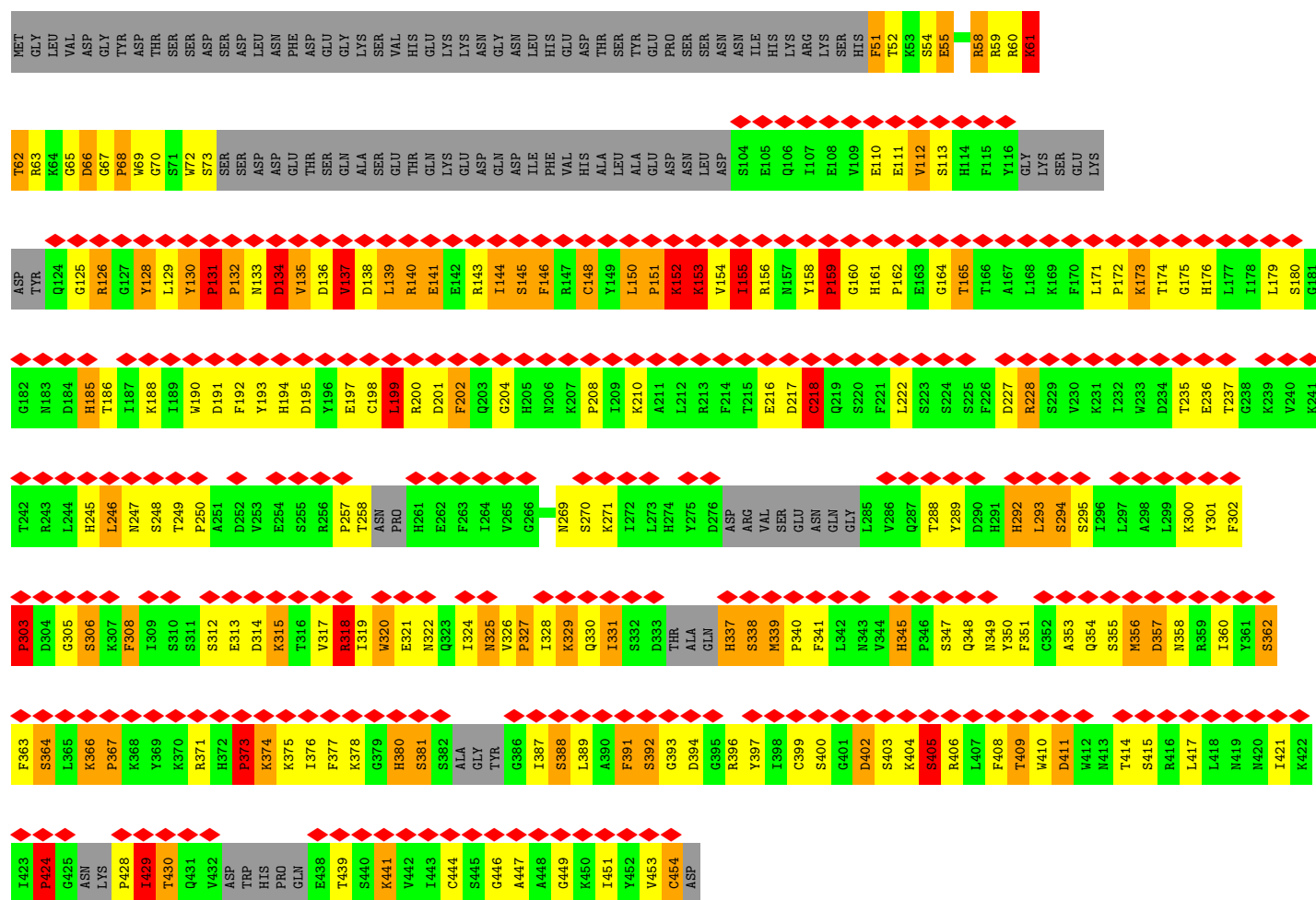




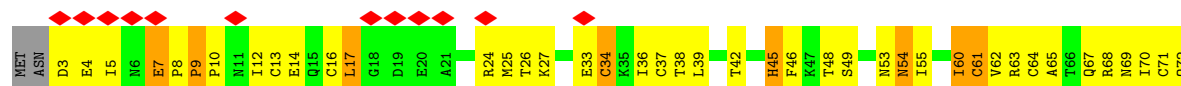
Chain L: 7% 62% 34%



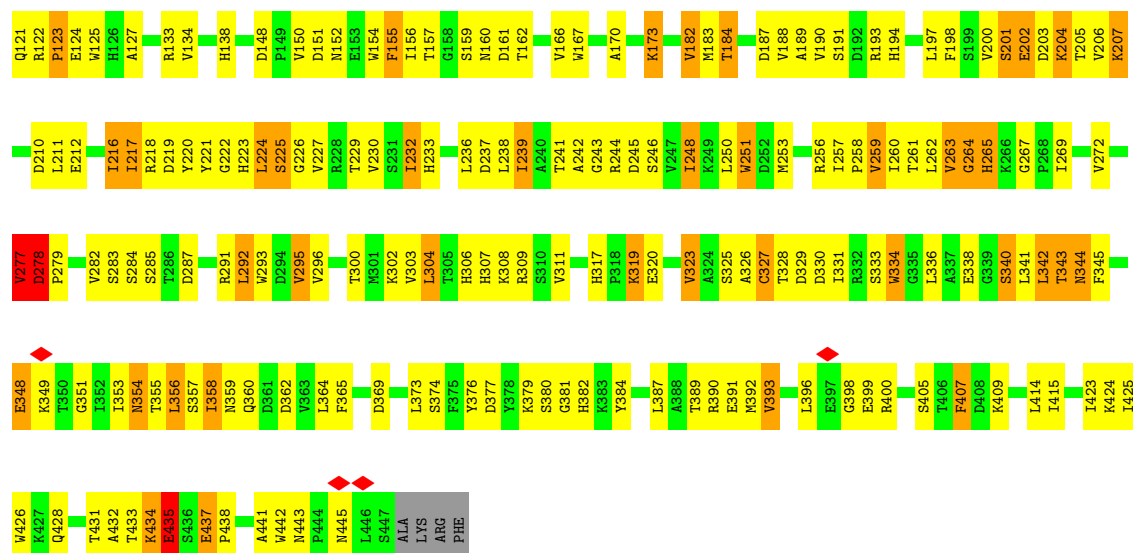
Chain T:



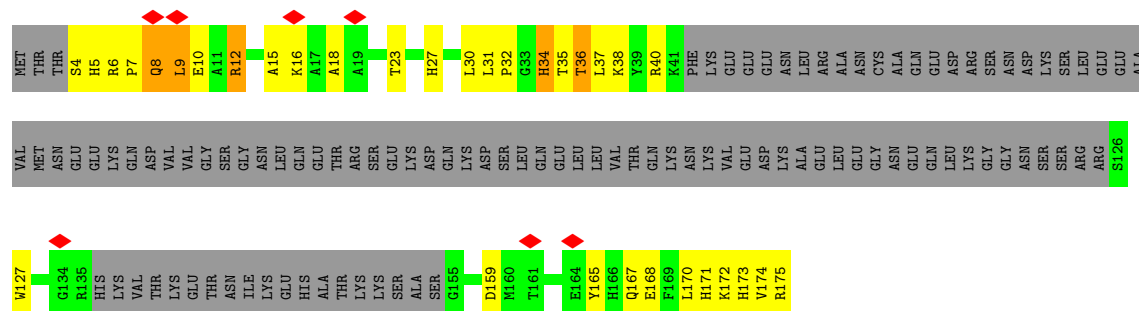
Chain M:



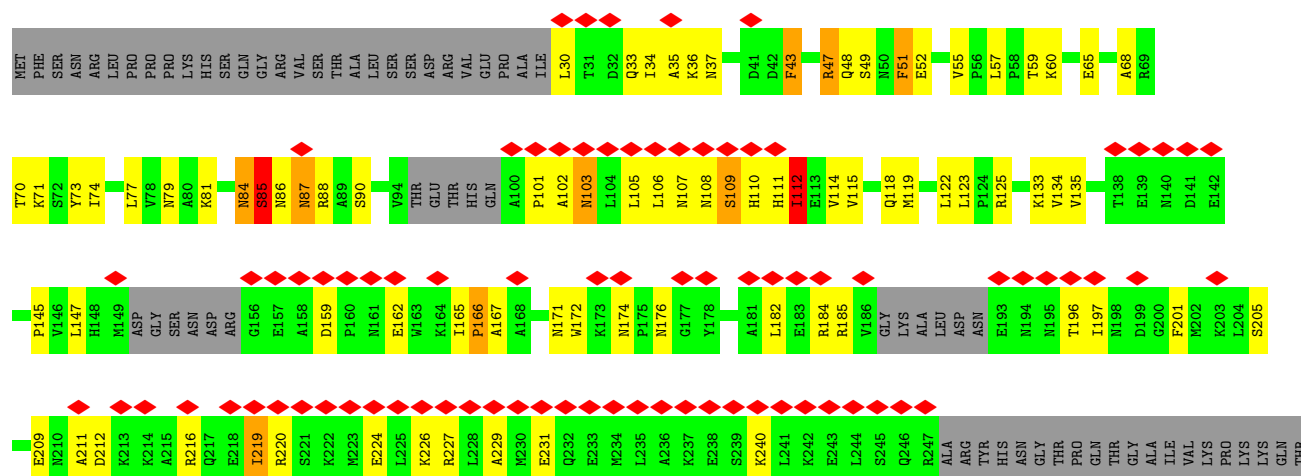
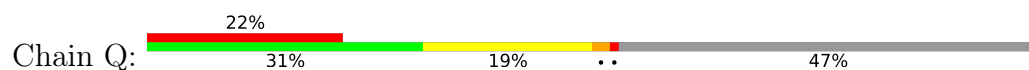


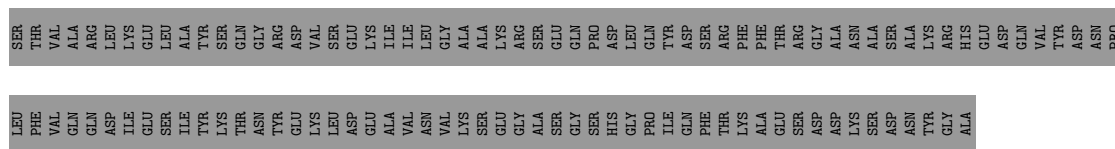


• Molecule 17: Pre-mRNA-splicing factor CWC15

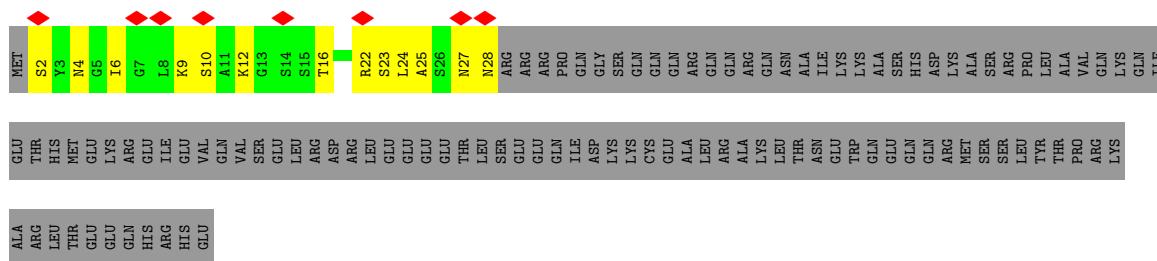


• Molecule 18: Pre-mRNA-processing protein 45

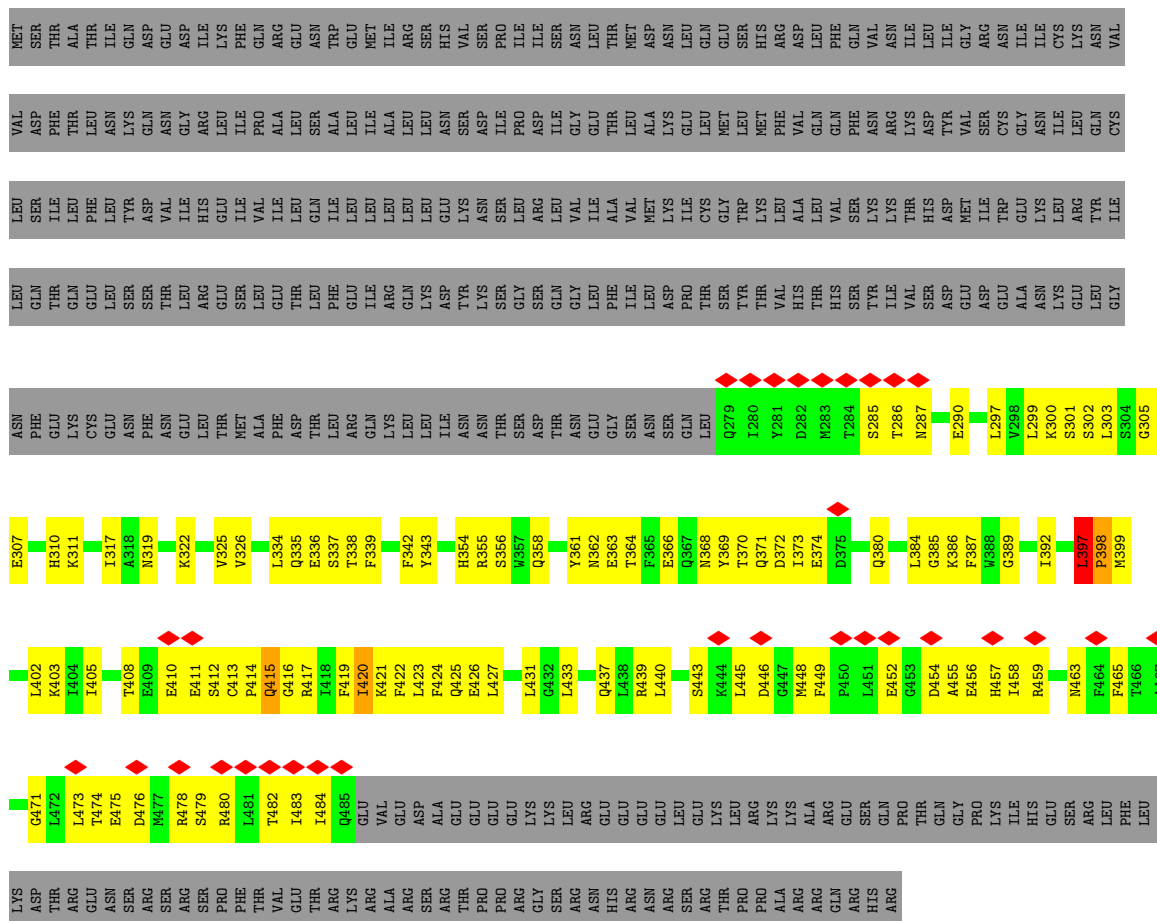




- Molecule 19: Pre-mRNA-splicing factor CWC21



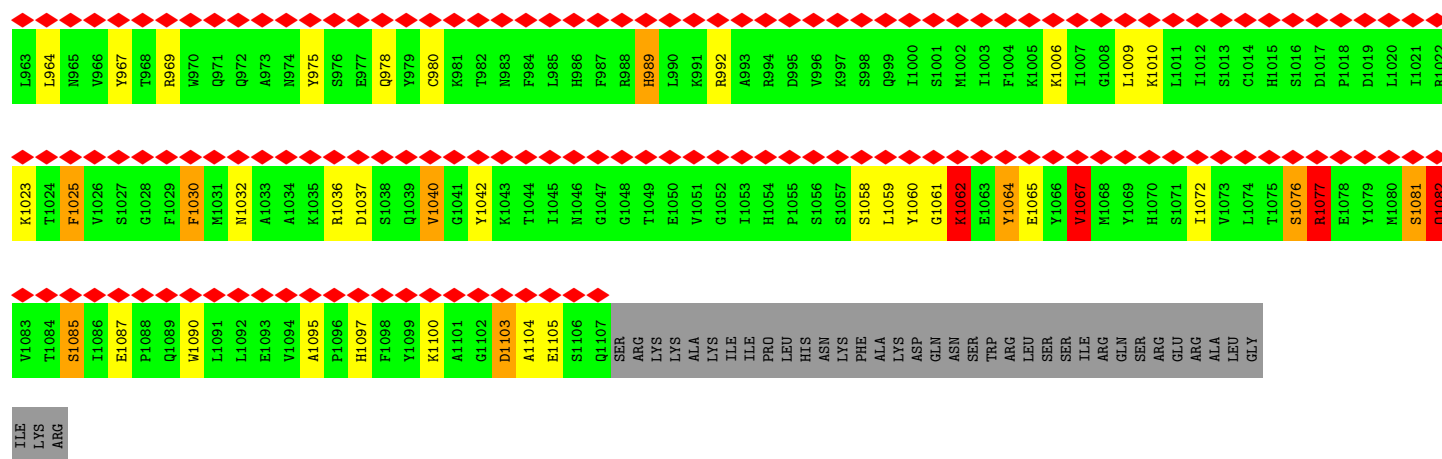
- Molecule 20: Pre-mRNA-splicing factor CWC22



- Molecule 21: Pre-mRNA-splicing factor 18



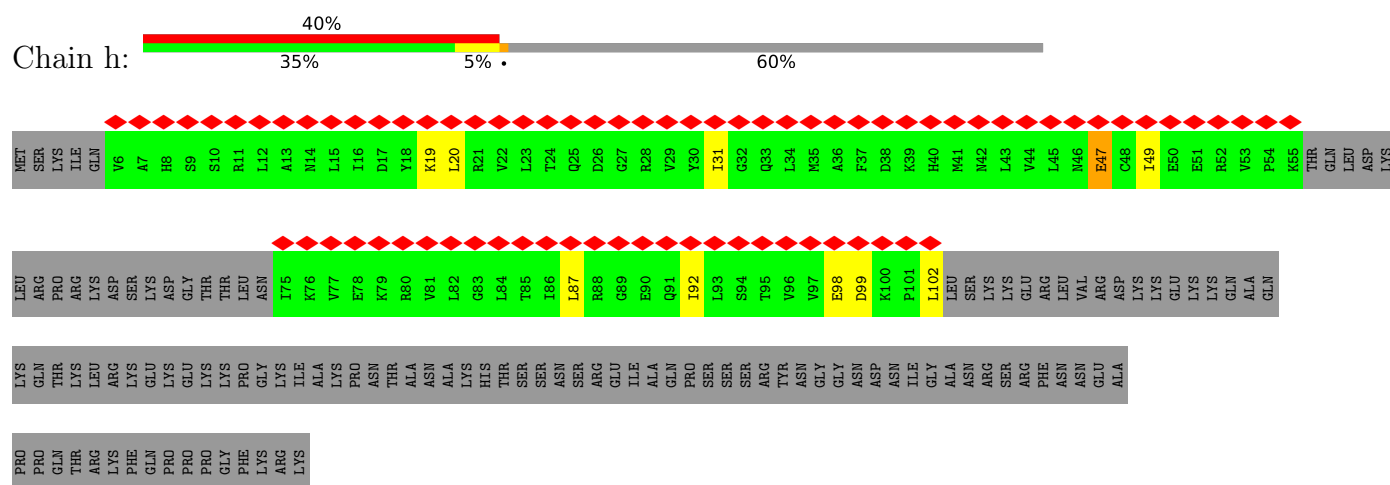




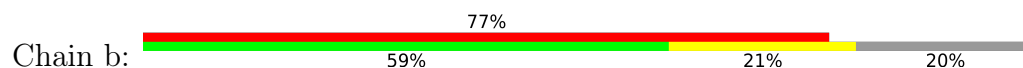
• Molecule 24: Small nuclear ribonucleoprotein-associated protein B

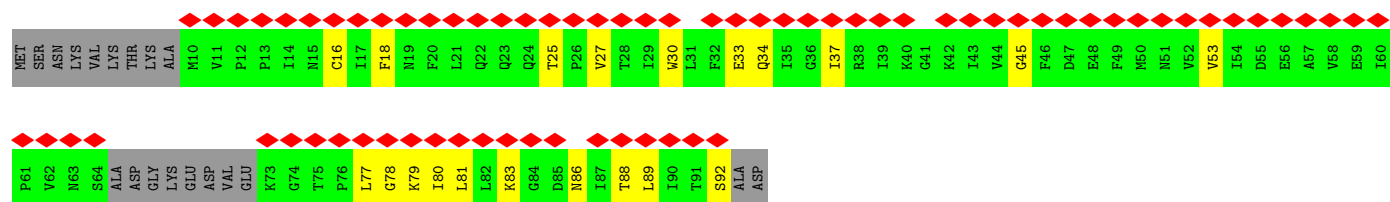


• Molecule 24: Small nuclear ribonucleoprotein-associated protein B

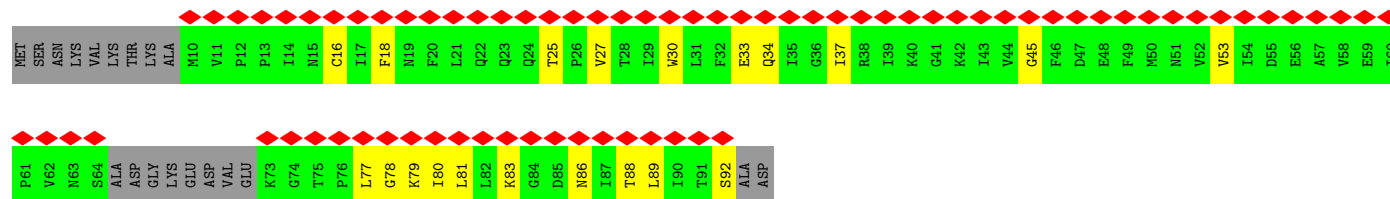
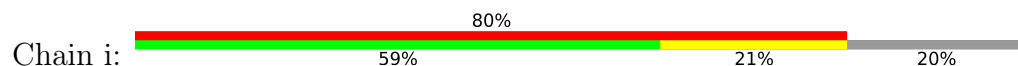


• Molecule 25: Small nuclear ribonucleoprotein E

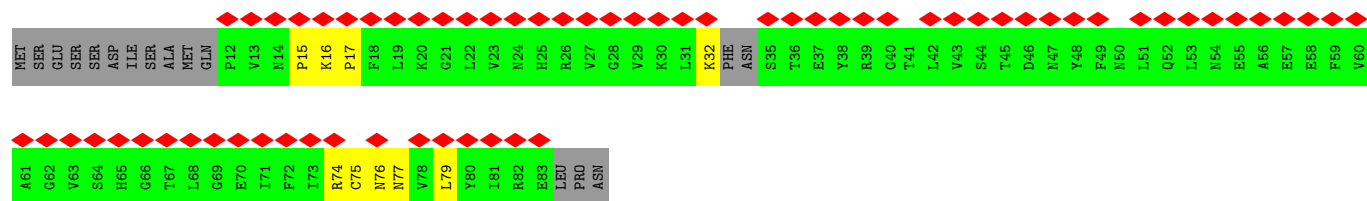
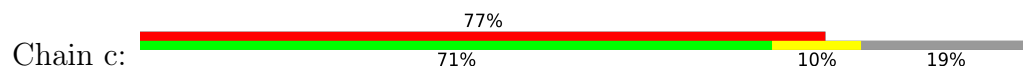




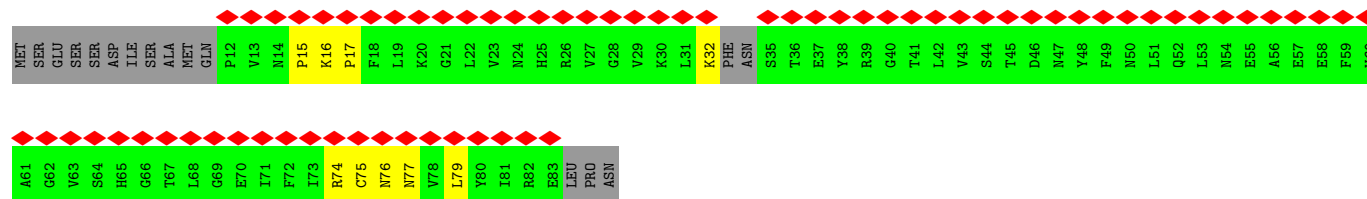
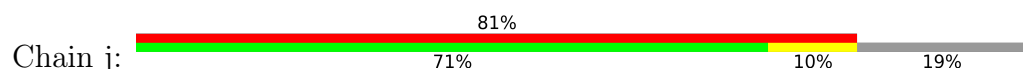
• Molecule 25: Small nuclear ribonucleoprotein E



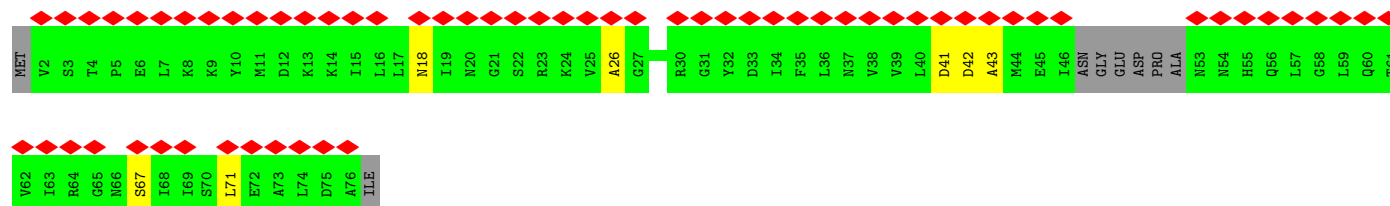
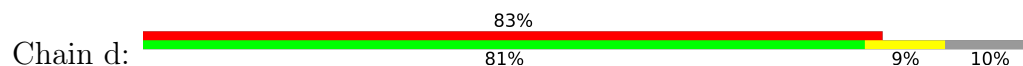
• Molecule 26: Small nuclear ribonucleoprotein F

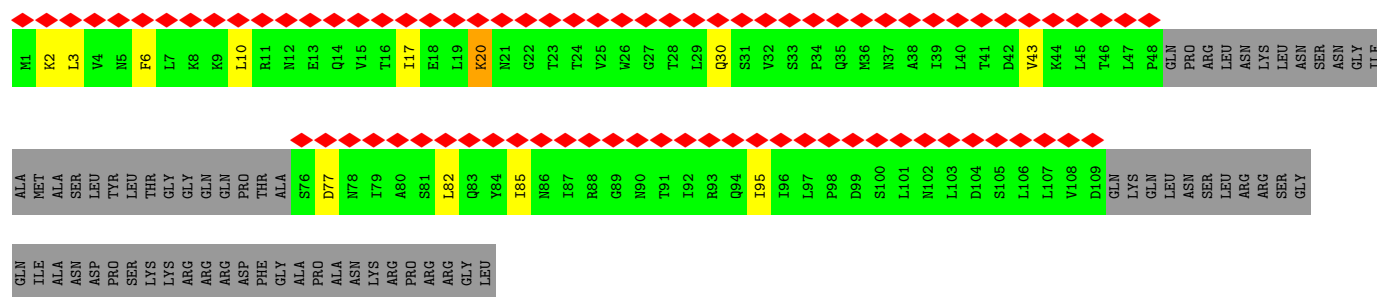


• Molecule 26: Small nuclear ribonucleoprotein F

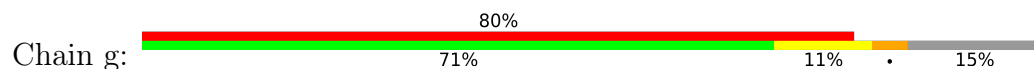


• Molecule 27: Small nuclear ribonucleoprotein G

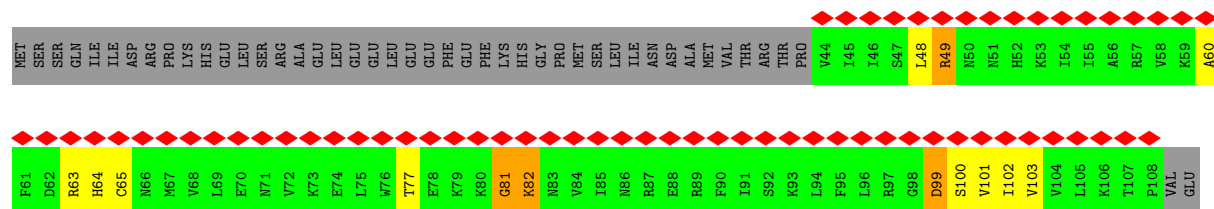




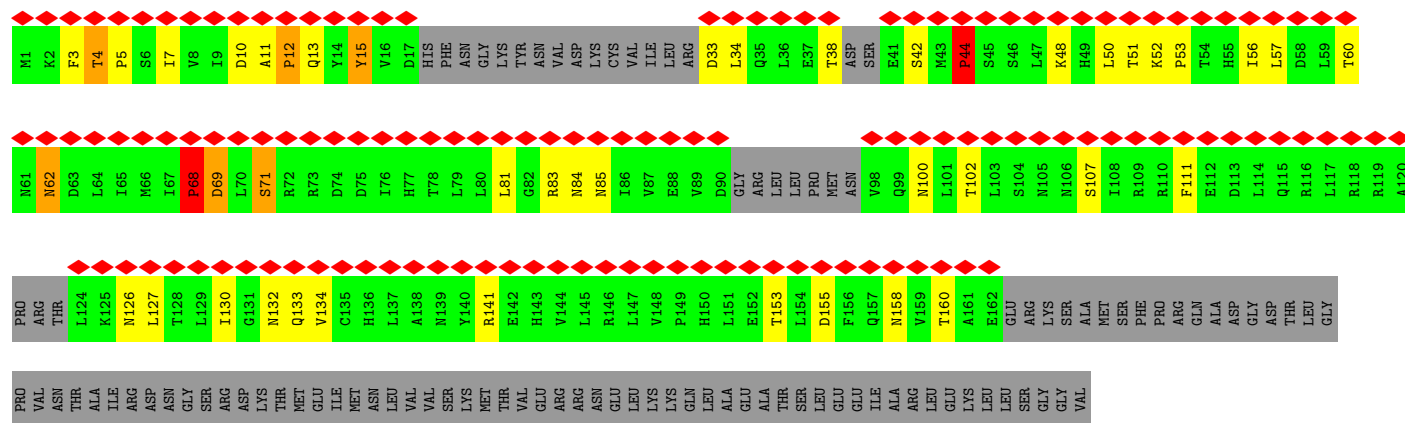
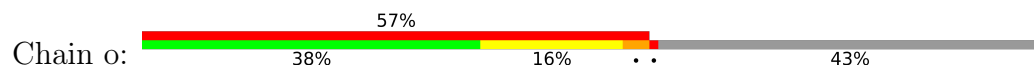
• Molecule 30: Small nuclear ribonucleoprotein Sm D2



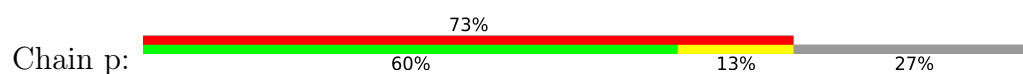
• Molecule 30: Small nuclear ribonucleoprotein Sm D2



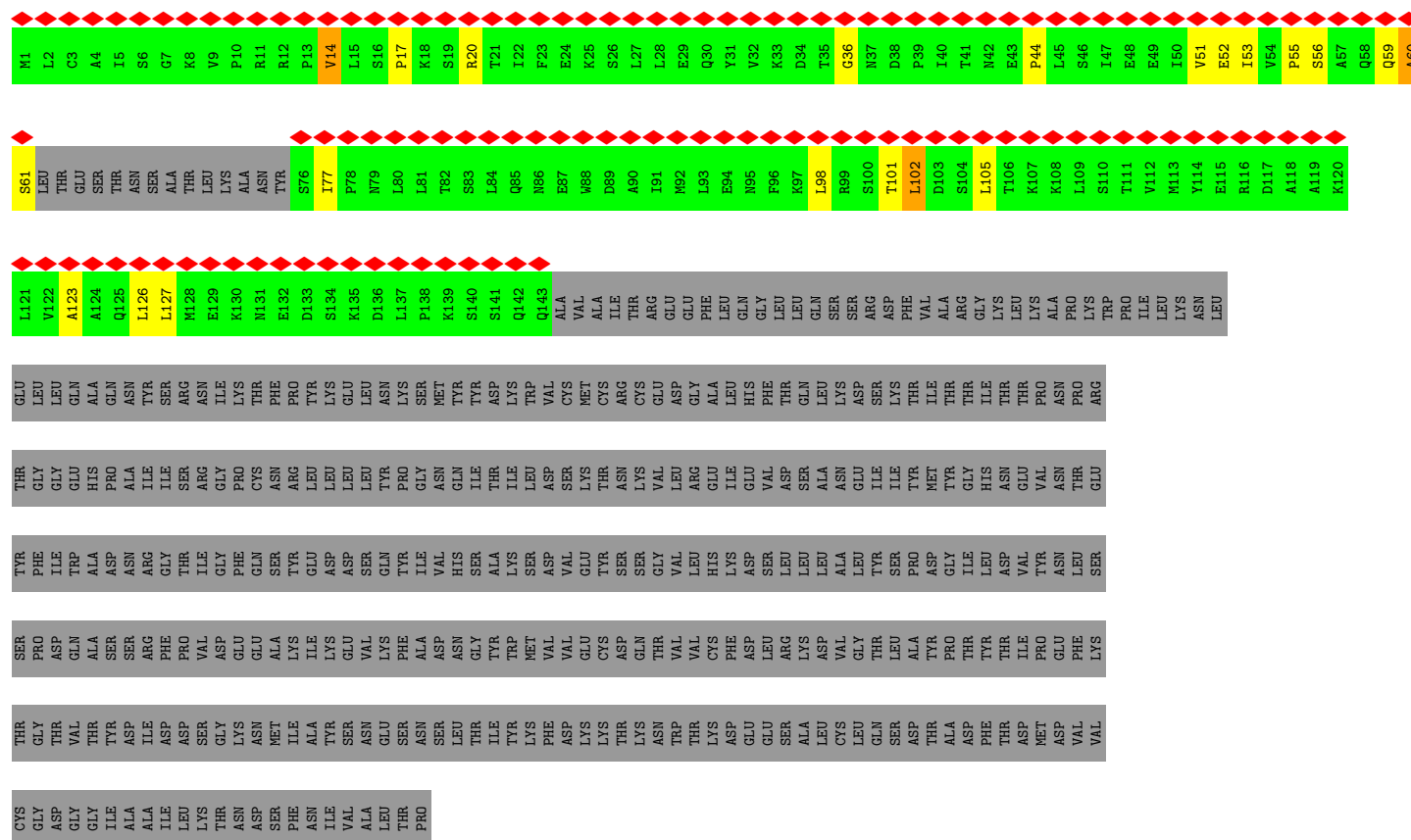
• Molecule 31: U2 small nuclear ribonucleoprotein A'



• Molecule 32: U2 small nuclear ribonucleoprotein B''



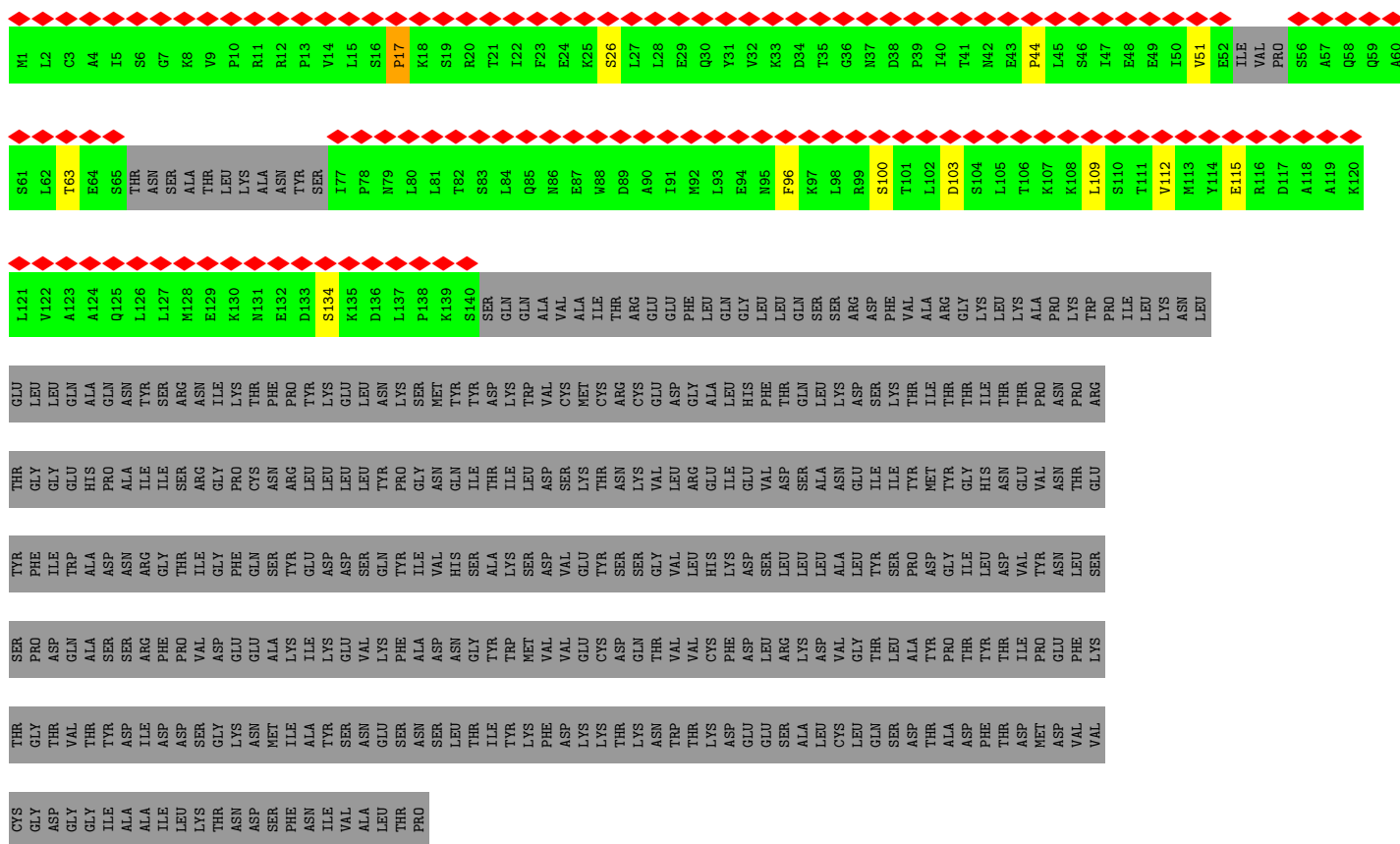
• Molecule 33: Pre-mRNA-processing factor 19



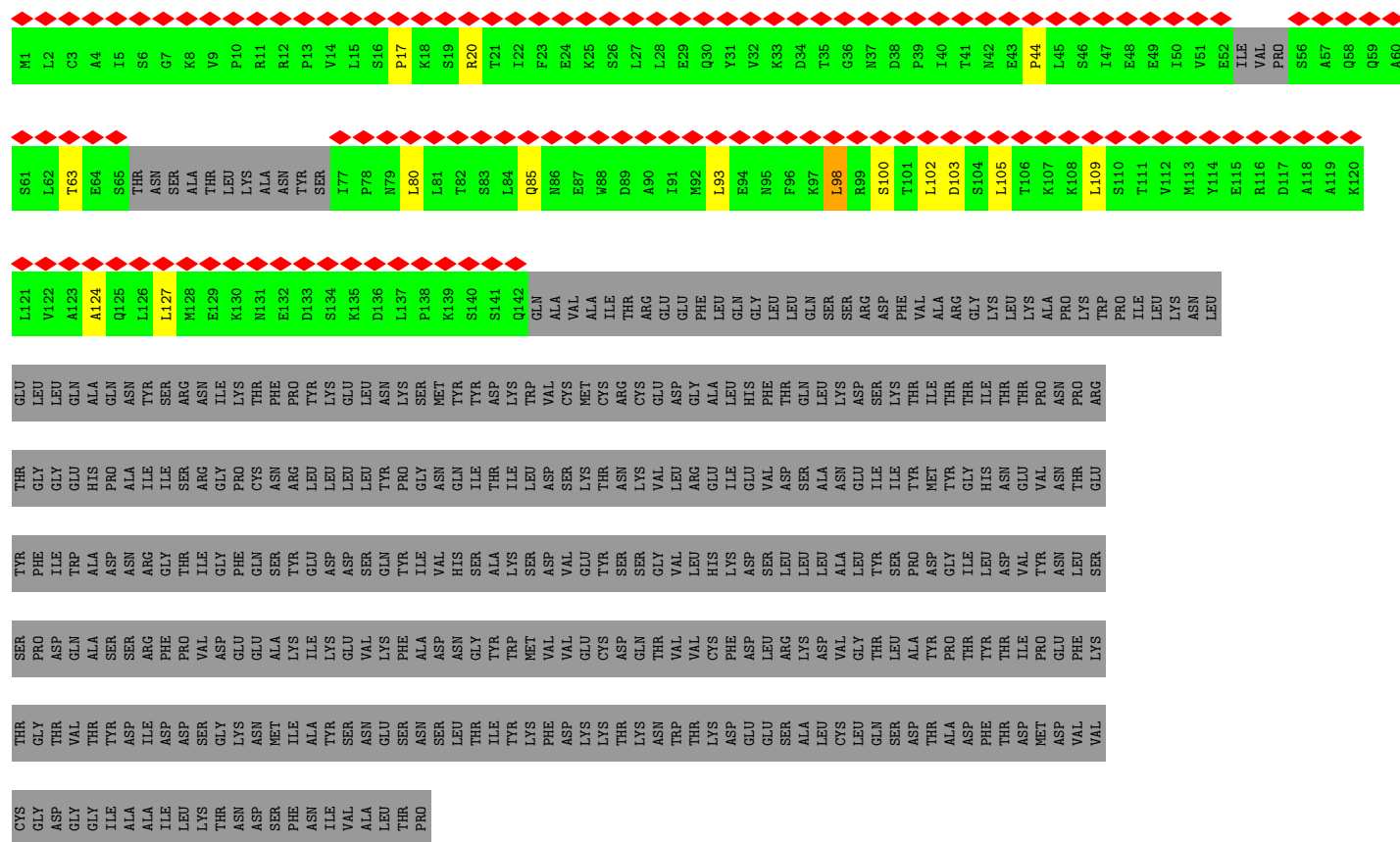
• Molecule 33: Pre-mRNA-processing factor 19



- Molecule 33: Pre-mRNA-processing factor 19



- Molecule 33: Pre-mRNA-processing factor 19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.230	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.034	Depositor
Map size ($\text{\AA}$)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, GTP, MG, 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	1.07	30/16338 (0.2%)	1.11	45/22145 (0.2%)
2	B	0.26	0/2747	0.33	0/4267
3	C	0.90	3/7168 (0.0%)	1.01	7/9707 (0.1%)
4	D	0.26	0/2452	0.24	0/3817
5	E	0.42	2/1461 (0.1%)	0.66	1/2260 (0.0%)
6	F	0.65	11/2123 (0.5%)	0.79	11/3295 (0.3%)
7	G	0.58	0/924	1.06	2/1244 (0.2%)
8	H	0.65	9/2991 (0.3%)	0.97	23/4072 (0.6%)
9	I	0.64	0/3459	0.87	7/4708 (0.1%)
10	J	0.63	1/2967 (0.0%)	1.01	12/3994 (0.3%)
11	K	0.59	0/780	0.85	0/1036
12	L	0.95	0/1315	1.08	7/1759 (0.4%)
13	T	1.20	27/2390 (1.1%)	1.53	43/3200 (1.3%)
14	M	0.81	0/1496	1.11	9/2014 (0.4%)
15	N	0.77	0/2135	0.97	2/2871 (0.1%)
16	O	1.61	42/2704 (1.6%)	1.43	15/3676 (0.4%)
17	P	1.20	6/574 (1.0%)	1.16	1/766 (0.1%)
18	Q	0.97	3/1604 (0.2%)	1.17	7/2160 (0.3%)
19	R	0.55	0/191	0.97	1/254 (0.4%)
20	S	0.79	0/1732	0.99	3/2330 (0.1%)
21	U	0.37	0/1227	0.81	3/1665 (0.2%)
22	V	1.07	2/555 (0.4%)	1.18	5/742 (0.7%)
23	W	0.83	4/5660 (0.1%)	1.59	81/7653 (1.1%)
24	a	0.55	0/636	0.76	0/856
24	h	0.55	0/615	0.76	0/829
25	b	0.64	0/585	0.86	0/795
25	i	0.64	0/585	0.86	0/795
26	c	0.60	0/564	0.87	0/761
26	j	0.61	0/564	0.87	0/761
27	d	0.53	0/532	0.82	1/715 (0.1%)
27	k	0.53	0/532	0.82	1/715 (0.1%)
28	e	0.55	0/634	0.96	0/859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	l	0.55	0/625	0.96	0/848
29	f	0.58	0/649	0.81	0/880
29	m	0.59	0/649	0.81	0/880
30	g	0.65	0/753	0.96	2/1013 (0.2%)
30	n	0.65	0/535	0.86	2/717 (0.3%)
31	o	1.24	6/839 (0.7%)	2.35	43/1127 (3.8%)
32	p	1.01	2/514 (0.4%)	1.86	8/686 (1.2%)
33	q	0.58	0/856	0.92	0/1155
33	r	0.53	0/828	0.86	0/1117
33	s	0.54	0/835	0.85	0/1126
33	t	0.54	0/848	0.92	0/1143
All	All	0.86	148/78171 (0.2%)	1.08	342/107413 (0.3%)

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	8
3	C	0	3
9	I	0	1
10	J	0	3
12	L	0	5
13	T	0	2
14	M	0	5
15	N	0	1
16	O	0	11
18	Q	0	3
20	S	0	3
23	W	0	35
27	d	0	1
27	k	0	1
28	e	0	2
28	l	0	2
30	g	0	2
30	n	0	2
All	All	0	90

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	185	HIS	CB-CG	23.63	1.83	1.50
22	V	302	LEU	CA-CB	-14.29	1.29	1.53
13	T	444	CYS	CB-SG	-11.49	1.43	1.81
31	o	69	ASP	CA-CB	-10.61	1.38	1.53
1	A	716	ARG	CD-NE	-10.07	1.32	1.46
16	O	202	GLU	CA-C	-9.71	1.39	1.52
13	T	454	CYS	CB-SG	-9.32	1.50	1.81
13	T	218	CYS	CA-CB	-8.91	1.38	1.53
13	T	399	CYS	CB-SG	-8.71	1.52	1.81
8	H	712	CYS	CB-SG	-8.50	1.53	1.81
1	A	753	TYR	N-CA	-8.39	1.36	1.46
23	W	563	THR	N-CA	8.25	1.56	1.45
6	F	1096	C	O3'-P	-8.03	1.49	1.61
3	C	172	TRP	N-CA	-7.97	1.38	1.46
6	F	1096	C	C1'-N1	7.68	1.59	1.48
1	A	743	LYS	CA-C	-7.63	1.43	1.52
6	F	1120	G	C1'-N9	-7.60	1.36	1.48
18	Q	55	VAL	N-CA	-7.59	1.40	1.45
6	F	1118	U	C1'-N1	7.52	1.59	1.48
1	A	551	LEU	CA-C	-7.43	1.43	1.52
16	O	239	ILE	N-CA	-7.34	1.38	1.46
1	A	559	GLN	N-CA	-7.21	1.36	1.46
16	O	194	HIS	CA-C	-7.15	1.42	1.52
17	P	38	LYS	CA-C	-7.09	1.43	1.52
6	F	1101	C	C1'-N1	7.06	1.59	1.48
6	F	1109	C	C1'-N1	6.98	1.57	1.47
6	F	1111	U	C1'-N1	6.97	1.58	1.48
16	O	201	SER	C-O	-6.97	1.15	1.24
16	O	224	LEU	CA-C	-6.96	1.43	1.52
16	O	327	CYS	CA-C	-6.95	1.44	1.53
6	F	1115	G	C1'-N9	-6.93	1.37	1.48
31	o	102	THR	CB-OG1	6.92	1.54	1.43
6	F	1119	C	C1'-N1	6.91	1.58	1.48
16	O	325	SER	CA-C	-6.89	1.44	1.52
16	O	257	ILE	CA-CB	-6.85	1.45	1.54
1	A	1376	ASN	CA-C	-6.74	1.46	1.53
17	P	32	PRO	N-CA	-6.74	1.39	1.47
16	O	259	VAL	N-CA	-6.64	1.39	1.46
13	T	288	THR	CB-OG1	6.63	1.54	1.43
31	o	51	THR	CB-OG1	6.57	1.54	1.43
13	T	430	THR	CA-CB	-6.54	1.42	1.53
13	T	409	THR	CB-OG1	6.53	1.54	1.43
5	E	301	A	C3'-O3'	6.41	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	O	263	VAL	CA-C	-6.31	1.44	1.52
32	p	75	THR	CB-OG1	6.23	1.53	1.43
1	A	657	LEU	C-O	-6.22	1.16	1.24
16	O	251	TRP	CA-C	-6.20	1.45	1.52
16	O	354	ASN	CA-C	-6.19	1.44	1.52
32	p	110	THR	CB-OG1	6.19	1.53	1.43
16	O	225	SER	CA-C	-6.18	1.44	1.52
13	T	345	HIS	CB-CG	-6.17	1.41	1.50
17	P	31	LEU	CA-C	-6.12	1.46	1.53
13	T	362	SER	CB-OG	6.09	1.54	1.42
1	A	208	VAL	C-O	-6.08	1.18	1.24
31	o	153	THR	CB-OG1	6.06	1.53	1.43
16	O	277	VAL	CA-C	-6.02	1.45	1.52
16	O	282	VAL	N-CA	-6.02	1.39	1.46
5	E	355	U	C1'-N1	6.01	1.56	1.47
16	O	207	LYS	C-O	-6.01	1.17	1.24
16	O	248	ILE	CA-C	-5.97	1.44	1.52
23	W	293	SER	C-N	5.97	1.41	1.34
13	T	403	SER	CA-CB	-5.96	1.44	1.53
6	F	1112	G	C1'-N9	-5.95	1.39	1.48
1	A	192	LEU	CA-C	-5.93	1.45	1.52
6	F	121	C	C1'-N1	5.92	1.57	1.48
13	T	306	SER	CB-OG	5.92	1.53	1.42
1	A	1547	ILE	CA-C	-5.90	1.46	1.52
16	O	326	ALA	CA-C	-5.87	1.45	1.53
13	T	249	THR	CB-OG1	5.87	1.53	1.43
16	O	204	LYS	N-CA	-5.87	1.38	1.46
13	T	143	ARG	C-N	5.86	1.41	1.33
1	A	175	LEU	CA-C	-5.85	1.45	1.53
1	A	742	VAL	CA-C	-5.84	1.45	1.52
31	o	38	THR	CB-OG1	5.84	1.53	1.43
1	A	745	THR	N-CA	-5.80	1.38	1.45
16	O	257	ILE	N-CA	-5.78	1.39	1.46
22	V	246	THR	CB-OG1	5.78	1.52	1.43
31	o	160	THR	CB-OG1	5.72	1.52	1.43
13	T	405	SER	CA-CB	-5.71	1.43	1.53
10	J	145	GLU	CD-OE2	5.68	1.36	1.25
17	P	27	HIS	CA-C	-5.66	1.45	1.53
8	H	723	SER	CB-OG	5.65	1.53	1.42
1	A	208	VAL	N-CA	-5.65	1.39	1.46
13	T	258	THR	CB-OG1	5.64	1.52	1.43
16	O	295	VAL	CA-C	-5.64	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	O	201	SER	CA-C	-5.62	1.45	1.52
23	W	562	TYR	CA-C	5.62	1.60	1.52
1	A	1439	THR	CA-C	-5.62	1.45	1.52
16	O	259	VAL	CA-CB	-5.62	1.48	1.54
16	O	202	GLU	N-CA	-5.61	1.39	1.46
18	Q	74	ILE	CA-CB	-5.60	1.47	1.54
1	A	185	GLN	N-CA	5.60	1.52	1.46
1	A	1610	TRP	CA-C	-5.60	1.47	1.53
16	O	358	ILE	CA-CB	-5.59	1.46	1.54
8	H	718	SER	CB-OG	5.58	1.53	1.42
1	A	656	ILE	CA-CB	-5.56	1.48	1.54
1	A	208	VAL	CA-C	-5.49	1.46	1.52
16	O	334	TRP	CA-C	-5.49	1.45	1.52
1	A	192	LEU	N-CA	-5.43	1.40	1.46
16	O	407	PHE	CA-C	-5.41	1.46	1.52
16	O	210	ASP	CA-C	-5.40	1.45	1.52
16	O	238	LEU	CA-C	-5.37	1.46	1.52
16	O	330	ASP	CA-C	-5.37	1.46	1.52
13	T	165	THR	CB-OG1	5.37	1.52	1.43
16	O	311	VAL	CA-C	-5.37	1.46	1.52
13	T	144	ILE	C-N	5.36	1.41	1.33
1	A	752	ALA	C-O	-5.36	1.17	1.24
17	P	34	HIS	CA-C	-5.36	1.47	1.53
1	A	519	LYS	C-O	5.35	1.30	1.24
16	O	204	LYS	CA-C	-5.35	1.45	1.52
13	T	388	SER	CB-OG	5.31	1.52	1.42
16	O	292	LEU	CA-C	-5.28	1.46	1.52
18	Q	79	ASN	CA-C	-5.26	1.45	1.52
13	T	364	SER	CA-CB	-5.25	1.46	1.53
16	O	253	MET	C-O	-5.25	1.17	1.23
13	T	131	PRO	C-N	5.24	1.41	1.34
13	T	318	ARG	CZ-NH1	5.21	1.40	1.32
1	A	1778	ASP	CA-C	-5.20	1.46	1.52
8	H	576	THR	CB-OG1	5.20	1.52	1.43
1	A	1602	PRO	N-CD	5.20	1.55	1.47
8	H	714	SER	CB-OG	5.20	1.52	1.42
16	O	277	VAL	CA-CB	-5.19	1.47	1.54
16	O	300	THR	N-CA	-5.18	1.39	1.46
13	T	113	SER	CB-OG	5.18	1.52	1.42
3	C	433	THR	CA-C	-5.18	1.48	1.52
16	O	356	LEU	CA-C	-5.18	1.46	1.52
1	A	743	LYS	N-CA	-5.17	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	186	THR	CB-OG1	5.17	1.52	1.43
16	O	184	THR	C-O	-5.16	1.17	1.23
16	O	283	SER	CA-C	-5.16	1.46	1.52
3	C	172	TRP	CA-C	-5.15	1.49	1.52
8	H	632	THR	CB-OG1	5.12	1.51	1.43
13	T	151	PRO	N-CD	5.11	1.54	1.47
16	O	217	ILE	N-CA	-5.10	1.40	1.46
23	W	294	PRO	N-CD	5.10	1.54	1.47
8	H	681	SER	CB-OG	5.08	1.52	1.42
8	H	719	THR	CB-OG1	5.08	1.51	1.43
1	A	1601	ILE	C-N	5.08	1.40	1.34
1	A	1509	ARG	C-O	5.07	1.29	1.24
16	O	216	ILE	CA-C	-5.06	1.47	1.53
1	A	1014	LYS	CA-C	-5.04	1.45	1.52
13	T	132	PRO	N-CD	5.04	1.54	1.47
1	A	168	LEU	N-CA	-5.02	1.42	1.46
1	A	300	LYS	C-O	-5.02	1.17	1.24
16	O	311	VAL	N-CA	-5.02	1.40	1.46
17	P	12	ARG	N-CA	-5.01	1.40	1.46
8	H	644	ILE	CB-CG1	-5.01	1.43	1.53
13	T	381	SER	CB-OG	5.01	1.52	1.42

All (342) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	152	LYS	CB-CA-C	-23.52	77.83	111.23
13	T	130	TYR	N-CA-C	21.07	156.37	109.81
31	o	44	PRO	N-CA-CB	15.87	113.86	103.23
13	T	153	LYS	N-CA-CB	13.74	133.71	110.49
13	T	424	PRO	N-CA-CB	12.19	116.05	103.25
31	o	81	LEU	CA-C-N	12.12	131.62	120.10
31	o	81	LEU	C-N-CA	12.12	131.62	120.10
13	T	130	TYR	CB-CA-C	-11.48	87.55	110.17
20	S	397	LEU	CA-C-N	10.59	133.08	119.84
20	S	397	LEU	C-N-CA	10.59	133.08	119.84
13	T	153	LYS	N-CA-C	-10.42	88.60	110.80
23	W	616	PHE	CA-CB-CG	10.32	124.12	113.80
23	W	522	GLU	CB-CA-C	10.20	125.71	111.74
13	T	131	PRO	N-CA-CB	-10.19	93.20	103.08
1	A	240	PRO	N-CA-C	10.10	123.02	110.70
23	W	750	SER	N-CA-C	9.99	119.97	108.49
13	T	325	ASN	CA-CB-CG	-9.37	103.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	o	12	PRO	N-CA-CB	9.15	111.43	103.19
13	T	125	GLY	N-CA-C	-9.01	91.84	113.18
13	T	155	ILE	N-CA-C	8.75	119.98	111.67
23	W	559	ASP	CA-CB-CG	8.65	121.25	112.60
13	T	131	PRO	N-CA-C	-8.57	100.24	110.70
3	C	171	GLY	N-CA-C	8.51	123.53	112.13
22	V	275	THR	CA-C-N	-8.47	105.04	122.07
22	V	275	THR	C-N-CA	-8.47	105.04	122.07
23	W	562	TYR	CA-C-N	8.46	136.82	121.85
23	W	562	TYR	C-N-CA	8.46	136.82	121.85
31	o	5	PRO	N-CA-CB	8.22	112.02	103.23
23	W	826	PHE	CA-CB-CG	8.19	121.98	113.80
23	W	440	ASP	CA-CB-CG	-8.14	104.46	112.60
10	J	334	PRO	N-CA-CB	8.14	110.92	103.19
13	T	208	PRO	N-CA-CB	8.07	110.49	103.31
31	o	15	TYR	CA-C-O	-8.02	111.78	120.36
31	o	107	SER	N-CA-C	8.01	122.84	112.26
18	Q	59	THR	CB-CA-C	-7.98	105.35	115.89
8	H	613	PRO	N-CA-CB	7.96	111.15	103.51
1	A	284	ARG	NE-CZ-NH2	7.70	126.13	119.20
23	W	1077	ARG	NE-CZ-NH2	7.69	126.12	119.20
16	O	342	LEU	CB-CA-C	-7.68	106.65	115.79
8	H	477	PRO	N-CA-CB	7.62	110.44	103.20
6	F	1111	U	P-O5'-C5'	-7.61	109.49	120.90
8	H	616	PRO	N-CA-CB	7.60	110.45	103.08
13	T	143	ARG	CA-C-N	-7.58	112.99	122.93
13	T	143	ARG	C-N-CA	-7.58	112.99	122.93
31	o	126	ASN	CA-C-O	7.57	128.34	120.40
16	O	232	ILE	CB-CA-C	-7.50	102.25	111.32
8	H	773	PRO	N-CA-CB	7.41	110.27	103.08
19	R	12	LYS	N-CA-C	-7.36	103.30	112.72
6	F	1110	U	O3'-P-O5'	-7.31	93.04	104.00
13	T	303	PRO	N-CA-CB	7.31	110.92	103.25
12	L	149	GLY	N-CA-C	-7.29	104.72	115.72
31	o	57	LEU	N-CA-CB	7.28	123.03	110.81
23	W	538	ARG	NE-CZ-NH2	7.25	125.72	119.20
32	p	65	PHE	CA-CB-CG	-7.24	106.56	113.80
9	I	421	PRO	N-CA-CB	7.18	110.14	103.46
13	T	162	PRO	N-CA-CB	7.17	110.79	102.33
18	Q	51	PHE	N-CA-C	-7.17	101.59	110.41
12	L	103	LEU	N-CA-C	7.16	120.37	110.35
31	o	33	ASP	CA-CB-CG	7.14	119.74	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1601	ILE	CB-CA-C	-7.11	106.81	114.35
3	C	416	ASP	CA-C-N	-7.11	110.95	119.84
3	C	416	ASP	C-N-CA	-7.11	110.95	119.84
31	o	10	ASP	CA-CB-CG	7.05	119.65	112.60
31	o	42	SER	N-CA-CB	-7.05	99.64	110.42
6	F	1113	U	C3'-C2'-O2'	-7.00	104.10	114.60
8	H	722	PRO	N-CA-CB	6.97	111.00	103.33
31	o	7	ILE	CA-CB-CG1	6.97	122.25	110.40
1	A	262	ASP	N-CA-C	6.95	125.16	109.81
1	A	287	GLU	N-CA-C	-6.94	103.79	111.36
9	I	213	GLY	N-CA-C	6.93	123.26	114.25
14	M	60	ILE	N-CA-C	6.92	118.12	108.23
16	O	331	ILE	CB-CA-C	-6.90	102.36	111.81
16	O	344	ASN	CB-CA-C	-6.89	102.39	111.42
8	H	223	PRO	N-CA-CB	6.89	110.58	103.00
32	p	73	PHE	CA-C-O	-6.89	112.74	120.32
18	Q	85	SER	N-CA-C	6.88	121.17	107.62
10	J	418	PRO	N-CA-CB	6.88	110.47	103.25
1	A	284	ARG	NE-CZ-NH1	-6.86	114.64	121.50
13	T	144	ILE	N-CA-CB	-6.84	102.86	111.41
31	o	3	PHE	N-CA-C	-6.84	98.07	108.67
8	H	299	PRO	N-CA-CB	6.83	110.51	103.00
13	T	441	LYS	N-CA-C	6.83	119.24	108.79
23	W	471	ARG	NE-CZ-NH2	6.82	125.33	119.20
31	o	4	THR	N-CA-CB	-6.79	98.28	110.37
3	C	172	TRP	N-CA-C	-6.78	100.72	111.02
13	T	148	CYS	N-CA-C	6.78	119.48	110.53
8	H	267	PRO	N-CA-CB	6.77	110.45	103.00
8	H	617	PRO	CA-CB-CG	6.74	117.31	104.50
8	H	479	PRO	N-CA-CB	6.73	110.65	103.52
1	A	745	THR	N-CA-C	-6.70	101.51	110.55
16	O	122	ARG	CA-C-N	6.69	126.92	119.90
16	O	122	ARG	C-N-CA	6.69	126.92	119.90
22	V	246	THR	CA-CB-OG1	6.69	119.63	109.60
1	A	1580	GLY	N-CA-C	6.66	120.72	112.73
5	E	301	A	C2'-C3'-O3'	-6.66	99.52	109.50
8	H	252	PRO	N-CA-CB	6.65	110.31	103.00
9	I	559	PRO	N-CA-CB	6.64	110.30	103.00
18	Q	55	VAL	CA-C-O	6.63	123.39	119.94
16	O	205	THR	CB-CA-C	-6.63	98.04	109.65
8	H	437	PRO	N-CA-CB	6.63	110.29	103.00
8	H	515	PRO	N-CA-CB	6.62	110.54	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1107	C	C5'-C4'-O4'	-6.62	99.18	109.10
23	W	640	SER	N-CA-C	6.61	124.89	110.80
13	T	366	LYS	CA-C-N	6.60	126.37	119.05
13	T	366	LYS	C-N-CA	6.60	126.37	119.05
23	W	862	ASP	CA-CB-CG	6.59	119.19	112.60
31	o	68	PRO	N-CA-CB	6.58	110.16	103.25
16	O	238	LEU	CB-CA-C	-6.57	98.15	109.65
30	n	82	LYS	N-CA-C	6.57	124.78	110.80
8	H	774	PRO	N-CA-CB	6.56	110.47	103.39
13	T	159	PRO	N-CA-CB	6.56	110.14	103.25
31	o	130	ILE	CA-C-O	6.54	128.96	120.78
30	g	82	LYS	N-CA-C	6.54	124.72	110.80
9	I	435	PRO	N-CA-CB	6.52	110.43	103.52
8	H	557	PRO	N-CA-CB	6.51	110.42	103.39
9	I	397	PRO	N-CA-CB	6.44	110.35	103.52
8	H	533	PRO	N-CA-CB	6.44	110.34	103.52
6	F	1112	G	P-O3'-C3'	6.43	129.85	120.20
1	A	1400	ILE	CB-CA-C	-6.43	103.09	111.25
1	A	260	PRO	N-CA-C	6.39	121.95	113.57
9	I	545	PRO	N-CA-CB	6.38	110.29	103.52
23	W	497	ARG	NE-CZ-NH2	6.38	124.94	119.20
23	W	1105	GLU	CB-CA-C	6.36	123.08	110.42
8	H	443	PRO	N-CA-CB	6.35	110.56	103.44
16	O	295	VAL	CB-CA-C	-6.34	103.72	112.02
23	W	729	PRO	CA-C-N	6.28	131.56	121.95
23	W	729	PRO	C-N-CA	6.28	131.56	121.95
8	H	161	PRO	N-CA-CB	6.24	110.43	103.44
8	H	518	PRO	N-CA-CB	6.24	110.13	103.52
23	W	442	ARG	NE-CZ-NH2	6.24	124.81	119.20
13	T	373	PRO	N-CA-CB	6.23	110.19	103.33
6	F	1111	U	C5'-C4'-C3'	-6.21	106.68	116.00
10	J	467	PRO	N-CA-CB	6.21	109.77	103.25
23	W	1104	ALA	N-CA-C	6.21	120.55	112.92
1	A	1488	ILE	CA-C-N	-6.20	112.10	119.84
1	A	1488	ILE	C-N-CA	-6.20	112.10	119.84
31	o	50	LEU	CA-C-N	6.19	131.38	122.40
31	o	50	LEU	C-N-CA	6.19	131.38	122.40
22	V	302	LEU	N-CA-C	6.17	123.95	110.80
31	o	83	ARG	N-CA-C	6.16	119.86	111.17
8	H	641	PRO	CA-CB-CG	6.15	116.19	104.50
8	H	262	PRO	N-CA-CB	6.14	110.32	103.44
10	J	447	PRO	N-CA-CB	6.14	109.69	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1410	SER	N-CA-C	6.11	119.46	110.30
9	I	351	PRO	N-CA-CB	6.10	110.27	103.44
31	o	111	PHE	CA-CB-CG	6.10	119.90	113.80
10	J	424	PRO	N-CA-CB	6.08	109.69	103.00
10	J	376	PRO	N-CA-CB	6.06	110.23	103.44
1	A	404	ASN	N-CA-C	6.04	118.35	109.24
13	T	367	PRO	N-CA-CB	6.03	109.96	103.33
31	o	85	ASN	N-CA-CB	-6.02	102.60	111.51
31	o	132	ASN	OD1-CG-ND2	6.01	128.61	122.60
23	W	506	GLY	CA-C-N	6.00	133.00	121.54
23	W	506	GLY	C-N-CA	6.00	133.00	121.54
23	W	725	LEU	CB-CA-C	6.00	119.67	109.53
31	o	127	LEU	CA-C-N	-5.98	114.34	122.77
31	o	127	LEU	C-N-CA	-5.98	114.34	122.77
1	A	1395	GLY	CA-C-O	5.97	124.38	118.77
1	A	742	VAL	CB-CA-C	-5.97	101.50	111.29
31	o	62	ASN	CA-CB-CG	5.97	118.57	112.60
6	F	1106	G	O3'-P-O5'	-5.96	95.07	104.00
7	G	105	PRO	CA-CB-CG	5.96	115.82	104.50
23	W	506	GLY	O-C-N	5.96	130.44	122.70
32	p	66	LYS	N-CA-C	-5.95	104.70	111.07
23	W	912	LEU	O-C-N	-5.95	114.68	122.59
23	W	1025	PHE	CA-CB-CG	5.91	119.71	113.80
14	M	7	GLU	CA-C-N	-5.88	114.32	120.38
14	M	7	GLU	C-N-CA	-5.88	114.32	120.38
18	Q	88	ARG	N-CA-C	-5.88	105.37	112.54
10	J	417	PRO	N-CA-CB	5.85	108.75	103.08
16	O	331	ILE	N-CA-C	5.84	115.75	106.88
8	H	617	PRO	N-CA-CB	5.83	109.38	103.25
10	J	432	PRO	N-CA-CB	5.83	109.70	103.52
23	W	1103	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	1319	ILE	CB-CA-C	-5.82	104.52	111.97
23	W	1032	ASN	CA-CB-CG	5.80	118.40	112.60
23	W	916	ASP	CB-CA-C	5.76	120.29	110.56
31	o	44	PRO	CB-CA-C	-5.73	106.19	111.40
31	o	60	THR	CA-C-O	5.73	127.62	121.55
13	T	345	HIS	CA-C-N	5.73	125.34	119.56
13	T	345	HIS	C-N-CA	5.73	125.34	119.56
18	Q	87	ASN	N-CA-C	-5.72	101.19	109.59
6	F	1107	C	P-O3'-C3'	5.71	128.76	120.20
12	L	118	SER	N-CA-C	5.71	117.15	108.07
13	T	131	PRO	CA-C-N	-5.70	112.72	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	131	PRO	C-N-CA	-5.70	112.72	119.05
10	J	80	LEU	CA-C-N	-5.70	112.71	119.84
10	J	80	LEU	C-N-CA	-5.70	112.71	119.84
10	J	339	PRO	N-CA-CB	5.68	109.80	103.44
16	O	123	PRO	N-CA-C	5.67	119.36	110.80
23	W	469	GLY	O-C-N	-5.67	118.64	123.23
23	W	525	PHE	CA-C-N	5.66	132.35	121.54
23	W	525	PHE	C-N-CA	5.66	132.35	121.54
14	M	62	VAL	N-CA-C	-5.66	107.26	113.43
6	F	1111	U	O4'-C1'-C2'	-5.65	101.95	107.60
1	A	742	VAL	CA-C-N	-5.65	112.48	122.20
1	A	742	VAL	C-N-CA	-5.65	112.48	122.20
1	A	1903	LYS	CB-CA-C	-5.65	109.06	115.79
23	W	730	VAL	CB-CA-C	-5.65	103.10	111.80
23	W	1067	VAL	CA-CB-CG2	5.65	120.00	110.40
10	J	374	PRO	N-CA-CB	5.64	109.50	103.52
13	T	424	PRO	CA-CB-CG	5.63	115.20	104.50
23	W	862	ASP	N-CA-CB	-5.63	101.80	110.25
1	A	1283	GLU	N-CA-C	5.63	120.02	113.20
31	o	158	ASN	CB-CA-C	-5.62	102.07	110.16
13	T	327	PRO	N-CA-CB	5.61	109.14	103.25
1	A	484	PHE	CA-C-N	-5.60	112.93	119.32
1	A	484	PHE	C-N-CA	-5.60	112.93	119.32
16	O	384	TYR	N-CA-C	5.56	119.76	112.92
1	A	1601	ILE	O-C-N	5.56	124.02	120.07
1	A	834	ILE	CB-CA-C	-5.54	104.57	112.22
23	W	513	THR	CA-C-N	5.54	128.50	120.79
23	W	513	THR	C-N-CA	5.54	128.50	120.79
6	F	1108	A	N9-C1'-C2'	5.54	120.31	112.00
23	W	989	HIS	CB-CG-CD2	-5.54	124.00	131.20
13	T	144	ILE	CA-C-N	-5.52	112.88	120.28
13	T	144	ILE	C-N-CA	-5.52	112.88	120.28
23	W	992	ARG	NE-CZ-NH2	5.52	124.17	119.20
13	T	428	PRO	N-CA-CB	5.52	109.07	103.00
13	T	345	HIS	CA-CB-CG	-5.51	108.29	113.80
13	T	68	PRO	N-CA-C	5.51	120.81	114.20
23	W	461	ARG	NE-CZ-NH2	5.50	124.15	119.20
23	W	883	GLN	OE1-CD-NE2	-5.49	117.11	122.60
23	W	1036	ARG	NE-CZ-NH2	5.48	124.14	119.20
23	W	293	SER	CA-C-N	-5.48	112.87	118.85
23	W	293	SER	C-N-CA	-5.48	112.87	118.85
1	A	1346	PHE	CB-CA-C	-5.48	101.90	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	77	PRO	CA-CB-CG	5.47	114.90	104.50
21	U	100	ILE	N-CA-C	5.47	116.10	110.36
1	A	401	PRO	N-CA-C	5.46	121.03	113.98
18	Q	77	LEU	CA-CB-CG	-5.46	97.20	116.30
3	C	926	GLY	N-CA-C	5.45	117.12	111.95
31	o	15	TYR	O-C-N	5.44	129.43	123.22
23	W	978	GLN	OE1-CD-NE2	-5.44	117.16	122.60
23	W	445	ILE	CA-C-N	5.43	131.91	121.54
23	W	445	ILE	C-N-CA	5.43	131.91	121.54
1	A	1089	VAL	N-CA-C	-5.43	104.14	110.05
31	o	71	SER	N-CA-CB	-5.43	102.64	110.45
31	o	141	ARG	CD-NE-CZ	5.42	131.99	124.40
1	A	1270	LEU	CB-CA-C	-5.41	103.92	110.15
30	n	81	GLY	N-CA-C	5.41	119.50	112.25
31	o	50	LEU	N-CA-C	-5.41	106.18	112.89
23	W	714	ARG	NE-CZ-NH2	5.41	124.07	119.20
23	W	805	ARG	NE-CZ-NH2	5.41	124.07	119.20
23	W	686	HIS	CA-CB-CG	5.41	119.21	113.80
23	W	506	GLY	N-CA-C	5.39	125.97	113.18
1	A	1547	ILE	N-CA-CB	5.39	116.49	110.62
30	g	81	GLY	N-CA-C	5.38	119.45	112.25
23	W	638	LEU	CA-C-N	5.37	127.79	120.54
23	W	638	LEU	C-N-CA	5.37	127.79	120.54
21	U	124	TRP	N-CA-C	-5.37	105.34	111.14
23	W	447	MET	CA-C-N	5.35	131.76	121.54
23	W	447	MET	C-N-CA	5.35	131.76	121.54
23	W	989	HIS	CB-CA-C	5.34	119.93	110.85
23	W	811	ARG	NE-CZ-NH2	5.34	124.00	119.20
23	W	1082	GLN	OE1-CD-NE2	-5.34	117.26	122.60
32	p	93	ARG	CA-CB-CG	-5.33	103.43	114.10
23	W	867	PRO	N-CA-CB	5.33	105.99	103.22
23	W	1097	HIS	CB-CG-CD2	-5.32	124.29	131.20
32	p	41	MET	N-CA-C	5.30	117.47	111.11
31	o	155	ASP	CA-C-N	5.30	130.08	122.40
31	o	155	ASP	C-N-CA	5.30	130.08	122.40
16	O	194	HIS	N-CA-C	-5.29	102.46	110.50
31	o	133	GLN	CA-CB-CG	-5.29	103.52	114.10
1	A	289	ASP	N-CA-C	-5.28	98.42	107.61
17	P	172	LYS	CB-CA-C	-5.28	102.99	111.39
3	C	589	LEU	N-CA-C	5.28	117.34	110.43
23	W	909	ARG	NE-CZ-NH2	5.28	123.95	119.20
16	O	264	GLY	N-CA-C	5.27	125.66	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	140	VAL	CA-C-N	-5.26	114.68	122.41
12	L	140	VAL	C-N-CA	-5.26	114.68	122.41
23	W	714	ARG	CA-C-N	5.26	127.89	120.42
23	W	714	ARG	C-N-CA	5.26	127.89	120.42
31	o	38	THR	CA-CB-OG1	5.26	117.49	109.60
31	o	134	VAL	CA-C-N	5.26	127.86	120.28
31	o	134	VAL	C-N-CA	5.26	127.86	120.28
14	M	99	VAL	N-CA-C	5.25	120.27	109.34
23	W	911	LEU	N-CA-C	5.24	116.85	111.03
14	M	95	ASN	N-CA-C	-5.24	100.25	108.00
23	W	448	LEU	N-CA-C	5.24	121.96	110.80
6	F	1113	U	O4'-C1'-C2'	-5.23	100.57	105.80
8	H	641	PRO	N-CA-CB	5.23	108.75	103.25
1	A	1523	SER	CA-C-N	5.21	126.36	119.84
1	A	1523	SER	C-N-CA	5.21	126.36	119.84
12	L	107	ARG	N-CA-CB	5.21	117.96	110.20
16	O	304	LEU	N-CA-C	-5.21	99.80	108.34
1	A	1021	PRO	N-CA-C	5.20	117.05	110.70
22	V	301	GLU	N-CA-C	5.20	117.77	110.23
23	W	441	SER	CA-C-N	5.19	128.91	120.60
23	W	441	SER	C-N-CA	5.19	128.91	120.60
31	o	44	PRO	CA-C-O	-5.19	114.41	120.85
23	W	1030	PHE	CA-CB-CG	-5.19	108.61	113.80
32	p	71	GLN	N-CA-C	5.19	117.56	109.52
14	M	54	ASN	N-CA-C	5.18	117.94	109.59
1	A	622	MET	CG-SD-CE	-5.18	89.50	100.90
1	A	1601	ILE	CA-C-N	-5.18	113.30	119.05
1	A	1601	ILE	C-N-CA	-5.18	113.30	119.05
1	A	511	ASP	CB-CA-C	-5.17	109.07	115.89
31	o	100	ASN	CA-CB-CG	5.16	117.76	112.60
13	T	271	LYS	N-CA-C	5.16	117.77	110.50
1	A	461	LEU	N-CA-C	5.15	119.28	112.89
15	N	25	GLN	N-CA-C	5.14	116.92	110.91
23	W	480	ARG	CB-CG-CD	5.14	123.11	111.30
20	S	397	LEU	C-N-CD	-5.11	104.04	125.00
23	W	869	LYS	CA-C-N	5.11	127.08	120.44
23	W	869	LYS	C-N-CA	5.11	127.08	120.44
23	W	751	ARG	NE-CZ-NH2	5.11	123.79	119.20
1	A	488	ARG	N-CA-C	5.10	118.94	111.04
13	T	134	ASP	N-CA-C	5.10	116.92	111.36
12	L	144	GLN	CA-C-O	5.09	125.97	120.32
15	N	34	TYR	N-CA-C	-5.09	103.81	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	594	MET	CA-C-N	5.09	127.81	120.38
23	W	594	MET	C-N-CA	5.09	127.81	120.38
23	W	443	ASN	CA-CB-CG	5.09	117.69	112.60
32	p	68	GLN	N-CA-C	5.09	119.48	113.28
23	W	591	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	1378	LYS	N-CA-C	-5.07	107.12	113.72
23	W	883	GLN	CB-CG-CD	5.07	121.22	112.60
27	d	42	ASP	N-CA-C	5.07	117.23	110.53
1	A	1527	TRP	N-CA-C	5.06	118.94	112.87
1	A	794	LYS	N-CA-C	-5.06	105.42	111.03
3	C	218	HIS	N-CA-C	-5.05	103.86	110.53
21	U	246	ASN	N-CA-C	5.05	116.28	109.11
23	W	1060	TYR	CA-C-N	5.05	131.31	121.41
23	W	1060	TYR	C-N-CA	5.05	131.31	121.41
27	k	42	ASP	N-CA-C	5.04	117.19	110.53
31	o	107	SER	N-CA-CB	-5.04	102.90	111.17
23	W	969	ARG	NE-CZ-NH2	5.04	123.73	119.20
13	T	339	MET	CA-C-N	-5.03	113.37	118.85
13	T	339	MET	C-N-CA	-5.03	113.37	118.85
13	T	171	LEU	CA-C-N	5.03	126.13	119.84
13	T	171	LEU	C-N-CA	5.03	126.13	119.84
14	M	9	PRO	CA-C-N	-5.03	114.77	119.85
14	M	9	PRO	C-N-CA	-5.03	114.77	119.85
13	T	210	LYS	N-CA-C	5.03	117.87	111.69
31	o	56	ILE	CA-C-O	-5.02	115.24	120.76
23	W	565	ARG	CA-C-N	5.01	131.12	121.54
23	W	565	ARG	C-N-CA	5.01	131.12	121.54
1	A	726	ILE	N-CA-C	5.01	115.78	110.72
13	T	325	ASN	N-CA-C	5.01	116.82	111.36
1	A	1528	THR	N-CA-C	5.01	116.99	109.23
32	p	103	PHE	CA-C-O	-5.01	115.34	121.05

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1014	LYS	Peptide
1	A	1375	LEU	Peptide
1	A	1432	GLU	Peptide
1	A	1809	ASN	Peptide
1	A	239	PHE	Peptide
1	A	288	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	539	PRO	Peptide
1	A	907	ASN	Peptide
3	C	170	LEU	Peptide
3	C	365	GLU	Peptide
3	C	70	TYR	Peptide
9	I	212	HIS	Peptide
10	J	224	MET	Peptide
10	J	65	PHE	Peptide
10	J	81	PRO	Peptide
12	L	1	MET	Peptide
12	L	104	CYS	Peptide
12	L	116	ASN	Peptide
12	L	118	SER	Peptide
12	L	5	LYS	Peptide
14	M	103	GLU	Peptide
14	M	291	ILE	Peptide
14	M	45	HIS	Peptide
14	M	94	VAL	Peptide
14	M	98	ASN	Peptide
15	N	203	THR	Peptide
16	O	123	PRO	Peptide
16	O	155	PHE	Peptide
16	O	278	ASP	Peptide
16	O	284	SER	Peptide
16	O	336	LEU	Peptide
16	O	351	GLY	Peptide
16	O	431	THR	Peptide
16	O	434	LYS	Peptide
16	O	435	GLU	Peptide
16	O	437	GLU	Peptide
16	O	441	ALA	Peptide
18	Q	103	ASN	Peptide
18	Q	84	ASN	Peptide
18	Q	85	SER	Peptide
20	S	335	GLN	Peptide
20	S	397	LEU	Mainchain,Peptide
13	T	366	LYS	Peptide
13	T	67	GLY	Peptide
23	W	1037	ASP	Peptide
23	W	1042	TYR	Sidechain
23	W	1064	TYR	Sidechain
23	W	1067	VAL	Peptide

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Mol	Chain	Res	Type	Group
23	W	1076	SER	Peptide
23	W	1077	ARG	Sidechain
23	W	1081	SER	Peptide
23	W	1103	ASP	Peptide
23	W	439	LYS	Peptide
23	W	440	ASP	Sidechain
23	W	446	GLN	Peptide
23	W	468	TYR	Peptide
23	W	474	LEU	Peptide
23	W	480	ARG	Sidechain
23	W	486	TYR	Sidechain
23	W	489	ARG	Sidechain
23	W	505	VAL	Peptide
23	W	512	LYS	Peptide
23	W	522	GLU	Peptide
23	W	537	ARG	Sidechain
23	W	562	TYR	Peptide
23	W	566	PHE	Peptide
23	W	575	ARG	Sidechain
23	W	646	TYR	Sidechain
23	W	666	TYR	Sidechain
23	W	729	PRO	Peptide
23	W	786	ARG	Peptide
23	W	808	ARG	Sidechain
23	W	811	ARG	Sidechain
23	W	840	ARG	Sidechain
23	W	911	LEU	Peptide
23	W	916	ASP	Peptide
23	W	940	LYS	Peptide
23	W	957	TYR	Sidechain
23	W	967	TYR	Sidechain
27	d	41	ASP	Peptide
28	e	81	ALA	Mainchain,Peptide
30	g	81	GLY	Mainchain,Peptide
27	k	41	ASP	Peptide
28	l	81	ALA	Mainchain,Peptide
30	n	81	GLY	Mainchain,Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15931	0	15900	1109	0
2	B	2465	0	1251	71	0
3	C	7019	0	7202	362	0
4	D	2192	0	1106	99	0
5	E	1310	0	658	124	0
6	F	1909	0	970	182	0
7	G	926	0	606	11	0
8	H	3012	0	1581	52	0
9	I	3424	0	2581	91	0
10	J	2949	0	2436	88	0
11	K	777	0	801	47	0
12	L	1291	0	1312	57	0
13	T	2357	0	1924	363	0
14	M	1472	0	1486	114	0
15	N	2089	0	2053	164	0
16	O	2646	0	2639	170	0
17	P	560	0	545	54	0
18	Q	1583	0	1608	81	0
19	R	190	0	186	12	0
20	S	1701	0	1712	87	0
21	U	1202	0	1248	95	0
22	V	554	0	416	74	0
23	W	5553	0	5532	50	0
24	a	631	0	670	3	0
24	h	610	0	640	17	0
25	b	575	0	597	21	0
25	i	575	0	597	21	0
26	c	554	0	556	17	0
26	j	554	0	556	17	0
27	d	529	0	557	2	0
27	k	529	0	557	2	0
28	e	625	0	647	5	0
28	l	616	0	634	9	0
29	f	644	0	686	14	0
29	m	644	0	686	14	0
30	g	741	0	778	17	0
30	n	528	0	573	16	0
31	o	841	0	614	19	0
32	p	513	0	402	12	0
33	q	850	0	682	10	0
33	r	823	0	654	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	s	830	0	663	6	0
33	t	843	0	675	8	0
34	A	36	0	6	9	0
35	C	32	0	12	6	0
36	C	1	0	0	0	0
36	D	5	0	0	0	0
37	L	3	0	0	0	0
37	M	2	0	0	2	0
37	N	1	0	0	0	0
All	All	76247	0	68195	3238	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 22.

All (3238) 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)
6:F:20:G:C2	17:P:6:ARG:HB3	1.23	1.63
13:T:185:HIS:CB	13:T:185:HIS:CG	1.83	1.62
13:T:317:VAL:CB	13:T:331:ILE:HD11	1.22	1.57
1:A:2003:THR:HB	22:V:333:PRO:CB	1.35	1.55
6:F:20:G:N2	17:P:6:ARG:CB	1.74	1.46
6:F:20:G:N2	17:P:6:ARG:HB3	1.22	1.44
4:D:40:A:C2	15:N:121:ARG:NE	1.74	1.42
1:A:1875:ILE:CD1	13:T:326:VAL:HG11	1.52	1.39
8:H:729:TYR:CZ	8:H:748:PHE:CB	2.03	1.39
1:A:511:ASP:HB2	1:A:514:TYR:CE2	1.58	1.38
1:A:2056:ARG:NH2	22:V:331:ALA:O	1.58	1.37
1:A:1988:LEU:CD1	21:U:180:VAL:HG12	1.55	1.36
1:A:659:HIS:CE1	34:A:3000:IHP:O22	1.78	1.34
1:A:1927:GLU:CG	21:U:135:LEU:HD11	1.56	1.33
6:F:20:G:C2	17:P:6:ARG:CB	2.09	1.32
13:T:126:ARG:NH1	13:T:131:PRO:CG	1.93	1.31
1:A:1875:ILE:HD13	13:T:326:VAL:CG1	1.60	1.31
1:A:511:ASP:HB2	1:A:514:TYR:CZ	1.64	1.30
13:T:139:LEU:HD12	13:T:174:THR:OG1	1.27	1.30
13:T:376:ILE:O	13:T:377:PHE:HD1	1.14	1.30
10:J:179:SER:HB3	13:T:337:HIS:CD2	1.67	1.30
8:H:729:TYR:CE1	8:H:748:PHE:CB	2.13	1.29
1:A:1875:ILE:CD1	13:T:326:VAL:CG1	2.11	1.29
1:A:1988:LEU:CD2	21:U:180:VAL:HG11	1.62	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:193:GLN:OE1	13:T:447:ALA:HB1	1.20	1.29
1:A:1986:MET:CB	21:U:184:MET:HB3	1.62	1.28
1:A:1875:ILE:CG2	13:T:326:VAL:HG21	1.63	1.27
1:A:1986:MET:CG	21:U:184:MET:HG3	1.63	1.27
6:F:20:G:N3	17:P:6:ARG:HB3	1.46	1.27
1:A:1988:LEU:HD22	21:U:180:VAL:CG1	1.64	1.27
1:A:1870:VAL:HG21	5:E:299:U:O2	1.18	1.26
1:A:1870:VAL:CG2	5:E:299:U:O2	1.83	1.26
1:A:2003:THR:CB	22:V:333:PRO:CB	2.13	1.25
4:D:40:A:N1	15:N:121:ARG:NE	1.86	1.24
13:T:139:LEU:CD1	13:T:174:THR:OG1	1.85	1.23
13:T:292:HIS:CE1	13:T:312:SER:HB3	1.72	1.23
13:T:317:VAL:CB	13:T:331:ILE:CD1	2.16	1.23
1:A:2056:ARG:NH2	22:V:331:ALA:C	1.97	1.22
1:A:1666:CYS:O	1:A:1670:ASP:HB2	1.32	1.22
13:T:132:PRO:HB3	13:T:176:HIS:ND1	1.54	1.19
1:A:1988:LEU:HD13	21:U:180:VAL:CG1	1.70	1.19
10:J:179:SER:CB	13:T:337:HIS:CD2	2.24	1.19
14:M:215:PRO:HG3	14:M:217:TRP:CE2	1.77	1.19
13:T:129:LEU:HD12	13:T:130:TYR:N	1.57	1.18
3:C:240:ASP:CG	3:C:269:LYS:HD2	1.68	1.18
1:A:1774:MET:O	1:A:1786:ALA:HA	1.45	1.16
1:A:2003:THR:CB	22:V:333:PRO:HB2	1.71	1.16
13:T:59:ARG:O	13:T:62:THR:HG23	1.41	1.16
1:A:1986:MET:HB3	21:U:184:MET:CG	1.74	1.16
13:T:317:VAL:CG1	13:T:331:ILE:HD11	1.75	1.15
24:h:98:GLU:O	31:o:53:PRO:CB	1.92	1.15
1:A:1986:MET:CB	21:U:184:MET:CG	2.25	1.15
10:J:193:GLN:OE1	13:T:447:ALA:CB	1.92	1.15
1:A:2002:TYR:CE1	22:V:307:ARG:CG	2.30	1.15
4:D:40:A:C2	15:N:121:ARG:CZ	2.28	1.15
13:T:126:ARG:HH12	13:T:131:PRO:CG	1.56	1.15
4:D:90:U:C5	9:I:104:ARG:NH2	2.15	1.14
1:A:1986:MET:CB	21:U:184:MET:CB	2.25	1.14
14:M:215:PRO:HG3	14:M:217:TRP:CZ2	1.83	1.14
1:A:1957:ARG:HH21	22:V:272:LEU:CB	1.61	1.13
6:F:20:G:H21	17:P:6:ARG:CB	1.49	1.13
1:A:2003:THR:HB	22:V:333:PRO:HB3	1.14	1.12
5:E:1:G:H2'	5:E:2:U:H5''	1.31	1.12
13:T:376:ILE:O	13:T:377:PHE:CD1	2.01	1.13
4:D:91:A:C4	9:I:99:ILE:HD11	1.84	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1109:C:N4	32:p:109:LYS:H	1.48	1.11
6:F:20:G:N3	17:P:7:PRO:HD2	1.65	1.11
1:A:511:ASP:HB2	1:A:514:TYR:OH	1.47	1.11
13:T:292:HIS:CE1	13:T:312:SER:CB	2.33	1.11
1:A:1488:ILE:HG23	1:A:1489:PRO:HD3	1.21	1.10
8:H:729:TYR:CE2	8:H:748:PHE:CB	2.33	1.10
1:A:2002:TYR:CZ	22:V:307:ARG:CG	2.34	1.10
13:T:129:LEU:HD12	13:T:130:TYR:H	0.96	1.10
6:F:1111:U:H5'	6:F:1111:U:C6	1.86	1.10
1:A:1494:LEU:CD2	23:W:298:GLU:HG2	1.82	1.09
1:A:2003:THR:HB	22:V:333:PRO:HB2	1.21	1.09
5:E:346:A:O2'	5:E:347:A:C8	2.02	1.09
7:G:7:VAL:HG11	7:G:154:VAL:CB	1.81	1.09
1:A:1875:ILE:HD13	13:T:326:VAL:CG2	1.82	1.08
1:A:1875:ILE:HG21	13:T:326:VAL:HG21	1.11	1.08
1:A:1986:MET:HB2	21:U:184:MET:HB3	1.12	1.08
21:U:183:TYR:CE2	21:U:234:LYS:HD2	1.88	1.08
6:F:20:G:N2	17:P:6:ARG:HB2	1.59	1.08
1:A:2003:THR:CB	22:V:333:PRO:HB3	1.78	1.08
1:A:1494:LEU:HD22	23:W:298:GLU:HG2	1.34	1.07
1:A:1927:GLU:HG2	21:U:135:LEU:HD11	1.15	1.07
1:A:1927:GLU:HG3	21:U:135:LEU:CD1	1.85	1.06
13:T:295:SER:N	13:T:313:GLU:HB2	1.69	1.05
6:F:1102:C:H2'	6:F:1103:C:C6	1.91	1.05
13:T:317:VAL:CG1	13:T:331:ILE:CD1	2.34	1.05
13:T:411:ASP:OD1	13:T:414:THR:N	1.90	1.05
1:A:1927:GLU:HG3	21:U:135:LEU:HD11	1.36	1.05
3:C:240:ASP:CG	3:C:269:LYS:CD	2.28	1.05
8:H:161:PRO:CB	31:o:48:LYS:CB	2.34	1.05
13:T:340:PRO:HG2	13:T:356:MET:CE	1.87	1.04
24:h:99:ASP:CB	31:o:53:PRO:CB	2.35	1.04
1:A:510:PRO:O	1:A:514:TYR:CZ	2.11	1.04
1:A:1875:ILE:HD13	13:T:326:VAL:HG11	1.17	1.04
6:F:1116:A:H2'	6:F:1117:G:H8	1.17	1.04
13:T:308:PHE:HE1	13:T:320:TRP:HB2	1.21	1.04
13:T:374:LYS:HZ3	13:T:374:LYS:HA	1.21	1.04
14:M:217:TRP:O	14:M:221:ASP:HB2	1.55	1.04
13:T:295:SER:O	13:T:313:GLU:N	1.89	1.04
1:A:1986:MET:HG3	21:U:184:MET:CG	1.88	1.03
13:T:111:GLU:CB	13:T:199:LEU:O	2.06	1.03
6:F:20:G:H1'	17:P:7:PRO:CD	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:135:VAL:HG11	13:T:193:TYR:CZ	1.93	1.03
1:A:511:ASP:CB	1:A:514:TYR:OH	2.04	1.03
33:s:51:VAL:HG21	33:t:20:ARG:CB	1.89	1.03
6:F:30:A:H3'	6:F:31:A:H5''	1.39	1.03
1:A:659:HIS:NE2	34:A:3000:IHP:O22	1.92	1.02
1:A:1927:GLU:CG	21:U:135:LEU:CD1	2.37	1.02
1:A:1986:MET:CG	21:U:184:MET:CG	2.38	1.02
2:B:165:A:H4'	2:B:166:U:C5'	1.89	1.02
23:W:295:GLU:O	23:W:299:ILE:HD12	1.56	1.02
1:A:511:ASP:CG	1:A:514:TYR:OH	2.03	1.02
4:D:51:A:C8	5:E:3:A:C2	2.48	1.02
6:F:110:A:H4'	6:F:111:C:C5'	1.89	1.02
5:E:1:G:H2'	5:E:2:U:C5'	1.89	1.01
13:T:139:LEU:HD13	13:T:174:THR:CB	1.90	1.01
1:A:1986:MET:HB2	21:U:184:MET:CB	1.88	1.00
1:A:1984:PRO:O	21:U:190:ASN:ND2	1.94	1.00
2:B:165:A:C4'	2:B:166:U:H5'	1.92	1.00
6:F:110:A:C4'	6:F:111:C:H5'	1.91	1.00
8:H:730:GLN:HA	8:H:733:ILE:HD11	1.37	1.00
1:A:1986:MET:HB3	21:U:184:MET:CB	1.87	1.00
6:F:1116:A:H2'	6:F:1117:G:C8	1.95	0.99
4:D:40:A:N1	15:N:121:ARG:CG	2.25	0.99
1:A:511:ASP:CB	1:A:514:TYR:CE2	2.43	0.99
1:A:1709:TRP:O	1:A:1728:ILE:HA	1.63	0.99
1:A:1986:MET:HB3	21:U:184:MET:HG2	1.40	0.99
1:A:910:LYS:HE3	1:A:1500:HIS:CE1	1.98	0.99
1:A:1875:ILE:HD13	13:T:326:VAL:CB	1.93	0.99
1:A:1875:ILE:CG2	13:T:326:VAL:CG2	2.40	0.99
13:T:200:ARG:NH2	13:T:237:THR:HA	1.77	0.99
1:A:910:LYS:HE3	1:A:1500:HIS:HE1	1.27	0.98
8:H:718:SER:OG	8:H:725:THR:HG21	1.61	0.98
3:C:240:ASP:OD1	3:C:269:LYS:CD	2.12	0.98
6:F:1114:G:O6	32:p:38:LYS:NZ	1.95	0.98
1:A:1875:ILE:HD13	13:T:326:VAL:HG21	1.43	0.97
1:A:928:ARG:NH2	1:A:1595:ARG:NH2	2.12	0.97
3:C:268:ASN:OD1	3:C:269:LYS:N	1.97	0.97
9:I:99:ILE:HG13	9:I:100:PRO:HD3	1.46	0.97
12:L:120:CYS:HB2	12:L:122:CYS:HB3	1.44	0.97
1:A:511:ASP:HB2	1:A:514:TYR:HE2	1.28	0.97
13:T:150:LEU:H	13:T:150:LEU:HD12	1.27	0.97
1:A:1955:ALA:HB2	22:V:271:ARG:O	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1097:G:N2	6:F:1119:C:O2	1.96	0.97
9:I:227:ASP:O	9:I:231:ASN:HB2	1.62	0.96
13:T:358:ASN:OD1	13:T:380:HIS:O	1.83	0.96
3:C:784:SER:HB2	3:C:787:LEU:HB3	1.47	0.96
1:A:2002:TYR:HE2	22:V:329:LEU:HD11	1.31	0.96
4:D:40:A:C2	15:N:121:ARG:NH2	2.32	0.96
1:A:1875:ILE:HG21	13:T:326:VAL:CG2	1.96	0.96
4:D:90:U:H5	9:I:104:ARG:HH22	1.10	0.95
13:T:340:PRO:HG2	13:T:356:MET:HE1	1.46	0.95
6:F:1111:U:H5''	6:F:1111:U:H6	1.25	0.95
13:T:317:VAL:HG13	13:T:331:ILE:CD1	1.95	0.95
4:D:40:A:N3	15:N:121:ARG:NH2	2.15	0.95
13:T:295:SER:CB	13:T:313:GLU:CG	2.44	0.95
4:D:84:C:C2	17:P:4:SER:OG	2.19	0.95
6:F:1111:U:O4'	28:l:30:ARG:HD3	1.67	0.95
13:T:351:PHE:N	13:T:363:PHE:O	2.00	0.95
1:A:488:ARG:NH1	2:B:81:A:N6	2.15	0.94
6:F:1116:A:C2	6:F:1117:G:C4	2.54	0.94
13:T:135:VAL:HG11	13:T:193:TYR:CE1	2.02	0.94
13:T:148:CYS:HB2	13:T:396:ARG:CG	1.98	0.94
1:A:1954:ILE:O	22:V:271:ARG:HD3	1.67	0.94
6:F:110:A:C2	29:m:2:LYS:CE	2.51	0.94
4:D:25:C:HO2'	12:L:98:THR:HG1	1.13	0.94
4:D:66:C:OP2	17:P:12:ARG:NH2	2.01	0.94
13:T:111:GLU:HB2	13:T:199:LEU:O	1.64	0.93
6:F:1102:C:H2'	6:F:1103:C:C5	2.03	0.93
1:A:1875:ILE:HD11	13:T:326:VAL:CG1	1.96	0.93
23:W:300:ARG:HA	23:W:303:ILE:HD12	1.48	0.93
10:J:65:PHE:HE1	10:J:101:ARG:HB2	1.33	0.93
2:B:165:A:C2	29:f:2:LYS:CE	2.51	0.93
1:A:1851:PHE:O	1:A:1881:THR:HA	1.69	0.92
6:F:1101:C:N4	32:p:38:LYS:HZ3	1.67	0.92
6:F:1116:A:C6	6:F:1117:G:C6	2.57	0.92
8:H:729:TYR:CD1	8:H:748:PHE:CB	2.52	0.92
1:A:1988:LEU:CD1	21:U:180:VAL:CG1	2.39	0.92
4:D:40:A:H61	15:N:121:ARG:HG3	1.35	0.92
13:T:363:PHE:HE1	13:T:371:ARG:HB3	1.31	0.92
13:T:139:LEU:HD12	13:T:174:THR:HG1	1.21	0.92
1:A:659:HIS:HE1	34:A:3000:IHP:O22	1.41	0.92
13:T:138:ASP:O	13:T:141:GLU:HB2	1.70	0.92
13:T:351:PHE:HB2	13:T:363:PHE:HB2	1.47	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ARG:NH2	2:B:83:C:OP1	2.02	0.92
13:T:376:ILE:C	13:T:377:PHE:CD1	2.47	0.92
1:A:2003:THR:CG2	22:V:333:PRO:HB3	1.98	0.92
6:F:110:A:H4'	6:F:111:C:H5'	0.95	0.92
6:F:1099:G:C5	6:F:1100:A:C8	2.58	0.92
13:T:132:PRO:O	13:T:134:ASP:N	2.00	0.92
3:C:132:ARG:NH2	28:e:13:GLU:O	2.02	0.91
6:F:20:G:H1'	17:P:7:PRO:HD3	1.50	0.91
7:G:81:ASP:CB	7:G:85:THR:CB	2.49	0.91
4:D:40:A:H2	15:N:121:ARG:HE	0.94	0.91
13:T:55:GLU:OE2	13:T:58:ARG:NE	2.02	0.91
1:A:168:LEU:HB3	1:A:622:MET:HE1	1.52	0.91
13:T:139:LEU:HB3	13:T:174:THR:OG1	1.70	0.91
8:H:682:LYS:O	8:H:685:GLU:CG	2.18	0.91
14:M:215:PRO:CG	14:M:217:TRP:CE2	2.54	0.91
4:D:50:G:O2'	5:E:2:U:O4	1.89	0.90
13:T:139:LEU:CD1	13:T:174:THR:CB	2.46	0.90
13:T:292:HIS:NE2	13:T:312:SER:HB3	1.85	0.90
1:A:1986:MET:HG3	21:U:184:MET:HG3	0.94	0.90
4:D:40:A:N1	15:N:121:ARG:CD	2.35	0.90
10:J:179:SER:CB	13:T:337:HIS:HD2	1.82	0.90
1:A:1988:LEU:CD2	21:U:180:VAL:CG1	2.35	0.90
1:A:2059:ILE:O	1:A:2063:TYR:HB2	1.71	0.90
3:C:240:ASP:OD1	3:C:269:LYS:HD3	1.70	0.90
1:A:542:HIS:C	1:A:544:LYS:H	1.79	0.89
2:B:165:A:C2	29:f:2:LYS:HE2	2.07	0.89
4:D:40:A:N1	15:N:121:ARG:HG3	1.85	0.89
8:H:730:GLN:HA	8:H:733:ILE:CD1	2.02	0.89
6:F:1099:G:C6	6:F:1100:A:N7	2.41	0.89
6:F:20:G:N3	17:P:6:ARG:CB	2.25	0.89
15:N:23:PRO:O	15:N:37:TRP:NE1	2.05	0.89
6:F:110:A:C2	29:m:2:LYS:HE2	2.08	0.89
5:E:-3:A:H2'	5:E:-2:A:C5'	2.02	0.89
6:F:15:C:H41	11:K:209:ARG:HG2	1.38	0.88
13:T:129:LEU:CD1	13:T:130:TYR:N	2.35	0.88
13:T:317:VAL:HG13	13:T:331:ILE:HD13	1.53	0.88
1:A:1988:LEU:H	21:U:181:GLN:HG2	1.36	0.88
9:I:99:ILE:HG13	9:I:100:PRO:CD	2.03	0.88
13:T:111:GLU:HB3	13:T:199:LEU:O	1.73	0.88
16:O:327:CYS:SG	16:O:328:THR:N	2.36	0.88
13:T:151:PRO:CB	13:T:454:CYS:C	2.45	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:128:TYR:OH	13:T:235:THR:O	1.91	0.88
1:A:1985:GLN:NE2	21:U:185:LYS:HE2	1.89	0.88
1:A:1875:ILE:HD11	13:T:326:VAL:HG13	1.55	0.87
5:E:346:A:O2'	5:E:347:A:O4'	1.92	0.87
13:T:374:LYS:HA	13:T:374:LYS:NZ	1.90	0.87
1:A:1592:HIS:CE1	5:E:353:A:C8	2.61	0.87
1:A:1608:LEU:HD12	1:A:1644:SER:OG	1.75	0.87
4:D:40:A:N6	15:N:121:ARG:HG3	1.89	0.87
4:D:90:U:C6	9:I:104:ARG:NH2	2.42	0.87
1:A:1663:PHE:HE2	22:V:247:ARG:HD2	1.38	0.87
1:A:1775:ILE:HA	1:A:1785:ASP:O	1.75	0.87
4:D:35:A:N6	15:N:81:CYS:SG	2.47	0.87
13:T:339:MET:SD	13:T:353:ALA:CB	2.63	0.87
6:F:110:A:C2	29:m:2:LYS:HE3	2.10	0.86
13:T:139:LEU:HD21	13:T:193:TYR:OH	1.73	0.86
13:T:300:LYS:O	13:T:308:PHE:HB2	1.74	0.86
23:W:299:ILE:HG22	23:W:303:ILE:HD11	1.55	0.86
6:F:1099:G:N7	6:F:1100:A:C8	2.43	0.86
2:B:165:A:H4'	2:B:166:U:H5'	0.95	0.86
13:T:376:ILE:C	13:T:377:PHE:HD1	1.82	0.86
1:A:1666:CYS:O	1:A:1670:ASP:CB	2.22	0.86
2:B:165:A:C2	29:f:2:LYS:HE3	2.10	0.86
13:T:152:LYS:HD2	13:T:152:LYS:C	2.00	0.86
1:A:514:TYR:HD2	1:A:514:TYR:H	1.19	0.86
10:J:179:SER:CA	13:T:337:HIS:CD2	2.57	0.86
13:T:159:PRO:CG	13:T:160:GLY:H	1.84	0.86
8:H:730:GLN:O	8:H:733:ILE:HD12	1.76	0.85
13:T:135:VAL:HG21	13:T:193:TYR:CE1	2.11	0.85
13:T:340:PRO:CG	13:T:356:MET:CE	2.54	0.85
1:A:2002:TYR:OH	22:V:307:ARG:CG	2.25	0.85
13:T:151:PRO:HB2	13:T:454:CYS:C	2.00	0.85
16:O:259:VAL:HG12	16:O:260:ILE:HG13	1.58	0.85
1:A:1082:ILE:HG21	1:A:1113:ILE:HD11	1.59	0.85
1:A:1365:THR:O	1:A:1369:ASN:ND2	2.10	0.85
1:A:2003:THR:CG2	22:V:333:PRO:CB	2.54	0.85
4:D:91:A:C4	9:I:99:ILE:CD1	2.60	0.85
3:C:340:LYS:O	3:C:343:ASP:HB3	1.77	0.84
16:O:263:VAL:HG12	16:O:264:GLY:H	1.41	0.84
1:A:934:ARG:HD3	6:F:31:A:C2	2.12	0.84
6:F:1099:G:C5	6:F:1100:A:N7	2.44	0.84
1:A:510:PRO:O	1:A:514:TYR:CE2	2.30	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ASP:CB	1:A:514:TYR:HE2	1.82	0.84
1:A:934:ARG:HD3	6:F:31:A:H2	1.39	0.84
1:A:1488:ILE:HG23	1:A:1489:PRO:CD	2.06	0.84
1:A:1670:ASP:HA	1:A:1681:VAL:HG21	1.60	0.84
1:A:751:ASP:OD1	1:A:752:ALA:N	2.11	0.84
1:A:2002:TYR:OH	22:V:329:LEU:HD21	1.77	0.84
1:A:1597:GLY:HA3	5:E:348:U:O2'	1.76	0.84
13:T:148:CYS:SG	13:T:393:GLY:O	2.35	0.84
13:T:200:ARG:NH2	13:T:236:GLU:O	2.11	0.84
1:A:1955:ALA:HA	22:V:271:ARG:HB2	1.60	0.83
6:F:1102:C:H2'	6:F:1103:C:H6	1.42	0.83
6:F:1109:C:H41	32:p:109:LYS:H	1.21	0.83
15:N:118:ALA:O	15:N:129:SER:OG	1.96	0.83
15:N:165:SER:HA	15:N:170:ILE:HD11	1.60	0.83
25:i:86:ASN:HD21	26:j:32:LYS:HD3	1.43	0.83
13:T:292:HIS:CE1	13:T:312:SER:OG	2.31	0.83
15:N:253:LEU:O	15:N:257:ASN:HB3	1.78	0.83
25:b:86:ASN:HD21	26:c:32:LYS:HD3	1.43	0.83
1:A:1986:MET:CE	21:U:184:MET:HG2	2.08	0.83
8:H:724:VAL:O	8:H:727:GLU:CG	2.27	0.83
3:C:240:ASP:OD2	3:C:269:LYS:CD	2.26	0.83
13:T:315:LYS:H	13:T:315:LYS:HD2	1.43	0.83
33:q:51:VAL:HG13	33:r:20:ARG:CB	2.09	0.83
1:A:1592:HIS:HE1	5:E:353:A:C8	1.97	0.83
13:T:317:VAL:H	13:T:331:ILE:HD12	1.41	0.83
1:A:320:ASP:OD1	1:A:508:GLN:NE2	2.11	0.83
3:C:472:VAL:HB	3:C:575:ALA:O	1.79	0.83
4:D:29:U:H1'	12:L:120:CYS:HB3	1.60	0.83
1:A:620:HIS:HB3	1:A:669:TYR:CE2	2.14	0.82
13:T:59:ARG:O	13:T:62:THR:CG2	2.25	0.82
13:T:128:TYR:CD2	13:T:199:LEU:HD12	2.14	0.82
1:A:488:ARG:NH1	2:B:81:A:H61	1.76	0.82
13:T:340:PRO:HG3	13:T:356:MET:SD	2.19	0.82
3:C:734:CYS:SG	3:C:755:TYR:OH	2.37	0.82
1:A:1405:ILE:HG22	1:A:1406:LEU:H	1.44	0.82
1:A:1592:HIS:HE1	5:E:353:A:H8	1.25	0.82
13:T:140:ARG:HG2	13:T:140:ARG:HH11	1.45	0.82
1:A:1955:ALA:CB	22:V:271:ARG:O	2.28	0.82
1:A:1748:ILE:O	1:A:1751:TYR:N	2.12	0.82
1:A:1863:HIS:O	1:A:1871:ALA:HB3	1.80	0.82
10:J:179:SER:HA	13:T:337:HIS:CD2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1988:LEU:H	21:U:181:GLN:CG	1.93	0.82
4:D:40:A:C6	15:N:121:ARG:HG3	2.14	0.82
7:G:114:LEU:O	7:G:117:VAL:HG22	1.78	0.82
5:E:299:U:O2'	5:E:300:A:OP1	1.98	0.81
5:E:-1:G:C6	5:E:351:U:O4	2.33	0.81
1:A:1339:LEU:HD21	1:A:1440:ILE:CD1	2.10	0.81
6:F:1101:C:H41	32:p:38:LYS:HZ3	1.26	0.81
1:A:137:GLU:OE2	1:A:140:ARG:NH2	2.13	0.81
1:A:1656:LYS:HD3	1:A:1949:LEU:HD12	1.62	0.81
6:F:30:A:C3'	6:F:31:A:H5''	2.10	0.81
13:T:68:PRO:HD2	13:T:69:TRP:CE3	2.15	0.81
24:h:19:LYS:NZ	31:o:34:LEU:CB	2.44	0.81
5:E:286:A:C2	13:T:414:THR:O	2.33	0.81
20:S:317:ILE:HD13	20:S:325:VAL:HG21	1.63	0.81
1:A:1335:TRP:HD1	1:A:1367:ILE:HD12	1.45	0.81
1:A:1711:VAL:HG13	1:A:1789:ASN:HB3	1.63	0.81
5:E:-3:A:C2'	5:E:-2:A:H5''	2.10	0.81
14:M:73:CYS:SG	14:M:74:CYS:N	2.53	0.81
15:N:253:LEU:O	15:N:257:ASN:CB	2.27	0.81
9:I:122:MET:HE2	9:I:122:MET:HA	1.63	0.81
1:A:370:ILE:HD13	3:C:954:LEU:HD21	1.61	0.80
1:A:1875:ILE:CD1	13:T:326:VAL:HG13	2.09	0.80
16:O:362:ASP:OD2	16:O:379:LYS:NZ	2.13	0.80
1:A:366:GLU:HG3	1:A:372:ARG:HH11	1.45	0.80
8:H:724:VAL:HA	8:H:727:GLU:CG	2.11	0.80
17:P:9:LEU:HD12	17:P:10:GLU:HB2	1.63	0.80
6:F:30:A:H4'	6:F:31:A:OP2	1.81	0.80
13:T:132:PRO:CB	13:T:176:HIS:ND1	2.42	0.80
13:T:363:PHE:CE1	13:T:371:ARG:HB3	2.14	0.80
26:j:74:ARG:NH2	30:n:64:HIS:O	2.14	0.80
1:A:1081:TYR:O	1:A:1085:LYS:HB2	1.82	0.80
1:A:1875:ILE:CD1	13:T:326:VAL:CG2	2.60	0.80
1:A:1875:ILE:HG23	13:T:326:VAL:CG2	2.11	0.80
19:R:2:SER:O	19:R:4:ASN:ND2	2.13	0.80
1:A:1335:TRP:CD1	1:A:1367:ILE:HD12	2.17	0.80
15:N:76:PHE:HB2	15:N:91:HIS:HD2	1.45	0.80
16:O:340:SER:OG	16:O:341:LEU:N	2.10	0.80
24:h:102:LEU:C	31:o:13:GLN:HB3	2.07	0.80
4:D:35:A:C8	15:N:75:PHE:CE2	2.70	0.80
4:D:85:C:OP1	4:D:85:C:O4'	2.00	0.80
1:A:1211:SER:O	1:A:1257:ASN:ND2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:G:C8	6:F:34:G:OP2	2.35	0.80
1:A:1456:ARG:NH2	1:A:1460:GLU:OE2	2.15	0.80
5:E:346:A:O2'	5:E:347:A:N9	2.10	0.79
6:F:1099:G:H5''	6:F:1099:G:N3	1.97	0.79
26:c:74:ARG:NH2	30:g:64:HIS:O	2.14	0.79
2:B:174:G:H5'	30:g:99:ASP:OD2	1.82	0.79
6:F:119:G:H5'	30:n:99:ASP:OD2	1.82	0.79
1:A:1281:ASN:HD22	1:A:1285:VAL:HG21	1.47	0.79
5:E:-3:A:H2'	5:E:-2:A:H5''	1.62	0.79
15:N:110:ASP:OD1	15:N:114:ARG:N	2.14	0.79
3:C:240:ASP:OD2	3:C:269:LYS:HD2	1.82	0.79
6:F:1109:C:N4	32:p:109:LYS:N	2.30	0.79
14:M:208:TYR:HB2	14:M:290:ILE:HD12	1.64	0.79
1:A:2034:ILE:HG12	1:A:2041:PRO:HA	1.65	0.79
1:A:1122:ASP:OD1	1:A:1161:TYR:OH	1.99	0.79
14:M:13:CYS:SG	14:M:16:CYS:HB3	2.23	0.79
1:A:1928:GLU:OE2	21:U:238:THR:CG2	2.31	0.78
3:C:779:LEU:O	3:C:782:GLU:N	2.16	0.78
20:S:440:LEU:HD12	20:S:473:LEU:HD13	1.64	0.78
1:A:376:ARG:NH2	3:C:962:LEU:HD21	1.99	0.78
14:M:104:ALA:HB1	14:M:110:LYS:HB3	1.65	0.78
1:A:1875:ILE:CD1	13:T:326:VAL:HG21	2.12	0.78
1:A:2002:TYR:CE2	22:V:329:LEU:HD11	2.17	0.78
1:A:1673:LEU:HA	1:A:1678:ILE:HB	1.66	0.78
13:T:408:PHE:HB2	13:T:410:TRP:CH2	2.18	0.78
1:A:416:GLU:HG2	1:A:418:ASP:H	1.47	0.78
6:F:1100:A:H61	6:F:1116:A:H61	1.30	0.78
1:A:1348:GLU:HG2	1:A:1446:THR:HB	1.65	0.78
1:A:1986:MET:CB	21:U:184:MET:HG3	2.05	0.78
5:E:-1:G:C6	5:E:351:U:C4	2.72	0.78
12:L:128:GLN:O	12:L:131:GLU:N	2.16	0.77
13:T:356:MET:HE2	13:T:356:MET:HA	1.66	0.77
4:D:39:G:O6	15:N:127:ILE:O	2.03	0.77
1:A:1335:TRP:CH2	1:A:1339:LEU:HD13	2.19	0.77
1:A:1500:HIS:HB2	23:W:293:SER:HB2	1.65	0.77
5:E:1:G:C2'	5:E:2:U:H5''	2.13	0.77
1:A:259:GLU:HG3	1:A:260:PRO:HD2	1.64	0.77
9:I:229:VAL:O	9:I:233:GLN:HB2	1.83	0.77
13:T:404:LYS:O	13:T:405:SER:CB	2.33	0.77
1:A:1889:LEU:O	1:A:1988:LEU:HA	1.83	0.77
21:U:183:TYR:CE2	21:U:234:LYS:CD	2.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:468:LEU:O	3:C:578:TYR:HA	1.85	0.77
6:F:1100:A:N1	6:F:1116:A:N1	2.33	0.77
1:A:1195:PHE:HB3	1:A:1217:ARG:HE	1.49	0.77
5:E:346:A:C2'	5:E:347:A:OP2	2.33	0.77
13:T:140:ARG:HG2	13:T:140:ARG:NH1	1.99	0.77
13:T:151:PRO:HB3	13:T:454:CYS:O	1.83	0.77
1:A:1988:LEU:CG	21:U:180:VAL:HG12	2.14	0.77
3:C:240:ASP:CG	3:C:269:LYS:HD3	2.08	0.77
6:F:1111:U:C6	6:F:1111:U:C5'	2.65	0.77
9:I:189:TYR:HB3	9:I:205:TRP:CD1	2.20	0.77
3:C:667:GLU:OE1	3:C:667:GLU:N	2.18	0.77
3:C:706:LEU:HD21	3:C:834:MET:HE1	1.67	0.77
1:A:1585:MET:O	1:A:1590:LEU:HD11	1.83	0.76
5:E:285:U:C6	5:E:285:U:OP2	2.38	0.76
20:S:421:LYS:HG3	20:S:468:ILE:HG12	1.66	0.76
1:A:1042:SER:OG	1:A:1043:ARG:NH1	2.17	0.76
3:C:770:ASN:OD1	3:C:771:GLY:N	2.18	0.76
13:T:135:VAL:HG21	13:T:193:TYR:CD1	2.20	0.76
1:A:1887:GLY:HA2	1:A:1991:ILE:HD12	1.68	0.76
5:E:1:G:C2	5:E:349:A:C2	2.72	0.76
13:T:392:SER:OG	13:T:397:TYR:N	2.18	0.76
14:M:209:ASN:HD22	14:M:288:ILE:HA	1.50	0.76
5:E:286:A:N1	13:T:414:THR:HB	2.01	0.76
6:F:1109:C:H41	32:p:109:LYS:N	1.84	0.76
9:I:103:ILE:HA	9:I:106:ILE:HD12	1.68	0.76
13:T:146:PHE:O	13:T:394:ASP:OD2	2.02	0.76
4:D:35:A:O2'	15:N:75:PHE:CZ	2.36	0.76
13:T:68:PRO:HD2	13:T:69:TRP:HE3	1.50	0.76
13:T:144:ILE:CB	13:T:394:ASP:OD1	2.34	0.76
1:A:404:ASN:ND2	3:C:927:MET:SD	2.59	0.75
8:H:729:TYR:CD2	8:H:748:PHE:CB	2.69	0.75
13:T:217:ASP:O	13:T:218:CYS:CB	2.33	0.75
13:T:308:PHE:CE1	13:T:320:TRP:HB2	2.13	0.75
1:A:796:ASN:ND2	1:A:861:GLN:OE1	2.19	0.75
14:M:9:PRO:HB2	14:M:10:PRO:HD2	1.67	0.75
16:O:230:VAL:HG22	16:O:241:THR:HG22	1.68	0.75
1:A:1957:ARG:NH2	22:V:272:LEU:CB	2.46	0.75
1:A:514:TYR:CD2	1:A:514:TYR:N	2.47	0.75
1:A:381:SER:O	1:A:384:LYS:N	2.19	0.75
1:A:971:MET:HE2	17:P:174:VAL:HG13	1.68	0.75
13:T:339:MET:SD	13:T:353:ALA:HB1	2.26	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1494:LEU:HD23	23:W:298:GLU:HG2	1.68	0.75
13:T:295:SER:N	13:T:313:GLU:CB	2.49	0.74
16:O:217:ILE:HG22	16:O:218:ARG:HG3	1.69	0.74
1:A:801:VAL:HG11	1:A:804:MET:HE3	1.69	0.74
1:A:1538:ASN:OD1	1:A:1539:LEU:N	2.20	0.74
3:C:712:ALA:HA	3:C:817:GLN:O	1.88	0.74
5:E:345:A:H3'	5:E:345:A:N3	2.03	0.74
16:O:309:ARG:HD2	16:O:328:THR:HG21	1.66	0.74
1:A:2018:ASN:ND2	1:A:2062:GLU:OE1	2.20	0.74
13:T:308:PHE:HE1	13:T:320:TRP:CB	1.98	0.74
15:N:108:VAL:HG23	15:N:109:LEU:HG	1.68	0.74
16:O:203:ASP:O	16:O:204:LYS:HB2	1.84	0.74
1:A:2059:ILE:O	1:A:2063:TYR:CB	2.36	0.74
5:E:-3:A:H2'	5:E:-2:A:H5'	1.70	0.74
13:T:350:TYR:HA	13:T:363:PHE:O	1.88	0.74
16:O:125:TRP:HE1	16:O:437:GLU:CD	1.95	0.74
1:A:1988:LEU:HD13	21:U:180:VAL:HG12	0.79	0.74
1:A:744:THR:O	1:A:749:ARG:NH2	2.20	0.74
1:A:934:ARG:HH22	6:F:30:A:H5'	1.53	0.74
1:A:1572:GLY:O	1:A:1827:GLN:HG3	1.88	0.74
1:A:709:ARG:HH22	2:B:83:C:P	2.10	0.74
1:A:1051:GLU:OE1	1:A:1204:ARG:NH2	2.21	0.74
1:A:1447:TRP:HB3	1:A:1451:PHE:HE2	1.53	0.74
13:T:388:SER:HB2	13:T:430:THR:HA	1.70	0.74
1:A:992:ASP:OD1	1:A:1085:LYS:NZ	2.21	0.74
3:C:711:ALA:HB3	3:C:819:LYS:O	1.88	0.74
18:Q:174:ASN:OD1	18:Q:185:ARG:NH1	2.21	0.74
1:A:1815:LEU:O	1:A:1818:ARG:N	2.21	0.73
4:D:35:A:C8	15:N:75:PHE:CD2	2.76	0.73
1:A:1046:SER:HA	1:A:1251:TYR:O	1.87	0.73
13:T:128:TYR:OH	13:T:236:GLU:HA	1.88	0.73
1:A:861:GLN:HE21	1:A:1097:HIS:HB3	1.54	0.73
3:C:748:SER:HB2	3:C:762:SER:HB3	1.70	0.73
8:H:669:TYR:HE2	8:H:686:ILE:HG13	1.53	0.73
13:T:340:PRO:HD2	13:T:354:GLN:O	1.88	0.73
1:A:1845:ASN:ND2	22:V:299:LEU:HA	2.02	0.73
1:A:2006:SER:HB2	22:V:330:VAL:O	1.88	0.73
1:A:1585:MET:HG3	1:A:1590:LEU:HD21	1.70	0.73
3:C:885:GLY:HA2	3:C:907:PRO:HD3	1.68	0.73
15:N:234:ALA:HA	15:N:237:ARG:HD3	1.70	0.73
4:D:66:C:H4'	18:Q:133:LYS:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:i:86:ASN:HD21	26:j:32:LYS:CD	2.02	0.73
1:A:2003:THR:HB	22:V:333:PRO:CG	2.15	0.73
5:E:353:A:H2'	5:E:353:A:N3	2.04	0.73
6:F:34:G:OP2	6:F:34:G:O4'	2.05	0.73
5:E:1:G:N2	5:E:349:A:O2'	2.21	0.73
13:T:317:VAL:CA	13:T:331:ILE:HD11	2.16	0.73
24:h:47:GLU:HG3	31:o:15:TYR:CB	2.18	0.73
13:T:155:ILE:HD12	13:T:155:ILE:N	2.04	0.73
16:O:152:ASN:HD21	16:O:409:LYS:HB3	1.53	0.73
1:A:1882:LEU:HB2	1:A:1991:ILE:HD11	1.71	0.72
5:E:1:G:N1	5:E:349:A:C2	2.56	0.72
1:A:1130:ARG:NH1	1:A:1133:ASP:OD2	2.22	0.72
10:J:65:PHE:CE1	10:J:101:ARG:HB2	2.21	0.72
13:T:338:SER:HB3	13:T:356:MET:HG2	1.70	0.72
1:A:1180:GLU:HA	1:A:1183:THR:HG22	1.70	0.72
12:L:44:LYS:O	12:L:47:GLU:N	2.22	0.72
13:T:191:ASP:CB	13:T:195:ASP:HB2	2.19	0.72
1:A:1056:GLU:OE1	1:A:1060:LYS:NZ	2.21	0.72
1:A:1305:SER:OG	1:A:1307:GLU:OE1	2.07	0.72
13:T:295:SER:CA	13:T:313:GLU:HB2	2.19	0.72
15:N:87:CYS:HB3	15:N:91:HIS:CE1	2.25	0.72
1:A:1736:VAL:HG22	1:A:1775:ILE:HB	1.72	0.72
16:O:358:ILE:HG22	16:O:359:ASN:H	1.54	0.72
25:b:86:ASN:HD21	26:c:32:LYS:CD	2.02	0.72
4:D:29:U:O4'	12:L:120:CYS:HA	1.89	0.72
13:T:315:LYS:H	13:T:315:LYS:CD	2.03	0.72
1:A:585:ARG:NH2	1:A:733:GLN:O	2.22	0.71
1:A:1945:GLU:O	1:A:1948:MET:N	2.23	0.71
4:D:89:U:H5	11:K:176:TYR:O	1.72	0.71
13:T:228:ARG:HG2	13:T:228:ARG:HH11	1.55	0.71
1:A:1926:LYS:NZ	22:V:250:GLU:HB2	2.04	0.71
6:F:1101:C:N4	32:p:38:LYS:NZ	2.36	0.71
10:J:78:ARG:NH2	10:J:79:GLU:OE2	2.24	0.71
15:N:76:PHE:HB2	15:N:91:HIS:CD2	2.25	0.71
16:O:357:SER:HG	16:O:405:SER:HG	1.38	0.71
1:A:928:ARG:HH22	1:A:1595:ARG:NH2	1.88	0.71
3:C:84:GLN:HE22	3:C:90:LEU:HA	1.54	0.71
14:M:77:ASP:OD1	14:M:78:SER:N	2.24	0.71
3:C:135:ASN:N	3:C:233:ASP:OD2	2.24	0.71
5:E:-1:G:C2	5:E:351:U:N3	2.58	0.71
1:A:1988:LEU:HD22	21:U:180:VAL:HG11	0.77	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:161:ARG:O	15:N:165:SER:CB	2.38	0.71
16:O:414:LEU:HB3	16:O:426:TRP:HB2	1.73	0.71
3:C:163:ASP:OD2	3:C:548:ARG:NH1	2.24	0.71
3:C:969:LYS:O	3:C:972:ARG:N	2.23	0.71
5:E:346:A:O2'	5:E:347:A:C1'	2.39	0.71
16:O:156:ILE:HG12	16:O:166:VAL:HG22	1.73	0.71
1:A:1810:PRO:O	1:A:1813:TYR:N	2.23	0.71
13:T:130:TYR:CG	13:T:130:TYR:O	2.41	0.71
21:U:183:TYR:HE2	21:U:234:LYS:HD2	1.55	0.71
2:B:174:G:H4'	2:B:174:G:OP1	1.90	0.71
4:D:65:U:OP2	17:P:16:LYS:HE3	1.91	0.71
13:T:293:LEU:O	13:T:293:LEU:HD23	1.91	0.71
13:T:295:SER:H	13:T:313:GLU:HB2	1.54	0.71
13:T:408:PHE:CB	13:T:410:TRP:CH2	2.74	0.71
15:N:245:GLU:HG3	15:N:249:MET:HE2	1.73	0.71
1:A:168:LEU:HB3	1:A:622:MET:CE	2.19	0.71
1:A:1315:ARG:O	1:A:1318:GLY:N	2.23	0.71
3:C:308:ASP:HB3	3:C:310:ASN:HD22	1.54	0.71
3:C:378:LEU:O	3:C:381:LEU:N	2.23	0.71
3:C:833:VAL:O	3:C:837:GLN:HB2	1.89	0.71
6:F:41:C:O2'	6:F:42:U:O5'	2.07	0.71
6:F:1116:A:C6	6:F:1117:G:C5	2.79	0.71
16:O:201:SER:OG	16:O:202:GLU:N	2.23	0.71
16:O:187:ASP:OD1	16:O:188:VAL:N	2.24	0.70
20:S:475:GLU:OE2	20:S:478:ARG:NH1	2.24	0.70
23:W:295:GLU:HA	23:W:295:GLU:OE2	1.90	0.70
1:A:929:LEU:O	1:A:934:ARG:NH1	2.24	0.70
3:C:265:PHE:CD2	3:C:295:ILE:HD12	2.25	0.70
3:C:856:ILE:HA	3:C:944:VAL:HG11	1.72	0.70
13:T:191:ASP:CG	13:T:195:ASP:HB2	2.16	0.70
1:A:997:GLN:OE1	1:A:1511:ARG:NH2	2.24	0.70
1:A:1663:PHE:CE2	22:V:247:ARG:HD2	2.25	0.70
3:C:307:ILE:HA	3:C:324:ILE:HD11	1.73	0.70
5:E:352:A:O2'	5:E:353:A:OP1	2.09	0.70
1:A:688:TYR:O	1:A:691:PHE:N	2.22	0.70
1:A:928:ARG:NH2	1:A:1595:ARG:HH22	1.88	0.70
2:B:173:U:H4'	2:B:174:G:OP1	1.91	0.70
3:C:67:GLU:CD	3:C:68:HIS:H	1.98	0.70
13:T:159:PRO:CG	13:T:160:GLY:N	2.47	0.70
13:T:126:ARG:HB3	13:T:126:ARG:CZ	2.20	0.70
5:E:-1:G:N1	5:E:351:U:C4	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2043:PHE:HB3	1:A:2047:GLN:HB2	1.73	0.70
6:F:119:G:OP1	6:F:119:G:H4'	1.90	0.70
13:T:293:LEU:HD21	13:T:314:ASP:CG	2.16	0.70
1:A:299:LYS:HA	1:A:493:MET:HG2	1.73	0.70
1:A:1924:LEU:HD22	21:U:234:LYS:HZ2	1.57	0.70
1:A:1924:LEU:CD2	21:U:234:LYS:NZ	2.55	0.70
1:A:1986:MET:HB3	21:U:184:MET:HB3	1.49	0.70
8:H:718:SER:OG	8:H:725:THR:CG2	2.38	0.70
1:A:1859:ARG:O	1:A:1874:ALA:HA	1.92	0.70
6:F:20:G:C2	17:P:6:ARG:CD	2.74	0.70
9:I:198:GLN:O	9:I:201:THR:OG1	2.09	0.70
10:J:68:GLU:O	10:J:72:GLN:HB2	1.92	0.70
1:A:1594:GLN:HG2	5:E:348:U:O2	1.91	0.69
6:F:20:G:C2	17:P:6:ARG:CG	2.75	0.69
15:N:161:ARG:HG2	15:N:173:ILE:HD12	1.72	0.69
25:i:86:ASN:HD21	26:j:32:LYS:CE	2.05	0.69
1:A:701:CYS:SG	1:A:702:GLY:N	2.66	0.69
1:A:1464:LYS:NZ	1:A:1479:GLU:O	2.23	0.69
8:H:616:PRO:CG	8:H:617:PRO:N	2.53	0.69
28:l:30:ARG:O	28:l:47:VAL:HG23	1.92	0.69
1:A:1379:MET:HE1	1:A:1620:TYR:H	1.57	0.69
1:A:1485:ASP:O	1:A:1490:ARG:NH2	2.25	0.69
15:N:206:LEU:HD12	15:N:207:PRO:HD2	1.75	0.69
16:O:391:GLU:HB3	16:O:400:ARG:HB2	1.74	0.69
1:A:1594:GLN:HG3	5:E:349:A:C8	2.28	0.69
5:E:3:A:C8	5:E:4:U:C5	2.80	0.69
6:F:1102:C:H6	6:F:1102:C:O5'	1.76	0.69
13:T:341:PHE:CB	13:T:387:ILE:O	2.40	0.69
14:M:217:TRP:O	14:M:221:ASP:CB	2.37	0.69
3:C:101:GLN:HA	3:C:104:THR:O	1.93	0.69
1:A:1151:GLU:O	1:A:1155:ALA:N	2.24	0.69
1:A:1454:SER:HA	1:A:1487:GLY:HA2	1.74	0.69
1:A:1493:THR:OG1	23:W:301:GLN:OE1	2.11	0.69
1:A:1889:LEU:HB2	1:A:1989:PHE:HB2	1.74	0.69
1:A:1902:GLN:OE1	1:A:1902:GLN:N	2.25	0.69
1:A:1986:MET:HE2	21:U:184:MET:HG2	1.73	0.69
3:C:123:MET:HB2	3:C:199:LEU:HD23	1.75	0.69
4:D:28:U:OP1	12:L:118:SER:OG	2.11	0.69
5:E:10:U:C6	5:E:10:U:OP2	2.46	0.69
13:T:345:HIS:CG	13:T:350:TYR:H	2.10	0.69
20:S:454:ASP:HB3	20:S:457:HIS:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ALA:HB2	18:Q:122:LEU:HD21	1.74	0.69
14:M:33:GLU:OE1	14:M:33:GLU:N	2.25	0.69
16:O:407:PHE:CE1	16:O:414:LEU:HD13	2.27	0.69
25:b:86:ASN:HD21	26:c:32:LYS:CE	2.05	0.69
1:A:333:LYS:O	1:A:336:PHE:N	2.25	0.69
1:A:623:ARG:NH2	1:A:624:GLU:OE2	2.26	0.69
1:A:1082:ILE:O	1:A:1085:LYS:N	2.24	0.69
1:A:1924:LEU:HD21	21:U:234:LYS:HZ1	1.57	0.69
6:F:1116:A:C2	6:F:1117:G:C5	2.80	0.69
13:T:292:HIS:CD2	13:T:318:ARG:HG3	2.28	0.69
20:S:319:ASN:HA	20:S:322:LYS:HD3	1.75	0.69
1:A:900:PHE:N	1:A:1075:ASP:OD2	2.25	0.68
1:A:1750:ARG:O	1:A:1754:ALA:HB2	1.93	0.68
5:E:294:G:O2'	5:E:295:A:P	2.51	0.68
6:F:110:A:H2	29:m:2:LYS:HE2	1.58	0.68
1:A:542:HIS:C	1:A:544:LYS:N	2.47	0.68
3:C:183:GLN:NE2	3:C:654:CYS:HA	2.09	0.68
3:C:646:GLY:HA3	3:C:652:MET:HE3	1.76	0.68
4:D:64:U:O2'	4:D:65:U:OP1	2.11	0.68
6:F:1116:A:C4	6:F:1117:G:C8	2.80	0.68
8:H:602:MET:HA	8:H:605:PHE:HD2	1.57	0.68
1:A:1626:GLN:HE21	1:A:1631:GLY:HA2	1.56	0.68
10:J:239:LYS:O	10:J:243:GLN:HB2	1.92	0.68
1:A:1526:TRP:CD1	1:A:1526:TRP:H	2.11	0.68
3:C:274:ILE:HG12	3:C:275:LEU:HD12	1.74	0.68
5:E:1:G:H21	5:E:349:A:H2'	1.59	0.68
6:F:119:G:N7	29:m:20:LYS:HE2	2.08	0.68
9:I:199:MET:HB2	9:I:242:GLU:HG3	1.75	0.68
2:B:174:G:N7	29:f:20:LYS:HE2	2.08	0.68
1:A:681:LYS:O	1:A:684:LYS:HB3	1.93	0.68
1:A:1025:VAL:HG21	1:A:1265:PHE:HD2	1.56	0.68
3:C:252:LEU:O	3:C:255:GLN:N	2.26	0.68
1:A:1748:ILE:HG22	1:A:1752:VAL:HG23	1.75	0.68
1:A:1852:VAL:HB	1:A:1935:VAL:HG22	1.76	0.68
3:C:271:ASP:OD2	35:C:1500:GTP:N1	2.26	0.68
3:C:326:GLU:HG2	3:C:330:TYR:CE2	2.28	0.68
8:H:709:TRP:HA	8:H:712:CYS:SG	2.34	0.68
15:N:161:ARG:O	15:N:165:SER:HB3	1.93	0.68
33:q:20:ARG:CB	33:r:53:ILE:HA	2.24	0.68
5:E:1:G:H21	5:E:349:A:C2'	2.07	0.68
5:E:346:A:H2'	5:E:347:A:OP2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:44:ARG:HD2	10:J:214:ASN:HD21	1.58	0.68
13:T:345:HIS:CG	13:T:349:ASN:H	2.12	0.68
26:c:74:ARG:NH1	30:g:65:CYS:SG	2.66	0.68
3:C:315:SER:O	3:C:319:GLY:N	2.27	0.68
6:F:118:U:H4'	6:F:119:G:OP1	1.91	0.68
9:I:209:GLU:O	9:I:213:GLY:N	2.23	0.68
3:C:365:GLU:HG3	3:C:366:ASN:H	1.59	0.67
3:C:407:ASN:OD1	3:C:408:LEU:N	2.26	0.67
5:E:1:G:N2	5:E:349:A:N3	2.42	0.67
13:T:374:LYS:HE2	13:T:374:LYS:N	2.09	0.67
1:A:1282:ASP:OD1	1:A:1283:GLU:N	2.28	0.67
1:A:1927:GLU:HG2	21:U:135:LEU:CD1	2.08	0.67
1:A:1990:ASN:ND2	1:A:1993:ASP:O	2.27	0.67
6:F:18:U:C6	11:K:202:GLN:CG	2.76	0.67
20:S:384:LEU:O	20:S:387:PHE:N	2.27	0.67
1:A:697:LYS:HE3	34:A:3000:IHP:O46	1.94	0.67
2:B:175:G:C2	25:b:33:GLU:HG3	2.29	0.67
26:j:74:ARG:NH1	30:n:65:CYS:SG	2.66	0.67
1:A:511:ASP:CG	1:A:514:TYR:HH	1.96	0.67
13:T:295:SER:H	13:T:313:GLU:CB	2.04	0.67
20:S:479:SER:O	20:S:482:THR:OG1	2.13	0.67
1:A:1717:LEU:HB2	1:A:1786:ALA:HB3	1.75	0.67
2:B:174:G:C5'	30:g:99:ASP:HB2	2.24	0.67
3:C:360:ARG:HG2	3:C:362:LYS:HB2	1.76	0.67
9:I:248:ASN:O	9:I:252:HIS:HB2	1.95	0.67
13:T:139:LEU:CB	13:T:174:THR:OG1	2.41	0.67
15:N:182:GLY:O	15:N:183:PHE:HD1	1.77	0.67
1:A:312:TYR:O	1:A:319:ARG:NH2	2.27	0.67
5:E:299:U:O2'	5:E:300:A:H5'	1.93	0.67
6:F:120:G:C2	25:i:33:GLU:HG3	2.29	0.67
3:C:214:ASP:OD1	3:C:215:ALA:N	2.27	0.67
3:C:760:LEU:O	3:C:764:ASN:ND2	2.28	0.67
4:D:92:C:O2'	4:D:93:A:O5'	2.11	0.67
8:H:601:VAL:O	8:H:604:SER:OG	2.09	0.67
10:J:69:GLU:HG3	10:J:93:ARG:HH21	1.58	0.67
10:J:243:GLN:O	10:J:247:LYS:HG2	1.95	0.67
13:T:154:VAL:HA	13:T:453:VAL:O	1.95	0.67
1:A:984:VAL:HG12	1:A:985:ASP:H	1.60	0.67
1:A:1063:PHE:HE1	1:A:1086:ASN:HD22	1.40	0.67
1:A:2022:ALA:HB1	1:A:2055:MET:HE1	1.76	0.67
3:C:129:ILE:HG22	3:C:131:GLU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:A:N3	9:I:99:ILE:HD13	2.10	0.67
6:F:1116:A:C4	6:F:1117:G:N7	2.63	0.67
13:T:111:GLU:C	13:T:112:VAL:HG23	2.18	0.67
16:O:343:THR:OG1	16:O:344:ASN:N	2.28	0.67
1:A:340:LYS:O	1:A:343:ASN:N	2.26	0.67
1:A:1608:LEU:HD12	1:A:1644:SER:CB	2.24	0.67
3:C:656:LEU:HD13	3:C:670:ILE:HD13	1.75	0.67
6:F:119:G:C5'	30:n:99:ASP:HB2	2.25	0.67
13:T:317:VAL:N	13:T:331:ILE:HD12	2.10	0.67
13:T:340:PRO:CG	13:T:356:MET:SD	2.81	0.67
33:q:20:ARG:CB	33:r:52:GLU:O	2.43	0.67
33:s:51:VAL:HG11	33:t:20:ARG:CB	2.25	0.67
1:A:1286:TRP:NE1	1:A:1348:GLU:OE1	2.27	0.67
3:C:183:GLN:HE22	3:C:654:CYS:HA	1.60	0.67
3:C:245:VAL:HG11	3:C:295:ILE:HG22	1.76	0.67
5:E:-3:A:C2'	5:E:-2:A:C5'	2.71	0.67
5:E:1:G:H5''	5:E:301:A:N3	2.10	0.67
20:S:471:GLY:O	20:S:478:ARG:NH2	2.28	0.67
1:A:1591:THR:H	1:A:1594:GLN:HE21	1.43	0.66
1:A:1875:ILE:HD12	13:T:326:VAL:HG11	1.69	0.66
3:C:362:LYS:O	3:C:364:PHE:N	2.27	0.66
6:F:18:U:C6	11:K:202:GLN:HG2	2.29	0.66
21:U:169:HIS:CE1	21:U:195:ILE:H	2.13	0.66
1:A:1494:LEU:CD2	23:W:298:GLU:CG	2.66	0.66
1:A:1899:TRP:HH2	1:A:1909:ALA:HA	1.59	0.66
13:T:128:TYR:HD1	13:T:129:LEU:H	1.43	0.66
1:A:1972:ASP:O	1:A:1975:SER:N	2.27	0.66
1:A:2013:ARG:HB3	1:A:2059:ILE:HD11	1.78	0.66
10:J:218:VAL:O	14:M:109:MET:SD	2.53	0.66
14:M:89:HIS:O	14:M:92:SER:OG	2.07	0.66
1:A:342:LEU:HD13	1:A:392:ASN:HD22	1.61	0.66
1:A:269:ASP:CG	1:A:271:GLN:H	2.04	0.66
1:A:847:LYS:O	1:A:850:GLY:N	2.28	0.66
1:A:1592:HIS:CE1	5:E:353:A:H8	2.03	0.66
1:A:1814:VAL:HG21	1:A:1949:LEU:HD21	1.76	0.66
2:B:79:C:H3'	2:B:79:C:O2	1.94	0.66
1:A:933:GLU:OE1	1:A:933:GLU:N	2.19	0.66
1:A:1142:ASN:OD1	1:A:1148:LYS:NZ	2.28	0.66
4:D:64:U:O2'	4:D:65:U:P	2.53	0.66
5:E:345:A:O2'	5:E:346:A:O5'	2.13	0.66
13:T:293:LEU:O	13:T:294:SER:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:87:CYS:HB3	15:N:91:HIS:HE1	1.61	0.66
15:N:124:MET:HE3	15:N:227:ASN:ND2	2.10	0.66
1:A:1034:ASN:ND2	1:A:1289:VAL:O	2.29	0.66
2:B:165:A:H2	29:f:2:LYS:HE2	1.58	0.66
11:K:184:GLN:HA	11:K:187:LYS:HZ3	1.61	0.66
13:T:293:LEU:H	13:T:293:LEU:CD2	2.09	0.66
15:N:209:ASP:H	15:N:212:TRP:HB2	1.61	0.66
16:O:354:ASN:ND2	16:O:369:ASP:OD1	2.29	0.66
18:Q:118:GLN:OE1	18:Q:118:GLN:N	2.29	0.66
1:A:1573:LEU:HD23	1:A:1825:ILE:HD13	1.77	0.66
1:A:1656:LYS:CD	1:A:1949:LEU:HD12	2.25	0.66
1:A:2077:THR:HA	1:A:2080:LYS:HG2	1.77	0.66
14:M:82:ILE:CD1	15:N:253:LEU:HD11	2.25	0.66
5:E:3:A:N7	5:E:4:U:C5	2.64	0.66
13:T:55:GLU:OE2	13:T:55:GLU:HA	1.96	0.66
14:M:24:ARG:NH1	18:Q:115:VAL:HG21	2.11	0.66
15:N:254:ILE:O	15:N:258:THR:CB	2.44	0.66
1:A:1955:ALA:HA	22:V:271:ARG:CB	2.26	0.65
4:D:56:A:O2'	4:D:57:U:OP1	2.14	0.65
13:T:54:SER:O	13:T:58:ARG:HG2	1.96	0.65
14:M:202:THR:OG1	14:M:252:ARG:NE	2.24	0.65
25:i:77:LEU:HD21	25:i:80:ILE:HD12	1.78	0.65
1:A:801:VAL:HG13	1:A:802:PRO:HD2	1.79	0.65
3:C:787:LEU:HD12	3:C:790:LYS:HD2	1.77	0.65
4:D:35:A:N7	15:N:75:PHE:CD2	2.64	0.65
29:m:82:LEU:HD12	29:m:85:ILE:HD11	1.77	0.65
3:C:706:LEU:HD23	3:C:825:VAL:HA	1.79	0.65
13:T:331:ILE:HD12	13:T:331:ILE:O	1.96	0.65
16:O:365:PHE:HZ	16:O:373:LEU:HD22	1.61	0.65
8:H:729:TYR:CG	8:H:748:PHE:CB	2.79	0.65
13:T:354:GLN:HG3	13:T:389:LEU:CG	2.27	0.65
15:N:173:ILE:HG12	15:N:184:VAL:HG13	1.77	0.65
23:W:290:ALA:N	23:W:1062:LYS:HD3	2.11	0.65
1:A:676:GLN:N	1:A:676:GLN:OE1	2.29	0.65
1:A:1928:GLU:OE2	21:U:238:THR:HG21	1.95	0.65
3:C:70:TYR:HB3	3:C:74:VAL:HG21	1.78	0.65
1:A:740:GLU:HG3	1:A:741:ILE:H	1.61	0.65
1:A:1926:LYS:HZ1	22:V:250:GLU:HB2	1.61	0.65
4:D:56:A:O2'	4:D:57:U:P	2.54	0.65
4:D:91:A:N3	9:I:99:ILE:CD1	2.59	0.65
14:M:86:LEU:O	14:M:89:HIS:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:MET:SD	1:A:1160:LEU:HD22	2.37	0.65
15:N:208:SER:HA	15:N:212:TRP:CG	2.31	0.65
25:b:77:LEU:HD21	25:b:80:ILE:HD12	1.79	0.65
1:A:541:ASN:ND2	2:B:40:C:C4	2.64	0.65
1:A:847:LYS:HG2	6:F:24:U:C6	2.32	0.65
1:A:1905:LEU:HA	1:A:1908:LEU:HB3	1.79	0.65
5:E:355:U:C2'	5:E:355:U:O2	2.44	0.65
9:I:99:ILE:O	9:I:102:TRP:N	2.28	0.65
10:J:193:GLN:CD	13:T:447:ALA:CB	2.69	0.65
20:S:433:LEU:O	20:S:437:GLN:HG3	1.97	0.65
4:D:90:U:C5	9:I:104:ARG:CZ	2.80	0.65
5:E:1:G:C2	5:E:349:A:N3	2.64	0.65
6:F:40:U:C4'	6:F:41:C:OP1	2.45	0.65
8:H:722:PRO:O	8:H:725:THR:OG1	2.15	0.65
14:M:205:PHE:HB2	14:M:251:LEU:HB3	1.79	0.65
16:O:443:ASN:O	16:O:445:ASN:ND2	2.29	0.65
21:U:184:MET:HA	21:U:184:MET:HE3	1.79	0.65
1:A:1064:THR:HG22	10:J:81:PRO:HD2	1.79	0.65
1:A:1539:LEU:O	1:A:1541:ALA:N	2.30	0.65
1:A:1801:SER:O	1:A:1804:THR:OG1	2.11	0.65
3:C:701:GLU:OE1	3:C:706:LEU:N	2.30	0.65
3:C:855:PRO:HG2	3:C:944:VAL:HG21	1.78	0.65
5:E:355:U:O2	5:E:355:U:H2'	1.96	0.65
13:T:136:ASP:O	13:T:137:VAL:HG13	1.97	0.65
1:A:269:ASP:OD1	1:A:270:SER:N	2.30	0.64
1:A:452:PHE:CE1	3:C:343:ASP:OD1	2.50	0.64
1:A:1842:GLU:OE1	1:A:1845:ASN:ND2	2.23	0.64
9:I:248:ASN:O	9:I:252:HIS:CB	2.45	0.64
13:T:289:TYR:HD2	13:T:320:TRP:CZ3	2.15	0.64
16:O:365:PHE:CZ	16:O:373:LEU:HD22	2.32	0.64
20:S:374:GLU:HA	20:S:415:GLN:OE1	1.97	0.64
23:W:715:VAL:HG21	23:W:725:LEU:HD22	1.79	0.64
13:T:136:ASP:O	13:T:137:VAL:HG22	1.97	0.64
29:f:82:LEU:HD12	29:f:85:ILE:HD11	1.77	0.64
3:C:201:THR:HG22	3:C:207:SER:HB3	1.79	0.64
9:I:227:ASP:O	9:I:231:ASN:CB	2.41	0.64
6:F:25:A:H2	10:J:31:HIS:HB3	1.61	0.64
10:J:185:LEU:O	10:J:188:ARG:N	2.31	0.64
1:A:401:PRO:O	1:A:402:TRP:HB3	1.97	0.64
3:C:682:SER:HA	3:C:714:PRO:HG3	1.80	0.64
8:H:724:VAL:C	8:H:727:GLU:CG	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:229:ASP:HB2	11:K:151:LYS:HB3	1.79	0.64
1:A:402:TRP:HE1	1:A:405:ASN:ND2	1.95	0.64
1:A:834:ILE:HG12	1:A:840:VAL:HG11	1.80	0.64
1:A:940:ILE:O	1:A:943:ALA:N	2.31	0.64
1:A:1435:LYS:NZ	1:A:1550:LEU:O	2.27	0.64
1:A:1664:ASP:OD1	22:V:247:ARG:NH1	2.27	0.64
1:A:1955:ALA:CA	22:V:271:ARG:HB2	2.27	0.64
3:C:833:VAL:O	3:C:837:GLN:CB	2.46	0.64
14:M:103:GLU:HG2	14:M:104:ALA:HB3	1.79	0.64
1:A:1279:VAL:O	1:A:1299:LYS:NZ	2.31	0.64
1:A:1860:VAL:HA	1:A:1873:LYS:O	1.98	0.64
3:C:266:VAL:HG22	3:C:312:ILE:HB	1.79	0.64
9:I:189:TYR:HB3	9:I:205:TRP:HD1	1.62	0.64
26:c:77:ASN:OD1	30:g:49:ARG:HD3	1.97	0.64
1:A:1988:LEU:CG	21:U:180:VAL:CG1	2.72	0.64
6:F:41:C:O2'	6:F:42:U:P	2.55	0.64
18:Q:101:PRO:O	18:Q:103:ASN:N	2.25	0.64
24:h:98:GLU:C	31:o:53:PRO:CB	2.70	0.64
1:A:1447:TRP:HB3	1:A:1451:PHE:CE2	2.33	0.64
1:A:1792:ASN:OD1	1:A:1793:GLY:N	2.31	0.64
3:C:428:ILE:HG22	3:C:429:PHE:HD1	1.61	0.64
10:J:179:SER:HA	13:T:337:HIS:HD2	1.62	0.64
13:T:138:ASP:O	13:T:141:GLU:CB	2.44	0.64
14:M:74:CYS:SG	37:M:400:ZN:ZN	1.85	0.64
16:O:229:THR:HG21	16:O:272:VAL:H	1.62	0.64
18:Q:226:LYS:O	18:Q:229:ALA:N	2.31	0.64
1:A:616:GLY:HA3	4:D:72:C:OP1	1.98	0.63
1:A:1498:ASP:O	1:A:1501:THR:OG1	2.14	0.63
1:A:1717:LEU:N	1:A:1786:ALA:O	2.28	0.63
1:A:2003:THR:OG1	22:V:333:PRO:HB2	1.96	0.63
8:H:602:MET:HA	8:H:605:PHE:CD2	2.33	0.63
13:T:338:SER:O	13:T:355:SER:HA	1.98	0.63
1:A:1850:LEU:HD13	1:A:1930:PRO:HB3	1.80	0.63
6:F:1107:C:H6	6:F:1107:C:H5'	1.63	0.63
7:G:81:ASP:CB	7:G:85:THR:OG1	2.46	0.63
16:O:358:ILE:HG22	16:O:359:ASN:N	2.12	0.63
3:C:736:ASP:OD1	3:C:737:ILE:N	2.31	0.63
13:T:60:ARG:O	13:T:62:THR:N	2.31	0.63
13:T:135:VAL:HG11	13:T:193:TYR:OH	1.98	0.63
16:O:204:LYS:HE2	16:O:225:SER:HA	1.81	0.63
20:S:334:LEU:HD22	20:S:380:GLN:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:ARG:NH2	3:C:156:ASP:O	2.31	0.63
1:A:933:GLU:HA	1:A:936:GLU:OE1	1.99	0.63
1:A:1875:ILE:CG1	13:T:326:VAL:HG21	2.27	0.63
8:H:611:THR:CB	8:H:623:LEU:HD13	2.29	0.63
1:A:1067:ASN:O	1:A:1071:ARG:HG2	1.99	0.63
1:A:1527:TRP:CE3	1:A:1528:THR:HG23	2.34	0.63
26:j:77:ASN:OD1	30:n:49:ARG:HD3	1.97	0.63
18:Q:108:ASN:O	18:Q:111:HIS:N	2.31	0.63
21:U:136:PHE:CE2	21:U:140:LYS:HD2	2.34	0.63
2:B:83:C:O2'	2:B:84:A:O5'	2.17	0.63
14:M:61:CYS:O	14:M:72:GLN:NE2	2.32	0.63
15:N:175:TYR:OH	15:N:180:ASN:OD1	2.16	0.63
14:M:87:ARG:NH2	14:M:126:THR:OG1	2.32	0.63
14:M:242:VAL:O	15:N:161:ARG:NH2	2.32	0.63
14:M:258:LEU:O	14:M:262:PHE:CB	2.47	0.63
15:N:254:ILE:O	15:N:258:THR:OG1	2.16	0.63
18:Q:111:HIS:O	18:Q:112:ILE:HG13	1.99	0.63
3:C:779:LEU:HD12	3:C:782:GLU:HB2	1.81	0.62
19:R:27:ASN:OD1	19:R:28:ASN:N	2.32	0.62
1:A:161:PHE:CE1	1:A:198:ALA:HA	2.33	0.62
1:A:1870:VAL:HG23	5:E:299:U:H1'	1.81	0.62
13:T:151:PRO:CB	13:T:454:CYS:O	2.44	0.62
1:A:1156:HIS:CG	1:A:1157:PRO:HD2	2.34	0.62
2:B:174:G:O5'	26:c:76:ASN:ND2	2.32	0.62
6:F:20:G:H1'	17:P:7:PRO:HD2	1.81	0.62
6:F:119:G:O5'	26:j:76:ASN:ND2	2.32	0.62
6:F:1098:C:O5'	6:F:1098:C:H6	1.83	0.62
6:F:1120:G:H5''	6:F:1120:G:H8	1.64	0.62
9:I:261:GLU:O	9:I:265:ALA:HB2	2.00	0.62
13:T:164:GLY:HA3	13:T:447:ALA:HA	1.81	0.62
13:T:374:LYS:HZ3	13:T:374:LYS:CA	2.05	0.62
1:A:296:THR:CG2	2:B:33:U:OP2	2.47	0.62
1:A:320:ASP:O	1:A:508:GLN:NE2	2.32	0.62
1:A:1445:THR:OG1	1:A:1450:GLU:OE2	2.17	0.62
1:A:2041:PRO:HG2	1:A:2043:PHE:CZ	2.35	0.62
4:D:41:A:C8	15:N:34:TYR:CE2	2.88	0.62
10:J:68:GLU:O	10:J:72:GLN:CB	2.47	0.62
13:T:55:GLU:OE2	13:T:58:ARG:CD	2.47	0.62
14:M:240:LEU:HD13	14:M:251:LEU:HD13	1.80	0.62
21:U:183:TYR:CZ	21:U:234:LYS:HD2	2.32	0.62
1:A:511:ASP:OD2	1:A:514:TYR:OH	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:ILE:HG23	1:A:1074:VAL:HG23	1.81	0.62
14:M:256:SER:C	14:M:259:GLY:H	2.07	0.62
23:W:1023:LYS:HZ3	23:W:1090:TRP:CG	2.17	0.62
1:A:260:PRO:O	1:A:261:LEU:HB3	2.00	0.62
1:A:1414:TRP:O	1:A:1417:GLN:N	2.28	0.62
3:C:67:GLU:HB3	3:C:69:PRO:HD2	1.82	0.62
5:E:1:G:C2'	5:E:2:U:C5'	2.73	0.62
6:F:18:U:C4	11:K:202:GLN:NE2	2.68	0.62
13:T:363:PHE:CE1	13:T:371:ARG:CB	2.82	0.62
16:O:345:PHE:HE2	16:O:364:LEU:HD22	1.63	0.62
1:A:744:THR:HG22	4:D:75:A:OP1	1.99	0.62
1:A:1857:VAL:HG13	1:A:1894:ILE:HD13	1.81	0.62
1:A:1928:GLU:OE2	21:U:238:THR:HG22	2.00	0.62
1:A:220:THR:O	1:A:224:MET:HG2	1.99	0.62
1:A:1026:TYR:HA	1:A:1286:TRP:HZ3	1.64	0.62
1:A:1393:GLU:OE1	1:A:1393:GLU:N	2.25	0.62
3:C:398:ASN:OD1	3:C:401:ARG:NH2	2.32	0.62
3:C:775:ILE:N	3:C:818:TYR:O	2.32	0.62
6:F:15:C:N4	11:K:209:ARG:HG2	2.10	0.62
17:P:7:PRO:O	17:P:8:GLN:HB3	1.98	0.62
20:S:287:ASN:O	20:S:290:GLU:HB3	1.99	0.62
25:i:86:ASN:ND2	26:j:32:LYS:HD3	2.13	0.62
4:D:14:C:H4'	4:D:15:C:O5'	1.99	0.62
6:F:1099:G:C8	6:F:1100:A:C8	2.87	0.62
13:T:349:ASN:O	13:T:364:SER:HA	1.99	0.62
4:D:85:C:OP1	4:D:85:C:C4'	2.47	0.61
13:T:338:SER:HB3	13:T:356:MET:CG	2.29	0.61
14:M:217:TRP:CD1	14:M:218:LYS:N	2.68	0.61
1:A:151:SER:OG	1:A:152:LYS:N	2.32	0.61
1:A:1449:ASN:O	1:A:1452:LEU:N	2.33	0.61
3:C:719:MET:O	3:C:722:ASP:N	2.31	0.61
4:D:89:U:C4	11:K:176:TYR:CE1	2.88	0.61
29:f:3:LEU:HD11	30:g:60:ALA:HB1	1.82	0.61
3:C:234:LEU:HB2	3:C:262:ALA:O	2.00	0.61
3:C:477:ASP:HB2	3:C:628:TYR:CE2	2.35	0.61
15:N:253:LEU:O	15:N:257:ASN:HB2	2.01	0.61
20:S:399:MET:SD	20:S:439:ARG:HB3	2.40	0.61
1:A:514:TYR:HB3	1:A:518:VAL:HG21	1.81	0.61
1:A:1386:ALA:O	1:A:1390:THR:HG23	2.00	0.61
1:A:1590:LEU:HB2	1:A:1595:ARG:HG2	1.82	0.61
2:B:174:G:H5''	30:g:99:ASP:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:703:LEU:O	3:C:705:GLY:N	2.32	0.61
9:I:154:SER:O	9:I:157:THR:HB	2.01	0.61
11:K:200:ASN:O	11:K:204:ASN:HB2	2.01	0.61
16:O:333:SER:OG	16:O:334:TRP:N	2.32	0.61
1:A:978:ILE:HB	17:P:174:VAL:HA	1.81	0.61
2:B:175:G:N7	26:c:32:LYS:HD2	2.15	0.61
3:C:869:HIS:HD2	3:C:925:LEU:HB3	1.64	0.61
6:F:119:G:H5''	30:n:99:ASP:HB2	1.82	0.61
6:F:120:G:N7	26:j:32:LYS:HD2	2.15	0.61
6:F:1116:A:N1	6:F:1117:G:C6	2.68	0.61
9:I:99:ILE:HG13	9:I:100:PRO:N	2.12	0.61
13:T:190:TRP:CE3	13:T:198:CYS:HB2	2.35	0.61
16:O:224:LEU:HB2	16:O:245:ASP:OD1	2.01	0.61
1:A:2050:THR:O	1:A:2053:SER:OG	2.12	0.61
3:C:829:VAL:O	3:C:830:ASN:ND2	2.34	0.61
15:N:161:ARG:O	15:N:165:SER:OG	2.17	0.61
16:O:285:SER:O	16:O:287:ASP:N	2.33	0.61
1:A:783:LEU:O	1:A:786:LEU:N	2.32	0.61
1:A:1212:ARG:HG2	1:A:1213:MET:H	1.65	0.61
20:S:437:GLN:HG2	20:S:473:LEU:HD21	1.82	0.61
1:A:1594:GLN:OE1	5:E:348:U:N3	2.34	0.61
3:C:292:ILE:O	3:C:295:ILE:HG12	2.01	0.61
6:F:34:G:OP2	6:F:34:G:H8	1.79	0.61
10:J:224:MET:HE3	10:J:225:PRO:HD2	1.82	0.61
13:T:201:ASP:C	13:T:202:PHE:HD1	2.09	0.61
25:b:86:ASN:ND2	26:c:32:LYS:HD3	2.13	0.61
13:T:140:ARG:HH11	13:T:140:ARG:CG	2.14	0.61
16:O:407:PHE:HE1	16:O:414:LEU:HD13	1.62	0.61
21:U:95:ILE:H	21:U:171:GLN:HE22	1.49	0.61
21:U:169:HIS:HE1	21:U:195:ILE:H	1.47	0.61
29:m:3:LEU:HD11	30:n:60:ALA:HB1	1.82	0.61
3:C:576:THR:HG22	3:C:592:PHE:HD2	1.66	0.61
4:D:89:U:C5	11:K:176:TYR:CD1	2.89	0.60
5:E:9:U:C4'	5:E:10:U:OP2	2.49	0.60
9:I:267:TYR:OH	9:I:310:GLU:O	2.19	0.60
12:L:88:ASP:CG	12:L:91:LEU:H	2.09	0.60
14:M:107:ASP:O	14:M:110:LYS:HG2	2.01	0.60
28:l:20:SER:OG	28:l:30:ARG:HD2	2.01	0.60
1:A:1052:THR:O	1:A:1167:ARG:HA	2.00	0.60
3:C:116:THR:HG21	3:C:120:ARG:NH2	2.16	0.60
6:F:30:A:OP1	6:F:30:A:C4'	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1928:GLU:OE1	21:U:234:LYS:HG2	2.01	0.60
1:A:2013:ARG:HB3	1:A:2059:ILE:CD1	2.31	0.60
3:C:817:GLN:HE21	3:C:819:LYS:HE3	1.66	0.60
4:D:35:A:O2'	15:N:75:PHE:CE1	2.49	0.60
6:F:119:G:OP2	26:j:76:ASN:CB	2.49	0.60
13:T:136:ASP:C	13:T:137:VAL:HG13	2.25	0.60
13:T:339:MET:SD	13:T:353:ALA:HB3	2.41	0.60
8:H:724:VAL:CA	8:H:727:GLU:CG	2.79	0.60
1:A:402:TRP:CG	1:A:402:TRP:O	2.54	0.60
1:A:1289:VAL:HA	1:A:1295:GLN:O	2.02	0.60
4:D:53:A:H5'	4:D:54:U:OP2	2.01	0.60
5:E:354:A:O2'	5:E:355:U:C4	2.50	0.60
13:T:188:LYS:HB2	13:T:190:TRP:CZ2	2.37	0.60
16:O:225:SER:OG	16:O:245:ASP:OD1	2.17	0.60
16:O:263:VAL:HG12	16:O:264:GLY:N	2.12	0.60
1:A:1882:LEU:HB3	1:A:1889:LEU:HD23	1.83	0.60
3:C:795:ILE:HG23	3:C:842:MET:HE3	1.84	0.60
4:D:41:A:C8	15:N:34:TYR:HE2	2.19	0.60
5:E:-12:U:H2'	5:E:-11:A:H4'	1.84	0.60
1:A:416:GLU:HG2	1:A:418:ASP:N	2.16	0.60
2:B:174:G:OP2	26:c:76:ASN:CB	2.49	0.60
3:C:636:VAL:HG12	3:C:637:GLU:H	1.66	0.60
3:C:832:ASP:HA	3:C:835:LYS:HG2	1.83	0.60
1:A:235:LYS:O	1:A:648:GLN:NE2	2.35	0.60
1:A:971:MET:HE2	17:P:174:VAL:CG1	2.32	0.60
9:I:136:TRP:CE3	9:I:159:TRP:HB2	2.36	0.60
10:J:179:SER:CA	13:T:337:HIS:HD2	2.08	0.60
13:T:161:HIS:NE2	13:T:188:LYS:HD2	2.16	0.60
1:A:1762:ASP:OD1	1:A:1763:ASN:N	2.35	0.60
1:A:1952:PRO:HG3	22:V:247:ARG:CZ	2.31	0.60
3:C:145:GLY:O	3:C:148:SER:OG	2.18	0.60
16:O:307:HIS:ND1	16:O:327:CYS:HB2	2.17	0.60
20:S:402:LEU:HD22	20:S:445:LEU:HD13	1.84	0.60
21:U:183:TYR:CE2	21:U:234:LYS:HE3	2.37	0.60
25:i:83:LYS:NZ	26:j:75:CYS:O	2.35	0.60
1:A:1362:LYS:O	1:A:1365:THR:OG1	2.17	0.60
4:D:91:A:N9	9:I:99:ILE:HD11	2.15	0.60
12:L:118:SER:HB2	12:L:119:THR:HG23	1.82	0.60
14:M:87:ARG:NH2	14:M:122:GLY:O	2.35	0.60
25:b:83:LYS:NZ	26:c:75:CYS:O	2.35	0.60
1:A:269:ASP:OD2	1:A:272:ASP:N	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:TYR:HD2	1:A:514:TYR:N	1.93	0.59
1:A:1372:LYS:HG2	1:A:1383:PHE:CD2	2.36	0.59
10:J:64:GLU:HG2	10:J:65:PHE:H	1.67	0.59
1:A:590:TYR:OH	1:A:609:GLU:OE1	2.07	0.59
1:A:909:THR:O	1:A:913:VAL:HG23	2.02	0.59
1:A:992:ASP:O	1:A:995:LEU:N	2.34	0.59
3:C:84:GLN:HG2	3:C:88:THR:OG1	2.02	0.59
5:E:-1:G:C2	5:E:351:U:C2	2.90	0.59
5:E:-1:G:N2	5:E:351:U:C2	2.70	0.59
5:E:299:U:H2'	5:E:300:A:C8	2.36	0.59
9:I:40:LEU:HB2	10:J:249:ASN:OD1	2.01	0.59
13:T:164:GLY:HA2	13:T:449:GLY:HA2	1.84	0.59
13:T:165:THR:O	13:T:429:ILE:HD11	2.02	0.59
14:M:258:LEU:O	14:M:262:PHE:HB2	2.02	0.59
1:A:542:HIS:O	1:A:544:LYS:N	2.36	0.59
19:R:22:ARG:NH1	19:R:23:SER:O	2.35	0.59
21:U:106:LYS:HB3	21:U:107:PRO:HD3	1.83	0.59
1:A:815:TYR:O	1:A:818:SER:N	2.35	0.59
1:A:1335:TRP:HH2	1:A:1339:LEU:HD13	1.66	0.59
1:A:1988:LEU:O	21:U:181:GLN:NE2	2.35	0.59
1:A:296:THR:HG22	2:B:33:U:OP2	2.01	0.59
1:A:1870:VAL:HG23	5:E:299:U:O2	1.92	0.59
3:C:500:ARG:NH1	3:C:536:SER:OG	2.35	0.59
4:D:42:A:O2'	4:D:43:C:OP1	2.21	0.59
1:A:1052:THR:OG1	1:A:1168:ILE:HB	2.02	0.59
1:A:1142:ASN:HB3	1:A:1146:GLN:HB2	1.83	0.59
1:A:1599:SER:O	1:A:1602:PRO:HD2	2.03	0.59
1:A:1668:ILE:HD11	22:V:256:LEU:CD2	2.32	0.59
6:F:16:U:C2	11:K:179:ARG:NE	2.64	0.59
9:I:54:TYR:O	9:I:57:TYR:N	2.36	0.59
13:T:305:GLY:O	13:T:322:ASN:HB2	2.03	0.59
14:M:67:GLN:NE2	14:M:114:SER:O	2.36	0.59
16:O:377:ASP:OD2	16:O:380:SER:N	2.33	0.59
23:W:299:ILE:O	23:W:303:ILE:HG13	2.02	0.59
1:A:1340:ILE:O	1:A:1344:THR:OG1	2.16	0.59
10:J:525:ARG:O	10:J:528:GLN:CG	2.51	0.59
13:T:308:PHE:CE1	13:T:320:TRP:CG	2.91	0.59
13:T:356:MET:CE	13:T:356:MET:HA	2.33	0.59
15:N:63:ARG:HG3	15:N:85:PRO:O	2.03	0.59
1:A:284:ARG:HB2	1:A:287:GLU:OE2	2.02	0.59
1:A:304:ASP:OD1	1:A:305:LEU:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:TYR:CZ	1:A:936:GLU:OE1	2.56	0.59
1:A:1275:MET:O	1:A:1276:GLU:HG2	2.02	0.59
1:A:1565:THR:HG22	1:A:1819:ILE:HG22	1.84	0.59
1:A:2070:ASN:OD1	1:A:2071:ILE:N	2.36	0.59
13:T:292:HIS:NE2	13:T:318:ARG:HG3	2.16	0.59
14:M:53:ASN:HD21	15:N:69:GLN:HA	1.67	0.59
14:M:71:CYS:HB3	14:M:74:CYS:HB2	1.85	0.59
14:M:82:ILE:HD12	15:N:253:LEU:HD11	1.84	0.59
15:N:91:HIS:O	15:N:92:HIS:HB3	2.01	0.59
15:N:115:GLU:OE1	15:N:115:GLU:N	2.36	0.59
16:O:187:ASP:OD2	16:O:230:VAL:N	2.33	0.59
28:e:66:GLY:HA2	28:e:69:ILE:HD12	1.85	0.59
1:A:486:PHE:O	1:A:488:ARG:N	2.36	0.59
15:N:75:PHE:O	15:N:81:CYS:N	2.36	0.59
1:A:1368:GLN:O	1:A:1372:LYS:HG3	2.03	0.58
1:A:1431:HIS:CG	1:A:1434:GLU:HA	2.38	0.58
2:B:167:A:N7	30:g:63:ARG:NE	2.51	0.58
3:C:234:LEU:HD23	3:C:443:TYR:HB2	1.84	0.58
3:C:340:LYS:O	3:C:344:PHE:N	2.31	0.58
3:C:355:HIS:CD2	3:C:360:ARG:HB3	2.37	0.58
9:I:115:ILE:O	9:I:118:ALA:N	2.36	0.58
13:T:320:TRP:CD1	13:T:320:TRP:N	2.71	0.58
15:N:54:GLN:HB2	15:N:58:HIS:CD2	2.37	0.58
9:I:140:LEU:O	9:I:143:GLU:N	2.36	0.58
13:T:295:SER:O	13:T:313:GLU:HB2	2.02	0.58
13:T:360:ILE:HB	13:T:377:PHE:HB2	1.85	0.58
23:W:926:ILE:HD11	23:W:964:LEU:HB2	1.83	0.58
1:A:288:GLU:OE1	1:A:288:GLU:N	2.36	0.58
1:A:905:TYR:HB3	1:A:908:ASP:HB2	1.84	0.58
6:F:1116:A:N1	6:F:1117:G:C5	2.71	0.58
10:J:219:TYR:CE1	18:Q:135:VAL:HG21	2.38	0.58
13:T:373:PRO:HB2	13:T:374:LYS:HE2	1.84	0.58
13:T:406:ARG:HB3	13:T:421:ILE:O	2.03	0.58
14:M:257:GLU:OE2	14:M:261:ARG:NH2	2.37	0.58
15:N:44:ASN:OD1	15:N:45:THR:N	2.37	0.58
1:A:299:LYS:HA	1:A:493:MET:CG	2.32	0.58
1:A:512:GLU:H	1:A:514:TYR:HE2	1.51	0.58
1:A:618:SER:OG	1:A:725:TYR:HB3	2.02	0.58
1:A:1739:ARG:HD2	1:A:1751:TYR:CZ	2.38	0.58
2:B:175:G:N1	25:b:33:GLU:O	2.36	0.58
3:C:397:LYS:HG2	3:C:401:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:600:GLU:HB2	3:C:935:LYS:HE3	1.86	0.58
8:H:611:THR:CB	8:H:623:LEU:CD1	2.81	0.58
9:I:237:ILE:HD11	9:I:238:TRP:CE2	2.38	0.58
16:O:157:THR:HG21	16:O:423:ILE:HD11	1.86	0.58
28:l:66:GLY:HA2	28:l:69:ILE:HD12	1.85	0.58
1:A:342:LEU:HD13	1:A:392:ASN:ND2	2.18	0.58
1:A:475:ASP:O	1:A:478:SER:N	2.30	0.58
2:B:174:G:C5	29:f:20:LYS:HE2	2.39	0.58
3:C:383:LYS:O	3:C:387:TYR:HB2	2.04	0.58
13:T:140:ARG:H	13:T:140:ARG:HD3	1.67	0.58
13:T:293:LEU:HD23	13:T:293:LEU:H	1.69	0.58
13:T:411:ASP:OD1	13:T:414:THR:OG1	2.21	0.58
1:A:1705:SER:HB3	1:A:1709:TRP:CE3	2.39	0.58
6:F:20:G:C4	17:P:7:PRO:HD2	2.39	0.58
6:F:120:G:N1	25:i:33:GLU:O	2.36	0.58
13:T:356:MET:O	13:T:358:ASN:N	2.37	0.58
14:M:125:ILE:CD1	14:M:126:THR:HG23	2.34	0.58
1:A:1111:SER:HA	1:A:1514:PHE:CE2	2.39	0.58
5:E:346:A:O2'	5:E:347:A:OP2	2.20	0.58
8:H:687:LEU:HD23	8:H:713:ILE:HA	1.84	0.58
10:J:184:GLU:O	10:J:187:LYS:HB2	2.04	0.58
12:L:46:ASN:OD1	12:L:47:GLU:N	2.36	0.58
13:T:308:PHE:CE1	13:T:320:TRP:CD1	2.92	0.58
16:O:263:VAL:O	16:O:293:TRP:CH2	2.56	0.58
20:S:355:ARG:O	20:S:358:GLN:N	2.37	0.58
21:U:134:GLU:OE2	21:U:135:LEU:HG	2.04	0.58
1:A:282:ASP:HB2	1:A:285:PRO:HA	1.86	0.58
1:A:563:ASP:OD1	1:A:564:TRP:N	2.37	0.58
1:A:1493:THR:CB	23:W:301:GLN:OE1	2.51	0.58
1:A:1591:THR:OG1	1:A:1594:GLN:HB2	2.03	0.58
1:A:1656:LYS:HD3	1:A:1949:LEU:CD1	2.34	0.58
1:A:1701:ILE:O	1:A:1733:TRP:HA	2.03	0.58
1:A:1893:ILE:HB	1:A:1985:GLN:H	1.66	0.58
1:A:2002:TYR:CZ	22:V:329:LEU:HD21	2.39	0.58
3:C:717:SER:O	3:C:721:GLN:HB2	2.04	0.58
5:E:346:A:C2'	5:E:347:A:C8	2.87	0.58
6:F:112:A:N7	30:n:63:ARG:NE	2.51	0.58
13:T:161:HIS:CD2	13:T:188:LYS:HE3	2.38	0.58
16:O:328:THR:OG1	16:O:329:ASP:N	2.35	0.58
1:A:1914:ALA:HB2	1:A:1943:PRO:HB2	1.85	0.58
16:O:200:VAL:HG11	16:O:230:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:GLU:HG3	1:A:758:LEU:N	2.18	0.58
1:A:971:MET:HE3	1:A:978:ILE:HG22	1.86	0.58
1:A:1899:TRP:HB3	1:A:1905:LEU:HD21	1.86	0.58
13:T:140:ARG:H	13:T:140:ARG:CD	2.17	0.58
24:h:47:GLU:HG3	31:o:15:TYR:CG	2.39	0.58
1:A:137:GLU:O	1:A:138:HIS:C	2.46	0.57
1:A:488:ARG:HH11	2:B:81:A:N6	2.01	0.57
1:A:1169:TYR:CE2	1:A:1262:MET:HG2	2.39	0.57
13:T:380:HIS:HB3	13:T:408:PHE:CG	2.39	0.57
1:A:923:TYR:OH	1:A:936:GLU:OE1	2.21	0.57
1:A:1209:LYS:HD2	1:A:1417:GLN:HG2	1.86	0.57
1:A:1338:SER:O	1:A:1341:SER:OG	2.10	0.57
1:A:1659:GLU:O	1:A:1663:PHE:HB3	2.04	0.57
6:F:16:U:H2'	11:K:179:ARG:HH21	1.68	0.57
11:K:164:LEU:O	11:K:167:SER:OG	2.20	0.57
1:A:1463:THR:O	1:A:1466:GLN:N	2.37	0.57
1:A:1594:GLN:CG	5:E:348:U:O2	2.53	0.57
1:A:2003:THR:HG21	22:V:333:PRO:CB	2.34	0.57
1:A:2024:MET:O	1:A:2028:SER:N	2.37	0.57
6:F:20:G:H21	17:P:6:ARG:CA	2.12	0.57
16:O:160:ASN:HA	16:O:184:THR:OG1	2.04	0.57
16:O:285:SER:OG	16:O:287:ASP:OD1	2.22	0.57
20:S:301:SER:O	20:S:302:SER:OG	2.22	0.57
20:S:419:PHE:HD2	20:S:420:ILE:HD12	1.69	0.57
33:q:98:LEU:HD23	33:t:98:LEU:HD12	1.85	0.57
1:A:688:TYR:O	1:A:689:TYR:C	2.46	0.57
1:A:1955:ALA:HB1	22:V:270:SER:O	2.04	0.57
1:A:684:LYS:HE3	34:A:3000:IHP:O31	2.04	0.57
2:B:78:A:O2'	2:B:79:C:P	2.61	0.57
2:B:174:G:O6	29:f:20:LYS:HB3	2.05	0.57
3:C:802:ALA:HB2	3:C:843:LYS:HA	1.87	0.57
11:K:116:THR:O	11:K:119:SER:OG	2.19	0.57
12:L:120:CYS:CB	12:L:122:CYS:HB3	2.28	0.57
1:A:934:ARG:CD	6:F:31:A:H2	2.15	0.57
1:A:1679:GLU:HG2	1:A:1706:VAL:HA	1.87	0.57
1:A:1952:PRO:HG3	22:V:247:ARG:NH2	2.19	0.57
9:I:158:LYS:O	9:I:161:SER:N	2.38	0.57
9:I:193:VAL:HG12	9:I:201:THR:HB	1.87	0.57
18:Q:216:ARG:HA	18:Q:219:ILE:HD12	1.86	0.57
21:U:169:HIS:HD2	21:U:175:GLU:OE2	1.87	0.57
1:A:779:ALA:O	1:A:782:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:ALA:C	1:A:1478:GLU:H	2.12	0.57
1:A:1986:MET:HE3	21:U:184:MET:HG2	1.84	0.57
3:C:135:ASN:O	3:C:233:ASP:N	2.33	0.57
5:E:-1:G:N1	5:E:351:U:N3	2.53	0.57
1:A:1338:SER:OG	1:A:1339:LEU:N	2.35	0.57
1:A:2002:TYR:CE2	22:V:329:LEU:HD21	2.40	0.57
1:A:2013:ARG:NH1	1:A:2085:GLY:O	2.28	0.57
3:C:277:LEU:HB3	3:C:279:LEU:HD13	1.85	0.57
16:O:134:VAL:HG22	16:O:424:LYS:HG2	1.86	0.57
18:Q:43:PHE:CD1	18:Q:43:PHE:N	2.70	0.57
1:A:138:HIS:O	1:A:142:ILE:HG12	2.04	0.57
1:A:1776:GLY:O	1:A:1784:TYR:HA	2.04	0.57
5:E:294:G:O2'	5:E:295:A:OP1	2.21	0.57
13:T:406:ARG:HA	13:T:421:ILE:O	2.05	0.57
1:A:676:GLN:HE21	1:A:714:PHE:HB2	1.68	0.56
1:A:839:HIS:ND1	1:A:839:HIS:O	2.37	0.56
3:C:116:THR:HG21	3:C:120:ARG:CZ	2.35	0.56
3:C:463:THR:O	3:C:465:GLU:HG2	2.05	0.56
3:C:716:ASP:CG	3:C:719:MET:H	2.13	0.56
6:F:119:G:C5	29:m:20:LYS:HE2	2.39	0.56
10:J:163:GLN:HB3	10:J:167:ALA:HB3	1.86	0.56
13:T:340:PRO:CG	13:T:356:MET:HE3	2.33	0.56
1:A:224:MET:HE3	1:A:702:GLY:O	2.05	0.56
1:A:713:ASN:O	1:A:716:ARG:N	2.37	0.56
1:A:1253:LYS:O	1:A:1274:ARG:NH2	2.38	0.56
3:C:829:VAL:HG12	3:C:830:ASN:H	1.70	0.56
6:F:20:G:N3	17:P:6:ARG:CG	2.68	0.56
12:L:120:CYS:HB2	12:L:122:CYS:CB	2.26	0.56
14:M:256:SER:O	14:M:259:GLY:N	2.37	0.56
15:N:254:ILE:O	15:N:258:THR:HB	2.04	0.56
16:O:125:TRP:HE1	16:O:437:GLU:CG	2.18	0.56
20:S:475:GLU:O	20:S:478:ARG:N	2.38	0.56
1:A:252:GLU:OE1	1:A:252:GLU:N	2.38	0.56
1:A:376:ARG:HD2	3:C:910:GLU:OE2	2.05	0.56
1:A:1051:GLU:O	1:A:1246:ALA:HA	2.06	0.56
1:A:1924:LEU:HD21	21:U:234:LYS:NZ	2.20	0.56
3:C:545:LEU:HD12	3:C:545:LEU:O	2.05	0.56
3:C:798:GLY:HA2	3:C:839:ILE:HG23	1.86	0.56
3:C:840:PRO:O	3:C:843:LYS:HB3	2.04	0.56
3:C:864:VAL:CG2	3:C:906:VAL:HG12	2.35	0.56
7:G:7:VAL:CG1	7:G:154:VAL:CB	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:114:THR:O	11:K:118:ASN:HB2	2.05	0.56
13:T:137:VAL:HG23	13:T:138:ASP:N	2.20	0.56
13:T:391:PHE:N	13:T:391:PHE:CD1	2.73	0.56
14:M:16:CYS:SG	15:N:104:LEU:HD21	2.45	0.56
15:N:146:LEU:HD23	15:N:147:ASN:H	1.69	0.56
16:O:148:ASP:OD1	16:O:150:VAL:N	2.29	0.56
16:O:358:ILE:HG12	16:O:364:LEU:CD1	2.34	0.56
1:A:382:GLU:H	1:A:382:GLU:CD	2.14	0.56
1:A:557:PHE:O	1:A:558:GLN:NE2	2.39	0.56
1:A:1581:PHE:HE1	1:A:1598:LEU:HD11	1.69	0.56
1:A:1667:GLN:O	1:A:1670:ASP:N	2.38	0.56
1:A:1682:THR:O	1:A:1702:THR:OG1	2.18	0.56
13:T:317:VAL:CA	13:T:331:ILE:CD1	2.80	0.56
20:S:392:ILE:HG12	20:S:397:LEU:HD22	1.87	0.56
1:A:954:ILE:O	1:A:957:TYR:N	2.38	0.56
1:A:1181:GLU:O	1:A:1184:ASP:HB2	2.06	0.56
1:A:1668:ILE:HD11	22:V:256:LEU:HD22	1.86	0.56
1:A:1777:ILE:HA	1:A:1783:MET:O	2.05	0.56
6:F:119:G:O6	29:m:20:LYS:HB3	2.05	0.56
14:M:219:ILE:O	14:M:222:THR:OG1	2.17	0.56
16:O:188:VAL:HG13	16:O:197:LEU:HD11	1.88	0.56
20:S:386:LYS:O	20:S:389:GLY:N	2.39	0.56
20:S:408:THR:HB	20:S:410:GLU:HB3	1.87	0.56
21:U:183:TYR:CE2	21:U:234:LYS:CE	2.88	0.56
1:A:512:GLU:N	1:A:514:TYR:HE2	2.04	0.56
1:A:880:THR:HG23	18:Q:211:ALA:HB2	1.86	0.56
3:C:398:ASN:HA	3:C:401:ARG:NH2	2.21	0.56
5:E:304:C:H6	5:E:304:C:H5''	1.70	0.56
20:S:307:GLU:OE2	20:S:311:LYS:HE3	2.05	0.56
4:D:32:U:H5'	14:M:45:HIS:CE1	2.40	0.56
13:T:392:SER:HG	13:T:397:TYR:N	2.02	0.56
18:Q:147:LEU:HD12	18:Q:147:LEU:O	2.06	0.56
20:S:405:ILE:HD13	20:S:420:ILE:HD11	1.88	0.56
24:h:19:LYS:HZ1	31:o:34:LEU:CB	2.15	0.56
1:A:1663:PHE:O	1:A:1666:CYS:HB3	2.05	0.56
3:C:682:SER:O	3:C:854:ILE:HB	2.06	0.56
4:D:55:G:N7	10:J:35:LYS:HG2	2.21	0.56
13:T:193:TYR:O	13:T:194:HIS:CB	2.52	0.56
15:N:237:ARG:O	15:N:240:GLU:HB3	2.06	0.56
16:O:380:SER:OG	16:O:381:GLY:N	2.39	0.56
1:A:890:LEU:O	1:A:894:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:ILE:HD13	1:A:1645:LEU:HD13	1.88	0.56
1:A:1881:THR:OG1	1:A:1890:PHE:HB2	2.05	0.56
3:C:448:LEU:O	3:C:451:ASN:N	2.39	0.56
3:C:677:PHE:HB2	3:C:811:GLU:OE1	2.05	0.56
3:C:711:ALA:CB	3:C:819:LYS:O	2.54	0.56
5:E:294:G:O2'	5:E:295:A:O5'	2.24	0.56
6:F:1105:C:N4	32:p:97:LYS:NZ	2.54	0.56
9:I:143:GLU:HG3	9:I:151:ILE:HG21	1.87	0.56
13:T:393:GLY:O	13:T:394:ASP:HB2	2.06	0.56
15:N:65:ASP:OD1	15:N:90:LEU:HD22	2.05	0.56
20:S:301:SER:OG	20:S:311:LYS:NZ	2.39	0.56
29:f:43:VAL:HG11	29:f:85:ILE:HD12	1.86	0.56
1:A:2084:LEU:HD21	22:V:330:VAL:HG21	1.88	0.56
3:C:132:ARG:HG3	3:C:206:LYS:HZ1	1.71	0.56
13:T:128:TYR:N	13:T:128:TYR:CD1	2.73	0.56
13:T:202:PHE:N	13:T:202:PHE:CD1	2.74	0.56
13:T:227:ASP:O	13:T:228:ARG:HB2	2.05	0.56
15:N:110:ASP:CG	15:N:114:ARG:H	2.11	0.56
1:A:382:GLU:OE1	1:A:382:GLU:N	2.35	0.55
1:A:589:THR:OG1	15:N:39:GLN:NE2	2.40	0.55
1:A:1940:MET:HE3	1:A:1944:LEU:HG	1.88	0.55
1:A:2043:PHE:HD2	1:A:2048:TRP:CD2	2.24	0.55
3:C:116:THR:HG22	3:C:158:HIS:CD2	2.42	0.55
4:D:92:C:H4'	4:D:92:C:OP1	2.06	0.55
13:T:317:VAL:N	13:T:331:ILE:CD1	2.69	0.55
16:O:202:GLU:OE1	16:O:226:GLY:HA3	2.07	0.55
25:i:77:LEU:HD21	25:i:80:ILE:CD1	2.35	0.55
1:A:556:TYR:HE2	18:Q:119:MET:O	1.89	0.55
1:A:841:GLU:HB2	1:A:844:MET:HG2	1.88	0.55
1:A:1739:ARG:O	1:A:1778:ASP:HA	2.07	0.55
3:C:680:SER:OG	3:C:681:CYS:N	2.39	0.55
5:E:11:A:H2	15:N:46:ARG:HD3	1.71	0.55
6:F:1116:A:N3	6:F:1117:G:C8	2.74	0.55
16:O:437:GLU:OE1	16:O:438:PRO:HA	2.07	0.55
21:U:234:LYS:O	21:U:238:THR:HG23	2.06	0.55
31:o:44:PRO:O	31:o:69:ASP:CB	2.54	0.55
1:A:1339:LEU:HD21	1:A:1440:ILE:HD13	1.88	0.55
1:A:1648:ILE:HG22	1:A:1649:PHE:CD1	2.41	0.55
1:A:1985:GLN:HB2	21:U:185:LYS:HG2	1.88	0.55
1:A:2019:GLU:O	1:A:2022:ALA:N	2.36	0.55
3:C:901:GLU:OE2	3:C:903:ARG:NE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:196:ILE:H	11:K:200:ASN:HD22	1.54	0.55
12:L:81:LEU:O	12:L:84:GLU:N	2.37	0.55
16:O:155:PHE:HZ	16:O:425:ILE:HD11	1.72	0.55
1:A:1183:THR:O	1:A:1187:LEU:HB2	2.07	0.55
1:A:1500:HIS:HB2	23:W:293:SER:CB	2.36	0.55
3:C:122:TYR:OH	3:C:126:MET:HE2	2.06	0.55
3:C:170:LEU:HD12	3:C:171:GLY:HA2	1.88	0.55
3:C:807:PRO:HG3	3:C:850:LEU:HD23	1.87	0.55
14:M:260:GLU:O	14:M:264:SER:N	2.35	0.55
1:A:1111:SER:O	1:A:1114:PHE:HB3	2.07	0.55
1:A:1995:TRP:HE3	1:A:2004:ALA:HB1	1.70	0.55
2:B:78:A:O2'	2:B:79:C:OP1	2.24	0.55
3:C:89:PRO:O	3:C:91:VAL:N	2.35	0.55
3:C:429:PHE:N	3:C:429:PHE:CD1	2.71	0.55
13:T:150:LEU:HD12	13:T:150:LEU:N	2.03	0.55
13:T:152:LYS:HD2	13:T:153:LYS:N	2.21	0.55
3:C:497:ASP:N	3:C:497:ASP:OD1	2.39	0.55
5:E:-10:A:H61	19:R:6:ILE:HD11	1.72	0.55
6:F:40:U:O4'	6:F:41:C:OP1	2.24	0.55
6:F:1100:A:C2	6:F:1101:C:C2	2.95	0.55
14:M:125:ILE:HG13	14:M:126:THR:H	1.71	0.55
18:Q:103:ASN:HD22	18:Q:114:VAL:HG21	1.72	0.55
20:S:456:GLU:HA	20:S:459:ARG:HH11	1.71	0.55
29:m:43:VAL:HG11	29:m:85:ILE:HD12	1.87	0.55
1:A:790:TRP:O	1:A:793:TRP:N	2.40	0.55
1:A:1561:LEU:O	1:A:1564:GLY:N	2.30	0.55
1:A:1955:ALA:CB	22:V:271:ARG:HB2	2.37	0.55
1:A:1988:LEU:N	21:U:181:GLN:HG2	2.13	0.55
1:A:2056:ARG:NE	22:V:331:ALA:HB1	2.22	0.55
12:L:121:ILE:HD11	12:L:129:LEU:HD21	1.87	0.55
16:O:198:PHE:CE1	16:O:239:ILE:HD11	2.41	0.55
20:S:459:ARG:O	20:S:463:ASN:HB3	2.07	0.55
1:A:1348:GLU:CG	1:A:1446:THR:HB	2.36	0.55
1:A:1884:PRO:O	1:A:1992:TYR:OH	2.13	0.55
1:A:2026:LEU:HB3	1:A:2041:PRO:HG3	1.87	0.55
2:B:31:G:C2'	2:B:32:G:H5'	2.37	0.55
10:J:179:SER:HB3	13:T:337:HIS:NE2	2.16	0.55
15:N:241:GLU:O	15:N:244:LEU:HG	2.05	0.55
16:O:307:HIS:HD1	16:O:327:CYS:HB2	1.71	0.55
1:A:395:PRO:HB2	1:A:398:VAL:HG21	1.88	0.55
1:A:634:ASP:O	1:A:637:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1712:SER:HB3	1:A:1724:PHE:HA	1.89	0.55
4:D:64:U:HO2'	4:D:65:U:P	2.30	0.55
16:O:242:ALA:HB2	16:O:248:ILE:HA	1.89	0.55
17:P:7:PRO:O	17:P:8:GLN:CB	2.55	0.55
1:A:180:PRO:HA	1:A:187:LYS:HE2	1.88	0.55
1:A:1755:LYS:HB3	1:A:1759:TYR:CE2	2.41	0.55
4:D:91:A:C2	9:I:99:ILE:HD13	2.42	0.55
8:H:606:GLN:HA	8:H:609:GLU:CG	2.37	0.55
13:T:329:LYS:HG3	13:T:330:GLN:N	2.21	0.55
1:A:308:MET:HE2	1:A:486:PHE:O	2.07	0.54
1:A:763:MET:SD	1:A:783:LEU:HD11	2.46	0.54
6:F:15:C:O2'	6:F:16:U:O4'	2.25	0.54
9:I:238:TRP:HD1	9:I:242:GLU:CD	2.15	0.54
13:T:292:HIS:ND1	13:T:312:SER:CB	2.68	0.54
1:A:1090:ILE:O	1:A:1096:SER:HA	2.07	0.54
1:A:1493:THR:HB	23:W:301:GLN:OE1	2.07	0.54
1:A:1797:LEU:O	1:A:1801:SER:OG	2.24	0.54
3:C:164:MET:HG2	3:C:175:LEU:CD1	2.38	0.54
3:C:179:ASP:OD1	3:C:184:GLU:HB3	2.07	0.54
3:C:277:LEU:CB	3:C:279:LEU:HD13	2.37	0.54
3:C:738:ASP:HA	3:C:768:PHE:CZ	2.42	0.54
13:T:126:ARG:HH11	13:T:131:PRO:CG	2.07	0.54
13:T:340:PRO:HG2	13:T:356:MET:HE3	1.81	0.54
25:b:77:LEU:HD21	25:b:80:ILE:CD1	2.36	0.54
1:A:683:LEU:HD13	1:A:706:PRO:HB2	1.87	0.54
1:A:1154:LYS:HA	1:A:1159:ARG:NH2	2.22	0.54
1:A:1875:ILE:CG1	13:T:326:VAL:CG2	2.86	0.54
3:C:242:VAL:HG13	3:C:897:THR:HG21	1.89	0.54
3:C:797:GLN:O	3:C:800:TYR:N	2.40	0.54
3:C:798:GLY:O	3:C:801:TRP:HB3	2.06	0.54
13:T:191:ASP:O	13:T:192:PHE:HB3	2.07	0.54
20:S:384:LEU:HB3	20:S:419:PHE:HE1	1.71	0.54
1:A:284:ARG:NE	2:B:33:U:O4	2.41	0.54
1:A:287:GLU:HB2	1:A:288:GLU:OE1	2.08	0.54
1:A:995:LEU:HD11	1:A:1078:ILE:HG23	1.90	0.54
1:A:1476:ALA:HB3	1:A:1479:GLU:HG2	1.90	0.54
3:C:133:ILE:HG22	3:C:209:MET:HB3	1.89	0.54
3:C:743:ASN:HB3	3:C:746:LYS:HB3	1.89	0.54
11:K:190:TYR:CZ	11:K:192:VAL:HB	2.43	0.54
13:T:202:PHE:HD1	13:T:202:PHE:N	2.04	0.54
13:T:305:GLY:O	13:T:322:ASN:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:408:PHE:HB2	13:T:410:TRP:CZ3	2.41	0.54
16:O:220:TYR:CE1	16:O:256:ARG:HG2	2.43	0.54
16:O:251:TRP:CZ3	16:O:258:PRO:HB3	2.42	0.54
23:W:957:TYR:CD2	23:W:1085:SER:CB	2.90	0.54
24:h:47:GLU:HG3	31:o:15:TYR:HB2	1.87	0.54
1:A:644:VAL:HG12	1:A:648:GLN:HB2	1.89	0.54
3:C:68:HIS:HA	3:C:71:GLY:HA2	1.88	0.54
3:C:501:ILE:HD13	3:C:567:ILE:HG21	1.90	0.54
3:C:676:VAL:HG12	3:C:677:PHE:N	2.23	0.54
20:S:326:VAL:CG1	20:S:364:THR:HG21	2.38	0.54
1:A:1875:ILE:CB	13:T:326:VAL:HG21	2.36	0.54
3:C:353:TYR:N	3:C:353:TYR:CD1	2.75	0.54
3:C:493:LEU:HB2	3:C:556:ALA:HB3	1.89	0.54
6:F:1114:G:H2'	6:F:1115:G:C8	2.43	0.54
10:J:90:MET:HE2	18:Q:197:ILE:HG23	1.90	0.54
20:S:355:ARG:O	20:S:358:GLN:HB3	2.07	0.54
20:S:446:ASP:O	20:S:449:PHE:N	2.41	0.54
23:W:957:TYR:CD2	23:W:1085:SER:HB3	2.43	0.54
1:A:928:ARG:CZ	1:A:1595:ARG:HH22	2.21	0.54
1:A:960:THR:O	1:A:962:ARG:NH1	2.41	0.54
1:A:1354:GLU:OE2	1:A:1408:PRO:HG2	2.08	0.54
1:A:2010:LEU:HD21	1:A:2083:ILE:HG23	1.90	0.54
5:E:3:A:C8	5:E:4:U:C6	2.95	0.54
8:H:726:ARG:HA	8:H:729:TYR:CD2	2.42	0.54
9:I:185:VAL:HA	9:I:188:ILE:HD12	1.90	0.54
15:N:48:VAL:HG11	15:N:203:THR:HG23	1.90	0.54
15:N:95:ASP:OD1	15:N:98:ASP:N	2.36	0.54
18:Q:43:PHE:N	18:Q:43:PHE:HD1	2.04	0.54
1:A:835:LYS:HD2	17:P:173:HIS:CE1	2.43	0.54
3:C:136:VAL:HA	3:C:234:LEU:O	2.08	0.54
3:C:767:SER:OG	3:C:796:ILE:HD13	2.08	0.54
6:F:1114:G:H8	6:F:1114:G:O5'	1.91	0.54
10:J:216:ASP:OD1	10:J:217:ILE:N	2.41	0.54
13:T:374:LYS:CA	13:T:374:LYS:CE	2.86	0.54
15:N:256:ASN:OD1	15:N:257:ASN:N	2.40	0.54
1:A:264:ILE:HG22	1:A:265:ASN:O	2.08	0.54
1:A:314:LEU:O	1:A:317:PRO:HD2	2.08	0.54
1:A:1581:PHE:C	1:A:1581:PHE:CD1	2.85	0.54
1:A:1888:HIS:HA	1:A:1989:PHE:O	2.08	0.54
3:C:360:ARG:C	3:C:362:LYS:H	2.15	0.54
3:C:746:LYS:O	3:C:749:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1102:C:C2'	6:F:1103:C:H6	2.15	0.54
8:H:560:ALA:HA	8:H:570:THR:HG21	1.89	0.54
14:M:53:ASN:OD1	14:M:54:ASN:N	2.41	0.54
18:Q:30:LEU:O	18:Q:33:GLN:N	2.41	0.54
24:a:31:ILE:HD11	24:a:49:ILE:HD12	1.90	0.54
1:A:1962:ARG:HG3	1:A:2085:GLY:HA3	1.89	0.54
3:C:105:ILE:HG12	3:C:106:PHE:H	1.73	0.54
10:J:207:TYR:CE2	10:J:210:ASP:HA	2.43	0.54
13:T:60:ARG:C	13:T:62:THR:N	2.64	0.54
13:T:191:ASP:CG	13:T:193:TYR:HB2	2.32	0.54
13:T:315:LYS:HD2	13:T:315:LYS:N	2.18	0.54
13:T:317:VAL:CG1	13:T:331:ILE:HD13	2.17	0.54
16:O:382:HIS:CE1	16:O:442:TRP:H	2.26	0.54
21:U:90:THR:HG22	21:U:90:THR:O	2.08	0.54
1:A:1376:ASN:O	1:A:1377:SER:OG	2.10	0.53
1:A:1865:THR:OG1	1:A:1869:ASN:N	2.41	0.53
13:T:350:TYR:CA	13:T:363:PHE:O	2.56	0.53
1:A:367:PHE:O	1:A:372:ARG:NH2	2.41	0.53
1:A:933:GLU:O	1:A:936:GLU:N	2.42	0.53
1:A:1063:PHE:HB2	10:J:83:GLN:NE2	2.24	0.53
4:D:67:C:OP2	9:I:59:LYS:HE3	2.08	0.53
5:E:354:A:H8	5:E:354:A:O5'	1.90	0.53
6:F:20:G:H21	17:P:6:ARG:C	2.15	0.53
10:J:179:SER:HB2	13:T:337:HIS:HD2	1.71	0.53
12:L:51:GLU:O	12:L:54:GLN:N	2.40	0.53
21:U:223:ASP:CG	21:U:224:GLU:H	2.16	0.53
31:o:68:PRO:O	31:o:69:ASP:CB	2.54	0.53
1:A:1405:ILE:HD13	1:A:1439:THR:HG21	1.90	0.53
2:B:174:G:H8	30:g:99:ASP:OD2	1.91	0.53
3:C:67:GLU:N	3:C:76:VAL:HG21	2.23	0.53
6:F:1102:C:C2'	6:F:1103:C:C6	2.80	0.53
8:H:682:LYS:O	8:H:686:ILE:HG12	2.08	0.53
13:T:55:GLU:O	13:T:59:ARG:HB2	2.08	0.53
14:M:13:CYS:N	14:M:71:CYS:SG	2.71	0.53
15:N:63:ARG:HD3	15:N:86:LYS:HA	1.90	0.53
20:S:410:GLU:OE1	20:S:411:GLU:N	2.41	0.53
1:A:722:LEU:O	1:A:723:GLU:C	2.51	0.53
1:A:1705:SER:HB3	1:A:1709:TRP:CD2	2.43	0.53
1:A:1872:THR:HG21	5:E:302:C:OP1	2.08	0.53
1:A:1926:LYS:CE	22:V:248:LEU:HB3	2.37	0.53
3:C:105:ILE:HG22	3:C:180:ASN:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1103:C:C6	6:F:1114:G:N2	2.76	0.53
13:T:55:GLU:O	13:T:58:ARG:HG3	2.09	0.53
13:T:356:MET:C	13:T:358:ASN:H	2.16	0.53
14:M:39:LEU:HD11	14:M:111:ARG:HG3	1.90	0.53
21:U:223:ASP:CG	21:U:224:GLU:N	2.66	0.53
33:t:102:LEU:O	33:t:105:LEU:CG	2.57	0.53
6:F:25:A:H2'	6:F:27:A:OP2	2.08	0.53
6:F:1105:C:H42	32:p:97:LYS:NZ	2.07	0.53
13:T:200:ARG:HH22	13:T:237:THR:HA	1.67	0.53
1:A:1955:ALA:HA	22:V:271:ARG:CD	2.39	0.53
3:C:715:MET:HB2	3:C:720:ILE:HD11	1.89	0.53
10:J:202:LYS:O	10:J:204:LYS:N	2.39	0.53
13:T:185:HIS:CG	13:T:185:HIS:CA	2.83	0.53
13:T:308:PHE:H	13:T:308:PHE:HD1	1.55	0.53
15:N:62:THR:OG1	15:N:63:ARG:N	2.42	0.53
1:A:484:PHE:O	1:A:485:PRO:C	2.50	0.53
1:A:1715:SER:HG	1:A:1790:TRP:CD1	2.26	0.53
1:A:2034:ILE:CG1	1:A:2041:PRO:HA	2.38	0.53
3:C:502:LEU:HD11	3:C:506:GLN:HB2	1.91	0.53
6:F:119:G:H8	30:n:99:ASP:OD2	1.91	0.53
15:N:46:ARG:NH2	15:N:220:GLY:O	2.42	0.53
15:N:249:MET:HA	15:N:252:HIS:HD2	1.72	0.53
1:A:456:GLU:OE1	1:A:456:GLU:N	2.42	0.53
1:A:1058:ALA:HB1	1:A:1103:LEU:HB3	1.90	0.53
1:A:1286:TRP:HD1	1:A:1448:GLU:OE2	1.92	0.53
1:A:1842:GLU:OE1	22:V:299:LEU:O	2.27	0.53
3:C:675:THR:OG1	3:C:676:VAL:N	2.40	0.53
9:I:99:ILE:CG1	9:I:100:PRO:HD3	2.31	0.53
9:I:265:ALA:O	9:I:269:ILE:HD12	2.09	0.53
13:T:60:ARG:C	13:T:62:THR:H	2.16	0.53
14:M:34:CYS:HB3	14:M:36:ILE:H	1.73	0.53
16:O:154:TRP:CD1	16:O:154:TRP:N	2.75	0.53
16:O:434:LYS:O	16:O:435:GLU:C	2.51	0.53
20:S:412:SER:O	20:S:417:ARG:NH1	2.41	0.53
24:h:98:GLU:O	31:o:53:PRO:CA	2.56	0.53
1:A:1813:TYR:CG	22:V:268:PRO:HG2	2.44	0.53
1:A:2013:ARG:O	1:A:2016:LYS:N	2.37	0.53
1:A:2080:LYS:O	1:A:2084:LEU:HG	2.08	0.53
1:A:2084:LEU:CD2	22:V:330:VAL:HG21	2.39	0.53
3:C:343:ASP:O	3:C:346:THR:OG1	2.26	0.53
3:C:865:ASP:OD1	3:C:866:ILE:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:16:U:N3	11:K:179:ARG:HD3	2.24	0.53
6:F:1116:A:C5	6:F:1117:G:C5	2.97	0.53
8:H:718:SER:HG	8:H:725:THR:HG21	1.70	0.53
9:I:126:ILE:HG13	9:I:127:SER:N	2.24	0.53
13:T:429:ILE:HG12	13:T:446:GLY:HA2	1.91	0.53
14:M:70:ILE:HB	14:M:76:LEU:O	2.09	0.53
14:M:119:LYS:HE3	14:M:123:ALA:HB1	1.91	0.53
18:Q:101:PRO:C	18:Q:103:ASN:H	2.15	0.53
20:S:452:GLU:OE1	20:S:452:GLU:N	2.41	0.53
21:U:246:ASN:O	21:U:247:HIS:ND1	2.42	0.53
1:A:143:ILE:HG13	1:A:144:ASN:N	2.23	0.53
1:A:1626:GLN:NE2	1:A:1631:GLY:HA2	2.23	0.53
13:T:354:GLN:CG	13:T:389:LEU:CG	2.87	0.53
13:T:392:SER:HG	13:T:397:TYR:HB2	1.73	0.53
15:N:150:HIS:O	15:N:152:LYS:N	2.42	0.53
21:U:225:ARG:NH1	21:U:225:ARG:HB2	2.24	0.53
24:h:31:ILE:HD11	24:h:49:ILE:HD12	1.90	0.53
1:A:834:ILE:O	1:A:837:GLY:N	2.42	0.52
1:A:905:TYR:HE2	1:A:907:ASN:HB2	1.72	0.52
1:A:1229:GLU:O	1:A:1232:SER:OG	2.11	0.52
1:A:1591:THR:HB	1:A:1594:GLN:H	1.74	0.52
1:A:1679:GLU:HB2	1:A:1704:GLU:O	2.09	0.52
1:A:1710:GLU:HA	1:A:1727:LEU:O	2.09	0.52
3:C:90:LEU:HD23	3:C:90:LEU:O	2.08	0.52
3:C:223:ASP:OD2	3:C:647:ASN:ND2	2.31	0.52
3:C:749:LYS:O	3:C:753:THR:OG1	2.22	0.52
13:T:301:TYR:HA	13:T:308:PHE:HA	1.91	0.52
1:A:735:GLU:OE1	17:P:23:THR:O	2.27	0.52
1:A:1699:ALA:HB2	1:A:1767:TYR:HD1	1.74	0.52
3:C:246:THR:O	3:C:249:VAL:N	2.41	0.52
3:C:325:LYS:NZ	3:C:437:ASP:OD2	2.42	0.52
3:C:863:GLU:OE2	3:C:934:HIS:ND1	2.43	0.52
5:E:12:U:OP2	15:N:138:TYR:OH	2.21	0.52
5:E:14:U:C5	15:N:183:PHE:CE2	2.98	0.52
6:F:16:U:C2'	11:K:179:ARG:HH21	2.22	0.52
10:J:179:SER:CA	13:T:337:HIS:NE2	2.72	0.52
13:T:139:LEU:CG	13:T:174:THR:OG1	2.55	0.52
15:N:76:PHE:O	15:N:79:GLY:N	2.31	0.52
20:S:361:TYR:O	20:S:364:THR:N	2.42	0.52
1:A:453:THR:HG22	3:C:358:ASN:HB3	1.91	0.52
1:A:897:PRO:O	1:A:1006:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:GLU:OE1	1:A:1247:PHE:HB2	2.10	0.52
1:A:1341:SER:HA	1:A:1525:PHE:CE1	2.45	0.52
3:C:477:ASP:HB2	3:C:628:TYR:CD2	2.44	0.52
13:T:411:ASP:CG	13:T:414:THR:HG1	2.15	0.52
15:N:72:PHE:HD1	15:N:90:LEU:HB2	1.74	0.52
18:Q:51:PHE:N	18:Q:51:PHE:CD1	2.75	0.52
3:C:801:TRP:HE1	3:C:843:LYS:HD2	1.73	0.52
6:F:1116:A:N6	6:F:1117:G:C6	2.78	0.52
13:T:51:PHE:HE1	13:T:55:GLU:HG3	1.75	0.52
14:M:111:ARG:HG2	18:Q:134:VAL:HG13	1.92	0.52
15:N:97:GLU:O	15:N:100:GLY:N	2.42	0.52
15:N:159:ARG:HD3	15:N:204:LEU:HB3	1.90	0.52
23:W:290:ALA:HA	23:W:1062:LYS:HG2	1.91	0.52
1:A:329:TYR:CE1	3:C:919:ARG:HD2	2.45	0.52
1:A:413:ASN:OD1	1:A:413:ASN:N	2.43	0.52
1:A:1624:LEU:HD21	1:A:1635:HIS:CE1	2.45	0.52
1:A:2003:THR:HG22	22:V:333:PRO:HB3	1.90	0.52
5:E:345:A:N3	5:E:345:A:C3'	2.73	0.52
13:T:126:ARG:NH1	13:T:126:ARG:CB	2.73	0.52
15:N:28:LEU:HG	15:N:29:THR:HG23	1.90	0.52
21:U:163:LEU:O	21:U:167:LEU:HD13	2.10	0.52
33:t:124:ALA:O	33:t:127:LEU:CG	2.57	0.52
1:A:905:TYR:CE2	1:A:907:ASN:HB2	2.43	0.52
1:A:953:ARG:HG2	1:A:957:TYR:CE2	2.45	0.52
1:A:1063:PHE:O	1:A:1066:LEU:N	2.43	0.52
1:A:1405:ILE:HG22	1:A:1406:LEU:N	2.21	0.52
1:A:1511:ARG:O	1:A:1515:LYS:HG2	2.10	0.52
1:A:2009:THR:O	1:A:2013:ARG:HG3	2.09	0.52
3:C:85:SER:O	3:C:88:THR:OG1	2.15	0.52
4:D:34:A:C6	15:N:89:TYR:CD1	2.98	0.52
13:T:411:ASP:OD1	13:T:414:THR:CA	2.58	0.52
16:O:156:ILE:HD13	16:O:197:LEU:HD22	1.91	0.52
1:A:164:ALA:HB2	18:Q:122:LEU:CD2	2.40	0.52
1:A:1489:PRO:HB3	23:W:301:GLN:NE2	2.24	0.52
3:C:701:GLU:HG2	3:C:703:LEU:H	1.74	0.52
3:C:718:LYS:HA	3:C:721:GLN:HB3	1.92	0.52
9:I:235:LEU:HD23	9:I:237:ILE:HG23	1.92	0.52
12:L:90:LEU:O	12:L:93:ALA:N	2.43	0.52
13:T:126:ARG:CZ	13:T:126:ARG:CB	2.86	0.52
13:T:374:LYS:N	13:T:374:LYS:CE	2.73	0.52
14:M:48:THR:OG1	14:M:49:SER:N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:139:VAL:O	15:N:181:CYS:HA	2.10	0.52
15:N:169:ASP:OD1	15:N:169:ASP:N	2.41	0.52
1:A:1572:GLY:HA3	1:A:1827:GLN:NE2	2.24	0.52
1:A:1604:ARG:O	1:A:1605:ARG:C	2.51	0.52
1:A:1852:VAL:HA	1:A:1881:THR:HG22	1.91	0.52
3:C:679:GLU:OE1	3:C:807:PRO:HD2	2.10	0.52
3:C:772:ASN:OD1	3:C:772:ASN:N	2.41	0.52
3:C:968:MET:HE2	3:C:971:ARG:HD3	1.91	0.52
6:F:31:A:N3	6:F:31:A:C5'	2.73	0.52
10:J:73:LEU:HD21	10:J:102:TYR:HB2	1.92	0.52
1:A:1094:ASP:OD1	1:A:1094:ASP:N	2.41	0.52
3:C:109:LEU:HD23	3:C:111:LYS:HG2	1.92	0.52
3:C:314:ALA:HB1	3:C:321:THR:HG22	1.91	0.52
3:C:429:PHE:HD1	3:C:429:PHE:N	2.07	0.52
6:F:1107:C:H5'	6:F:1107:C:C6	2.44	0.52
14:M:215:PRO:CG	14:M:217:TRP:CD2	2.92	0.52
1:A:149:MET:HB2	1:A:154:TYR:CD2	2.45	0.52
1:A:484:PHE:HB2	2:B:81:A:N7	2.25	0.52
1:A:865:ARG:O	1:A:868:GLN:N	2.40	0.52
1:A:878:GLU:O	1:A:881:THR:OG1	2.28	0.52
1:A:1232:SER:OG	1:A:1233:ARG:N	2.41	0.52
1:A:1286:TRP:CZ2	1:A:1302:LEU:HD11	2.45	0.52
1:A:1457:VAL:HG21	1:A:1486:ARG:HB2	1.92	0.52
3:C:916:THR:O	3:C:917:ASP:C	2.53	0.52
6:F:25:A:H3'	6:F:26:G:H5''	1.91	0.52
13:T:155:ILE:N	13:T:155:ILE:CD1	2.73	0.52
13:T:228:ARG:HH11	13:T:228:ARG:CG	2.22	0.52
14:M:9:PRO:HB2	14:M:10:PRO:CD	2.39	0.52
16:O:150:VAL:HG12	16:O:151:ASP:OD1	2.10	0.52
16:O:359:ASN:CG	16:O:360:GLN:H	2.18	0.52
24:h:99:ASP:CA	31:o:53:PRO:CB	2.88	0.52
25:i:27:VAL:HG22	25:i:92:SER:HB2	1.91	0.52
1:A:209:ILE:HG23	1:A:301:TRP:CD1	2.45	0.51
1:A:412:GLN:OE1	1:A:412:GLN:N	2.41	0.51
1:A:936:GLU:O	1:A:939:LEU:N	2.43	0.51
1:A:954:ILE:HG12	1:A:991:THR:HG22	1.91	0.51
1:A:1203:ASN:ND2	1:A:1213:MET:O	2.43	0.51
1:A:1451:PHE:O	1:A:1454:SER:OG	2.23	0.51
1:A:1490:ARG:O	1:A:1492:SER:N	2.43	0.51
3:C:734:CYS:SG	3:C:735:LEU:N	2.84	0.51
6:F:30:A:H4'	6:F:30:A:OP1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:A:N3	6:F:31:A:H5'	2.26	0.51
13:T:139:LEU:HD12	13:T:174:THR:CB	2.24	0.51
1:A:713:ASN:ND2	2:B:83:C:H4'	2.24	0.51
1:A:895:PHE:HE2	1:A:1073:ILE:HG13	1.75	0.51
1:A:1082:ILE:HG21	1:A:1113:ILE:CD1	2.37	0.51
1:A:1281:ASN:HD22	1:A:1285:VAL:CG2	2.21	0.51
1:A:1581:PHE:CD1	1:A:1582:GLU:N	2.78	0.51
1:A:1857:VAL:HG13	1:A:1894:ILE:CD1	2.40	0.51
2:B:78:A:H4'	2:B:79:C:OP1	2.10	0.51
3:C:363:PRO:O	3:C:364:PHE:HB3	2.10	0.51
3:C:733:ASN:OD1	3:C:734:CYS:N	2.43	0.51
5:E:1:G:C2'	5:E:2:U:O5'	2.59	0.51
13:T:293:LEU:CD2	13:T:314:ASP:CB	2.88	0.51
16:O:161:ASP:O	16:O:162:THR:OG1	2.24	0.51
16:O:216:ILE:HG22	16:O:217:ILE:N	2.25	0.51
18:Q:87:ASN:HD22	18:Q:90:SER:HB2	1.75	0.51
23:W:457:TRP:CD1	23:W:489:ARG:HH22	2.29	0.51
1:A:1147:PHE:C	1:A:1148:LYS:HD2	2.35	0.51
1:A:1488:ILE:CG2	1:A:1489:PRO:HD3	2.14	0.51
1:A:2014:ALA:HB3	1:A:2055:MET:HE3	1.91	0.51
3:C:324:ILE:O	3:C:328:VAL:HG23	2.09	0.51
3:C:347:ARG:O	3:C:352:VAL:HG11	2.10	0.51
3:C:428:ILE:HG22	3:C:429:PHE:CD1	2.43	0.51
3:C:585:ASP:O	3:C:588:GLN:HB3	2.10	0.51
14:M:125:ILE:HD11	14:M:126:THR:HG23	1.92	0.51
21:U:100:ILE:HD12	21:U:194:PRO:HG3	1.91	0.51
25:b:27:VAL:HG22	25:b:92:SER:HB2	1.91	0.51
1:A:452:PHE:CZ	3:C:347:ARG:HG3	2.45	0.51
3:C:471:HIS:N	3:C:487:ARG:O	2.39	0.51
3:C:831:ILE:O	3:C:835:LYS:HE2	2.11	0.51
10:J:21:LEU:O	10:J:24:ALA:N	2.43	0.51
14:M:111:ARG:HD3	18:Q:134:VAL:HG22	1.92	0.51
14:M:202:THR:HG1	14:M:252:ARG:HE	1.51	0.51
16:O:111:ILE:HB	16:O:114:ARG:HH21	1.76	0.51
16:O:203:ASP:O	16:O:204:LYS:CB	2.52	0.51
16:O:380:SER:OG	16:O:382:HIS:N	2.41	0.51
18:Q:182:LEU:O	18:Q:185:ARG:N	2.40	0.51
1:A:430:PRO:O	1:A:431:ILE:HG22	2.11	0.51
1:A:615:LEU:HD23	1:A:619:PHE:CD2	2.45	0.51
1:A:1292:ARG:HG3	1:A:1293:THR:HG23	1.93	0.51
1:A:1711:VAL:HG21	1:A:1771:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1716:LEU:N	1:A:1719:GLU:OE1	2.33	0.51
1:A:1843:LEU:O	1:A:1849:LYS:HD2	2.11	0.51
1:A:2002:TYR:HE2	22:V:329:LEU:CD1	2.16	0.51
3:C:265:PHE:CE2	3:C:295:ILE:HD12	2.46	0.51
3:C:737:ILE:HG23	3:C:768:PHE:CD2	2.46	0.51
9:I:81:MET:O	9:I:84:ALA:N	2.43	0.51
10:J:223:PRO:O	10:J:224:MET:HG2	2.09	0.51
13:T:315:LYS:CD	13:T:315:LYS:N	2.73	0.51
14:M:222:THR:HA	14:M:225:GLN:OE1	2.09	0.51
15:N:72:PHE:O	15:N:112:PHE:HD1	1.93	0.51
18:Q:108:ASN:O	18:Q:110:HIS:N	2.44	0.51
22:V:305:PHE:O	22:V:308:SER:N	2.43	0.51
24:h:47:GLU:CB	31:o:15:TYR:CG	2.93	0.51
1:A:472:ASN:O	1:A:474:LYS:N	2.44	0.51
1:A:1538:ASN:C	1:A:1539:LEU:HD12	2.36	0.51
1:A:1703:MET:HB2	1:A:1732:MET:HB2	1.93	0.51
1:A:1952:PRO:HD3	22:V:247:ARG:HH21	1.75	0.51
6:F:1116:A:C5	6:F:1117:G:N7	2.79	0.51
10:J:39:LEU:HD12	10:J:158:ARG:HH11	1.75	0.51
15:N:185:LYS:C	15:N:186:PHE:HD1	2.19	0.51
1:A:416:GLU:HB3	1:A:419:THR:HG23	1.93	0.51
1:A:1753:ARG:O	1:A:1757:LEU:HG	2.10	0.51
3:C:897:THR:O	3:C:899:LEU:N	2.41	0.51
10:J:179:SER:HB2	13:T:337:HIS:CD2	2.36	0.51
11:K:106:GLU:O	11:K:109:LEU:HB2	2.11	0.51
12:L:29:GLN:HA	12:L:32:ASP:OD2	2.11	0.51
13:T:145:SER:OG	13:T:439:THR:CG2	2.58	0.51
13:T:161:HIS:HE1	13:T:180:SER:OG	1.94	0.51
13:T:411:ASP:CG	13:T:414:THR:OG1	2.53	0.51
15:N:157:GLU:OE2	15:N:161:ARG:NE	2.44	0.51
16:O:263:VAL:O	16:O:293:TRP:HH2	1.93	0.51
1:A:149:MET:HB2	1:A:154:TYR:HD2	1.76	0.51
1:A:556:TYR:CE2	18:Q:119:MET:O	2.64	0.51
1:A:1588:LYS:HG3	1:A:1589:LYS:N	2.24	0.51
2:B:44:A:OP2	2:B:44:A:H4'	2.10	0.51
3:C:699:GLY:O	3:C:707:SER:OG	2.28	0.51
6:F:40:U:H2'	6:F:40:U:OP2	2.11	0.51
6:F:1102:C:O2'	6:F:1103:C:H5'	2.10	0.51
9:I:174:ASP:O	9:I:178:ARG:NH1	2.44	0.51
13:T:293:LEU:HD21	13:T:314:ASP:CB	2.41	0.51
20:S:336:GLU:O	20:S:337:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:TYR:CD2	1:A:1317:ARG:HD2	2.46	0.51
1:A:1082:ILE:O	1:A:1083:THR:C	2.54	0.51
1:A:1117:TYR:OH	1:A:1238:LEU:HD22	2.11	0.51
1:A:2049:ILE:O	1:A:2052:GLU:HB2	2.10	0.51
16:O:138:HIS:CE1	16:O:159:SER:HB2	2.46	0.51
33:r:124:ALA:O	33:r:127:LEU:CG	2.59	0.51
1:A:284:ARG:CZ	2:B:33:U:O4	2.59	0.51
1:A:580:ASN:O	1:A:581:LEU:C	2.54	0.51
1:A:763:MET:HE2	1:A:779:ALA:HB1	1.92	0.51
1:A:856:TRP:CG	17:P:174:VAL:HG11	2.46	0.51
1:A:934:ARG:NH2	6:F:30:A:H5'	2.25	0.51
3:C:793:GLU:HA	3:C:796:ILE:HG22	1.92	0.51
10:J:25:VAL:HG11	10:J:52:TRP:CH2	2.46	0.51
10:J:162:THR:HB	18:Q:176:ASN:O	2.11	0.51
1:A:452:PHE:HE1	3:C:347:ARG:NE	2.08	0.50
1:A:926:LYS:HD2	1:A:1521:ARG:HH22	1.75	0.50
3:C:184:GLU:OE2	3:C:192:LYS:N	2.44	0.50
5:E:9:U:H4'	5:E:10:U:OP2	2.11	0.50
6:F:18:U:C6	11:K:202:GLN:HG3	2.46	0.50
13:T:190:TRP:CE3	13:T:198:CYS:CB	2.94	0.50
13:T:411:ASP:OD1	13:T:414:THR:CB	2.59	0.50
15:N:15:GLU:HA	15:N:18:LEU:HG	1.92	0.50
15:N:207:PRO:O	15:N:212:TRP:NE1	2.44	0.50
1:A:511:ASP:CB	1:A:514:TYR:CZ	2.59	0.50
1:A:1039:TRP:CD2	1:A:1271:PRO:HB3	2.47	0.50
1:A:1182:LEU:O	1:A:1185:GLU:N	2.45	0.50
1:A:1468:ALA:HA	1:A:1473:ARG:HG2	1.93	0.50
1:A:1602:PRO:O	1:A:1605:ARG:HG2	2.12	0.50
6:F:1097:G:N1	6:F:1119:C:N3	2.50	0.50
12:L:131:GLU:OE2	12:L:135:LYS:NZ	2.36	0.50
14:M:4:GLU:O	14:M:8:PRO:HD2	2.11	0.50
14:M:217:TRP:CD1	14:M:217:TRP:C	2.89	0.50
20:S:476:ASP:O	20:S:479:SER:OG	2.19	0.50
23:W:894:LEU:C	23:W:894:LEU:HD12	2.36	0.50
1:A:139:LEU:HG	1:A:570:GLN:HE22	1.76	0.50
1:A:551:LEU:HG	1:A:557:PHE:CE2	2.46	0.50
1:A:688:TYR:O	1:A:690:LYS:N	2.44	0.50
1:A:929:LEU:HD23	1:A:937:LEU:HD12	1.93	0.50
1:A:1156:HIS:HD2	1:A:1158:ILE:HB	1.76	0.50
1:A:1232:SER:O	1:A:1234:VAL:N	2.45	0.50
3:C:655:LEU:O	3:C:658:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:A:HI1'	15:N:34:TYR:OH	2.10	0.50
9:I:136:TRP:CZ3	9:I:159:TRP:HB2	2.47	0.50
10:J:12:VAL:HG22	10:J:13:TRP:H	1.76	0.50
13:T:190:TRP:CZ3	13:T:198:CYS:CB	2.94	0.50
16:O:161:ASP:C	16:O:162:THR:HG23	2.36	0.50
16:O:414:LEU:HD12	16:O:415:ILE:H	1.76	0.50
21:U:155:LEU:HD22	21:U:159:LEU:HD23	1.94	0.50
1:A:861:GLN:NE2	1:A:1097:HIS:HB3	2.26	0.50
1:A:1129:GLU:O	1:A:1132:THR:N	2.44	0.50
3:C:120:ARG:O	3:C:123:MET:HB3	2.10	0.50
3:C:702:ASN:OD1	3:C:844:LYS:NZ	2.42	0.50
3:C:722:ASP:OD2	3:C:755:TYR:OH	2.17	0.50
3:C:864:VAL:HG22	3:C:906:VAL:HG12	1.93	0.50
5:E:14:U:C6	15:N:183:PHE:CE2	2.99	0.50
10:J:16:VAL:O	10:J:20:ILE:HD12	2.10	0.50
10:J:66:SER:O	10:J:70:ASP:N	2.44	0.50
13:T:374:LYS:HA	13:T:374:LYS:CE	2.41	0.50
13:T:408:PHE:HB3	13:T:410:TRP:CH2	2.46	0.50
1:A:168:LEU:N	1:A:169:PRO:HD2	2.26	0.50
1:A:1144:PHE:CE2	1:A:1145:MET:HE2	2.46	0.50
1:A:1494:LEU:HD22	23:W:298:GLU:CG	2.24	0.50
1:A:1716:LEU:HD23	1:A:1787:TYR:HB2	1.92	0.50
3:C:122:TYR:O	3:C:125:SER:HB3	2.12	0.50
3:C:946:ASP:HB3	3:C:949:ALA:HB2	1.92	0.50
8:H:606:GLN:HA	8:H:609:GLU:HG3	1.94	0.50
10:J:230:THR:O	10:J:232:THR:N	2.38	0.50
13:T:140:ARG:CD	13:T:140:ARG:N	2.75	0.50
13:T:191:ASP:HB3	13:T:195:ASP:HB2	1.94	0.50
33:s:100:SER:O	33:s:103:ASP:CG	2.55	0.50
1:A:857:ILE:O	1:A:858:LYS:C	2.54	0.50
3:C:139:ILE:O	3:C:237:ILE:HA	2.11	0.50
3:C:326:GLU:O	3:C:329:SER:OG	2.23	0.50
12:L:120:CYS:C	12:L:122:CYS:N	2.67	0.50
13:T:406:ARG:CA	13:T:421:ILE:O	2.60	0.50
15:N:109:LEU:HB2	15:N:114:ARG:O	2.11	0.50
15:N:233:ALA:O	15:N:237:ARG:HG3	2.12	0.50
18:Q:167:ALA:O	18:Q:184:ARG:NH2	2.45	0.50
20:S:454:ASP:O	20:S:458:ILE:HG13	2.12	0.50
1:A:784:GLN:HE22	6:F:19:U:H2'	1.76	0.50
1:A:852:LEU:O	1:A:855:LEU:N	2.44	0.50
1:A:931:ALA:HA	1:A:934:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2014:ALA:HB1	1:A:2058:LEU:HD12	1.94	0.50
2:B:174:G:OP2	26:c:76:ASN:HB2	2.12	0.50
12:L:123:ARG:O	12:L:154:ALA:HB2	2.12	0.50
13:T:402:ASP:OD1	13:T:404:LYS:N	2.45	0.50
20:S:326:VAL:HG11	20:S:364:THR:HG21	1.92	0.50
33:s:51:VAL:CG2	33:t:20:ARG:CB	2.77	0.50
1:A:224:MET:O	1:A:225:ARG:C	2.54	0.50
1:A:526:LEU:O	1:A:529:TYR:N	2.45	0.50
1:A:746:THR:OG1	1:A:749:ARG:NH2	2.44	0.50
1:A:1011:ASN:ND2	1:A:1143:GLU:O	2.45	0.50
1:A:1424:HIS:CD2	19:R:6:ILE:HG21	2.47	0.50
3:C:147:THR:OG1	3:C:214:ASP:OD2	2.30	0.50
3:C:240:ASP:OD2	3:C:269:LYS:HD3	2.05	0.50
5:E:303:A:C4	6:F:34:G:N2	2.80	0.50
16:O:323:VAL:O	16:O:323:VAL:HG13	2.10	0.50
23:W:938:ARG:HH22	23:W:947:ASP:CG	2.20	0.50
1:A:284:ARG:CZ	2:B:33:U:C4	2.95	0.50
1:A:923:TYR:HD1	1:A:926:LYS:HD3	1.77	0.50
1:A:1347:ARG:HD2	1:A:1447:TRP:CE2	2.47	0.50
1:A:1720:THR:OG1	1:A:1721:ASN:N	2.45	0.50
3:C:355:HIS:HD2	3:C:360:ARG:HB3	1.76	0.50
3:C:415:TYR:O	3:C:416:ASP:CG	2.55	0.50
3:C:468:LEU:HD12	3:C:490:SER:O	2.12	0.50
10:J:79:GLU:OE1	18:Q:205:SER:OG	2.29	0.50
13:T:132:PRO:HG3	13:T:139:LEU:HG	1.93	0.50
13:T:144:ILE:CA	13:T:394:ASP:OD1	2.59	0.50
15:N:72:PHE:CD1	15:N:90:LEU:HB2	2.47	0.50
15:N:105:ARG:HG2	15:N:109:LEU:HD11	1.92	0.50
26:j:74:ARG:HD3	30:n:101:VAL:O	2.12	0.50
1:A:453:THR:HG22	3:C:358:ASN:CB	2.42	0.49
1:A:709:ARG:NH2	2:B:83:C:P	2.81	0.49
1:A:1161:TYR:HD1	1:A:1170:MET:HG2	1.76	0.49
1:A:1494:LEU:HD23	23:W:298:GLU:CG	2.39	0.49
3:C:778:THR:HG23	3:C:781:ASP:H	1.76	0.49
5:E:1:G:H2'	5:E:2:U:O5'	2.10	0.49
6:F:1105:C:N4	32:p:97:LYS:HZ1	2.10	0.49
13:T:128:TYR:HD1	13:T:129:LEU:N	2.10	0.49
13:T:354:GLN:OE1	13:T:387:ILE:CB	2.60	0.49
18:Q:209:GLU:O	18:Q:212:ASP:HB3	2.11	0.49
1:A:289:ASP:O	1:A:290:SER:C	2.52	0.49
1:A:376:ARG:O	1:A:377:VAL:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ASN:HD21	1:A:1142:ASN:HB2	1.78	0.49
1:A:1403:SER:OG	1:A:1404:HIS:N	2.43	0.49
3:C:271:ASP:CG	35:C:1500:GTP:HN1	2.20	0.49
9:I:102:TRP:O	9:I:106:ILE:HG13	2.13	0.49
14:M:37:CYS:HB3	14:M:64:CYS:SG	2.51	0.49
15:N:234:ALA:O	15:N:237:ARG:HB2	2.12	0.49
16:O:127:ALA:HB3	16:O:428:GLN:HE21	1.77	0.49
23:W:1030:PHE:CE2	23:W:1095:ALA:HB3	2.46	0.49
25:b:86:ASN:HD21	26:c:32:LYS:NZ	2.09	0.49
1:A:307:GLU:O	1:A:310:ASN:N	2.45	0.49
1:A:745:THR:O	1:A:746:THR:HG23	2.12	0.49
1:A:776:GLN:HG2	1:A:777:LYS:H	1.77	0.49
1:A:1229:GLU:OE2	17:P:127:TRP:CZ3	2.65	0.49
1:A:1323:SER:HB2	1:A:1326:THR:OG1	2.12	0.49
4:D:84:C:O2'	4:D:85:C:OP1	2.24	0.49
9:I:149:VAL:HA	9:I:152:VAL:HG22	1.94	0.49
14:M:221:ASP:OD1	14:M:225:GLN:NE2	2.46	0.49
16:O:125:TRP:HE1	16:O:437:GLU:HG3	1.77	0.49
16:O:221:TYR:CG	16:O:222:GLY:N	2.77	0.49
16:O:306:HIS:NE2	18:Q:147:LEU:HD11	2.27	0.49
1:A:389:HIS:HB2	3:C:653:ASP:OD1	2.12	0.49
1:A:1339:LEU:HD21	1:A:1440:ILE:HD12	1.94	0.49
3:C:700:GLU:HG2	3:C:701:GLU:O	2.11	0.49
3:C:831:ILE:HG13	3:C:832:ASP:H	1.76	0.49
3:C:860:PRO:O	3:C:861:ILE:HG13	2.12	0.49
5:E:14:U:C4	15:N:183:PHE:HD2	2.30	0.49
6:F:1120:G:H8	6:F:1120:G:C5'	2.25	0.49
13:T:308:PHE:N	13:T:308:PHE:CD1	2.81	0.49
14:M:95:ASN:CG	14:M:96:GLU:H	2.20	0.49
15:N:4:TRP:NE1	15:N:60:GLY:O	2.45	0.49
15:N:22:ILE:HG22	15:N:30:PHE:CZ	2.46	0.49
16:O:148:ASP:CG	16:O:150:VAL:H	2.17	0.49
1:A:1041:VAL:HG11	1:A:1253:LYS:HA	1.95	0.49
1:A:1113:ILE:O	1:A:1116:TYR:HB3	2.12	0.49
1:A:1682:THR:OG1	1:A:1702:THR:OG1	2.13	0.49
1:A:1775:ILE:HG12	1:A:1786:ALA:HB2	1.94	0.49
1:A:1927:GLU:HG3	21:U:135:LEU:HD12	1.84	0.49
9:I:85:ARG:HH22	10:J:237:ILE:HD11	1.77	0.49
9:I:198:GLN:HB2	9:I:201:THR:HG23	1.95	0.49
10:J:513:ILE:HA	10:J:516:LYS:CG	2.43	0.49
11:K:187:LYS:HA	11:K:201:LYS:HZ1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:193:GLU:OE1	11:K:204:ASN:HB3	2.11	0.49
12:L:98:THR:OG1	12:L:99:GLY:N	2.45	0.49
13:T:55:GLU:OE2	13:T:58:ARG:HD2	2.13	0.49
15:N:249:MET:HA	15:N:252:HIS:CD2	2.47	0.49
1:A:801:VAL:CG1	1:A:802:PRO:HD2	2.42	0.49
1:A:1813:TYR:CE2	22:V:269:LYS:HB2	2.48	0.49
1:A:1910:LYS:O	1:A:1913:THR:OG1	2.30	0.49
3:C:775:ILE:HG22	3:C:776:ASN:H	1.78	0.49
4:D:31:G:N1	14:M:53:ASN:O	2.46	0.49
5:E:283:U:H4'	5:E:284:U:OP1	2.12	0.49
10:J:148:GLU:HA	10:J:151:MET:HE3	1.94	0.49
13:T:132:PRO:CG	13:T:139:LEU:HG	2.42	0.49
1:A:140:ARG:O	1:A:144:ASN:HB2	2.12	0.49
1:A:332:ASP:N	1:A:332:ASP:OD1	2.44	0.49
1:A:381:SER:OG	1:A:382:GLU:N	2.42	0.49
1:A:971:MET:HB3	1:A:978:ILE:CG2	2.42	0.49
1:A:1176:GLU:O	1:A:1180:GLU:HB2	2.11	0.49
1:A:1375:LEU:O	1:A:1376:ASN:ND2	2.45	0.49
1:A:1390:THR:OG1	1:A:1396:GLY:HA3	2.12	0.49
3:C:606:VAL:HG12	3:C:607:LEU:N	2.28	0.49
3:C:716:ASP:HB3	3:C:719:MET:HB2	1.95	0.49
9:I:117:HIS:ND1	10:J:230:THR:HG21	2.28	0.49
9:I:119:ARG:O	9:I:122:MET:N	2.43	0.49
10:J:26:GLN:HA	18:Q:182:LEU:HD23	1.93	0.49
12:L:100:TYR:O	12:L:102:LYS:N	2.45	0.49
20:S:305:GLY:HA2	20:S:342:PHE:CE1	2.47	0.49
20:S:459:ARG:O	20:S:463:ASN:CB	2.60	0.49
1:A:168:LEU:HD11	1:A:571:LEU:HD11	1.93	0.49
1:A:488:ARG:NH1	2:B:81:A:H62	2.08	0.49
3:C:778:THR:HG21	3:C:822:SER:HB2	1.94	0.49
8:H:726:ARG:HA	8:H:729:TYR:CE2	2.48	0.49
10:J:63:THR:HG22	10:J:93:ARG:HH12	1.76	0.49
17:P:37:LEU:HD23	17:P:37:LEU:HA	1.65	0.49
20:S:439:ARG:O	20:S:443:SER:OG	2.18	0.49
26:c:74:ARG:HD3	30:g:101:VAL:O	2.12	0.49
1:A:594:ASP:OD1	1:A:594:ASP:N	2.45	0.49
1:A:1153:GLU:O	1:A:1159:ARG:NE	2.46	0.49
1:A:1624:LEU:HD21	1:A:1635:HIS:ND1	2.28	0.49
1:A:1986:MET:HE2	21:U:184:MET:CG	2.40	0.49
4:D:41:A:N9	15:N:34:TYR:CE2	2.81	0.49
6:F:119:G:OP2	26:j:76:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1109:C:N4	32:p:108:THR:HA	2.28	0.49
10:J:218:VAL:HG12	10:J:219:TYR:CD2	2.47	0.49
13:T:222:LEU:HD23	13:T:222:LEU:C	2.38	0.49
14:M:118:VAL:HG23	14:M:119:LYS:O	2.12	0.49
16:O:216:ILE:CG2	16:O:217:ILE:N	2.76	0.49
18:Q:65:GLU:O	18:Q:68:ALA:N	2.46	0.49
22:V:336:TYR:O	22:V:339:LEU:HB2	2.13	0.49
1:A:1286:TRP:CE2	1:A:1302:LEU:HD11	2.48	0.49
1:A:1677:GLN:HB3	1:A:1706:VAL:HB	1.94	0.49
6:F:20:G:C2	17:P:6:ARG:HD3	2.47	0.49
7:G:86:LEU:O	7:G:89:GLU:CG	2.61	0.49
11:K:185:ASN:O	11:K:189:LEU:HG	2.13	0.49
13:T:132:PRO:HB3	13:T:176:HIS:CE1	2.39	0.49
13:T:164:GLY:HA2	13:T:449:GLY:CA	2.43	0.49
14:M:216:GLU:HG3	14:M:240:LEU:HD23	1.94	0.49
1:A:676:GLN:NE2	1:A:714:PHE:HB2	2.27	0.48
1:A:953:ARG:HG2	1:A:957:TYR:HE2	1.78	0.48
3:C:225:THR:O	3:C:228:ALA:N	2.46	0.48
3:C:268:ASN:HA	3:C:314:ALA:O	2.12	0.48
3:C:316:THR:OG1	35:C:1500:GTP:N7	2.46	0.48
3:C:636:VAL:HG12	3:C:637:GLU:N	2.27	0.48
3:C:711:ALA:O	3:C:818:TYR:HA	2.13	0.48
5:E:-1:G:C2	5:E:351:U:C4	3.00	0.48
9:I:106:ILE:HG12	9:I:122:MET:HE3	1.95	0.48
9:I:182:TRP:O	9:I:186:ARG:NH1	2.46	0.48
10:J:14:THR:HG23	10:J:17:GLU:H	1.78	0.48
12:L:140:VAL:O	12:L:140:VAL:HG13	2.13	0.48
13:T:406:ARG:CB	13:T:421:ILE:O	2.61	0.48
15:N:93:ILE:HG23	15:N:94:PRO:HD2	1.95	0.48
18:Q:84:ASN:O	18:Q:125:ARG:NH1	2.32	0.48
25:i:86:ASN:HD21	26:j:32:LYS:NZ	2.09	0.48
1:A:1585:MET:O	1:A:1590:LEU:CD1	2.57	0.48
1:A:2056:ARG:NH2	22:V:332:ASN:N	2.54	0.48
3:C:291:ILE:O	3:C:294:ASN:N	2.46	0.48
3:C:947:LYS:HD2	3:C:947:LYS:N	2.28	0.48
5:E:293:A:H2'	5:E:294:G:C1'	2.44	0.48
10:J:31:HIS:HD2	18:Q:171:ASN:HB3	1.78	0.48
13:T:135:VAL:CG1	13:T:193:TYR:CE1	2.86	0.48
13:T:302:PHE:CG	13:T:303:PRO:N	2.81	0.48
13:T:414:THR:O	13:T:415:SER:OG	2.29	0.48
16:O:414:LEU:O	16:O:425:ILE:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:THR:O	1:A:1032:ILE:N	2.46	0.48
1:A:1080:ASP:HB3	10:J:82:ASN:ND2	2.28	0.48
1:A:1699:ALA:HB1	1:A:1733:TRP:CG	2.48	0.48
1:A:1748:ILE:HD11	1:A:1783:MET:HB2	1.95	0.48
2:B:79:C:O2	2:B:79:C:C3'	2.59	0.48
3:C:233:ASP:OD1	3:C:487:ARG:NH2	2.47	0.48
8:H:712:CYS:O	8:H:713:ILE:C	2.57	0.48
11:K:187:LYS:HA	11:K:201:LYS:NZ	2.27	0.48
13:T:150:LEU:H	13:T:150:LEU:CD1	2.09	0.48
13:T:295:SER:C	13:T:313:GLU:HB2	2.39	0.48
14:M:104:ALA:HB1	14:M:110:LYS:CB	2.40	0.48
22:V:339:LEU:O	22:V:342:LYS:N	2.46	0.48
1:A:783:LEU:HD12	1:A:783:LEU:H	1.78	0.48
1:A:872:PRO:HD3	18:Q:201:PHE:CE1	2.49	0.48
1:A:1050:LEU:HD23	1:A:1248:VAL:HG22	1.94	0.48
1:A:2056:ARG:HE	22:V:331:ALA:HB1	1.77	0.48
3:C:602:VAL:HG12	3:C:908:VAL:HG21	1.94	0.48
13:T:191:ASP:CG	13:T:195:ASP:CB	2.86	0.48
13:T:373:PRO:C	13:T:374:LYS:HE2	2.38	0.48
1:A:603:LYS:O	1:A:604:THR:C	2.56	0.48
1:A:1372:LYS:HG2	1:A:1383:PHE:CE2	2.48	0.48
1:A:1624:LEU:HD11	1:A:1635:HIS:CE1	2.49	0.48
1:A:1999:ILE:HD11	1:A:2007:ARG:NH2	2.28	0.48
4:D:50:G:OP2	4:D:50:G:H8	1.97	0.48
13:T:179:LEU:HD23	13:T:179:LEU:C	2.38	0.48
13:T:190:TRP:CZ3	13:T:198:CYS:HB2	2.48	0.48
14:M:220:THR:HG23	14:M:240:LEU:HD22	1.94	0.48
1:A:266:LEU:HG	1:A:267:PRO:HD2	1.96	0.48
1:A:531:LEU:HA	1:A:531:LEU:HD23	1.65	0.48
1:A:1955:ALA:HA	22:V:271:ARG:HD2	1.95	0.48
3:C:167:ASN:O	3:C:171:GLY:HA3	2.14	0.48
3:C:927:MET:HG3	3:C:928:CYS:N	2.27	0.48
13:T:110:GLU:HA	13:T:200:ARG:CD	2.43	0.48
13:T:308:PHE:HD1	13:T:308:PHE:N	2.10	0.48
20:S:338:THR:HG22	20:S:339:PHE:N	2.29	0.48
1:A:999:LEU:O	1:A:1000:TRP:C	2.56	0.48
1:A:1986:MET:CB	21:U:184:MET:HG2	2.16	0.48
1:A:2002:TYR:HE1	22:V:307:ARG:CG	2.12	0.48
1:A:2052:GLU:OE1	22:V:333:PRO:HD2	2.13	0.48
1:A:2064:GLY:HA2	1:A:2069:VAL:O	2.13	0.48
1:A:2075:THR:O	1:A:2079:ILE:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:ILE:O	3:C:380:PRO:HG2	2.13	0.48
3:C:418:GLN:HB3	3:C:419:PRO:HD3	1.95	0.48
4:D:29:U:C1'	12:L:120:CYS:HB3	2.39	0.48
5:E:-3:A:C3'	5:E:-2:A:C5'	2.91	0.48
6:F:25:A:H3'	6:F:26:G:C5'	2.43	0.48
6:F:39:A:H2'	6:F:40:U:H5'	1.95	0.48
9:I:172:PHE:CE2	9:I:188:ILE:HG12	2.49	0.48
15:N:55:PRO:HG2	15:N:166:ARG:HD2	1.94	0.48
1:A:137:GLU:O	1:A:140:ARG:N	2.45	0.48
1:A:223:ALA:HB2	1:A:266:LEU:HD12	1.95	0.48
1:A:1339:LEU:HD11	1:A:1343:PHE:CE2	2.49	0.48
1:A:1648:ILE:HG22	1:A:1649:PHE:CE1	2.49	0.48
10:J:39:LEU:HD21	10:J:159:LEU:HD21	1.96	0.48
14:M:26:THR:HG22	14:M:27:LYS:N	2.27	0.48
16:O:211:LEU:O	16:O:212:GLU:C	2.57	0.48
17:P:167:GLN:O	17:P:171:HIS:HB2	2.14	0.48
21:U:89:LYS:HD2	21:U:89:LYS:N	2.29	0.48
1:A:974:ASN:C	1:A:976:GLN:H	2.22	0.48
1:A:1797:LEU:O	1:A:1801:SER:CB	2.62	0.48
1:A:1902:GLN:HE21	1:A:1908:LEU:HD21	1.78	0.48
1:A:1925:PRO:O	1:A:1929:GLN:HG3	2.13	0.48
2:B:96:U:O2	5:E:351:U:O2	2.31	0.48
3:C:706:LEU:HD21	3:C:834:MET:CE	2.41	0.48
4:D:49:A:H2'	4:D:50:G:H5'	1.96	0.48
4:D:56:A:H2'	4:D:57:U:C6	2.49	0.48
6:F:1116:A:N6	6:F:1117:G:O6	2.46	0.48
16:O:118:LEU:HD11	18:Q:48:GLN:HG2	1.96	0.48
16:O:155:PHE:CD2	16:O:167:TRP:HB2	2.49	0.48
16:O:265:HIS:CE1	16:O:291:ARG:HG2	2.49	0.48
20:S:285:SER:O	20:S:287:ASN:N	2.47	0.48
25:i:34:GLN:HE21	25:i:37:ILE:HD12	1.79	0.48
1:A:255:ILE:HD11	1:A:637:VAL:HG13	1.95	0.48
1:A:779:ALA:O	1:A:782:ILE:N	2.47	0.48
1:A:852:LEU:HD23	1:A:852:LEU:HA	1.56	0.48
1:A:1047:ALA:HA	1:A:1172:PHE:O	2.14	0.48
1:A:1899:TRP:CH2	1:A:1909:ALA:HA	2.45	0.48
1:A:1944:LEU:O	1:A:1948:MET:HG2	2.13	0.48
12:L:119:THR:O	12:L:120:CYS:C	2.55	0.48
13:T:63:ARG:NH1	13:T:70:GLY:O	2.40	0.48
13:T:112:VAL:HG21	13:T:197:GLU:CG	2.43	0.48
15:N:69:GLN:HG2	15:N:70:LEU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:348:GLU:HG2	16:O:349:LYS:H	1.78	0.48
18:Q:105:LEU:HD12	18:Q:106:LEU:H	1.78	0.48
1:A:783:LEU:HD12	1:A:783:LEU:N	2.29	0.47
1:A:1748:ILE:O	1:A:1749:SER:C	2.57	0.47
1:A:1880:PHE:CZ	1:A:1882:LEU:HD23	2.49	0.47
3:C:277:LEU:HB3	3:C:279:LEU:CD1	2.43	0.47
3:C:717:SER:O	3:C:721:GLN:CB	2.62	0.47
6:F:18:U:C5	11:K:202:GLN:CG	2.97	0.47
13:T:144:ILE:HA	13:T:394:ASP:OD1	2.14	0.47
14:M:24:ARG:HH11	18:Q:115:VAL:HG21	1.78	0.47
15:N:152:LYS:HG2	15:N:154:ALA:H	1.78	0.47
16:O:304:LEU:HD13	16:O:334:TRP:CE3	2.49	0.47
23:W:883:GLN:HB2	23:W:894:LEU:HD21	1.94	0.47
1:A:1878:CYS:SG	1:A:1891:LEU:HD22	2.54	0.47
1:A:1969:MET:HE1	1:A:1978:VAL:HG21	1.97	0.47
4:D:25:C:O2'	12:L:98:THR:OG1	2.03	0.47
15:N:134:ASN:ND2	15:N:226:ALA:O	2.47	0.47
15:N:255:ASN:O	15:N:259:ASN:ND2	2.36	0.47
16:O:125:TRP:HZ2	16:O:432:ALA:HB1	1.78	0.47
1:A:582:LEU:HD23	1:A:582:LEU:C	2.40	0.47
1:A:677:ILE:O	1:A:681:LYS:HG3	2.14	0.47
1:A:1026:TYR:HA	1:A:1286:TRP:CZ3	2.48	0.47
1:A:1540:ASN:O	1:A:1543:ARG:N	2.47	0.47
6:F:34:G:H2'	6:F:35:U:C6	2.49	0.47
6:F:1099:G:N3	6:F:1099:G:C5'	2.73	0.47
6:F:1100:A:C2	6:F:1101:C:N1	2.82	0.47
13:T:201:ASP:C	13:T:202:PHE:CD1	2.91	0.47
15:N:231:ASP:C	15:N:231:ASP:OD1	2.56	0.47
16:O:333:SER:C	16:O:334:TRP:CD1	2.92	0.47
16:O:348:GLU:CG	16:O:349:LYS:N	2.78	0.47
20:S:339:PHE:HE2	20:S:387:PHE:HA	1.78	0.47
1:A:380:ARG:NH2	1:A:382:GLU:OE2	2.47	0.47
1:A:2063:TYR:HA	1:A:2067:TYR:CD1	2.49	0.47
3:C:265:PHE:HD2	3:C:295:ILE:HD12	1.77	0.47
3:C:885:GLY:HA3	3:C:906:VAL:HA	1.95	0.47
10:J:152:LEU:O	10:J:156:ARG:CB	2.62	0.47
14:M:12:ILE:HB	18:Q:105:LEU:HD21	1.96	0.47
15:N:188:TYR:O	15:N:189:GLN:C	2.57	0.47
21:U:229:TRP:O	21:U:233:ILE:HG12	2.14	0.47
1:A:503:LYS:HA	1:A:506:PHE:CE2	2.50	0.47
1:A:1049:LEU:HB2	1:A:1249:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:GLU:HA	1:A:1481:GLU:HB2	1.96	0.47
3:C:75:GLU:OE1	16:O:133:ARG:NE	2.47	0.47
3:C:315:SER:HB3	3:C:320:PHE:CE2	2.49	0.47
3:C:716:ASP:HB3	3:C:719:MET:CB	2.45	0.47
4:D:34:A:N1	15:N:73:CYS:HA	2.29	0.47
4:D:89:U:C5	11:K:176:TYR:O	2.62	0.47
9:I:99:ILE:HA	9:I:102:TRP:HD1	1.79	0.47
10:J:152:LEU:O	10:J:156:ARG:HB3	2.14	0.47
13:T:111:GLU:O	13:T:112:VAL:HG23	2.14	0.47
14:M:13:CYS:SG	14:M:17:LEU:N	2.86	0.47
14:M:98:ASN:O	14:M:99:VAL:HG12	2.15	0.47
16:O:229:THR:HG22	16:O:230:VAL:N	2.29	0.47
16:O:303:VAL:O	16:O:304:LEU:HD23	2.15	0.47
22:V:267:ASP:OD1	22:V:267:ASP:N	2.44	0.47
1:A:258:ILE:HG12	1:A:641:LEU:HA	1.97	0.47
1:A:308:MET:HE3	1:A:486:PHE:HD1	1.80	0.47
1:A:828:HIS:O	1:A:829:TYR:C	2.58	0.47
1:A:978:ILE:O	17:P:175:ARG:HB3	2.15	0.47
1:A:1031:GLY:HA3	1:A:1145:MET:HE3	1.97	0.47
1:A:1372:LYS:HB3	1:A:1377:SER:O	2.14	0.47
5:E:-2:A:H5'	5:E:-2:A:H8	1.79	0.47
9:I:117:HIS:CE1	10:J:230:THR:HG21	2.49	0.47
9:I:189:TYR:O	9:I:193:VAL:HG22	2.14	0.47
10:J:103:ASN:O	10:J:107:GLU:HG3	2.15	0.47
10:J:581:GLN:O	10:J:584:LEU:CG	2.63	0.47
12:L:102:LYS:N	12:L:155:SER:OG	2.47	0.47
14:M:123:ALA:O	14:M:124:GLN:C	2.58	0.47
16:O:328:THR:O	16:O:353:ILE:HG12	2.15	0.47
20:S:361:TYR:O	20:S:362:ASN:C	2.56	0.47
1:A:366:GLU:HG3	1:A:372:ARG:NH1	2.23	0.47
1:A:665:GLY:HA2	1:A:667:TYR:CE1	2.49	0.47
1:A:823:TRP:CZ2	1:A:851:ARG:HG2	2.50	0.47
1:A:1423:THR:HB	1:A:1424:HIS:CD2	2.49	0.47
1:A:1431:HIS:HB2	1:A:1433:ASP:O	2.14	0.47
1:A:1458:TRP:CZ2	1:A:1491:ILE:HD13	2.50	0.47
1:A:1559:HIS:O	1:A:1612:PRO:HG2	2.15	0.47
1:A:1870:VAL:HB	5:E:300:A:O4'	2.14	0.47
1:A:1955:ALA:CB	22:V:271:ARG:CB	2.93	0.47
2:B:44:A:OP2	2:B:44:A:C4'	2.62	0.47
2:B:79:C:H3'	2:B:80:G:H5'	1.95	0.47
3:C:148:SER:OG	3:C:149:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:355:HIS:CE1	3:C:360:ARG:HH21	2.33	0.47
3:C:794:GLN:HE22	3:C:835:LYS:HD2	1.80	0.47
3:C:908:VAL:HG13	3:C:909:ILE:N	2.29	0.47
4:D:45:A:O5'	4:D:45:A:H8	1.98	0.47
11:K:106:GLU:HA	11:K:109:LEU:HD12	1.96	0.47
13:T:216:GLU:CG	13:T:257:PRO:HA	2.45	0.47
15:N:64:GLY:O	15:N:68:GLY:N	2.47	0.47
15:N:163:VAL:HG11	15:N:199:MET:HE2	1.96	0.47
15:N:244:LEU:O	15:N:247:LEU:HB3	2.14	0.47
20:S:386:LYS:HG2	20:S:426:GLU:HB2	1.96	0.47
1:A:960:THR:OG1	1:A:961:GLN:N	2.47	0.47
1:A:1025:VAL:HG21	1:A:1265:PHE:CD2	2.43	0.47
1:A:1613:THR:OG1	1:A:1614:ILE:N	2.46	0.47
1:A:1751:TYR:O	1:A:1755:LYS:HG2	2.15	0.47
3:C:241:VAL:HG13	3:C:242:VAL:N	2.30	0.47
3:C:314:ALA:CB	3:C:321:THR:HG22	2.45	0.47
3:C:320:PHE:CD2	3:C:425:LEU:HD13	2.50	0.47
5:E:294:G:HO2'	5:E:295:A:P	2.27	0.47
12:L:44:LYS:O	12:L:45:SER:C	2.56	0.47
13:T:154:VAL:C	13:T:155:ILE:HD12	2.40	0.47
16:O:211:LEU:HD23	16:O:211:LEU:HA	1.74	0.47
20:S:310:HIS:O	20:S:311:LYS:C	2.57	0.47
1:A:1320:LEU:HD23	1:A:1320:LEU:HA	1.78	0.47
5:E:286:A:C2	13:T:414:THR:HB	2.50	0.47
6:F:21:G:N7	17:P:5:HIS:HB3	2.29	0.47
13:T:356:MET:CE	13:T:356:MET:CA	2.93	0.47
14:M:38:THR:O	14:M:39:LEU:HD12	2.14	0.47
16:O:217:ILE:HG22	16:O:218:ARG:CG	2.43	0.47
18:Q:35:ALA:O	18:Q:37:ASN:N	2.48	0.47
1:A:225:ARG:NH2	1:A:693:LYS:O	2.48	0.47
1:A:634:ASP:O	1:A:635:THR:C	2.58	0.47
1:A:666:ILE:O	1:A:666:ILE:HG12	2.14	0.47
1:A:1111:SER:HA	1:A:1514:PHE:HE2	1.79	0.47
1:A:1144:PHE:HE2	1:A:1145:MET:HE2	1.80	0.47
1:A:1343:PHE:CD1	1:A:1350:ILE:HD13	2.50	0.47
1:A:1423:THR:C	1:A:1424:HIS:CG	2.93	0.47
2:B:167:A:N7	30:g:63:ARG:CZ	2.78	0.47
3:C:490:SER:HA	3:C:558:LYS:HD3	1.96	0.47
4:D:48:C:H4'	13:T:293:LEU:CD1	2.44	0.47
6:F:112:A:N7	30:n:63:ARG:CZ	2.78	0.47
8:H:645:ARG:NE	8:H:669:TYR:OH	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:250:LEU:HD23	16:O:250:LEU:HA	1.63	0.47
16:O:320:GLU:OE2	18:Q:47:ARG:NH1	2.40	0.47
20:S:369:TYR:CZ	20:S:405:ILE:HG12	2.50	0.47
1:A:353:GLU:HG2	2:B:104:G:O5'	2.15	0.46
1:A:461:LEU:H	1:A:461:LEU:HG	1.56	0.46
1:A:620:HIS:HB3	1:A:669:TYR:CZ	2.49	0.46
1:A:991:THR:O	1:A:992:ASP:C	2.58	0.46
1:A:1203:ASN:HD22	1:A:1213:MET:HB3	1.78	0.46
1:A:1471:GLN:OE1	1:A:1473:ARG:NE	2.48	0.46
1:A:1678:ILE:N	1:A:1706:VAL:HG23	2.30	0.46
1:A:1708:GLU:HA	1:A:1730:ASN:OD1	2.15	0.46
6:F:40:U:H4'	6:F:41:C:OP1	2.15	0.46
8:H:642:GLU:HG3	9:I:324:TRP:CB	2.44	0.46
16:O:345:PHE:CE2	16:O:364:LEU:HD22	2.49	0.46
25:b:34:GLN:HE21	25:b:37:ILE:HD12	1.78	0.46
28:l:30:ARG:C	28:l:47:VAL:HG23	2.40	0.46
1:A:239:PHE:CD1	1:A:241:PRO:HD3	2.50	0.46
1:A:385:VAL:O	1:A:385:VAL:HG12	2.15	0.46
1:A:526:LEU:O	1:A:527:LYS:C	2.57	0.46
1:A:758:LEU:HD23	1:A:759:ARG:N	2.30	0.46
1:A:790:TRP:CD1	1:A:819:LYS:HZ3	2.34	0.46
1:A:1689:ARG:HA	1:A:1692:TYR:CE1	2.51	0.46
1:A:1716:LEU:HA	1:A:1787:TYR:HA	1.97	0.46
2:B:179:U:OP1	30:g:79:LYS:HG2	2.16	0.46
3:C:745:ARG:O	3:C:748:SER:OG	2.20	0.46
5:E:296:U:C3'	5:E:297:A:H5''	2.45	0.46
10:J:181:ARG:O	10:J:185:LEU:HG	2.15	0.46
13:T:135:VAL:CG2	13:T:193:TYR:CE1	2.93	0.46
13:T:188:LYS:CB	13:T:190:TRP:CZ2	2.99	0.46
15:N:182:GLY:C	15:N:183:PHE:HD1	2.22	0.46
16:O:189:ALA:O	16:O:197:LEU:HD12	2.16	0.46
21:U:183:TYR:HE2	21:U:234:LYS:HE3	1.79	0.46
23:W:542:VAL:HG23	23:W:564:ILE:CD1	2.45	0.46
1:A:215:ALA:O	1:A:216:GLN:C	2.57	0.46
1:A:1888:HIS:HB3	1:A:1988:LEU:HD23	1.97	0.46
3:C:307:ILE:HG12	3:C:346:THR:HA	1.96	0.46
5:E:299:U:H4'	5:E:300:A:OP1	2.15	0.46
6:F:40:U:C1'	6:F:41:C:OP1	2.64	0.46
6:F:120:G:H4'	6:F:121:C:O4'	2.15	0.46
6:F:1115:G:H2'	6:F:1116:A:C8	2.50	0.46
6:F:1115:G:H2'	6:F:1116:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:106:ILE:O	9:I:109:GLU:N	2.46	0.46
12:L:50:TRP:CD1	12:L:148:CYS:O	2.68	0.46
13:T:139:LEU:HD11	13:T:175:GLY:C	2.40	0.46
14:M:33:GLU:HG2	14:M:34:CYS:O	2.15	0.46
16:O:341:LEU:HG	16:O:342:LEU:O	2.15	0.46
16:O:348:GLU:CD	16:O:349:LYS:N	2.73	0.46
17:P:8:GLN:C	17:P:9:LEU:HG	2.39	0.46
21:U:97:PRO:HB2	21:U:197:VAL:HG21	1.97	0.46
23:W:888:GLU:CD	23:W:890:LYS:HZ1	2.23	0.46
26:c:16:LYS:N	26:c:17:PRO:CD	2.79	0.46
1:A:428:LEU:HD22	3:C:896:GLY:O	2.16	0.46
1:A:470:LEU:HB3	1:A:471:PRO:HD2	1.97	0.46
1:A:1286:TRP:CD1	1:A:1448:GLU:OE2	2.68	0.46
1:A:1346:PHE:O	1:A:1347:ARG:C	2.56	0.46
1:A:1427:ALA:O	19:R:16:THR:HB	2.16	0.46
1:A:1581:PHE:CE1	1:A:1598:LEU:HD11	2.49	0.46
2:B:175:G:H4'	2:B:176:A:O4'	2.15	0.46
3:C:440:THR:HG22	3:C:441:ARG:N	2.29	0.46
4:D:15:C:OP2	4:D:15:C:C6	2.68	0.46
5:E:1:G:C5'	5:E:301:A:C4	2.98	0.46
6:F:18:U:C5	11:K:202:GLN:CD	2.94	0.46
14:M:60:ILE:HD12	14:M:65:ALA:HB2	1.97	0.46
18:Q:159:ASP:O	18:Q:162:GLU:N	2.49	0.46
1:A:404:ASN:CG	1:A:405:ASN:N	2.73	0.46
1:A:737:ARG:HG2	4:D:69:C:OP2	2.16	0.46
1:A:742:VAL:HG23	1:A:743:LYS:N	2.30	0.46
1:A:1505:ASP:OD1	1:A:1506:ARG:N	2.48	0.46
1:A:1861:THR:HG21	1:A:1875:ILE:HG13	1.97	0.46
2:B:174:G:N7	29:f:20:LYS:CE	2.77	0.46
3:C:317:LYS:N	35:C:1500:GTP:O6	2.35	0.46
3:C:480:GLY:O	3:C:481:ALA:C	2.58	0.46
5:E:345:A:HO2'	5:E:346:A:C5'	2.28	0.46
12:L:32:ASP:O	12:L:35:LYS:HD3	2.15	0.46
13:T:132:PRO:CA	13:T:176:HIS:CE1	2.98	0.46
13:T:340:PRO:CD	13:T:356:MET:HE3	2.46	0.46
13:T:391:PHE:HA	13:T:397:TYR:O	2.15	0.46
15:N:18:LEU:HD11	15:N:82:CYS:SG	2.55	0.46
15:N:74:LEU:HB3	15:N:112:PHE:CD1	2.50	0.46
16:O:306:HIS:N	16:O:306:HIS:CD2	2.80	0.46
21:U:136:PHE:CZ	21:U:140:LYS:HD2	2.50	0.46
25:i:86:ASN:ND2	26:j:32:LYS:NZ	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:l:39:SER:O	28:l:41:ASN:N	2.48	0.46
1:A:153:MET:HE2	1:A:154:TYR:CE1	2.51	0.46
1:A:304:ASP:CG	1:A:306:PRO:HD2	2.40	0.46
1:A:814:ARG:HD3	16:O:398:GLY:O	2.16	0.46
1:A:988:GLU:O	1:A:991:THR:OG1	2.34	0.46
1:A:1782:ASN:ND2	1:A:1816:ARG:HH21	2.14	0.46
3:C:391:MET:HE1	3:C:395:LYS:HG2	1.97	0.46
3:C:394:ASP:C	3:C:394:ASP:OD1	2.59	0.46
6:F:119:G:N7	29:m:20:LYS:CE	2.77	0.46
8:H:730:GLN:C	8:H:733:ILE:HD12	2.38	0.46
17:P:30:LEU:HD23	17:P:30:LEU:HA	1.78	0.46
20:S:413:CYS:O	20:S:416:GLY:N	2.48	0.46
20:S:465:PHE:HB2	20:S:474:THR:HG21	1.97	0.46
23:W:933:GLN:H	23:W:989:HIS:CD2	2.33	0.46
1:A:228:LYS:HD2	1:A:700:GLY:HA3	1.98	0.46
1:A:1365:THR:HG22	1:A:1429:MET:HE3	1.98	0.46
1:A:1750:ARG:O	1:A:1754:ALA:CB	2.60	0.46
1:A:1893:ILE:HD12	1:A:1985:GLN:HG2	1.96	0.46
3:C:825:VAL:HG13	3:C:826:PRO:HD2	1.97	0.46
5:E:14:U:C5	15:N:183:PHE:HE2	2.33	0.46
5:E:14:U:C6	15:N:183:PHE:HE2	2.33	0.46
11:K:207:LEU:HD21	18:Q:167:ALA:HB3	1.97	0.46
13:T:289:TYR:CD2	13:T:320:TRP:CZ3	3.01	0.46
15:N:69:GLN:CG	15:N:70:LEU:H	2.28	0.46
24:a:20:LEU:O	24:a:31:ILE:HA	2.16	0.46
1:A:1066:LEU:O	1:A:1067:ASN:C	2.59	0.46
1:A:1077:ASN:O	1:A:1080:ASP:N	2.48	0.46
1:A:1585:MET:HE2	1:A:1585:MET:CA	2.46	0.46
1:A:1863:HIS:O	1:A:1871:ALA:CB	2.59	0.46
1:A:1877:GLY:C	1:A:1894:ILE:HB	2.40	0.46
1:A:1907:GLN:O	1:A:1911:TRP:HD1	1.98	0.46
3:C:268:ASN:C	3:C:269:LYS:HG3	2.40	0.46
5:E:296:U:H3'	5:E:297:A:H5''	1.98	0.46
13:T:190:TRP:CZ3	13:T:198:CYS:HB3	2.51	0.46
14:M:16:CYS:SG	15:N:104:LEU:HD11	2.56	0.46
16:O:245:ASP:O	16:O:246:SER:HB2	2.16	0.46
16:O:308:LYS:C	16:O:309:ARG:HG3	2.40	0.46
16:O:317:HIS:CG	16:O:320:GLU:HB3	2.51	0.46
18:Q:220:ARG:O	18:Q:224:GLU:HG2	2.16	0.46
23:W:957:TYR:CD2	23:W:1064:TYR:CD1	3.04	0.46
25:i:30:TRP:CE2	25:i:89:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:j:16:LYS:N	26:j:17:PRO:CD	2.79	0.46
1:A:249:LEU:HD12	1:A:249:LEU:O	2.16	0.46
1:A:285:PRO:HD2	1:A:298:TYR:OH	2.16	0.46
1:A:859:ASN:ND2	17:P:170:LEU:HD12	2.30	0.46
1:A:901:PRO:HB2	1:A:955:LYS:HE3	1.98	0.46
1:A:1049:LEU:HA	1:A:1170:MET:O	2.15	0.46
1:A:1144:PHE:HD2	1:A:1145:MET:HG2	1.80	0.46
1:A:1282:ASP:CG	1:A:1283:GLU:H	2.23	0.46
1:A:1447:TRP:O	1:A:1448:GLU:C	2.59	0.46
1:A:1498:ASP:OD1	1:A:1498:ASP:N	2.48	0.46
3:C:761:ALA:O	3:C:764:ASN:N	2.49	0.46
4:D:44:A:H2'	4:D:45:A:C8	2.50	0.46
6:F:119:G:C8	30:n:99:ASP:OD2	2.69	0.46
8:H:606:GLN:HA	8:H:609:GLU:HG2	1.98	0.46
12:L:88:ASP:HB3	12:L:91:LEU:HB3	1.98	0.46
14:M:14:GLU:CG	18:Q:106:LEU:HD13	2.46	0.46
14:M:14:GLU:HG3	18:Q:106:LEU:HD13	1.97	0.46
16:O:224:LEU:HB2	16:O:245:ASP:CG	2.41	0.46
21:U:82:GLN:HA	21:U:85:ILE:HG12	1.97	0.46
1:A:332:ASP:OD1	1:A:335:SER:OG	2.22	0.46
1:A:488:ARG:NH2	3:C:172:TRP:CZ2	2.84	0.46
1:A:1413:SER:OG	1:A:1414:TRP:N	2.47	0.46
3:C:184:GLU:CD	3:C:191:ILE:H	2.23	0.46
11:K:99:GLN:O	11:K:103:LEU:HG	2.16	0.46
14:M:206:PHE:HB3	14:M:208:TYR:CZ	2.51	0.46
15:N:48:VAL:HG13	15:N:218:GLY:O	2.16	0.46
15:N:91:HIS:O	15:N:92:HIS:CB	2.63	0.46
20:S:413:CYS:SG	20:S:415:GLN:HB2	2.56	0.46
25:b:30:TRP:CE2	25:b:89:LEU:HD22	2.51	0.46
1:A:275:TYR:CE2	1:A:306:PRO:HB2	2.51	0.45
1:A:902:PRO:HG2	1:A:905:TYR:HD1	1.81	0.45
1:A:976:GLN:HE22	1:A:1310:LYS:HD3	1.81	0.45
1:A:1077:ASN:O	1:A:1078:ILE:C	2.59	0.45
1:A:1130:ARG:HD2	1:A:1133:ASP:OD2	2.16	0.45
1:A:1275:MET:C	1:A:1277:GLU:H	2.23	0.45
1:A:1382:ARG:HD3	1:A:1614:ILE:O	2.16	0.45
1:A:1986:MET:CE	21:U:184:MET:CG	2.88	0.45
2:B:75:A:H4'	2:B:76:U:C5'	2.46	0.45
3:C:271:ASP:OD1	3:C:272:ARG:N	2.49	0.45
4:D:84:C:N3	17:P:4:SER:OG	2.42	0.45
5:E:352:A:O3'	5:E:353:A:O4'	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:20:G:H21	17:P:6:ARG:HB3	1.21	0.45
6:F:20:G:C6	17:P:6:ARG:HD3	2.51	0.45
12:L:51:GLU:O	12:L:52:ILE:C	2.59	0.45
13:T:248:SER:OG	13:T:269:ASN:HB2	2.16	0.45
13:T:392:SER:HG	13:T:397:TYR:CB	2.29	0.45
16:O:200:VAL:CG2	16:O:206:VAL:HG22	2.46	0.45
25:b:86:ASN:ND2	26:c:32:LYS:NZ	2.64	0.45
29:f:6:PHE:CZ	29:f:10:LEU:HD11	2.51	0.45
29:m:6:PHE:CZ	29:m:10:LEU:HD11	2.51	0.45
1:A:1001:TYR:O	1:A:1005:GLN:HB2	2.16	0.45
1:A:1147:PHE:CD2	1:A:1153:GLU:HG2	2.51	0.45
1:A:1259:LEU:O	1:A:1260:PHE:HB3	2.16	0.45
1:A:1608:LEU:HD12	1:A:1644:SER:HB2	1.94	0.45
2:B:60:U:O2	2:B:60:U:O4'	2.34	0.45
3:C:137:GLY:O	3:C:235:VAL:HA	2.17	0.45
3:C:607:LEU:HD22	3:C:668:ILE:HD12	1.98	0.45
6:F:20:G:H1'	17:P:7:PRO:CG	2.45	0.45
13:T:357:ASP:OD1	13:T:357:ASP:C	2.59	0.45
14:M:258:LEU:O	14:M:262:PHE:HB3	2.15	0.45
20:S:473:LEU:HD23	20:S:473:LEU:HA	1.80	0.45
1:A:782:ILE:HD12	1:A:782:ILE:HA	1.81	0.45
2:B:167:A:N7	30:g:63:ARG:NH1	2.65	0.45
3:C:700:GLU:HG2	3:C:701:GLU:N	2.32	0.45
13:T:135:VAL:CG1	13:T:193:TYR:CZ	2.83	0.45
13:T:228:ARG:CG	13:T:228:ARG:NH1	2.79	0.45
14:M:94:VAL:O	14:M:95:ASN:HB3	2.17	0.45
16:O:243:GLY:O	16:O:245:ASP:N	2.49	0.45
16:O:396:LEU:O	16:O:399:GLU:N	2.23	0.45
23:W:911:LEU:C	23:W:912:LEU:O	2.59	0.45
1:A:234:PHE:CE2	1:A:700:GLY:HA2	2.51	0.45
1:A:860:GLU:OE2	1:A:863:ARG:NH2	2.50	0.45
1:A:1122:ASP:OD2	1:A:1163:ARG:NE	2.50	0.45
1:A:1748:ILE:HG22	1:A:1752:VAL:CG2	2.45	0.45
1:A:2043:PHE:HB2	1:A:2048:TRP:CD1	2.51	0.45
3:C:608:GLN:HG3	3:C:609:PRO:HD2	1.98	0.45
4:D:49:A:C2'	4:D:50:G:H5'	2.47	0.45
8:H:730:GLN:CA	8:H:733:ILE:CD1	2.86	0.45
13:T:191:ASP:CG	13:T:193:TYR:H	2.24	0.45
20:S:437:GLN:HA	20:S:473:LEU:HD21	1.98	0.45
28:e:39:SER:O	28:e:41:ASN:N	2.48	0.45
30:g:49:ARG:HD2	30:g:49:ARG:HA	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:q:102:LEU:HD12	33:t:98:LEU:HD21	1.99	0.45
1:A:660:ILE:C	1:A:662:GLN:H	2.23	0.45
1:A:728:ASN:O	1:A:729:LEU:C	2.59	0.45
1:A:1988:LEU:HD11	21:U:184:MET:SD	2.57	0.45
5:E:303:A:C2	6:F:34:G:C2	3.05	0.45
8:H:624:TRP:HE1	8:H:651:ALA:CB	2.30	0.45
10:J:94:PRO:HG2	10:J:97:VAL:HB	1.98	0.45
10:J:96:GLN:OE1	10:J:96:GLN:N	2.44	0.45
12:L:16:PHE:O	12:L:19:ILE:HG12	2.17	0.45
14:M:25:MET:HB2	14:M:45:HIS:O	2.15	0.45
1:A:1041:VAL:HG21	1:A:1274:ARG:NH1	2.31	0.45
1:A:1077:ASN:O	1:A:1080:ASP:HB2	2.16	0.45
1:A:1489:PRO:HB3	23:W:301:GLN:HE22	1.81	0.45
1:A:1540:ASN:O	1:A:1541:ALA:C	2.59	0.45
1:A:1794:LEU:O	1:A:1795:LYS:C	2.59	0.45
3:C:323:THR:O	3:C:326:GLU:N	2.49	0.45
5:E:-2:A:H5'	5:E:-2:A:C8	2.51	0.45
5:E:353:A:N3	5:E:353:A:C2'	2.78	0.45
9:I:205:TRP:O	9:I:208:PHE:HB3	2.16	0.45
12:L:122:CYS:HB2	12:L:145:CYS:HB2	1.98	0.45
13:T:306:SER:O	13:T:321:GLU:HA	2.16	0.45
15:N:117:PHE:O	15:N:129:SER:HA	2.17	0.45
18:Q:111:HIS:O	18:Q:112:ILE:CG1	2.64	0.45
1:A:466:GLU:OE1	1:A:466:GLU:N	2.41	0.45
3:C:151:ASP:OD1	3:C:175:LEU:HD22	2.17	0.45
3:C:637:GLU:HB2	3:C:639:SER:OG	2.16	0.45
3:C:879:LEU:O	3:C:883:ARG:HG2	2.17	0.45
6:F:1098:C:H2'	6:F:1099:G:H5''	1.98	0.45
6:F:1103:C:N1	6:F:1114:G:N2	2.64	0.45
13:T:111:GLU:HB2	13:T:200:ARG:HA	1.99	0.45
13:T:300:LYS:O	13:T:308:PHE:CB	2.56	0.45
17:P:34:HIS:C	17:P:36:THR:H	2.25	0.45
20:S:384:LEU:O	20:S:385:GLY:C	2.59	0.45
1:A:153:MET:HE2	1:A:154:TYR:HE1	1.81	0.45
1:A:645:ASP:OD1	1:A:646:ALA:N	2.50	0.45
1:A:682:ASP:O	1:A:683:LEU:C	2.60	0.45
3:C:737:ILE:HG12	3:C:768:PHE:HB3	1.99	0.45
3:C:777:ASP:O	3:C:778:THR:HB	2.17	0.45
6:F:1116:A:C4	6:F:1117:G:C5	3.05	0.45
6:F:1120:G:C5'	6:F:1120:G:C8	3.00	0.45
8:H:729:TYR:O	8:H:733:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:16:CYS:HB2	15:N:104:LEU:HD21	1.99	0.45
14:M:25:MET:HE2	14:M:46:PHE:CD2	2.52	0.45
16:O:203:ASP:C	16:O:203:ASP:OD1	2.58	0.45
18:Q:227:ARG:O	18:Q:231:GLU:HB2	2.17	0.45
23:W:1058:SER:HA	23:W:1059:LEU:HD12	1.98	0.45
33:r:62:LEU:O	33:r:63:THR:C	2.59	0.45
1:A:687:ILE:HD11	1:A:706:PRO:HG2	1.99	0.45
1:A:1326:THR:O	1:A:1327:THR:OG1	2.27	0.45
1:A:1751:TYR:CZ	1:A:1755:LYS:HG3	2.52	0.45
3:C:215:ALA:HB1	3:C:225:THR:HG22	1.98	0.45
5:E:292:U:H2'	5:E:293:A:C8	2.52	0.45
6:F:112:A:N7	30:n:63:ARG:NH1	2.65	0.45
8:H:673:GLU:CB	8:H:683:SER:HB3	2.47	0.45
14:M:246:ALA:HB3	14:M:248:CYS:SG	2.57	0.45
15:N:95:ASP:OD1	15:N:97:GLU:N	2.49	0.45
22:V:256:LEU:HD23	22:V:256:LEU:HA	1.63	0.45
1:A:295:GLY:O	1:A:298:TYR:N	2.36	0.45
1:A:664:THR:OG1	1:A:665:GLY:N	2.49	0.45
1:A:910:LYS:O	1:A:913:VAL:HB	2.17	0.45
1:A:1051:GLU:HG2	1:A:1169:TYR:HE1	1.82	0.45
1:A:1611:SER:N	1:A:1612:PRO:CD	2.80	0.45
1:A:1849:LYS:O	1:A:1884:PRO:HD2	2.17	0.45
3:C:106:PHE:CZ	3:C:478:TYR:HD2	2.35	0.45
3:C:236:LEU:HD11	3:C:439:ILE:HG12	2.00	0.45
3:C:660:ARG:HH22	3:C:670:ILE:HD12	1.81	0.45
5:E:289:A:OP1	13:T:375:LYS:HE3	2.17	0.45
13:T:172:PRO:O	13:T:173:LYS:CB	2.65	0.45
14:M:206:PHE:HB3	14:M:208:TYR:OH	2.17	0.45
15:N:110:ASP:OD1	15:N:113:GLY:N	2.49	0.45
16:O:119:LEU:HA	16:O:119:LEU:HD23	1.71	0.45
16:O:304:LEU:HB3	16:O:334:TRP:CZ3	2.51	0.45
1:A:667:TYR:CD2	1:A:667:TYR:C	2.95	0.44
1:A:1379:MET:HE2	1:A:1379:MET:HB3	1.90	0.44
1:A:2011:LEU:HD13	1:A:2040:TRP:CE3	2.53	0.44
3:C:194:ASN:OD1	3:C:195:GLY:N	2.50	0.44
3:C:743:ASN:O	3:C:747:LEU:N	2.42	0.44
3:C:817:GLN:NE2	3:C:819:LYS:HE3	2.32	0.44
10:J:22:LYS:O	10:J:26:GLN:HB2	2.17	0.44
15:N:135:LYS:HD3	15:N:187:LYS:O	2.17	0.44
18:Q:70:THR:O	18:Q:71:LYS:C	2.60	0.44
20:S:414:PRO:HA	20:S:417:ARG:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:1059:LEU:HA	23:W:1064:TYR:CE1	2.51	0.44
25:i:30:TRP:CD2	25:i:89:LEU:HD22	2.52	0.44
1:A:1130:ARG:NH2	1:A:1158:ILE:O	2.51	0.44
1:A:1736:VAL:HA	1:A:1775:ILE:O	2.17	0.44
3:C:624:LYS:O	3:C:628:TYR:HD1	2.00	0.44
13:T:308:PHE:CE1	13:T:320:TRP:CB	2.86	0.44
13:T:319:ILE:O	13:T:328:ILE:N	2.49	0.44
13:T:347:SER:O	13:T:348:GLN:CB	2.65	0.44
14:M:86:LEU:O	14:M:87:ARG:C	2.58	0.44
16:O:262:LEU:HD22	16:O:293:TRP:CE3	2.52	0.44
18:Q:196:THR:OG1	18:Q:197:ILE:N	2.50	0.44
1:A:157:ASP:O	1:A:160:ALA:HB3	2.17	0.44
1:A:514:TYR:HB3	1:A:518:VAL:CG2	2.44	0.44
1:A:779:ALA:O	1:A:780:ARG:C	2.59	0.44
1:A:1008:LEU:HD22	1:A:1073:ILE:HD11	1.98	0.44
1:A:1082:ILE:C	1:A:1085:LYS:H	2.24	0.44
1:A:1343:PHE:HE1	1:A:1350:ILE:HG21	1.81	0.44
3:C:809:ALA:HB3	3:C:811:GLU:HB2	1.99	0.44
3:C:916:THR:O	3:C:919:ARG:N	2.50	0.44
9:I:122:MET:HA	9:I:122:MET:CE	2.40	0.44
9:I:200:GLN:HA	9:I:203:LEU:HB3	1.98	0.44
10:J:230:THR:OG1	10:J:231:SER:N	2.50	0.44
13:T:293:LEU:CD2	13:T:293:LEU:N	2.73	0.44
16:O:358:ILE:HG12	16:O:364:LEU:HD11	1.99	0.44
16:O:391:GLU:O	16:O:392:MET:HB2	2.17	0.44
18:Q:105:LEU:HG	18:Q:106:LEU:HG	1.99	0.44
19:R:23:SER:HA	20:S:310:HIS:HD2	1.81	0.44
20:S:368:ASN:HA	20:S:372:ASP:HB3	1.98	0.44
23:W:1030:PHE:CZ	23:W:1095:ALA:HB3	2.51	0.44
33:q:14:VAL:HG12	33:q:52:GLU:HA	1.99	0.44
1:A:889:TRP:HD1	1:A:890:LEU:HG	1.81	0.44
1:A:1709:TRP:O	1:A:1728:ILE:CA	2.50	0.44
3:C:81:LYS:O	3:C:82:ASN:ND2	2.51	0.44
3:C:727:THR:HG22	3:C:736:ASP:HB2	2.00	0.44
3:C:772:ASN:HB3	3:C:816:VAL:H	1.82	0.44
6:F:1100:A:H61	6:F:1116:A:N6	2.07	0.44
8:H:433:LEU:O	8:H:437:PRO:N	2.50	0.44
8:H:712:CYS:O	8:H:715:LYS:N	2.49	0.44
9:I:99:ILE:N	9:I:100:PRO:CD	2.80	0.44
9:I:149:VAL:O	9:I:150:GLU:C	2.61	0.44
13:T:400:SER:HB3	13:T:410:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:81:HIS:O	14:M:82:ILE:HG13	2.18	0.44
15:N:96:GLU:OE2	15:N:187:LYS:NZ	2.50	0.44
15:N:127:ILE:HG22	15:N:128:GLY:N	2.32	0.44
18:Q:70:THR:O	18:Q:73:TYR:N	2.51	0.44
18:Q:85:SER:O	18:Q:87:ASN:N	2.48	0.44
23:W:960:HIS:HB2	23:W:1025:PHE:CE2	2.53	0.44
33:t:100:SER:O	33:t:103:ASP:CG	2.60	0.44
1:A:194:HIS:CD2	18:Q:122:LEU:HD22	2.52	0.44
1:A:422:LEU:HD12	1:A:469:ILE:HD11	1.98	0.44
1:A:517:LYS:NZ	34:A:3000:IHP:O43	2.48	0.44
1:A:580:ASN:O	1:A:583:ILE:N	2.50	0.44
1:A:636:HIS:O	1:A:637:VAL:C	2.59	0.44
1:A:867:ILE:HG21	1:A:1101:TYR:CD1	2.51	0.44
1:A:1306:GLU:HA	1:A:1309:ILE:HD12	1.99	0.44
1:A:1952:PRO:HD3	22:V:247:ARG:NH2	2.33	0.44
3:C:221:PHE:O	3:C:222:MET:C	2.61	0.44
3:C:920:LEU:O	3:C:922:THR:N	2.50	0.44
4:D:97:A:H2'	4:D:98:G:C8	2.52	0.44
6:F:20:G:C4	17:P:6:ARG:HD3	2.53	0.44
10:J:148:GLU:HG2	10:J:151:MET:HE3	1.99	0.44
12:L:55:LEU:O	12:L:56:HIS:C	2.61	0.44
12:L:88:ASP:OD1	12:L:90:LEU:N	2.50	0.44
13:T:60:ARG:O	13:T:61:LYS:C	2.60	0.44
14:M:38:THR:C	14:M:39:LEU:HD12	2.43	0.44
20:S:297:LEU:HA	20:S:297:LEU:HD12	1.68	0.44
20:S:363:GLU:O	20:S:366:GLU:N	2.50	0.44
20:S:408:THR:CB	20:S:410:GLU:HB3	2.47	0.44
33:r:5:ILE:HG23	33:s:96:PHE:HD2	1.80	0.44
1:A:1347:ARG:O	1:A:1441:PHE:CE1	2.71	0.44
1:A:1557:LEU:HD13	1:A:1562:PHE:CD2	2.53	0.44
3:C:363:PRO:O	3:C:364:PHE:CB	2.66	0.44
4:D:29:U:C4'	12:L:120:CYS:HA	2.47	0.44
4:D:64:U:C2'	4:D:65:U:O5'	2.66	0.44
8:H:574:TYR:CZ	8:H:591:PHE:HB2	2.52	0.44
16:O:217:ILE:HD13	16:O:217:ILE:HA	1.49	0.44
18:Q:34:ILE:HG23	18:Q:35:ALA:H	1.83	0.44
18:Q:216:ARG:HA	18:Q:219:ILE:CD1	2.48	0.44
20:S:364:THR:O	20:S:368:ASN:ND2	2.50	0.44
24:h:20:LEU:O	24:h:31:ILE:HA	2.16	0.44
1:A:591:LEU:HA	1:A:591:LEU:HD23	1.68	0.44
1:A:926:LYS:HE3	1:A:929:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:ARG:O	1:A:956:LYS:HB3	2.18	0.44
1:A:1542:TYR:O	1:A:1543:ARG:C	2.61	0.44
1:A:1570:TRP:CG	1:A:1571:GLU:N	2.82	0.44
1:A:1699:ALA:HB2	1:A:1767:TYR:CD1	2.53	0.44
1:A:2013:ARG:NH2	1:A:2083:ILE:O	2.50	0.44
4:D:41:A:H1'	15:N:34:TYR:CZ	2.53	0.44
6:F:19:U:O4	18:Q:174:ASN:OD1	2.35	0.44
6:F:20:G:N3	17:P:7:PRO:CD	2.58	0.44
10:J:90:MET:CE	18:Q:197:ILE:HG23	2.47	0.44
13:T:358:ASN:CG	13:T:358:ASN:O	2.60	0.44
14:M:119:LYS:O	14:M:120:LEU:HG	2.17	0.44
16:O:200:VAL:CG1	16:O:230:VAL:HG23	2.47	0.44
16:O:206:VAL:HG21	16:O:241:THR:HG21	2.00	0.44
16:O:217:ILE:HG23	16:O:217:ILE:HD12	1.48	0.44
16:O:295:VAL:HG23	16:O:296:VAL:N	2.33	0.44
20:S:422:PHE:O	20:S:423:LEU:C	2.59	0.44
25:b:30:TRP:CD2	25:b:89:LEU:HD22	2.52	0.44
9:I:99:ILE:O	9:I:100:PRO:C	2.61	0.44
13:T:126:ARG:NH1	13:T:126:ARG:HB2	2.32	0.44
13:T:392:SER:OG	13:T:397:TYR:HB2	2.17	0.44
21:U:81:ILE:HD12	21:U:81:ILE:H	1.83	0.44
1:A:266:LEU:HD23	1:A:268:LEU:H	1.83	0.44
1:A:525:LEU:HD23	1:A:525:LEU:HA	1.72	0.44
1:A:569:LEU:O	1:A:572:CYS:N	2.51	0.44
1:A:853:THR:HB	1:A:971:MET:HG3	2.00	0.44
1:A:1555:THR:O	1:A:1556:ILE:C	2.61	0.44
3:C:172:TRP:CD1	3:C:172:TRP:N	2.86	0.44
4:D:35:A:H8	15:N:75:PHE:CE2	2.33	0.44
6:F:1102:C:C2	6:F:1103:C:C5	3.06	0.44
9:I:248:ASN:O	9:I:252:HIS:HB3	2.17	0.44
10:J:104:ARG:HA	10:J:107:GLU:HB2	2.00	0.44
13:T:192:PHE:CG	13:T:192:PHE:O	2.70	0.44
15:N:176:VAL:HG12	15:N:179:LYS:H	1.83	0.44
15:N:189:GLN:HG3	15:N:193:GLU:OE2	2.18	0.44
16:O:125:TRP:NE1	16:O:437:GLU:OE1	2.51	0.44
16:O:193:ARG:HH22	16:O:237:ASP:H	1.63	0.44
18:Q:60:LYS:HD2	18:Q:60:LYS:HA	1.81	0.44
20:S:368:ASN:O	20:S:373:ILE:HG12	2.17	0.44
1:A:400:ILE:HA	1:A:401:PRO:HD2	1.87	0.43
1:A:472:ASN:O	1:A:475:ASP:N	2.47	0.43
1:A:512:GLU:N	1:A:514:TYR:CE2	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:GLU:O	1:A:934:ARG:C	2.61	0.43
1:A:1490:ARG:O	1:A:1491:ILE:C	2.61	0.43
1:A:1509:ARG:O	1:A:1510:ILE:C	2.59	0.43
1:A:1710:GLU:HB2	1:A:1724:PHE:HB3	2.00	0.43
1:A:1716:LEU:HB2	1:A:1719:GLU:HG3	1.99	0.43
1:A:1782:ASN:OD1	1:A:1782:ASN:O	2.35	0.43
1:A:1855:THR:HA	1:A:1937:ARG:NH2	2.33	0.43
3:C:501:ILE:HD11	3:C:577:LEU:HD12	1.99	0.43
6:F:39:A:C2'	6:F:40:U:H5'	2.48	0.43
12:L:32:ASP:HA	12:L:35:LYS:HD3	2.00	0.43
13:T:357:ASP:O	13:T:358:ASN:HB3	2.17	0.43
14:M:34:CYS:HB2	14:M:37:CYS:SG	2.58	0.43
15:N:31:ASN:C	15:N:31:ASN:OD1	2.61	0.43
15:N:102:LEU:O	15:N:105:ARG:N	2.39	0.43
15:N:234:ALA:O	15:N:238:LEU:HG	2.18	0.43
33:q:102:LEU:O	33:q:105:LEU:CG	2.66	0.43
1:A:237:MET:HB2	1:A:237:MET:HE3	1.80	0.43
1:A:402:TRP:HE1	1:A:405:ASN:HD21	1.63	0.43
1:A:564:TRP:O	1:A:567:ALA:N	2.51	0.43
1:A:1023:LEU:HD13	1:A:1451:PHE:CE1	2.53	0.43
1:A:1562:PHE:HB2	1:A:1609:TRP:HH2	1.83	0.43
1:A:1613:THR:O	1:A:1614:ILE:C	2.61	0.43
1:A:1805:ILE:HG23	1:A:1809:ASN:HD22	1.82	0.43
5:E:299:U:O2'	5:E:300:A:P	2.76	0.43
8:H:508:LEU:O	8:H:511:ALA:HB3	2.19	0.43
9:I:88:PHE:O	9:I:89:GLU:C	2.60	0.43
13:T:151:PRO:CG	13:T:454:CYS:C	2.91	0.43
13:T:191:ASP:CG	13:T:195:ASP:CG	2.86	0.43
13:T:228:ARG:NH1	13:T:247:ASN:O	2.51	0.43
13:T:289:TYR:CE2	13:T:325:ASN:HA	2.53	0.43
14:M:3:ASP:O	14:M:5:ILE:N	2.51	0.43
15:N:144:GLY:O	15:N:203:THR:HA	2.18	0.43
16:O:262:LEU:HA	16:O:262:LEU:HD23	1.79	0.43
16:O:295:VAL:HG23	16:O:296:VAL:HG23	2.00	0.43
16:O:379:LYS:HD2	18:Q:47:ARG:HH21	1.82	0.43
18:Q:103:ASN:ND2	18:Q:114:VAL:HG21	2.33	0.43
20:S:424:PHE:CZ	20:S:448:MET:HE1	2.54	0.43
1:A:275:TYR:HD2	1:A:310:ASN:HD21	1.65	0.43
1:A:574:GLN:O	1:A:575:GLY:C	2.61	0.43
1:A:605:LEU:HA	1:A:605:LEU:HD23	1.73	0.43
1:A:708:TRP:O	1:A:712:LEU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:LEU:O	1:A:853:THR:C	2.61	0.43
1:A:936:GLU:O	1:A:937:LEU:C	2.60	0.43
1:A:950:THR:O	1:A:953:ARG:N	2.52	0.43
1:A:1411:ASP:H	19:R:6:ILE:HG22	1.83	0.43
3:C:510:ARG:HD2	3:C:591:PHE:CE2	2.53	0.43
4:D:40:A:H2	15:N:121:ARG:NE	1.66	0.43
11:K:146:ASP:HB2	11:K:149:THR:O	2.18	0.43
11:K:169:GLN:O	11:K:172:SER:OG	2.33	0.43
12:L:121:ILE:HD12	12:L:121:ILE:HA	1.77	0.43
13:T:393:GLY:O	13:T:394:ASP:CB	2.66	0.43
13:T:411:ASP:O	13:T:415:SER:N	2.51	0.43
16:O:120:SER:OG	16:O:121:GLN:OE1	2.36	0.43
16:O:437:GLU:N	16:O:438:PRO:HD3	2.33	0.43
17:P:170:LEU:HD23	17:P:170:LEU:HA	1.74	0.43
20:S:480:ARG:HD3	20:S:483:ILE:HD12	2.00	0.43
26:c:16:LYS:CG	26:c:17:PRO:HD3	2.49	0.43
29:f:17:ILE:HG12	29:f:95:ILE:HG23	2.00	0.43
24:h:87:LEU:HG	24:h:92:ILE:HD11	2.00	0.43
25:i:88:THR:HG23	27:k:67:SER:CB	2.49	0.43
29:m:17:ILE:HG12	29:m:95:ILE:HG23	2.00	0.43
1:A:235:LYS:NZ	1:A:1758:ASP:OD1	2.50	0.43
1:A:361:GLU:OE1	1:A:361:GLU:N	2.52	0.43
1:A:644:VAL:O	1:A:645:ASP:HB2	2.18	0.43
1:A:962:ARG:HA	1:A:962:ARG:HD3	1.82	0.43
1:A:1400:ILE:HG23	1:A:1542:TYR:CE2	2.53	0.43
3:C:152:LEU:HD23	3:C:152:LEU:HA	1.74	0.43
3:C:254:LYS:O	3:C:258:LYS:HB2	2.19	0.43
3:C:317:LYS:HB2	35:C:1500:GTP:C6	2.54	0.43
3:C:786:GLU:O	3:C:789:SER:OG	2.28	0.43
6:F:120:G:C2	25:i:33:GLU:O	2.71	0.43
7:G:81:ASP:C	7:G:82:ASP:CG	2.86	0.43
11:K:203:PHE:O	11:K:206:LYS:HB3	2.18	0.43
12:L:106:LEU:HD23	12:L:106:LEU:HA	1.80	0.43
13:T:409:THR:O	13:T:417:LEU:HD12	2.18	0.43
15:N:145:ALA:HB2	15:N:204:LEU:HD12	2.00	0.43
16:O:292:LEU:HD23	16:O:292:LEU:HA	1.78	0.43
17:P:8:GLN:O	17:P:10:GLU:N	2.50	0.43
23:W:725:LEU:HD21	23:W:753:VAL:CG2	2.49	0.43
23:W:1023:LYS:HZ3	23:W:1090:TRP:CD1	2.35	0.43
24:h:47:GLU:HB3	31:o:15:TYR:CG	2.52	0.43
1:A:160:ALA:HA	18:Q:123:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:CB	1:A:299:LYS:O	2.67	0.43
1:A:570:GLN:O	1:A:574:GLN:HG2	2.18	0.43
1:A:683:LEU:O	1:A:684:LYS:C	2.60	0.43
1:A:1418:THR:O	1:A:1419:ASP:CG	2.61	0.43
1:A:2017:THR:HB	1:A:2062:GLU:OE2	2.18	0.43
2:B:83:C:HO2'	2:B:84:A:P	2.40	0.43
3:C:353:TYR:CD2	3:C:364:PHE:HA	2.53	0.43
5:E:-1:G:O6	5:E:351:U:O4	2.36	0.43
9:I:192:TYR:CZ	9:I:201:THR:HG22	2.52	0.43
13:T:200:ARG:NH2	13:T:237:THR:CA	2.67	0.43
14:M:48:THR:HG1	14:M:49:SER:H	1.65	0.43
16:O:133:ARG:NH1	16:O:170:ALA:O	2.50	0.43
16:O:162:THR:HG22	16:O:183:MET:C	2.43	0.43
19:R:9:LYS:O	19:R:10:SER:OG	2.30	0.43
19:R:23:SER:HA	20:S:310:HIS:CD2	2.53	0.43
21:U:220:ILE:HG22	21:U:221:MET:N	2.34	0.43
25:b:45:GLY:HA3	25:b:53:VAL:HG12	2.00	0.43
28:l:14:ALA:HA	28:l:78:LEU:HD21	2.01	0.43
33:s:112:VAL:O	33:s:115:GLU:CG	2.66	0.43
1:A:193:TYR:HD1	1:A:194:HIS:O	2.02	0.43
1:A:194:HIS:HA	1:A:557:PHE:CD1	2.54	0.43
1:A:937:LEU:HD23	1:A:937:LEU:HA	1.86	0.43
2:B:96:U:C2	5:E:351:U:O2	2.71	0.43
3:C:495:ARG:N	3:C:554:HIS:O	2.51	0.43
3:C:758:ASP:CG	3:C:761:ALA:H	2.27	0.43
4:D:64:U:O2'	4:D:65:U:O5'	2.37	0.43
5:E:1:G:N2	5:E:349:A:HO2'	2.14	0.43
6:F:20:G:C5	17:P:6:ARG:HD3	2.54	0.43
9:I:233:GLN:HG2	9:I:274:TRP:CZ2	2.54	0.43
13:T:320:TRP:CZ3	13:T:325:ASN:O	2.72	0.43
21:U:81:ILE:H	21:U:81:ILE:CD1	2.32	0.43
1:A:751:ASP:O	1:A:752:ALA:C	2.56	0.43
1:A:790:TRP:CG	1:A:819:LYS:HZ3	2.37	0.43
1:A:803:GLY:O	18:Q:166:PRO:HG3	2.19	0.43
1:A:1023:LEU:HD13	1:A:1451:PHE:CD1	2.54	0.43
1:A:1051:GLU:HG2	1:A:1169:TYR:CE1	2.54	0.43
3:C:110:LYS:NZ	3:C:552:PRO:HG2	2.34	0.43
3:C:200:CYS:SG	3:C:210:ILE:HD12	2.58	0.43
3:C:246:THR:HG23	3:C:248:VAL:HG12	2.00	0.43
5:E:11:A:C2	15:N:46:ARG:HD3	2.52	0.43
6:F:121:C:O2'	29:m:20:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:172:PRO:O	13:T:173:LYS:HB3	2.19	0.43
14:M:87:ARG:HH22	14:M:122:GLY:C	2.26	0.43
16:O:125:TRP:CE2	16:O:433:THR:O	2.72	0.43
16:O:155:PHE:HD2	16:O:167:TRP:CD1	2.37	0.43
18:Q:165:ILE:HG22	18:Q:166:PRO:O	2.19	0.43
22:V:267:ASP:O	22:V:269:LYS:N	2.51	0.43
25:b:88:THR:HG23	27:d:67:SER:CB	2.49	0.43
25:i:34:GLN:NE2	25:i:37:ILE:HD12	2.34	0.43
1:A:143:ILE:O	1:A:147:SER:OG	2.31	0.43
1:A:638:GLN:O	1:A:639:PHE:C	2.61	0.43
1:A:1130:ARG:O	1:A:1133:ASP:HB2	2.18	0.43
1:A:1180:GLU:O	1:A:1184:ASP:CG	2.60	0.43
1:A:1795:LYS:O	1:A:1799:GLN:HG3	2.17	0.43
2:B:75:A:H4'	2:B:76:U:H5'	2.00	0.43
3:C:766:TRP:CD1	3:C:776:ASN:ND2	2.87	0.43
5:E:-10:A:N6	19:R:6:ILE:HD11	2.34	0.43
9:I:85:ARG:NH2	10:J:237:ILE:HD11	2.33	0.43
13:T:200:ARG:HH21	13:T:236:GLU:C	2.27	0.43
15:N:186:PHE:N	15:N:186:PHE:CD1	2.87	0.43
18:Q:65:GLU:OE1	18:Q:65:GLU:HA	2.19	0.43
20:S:414:PRO:N	20:S:417:ARG:HH11	2.17	0.43
21:U:114:ASN:HD21	21:U:151:ARG:HH21	1.65	0.43
28:e:14:ALA:HA	28:e:78:LEU:HD21	2.01	0.43
26:j:16:LYS:CG	26:j:17:PRO:HD3	2.49	0.43
30:n:49:ARG:HA	30:n:49:ARG:HD2	1.64	0.43
1:A:265:ASN:O	1:A:266:LEU:HB2	2.17	0.43
1:A:452:PHE:CZ	3:C:343:ASP:OD1	2.72	0.43
1:A:462:LEU:HB3	3:C:383:LYS:HD3	2.01	0.43
1:A:683:LEU:HD23	1:A:683:LEU:HA	1.79	0.43
1:A:766:ILE:HG21	1:A:782:ILE:HG21	2.00	0.43
1:A:954:ILE:O	1:A:955:LYS:C	2.62	0.43
1:A:992:ASP:HB3	1:A:1108:LYS:HB2	2.00	0.43
1:A:1068:ARG:O	1:A:1071:ARG:N	2.51	0.43
1:A:1573:LEU:HD23	1:A:1825:ILE:HG21	2.01	0.43
1:A:1668:ILE:HD11	22:V:256:LEU:HD21	2.00	0.43
2:B:175:G:C2	25:b:33:GLU:O	2.71	0.43
4:D:53:A:C5'	4:D:54:U:OP2	2.67	0.43
5:E:6:U:H2'	5:E:7:A:C8	2.54	0.43
13:T:351:PHE:O	13:T:362:SER:HA	2.18	0.43
14:M:5:ILE:HG22	14:M:42:THR:HG23	2.00	0.43
14:M:223:VAL:O	14:M:227:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:445:LEU:O	20:S:449:PHE:HB2	2.18	0.43
23:W:957:TYR:CE2	23:W:1064:TYR:HA	2.54	0.43
1:A:797:ILE:HD12	18:Q:172:TRP:HH2	1.84	0.43
1:A:1033:ASN:C	1:A:1033:ASN:OD1	2.62	0.43
1:A:1476:ALA:C	1:A:1478:GLU:N	2.76	0.43
3:C:355:HIS:ND1	3:C:366:ASN:HB2	2.34	0.43
3:C:362:LYS:HD3	3:C:365:GLU:HB3	2.01	0.43
3:C:648:GLY:O	3:C:651:TYR:HB3	2.18	0.43
3:C:716:ASP:OD2	3:C:718:LYS:HB3	2.19	0.43
3:C:872:LEU:HB3	3:C:875:ILE:HD12	2.00	0.43
4:D:87:U:C5	4:D:88:U:C4	3.06	0.43
6:F:15:C:C2'	6:F:16:U:H5''	2.48	0.43
6:F:1097:G:H2'	6:F:1098:C:C6	2.54	0.43
7:G:136:VAL:O	7:G:139:GLN:CG	2.67	0.43
9:I:158:LYS:HA	9:I:158:LYS:HD2	1.83	0.43
10:J:204:LYS:HG2	10:J:205:LYS:H	1.83	0.43
12:L:47:GLU:O	12:L:50:TRP:N	2.51	0.43
13:T:139:LEU:CD2	13:T:193:TYR:OH	2.57	0.43
14:M:4:GLU:O	14:M:7:GLU:N	2.47	0.43
16:O:162:THR:HG21	16:O:182:VAL:O	2.18	0.43
16:O:360:GLN:HE22	16:O:409:LYS:C	2.26	0.43
18:Q:52:GLU:HG3	18:Q:52:GLU:O	2.19	0.43
25:b:88:THR:HG22	25:b:89:LEU:HD12	2.01	0.43
25:i:45:GLY:HA3	25:i:53:VAL:HG12	2.00	0.43
1:A:239:PHE:HD1	1:A:241:PRO:HD3	1.84	0.42
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.82	0.42
1:A:562:ILE:HD11	1:A:566:GLU:CD	2.43	0.42
1:A:932:SER:O	1:A:935:GLU:HB3	2.18	0.42
1:A:1020:ILE:HG13	1:A:1022:PRO:HD2	1.99	0.42
1:A:1123:LEU:HD23	1:A:1123:LEU:HA	1.76	0.42
1:A:1431:HIS:NE2	1:A:1434:GLU:HB3	2.34	0.42
1:A:1924:LEU:HD22	21:U:234:LYS:NZ	2.20	0.42
1:A:1926:LYS:HZ2	22:V:250:GLU:HB2	1.82	0.42
2:B:176:A:O2'	29:f:20:LYS:HE3	2.19	0.42
3:C:711:ALA:HB3	3:C:819:LYS:HB2	2.01	0.42
12:L:46:ASN:OD1	12:L:46:ASN:C	2.62	0.42
12:L:144:GLN:HB3	12:L:149:GLY:HA2	2.00	0.42
17:P:8:GLN:O	17:P:9:LEU:HG	2.19	0.42
20:S:337:SER:O	20:S:338:THR:OG1	2.35	0.42
23:W:683:ILE:HG23	23:W:718:LEU:HD11	2.00	0.42
23:W:932:VAL:HB	23:W:989:HIS:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:34:GLN:NE2	25:b:37:ILE:HD12	2.34	0.42
28:l:6:ILE:N	28:l:7:PRO:CD	2.82	0.42
33:q:123:ALA:O	33:q:127:LEU:CG	2.67	0.42
1:A:294:ASN:HB2	1:A:299:LYS:O	2.19	0.42
1:A:409:CYS:O	1:A:410:ILE:C	2.61	0.42
1:A:686:ILE:HD12	1:A:686:ILE:HG23	1.75	0.42
1:A:929:LEU:HD21	1:A:937:LEU:CD1	2.49	0.42
1:A:1033:ASN:O	1:A:1035:LEU:N	2.52	0.42
1:A:1422:ILE:HD13	1:A:1425:PHE:CZ	2.54	0.42
1:A:1678:ILE:C	1:A:1706:VAL:HG23	2.45	0.42
1:A:1679:GLU:HG2	1:A:1705:SER:O	2.19	0.42
1:A:1865:THR:O	1:A:1866:PHE:C	2.62	0.42
2:B:167:A:N7	30:g:63:ARG:HB3	2.34	0.42
2:B:174:G:C8	30:g:99:ASP:OD2	2.69	0.42
3:C:164:MET:HG2	3:C:175:LEU:HD12	2.00	0.42
3:C:251:GLN:NE2	3:C:255:GLN:HG2	2.34	0.42
3:C:769:TYR:HD2	3:C:803:VAL:HG11	1.84	0.42
3:C:769:TYR:O	3:C:770:ASN:C	2.60	0.42
4:D:73:A:OP2	4:D:73:A:H8	2.02	0.42
8:H:605:PHE:O	8:H:609:GLU:HG2	2.19	0.42
13:T:308:PHE:HE1	13:T:320:TRP:CG	2.32	0.42
16:O:207:LYS:HG2	16:O:219:ASP:OD1	2.18	0.42
18:Q:107:ASN:OD1	18:Q:109:SER:HB2	2.18	0.42
20:S:427:LEU:HD21	20:S:431:LEU:HD12	2.00	0.42
1:A:192:LEU:HA	1:A:192:LEU:HD12	1.82	0.42
1:A:312:TYR:CE2	1:A:319:ARG:NH1	2.88	0.42
1:A:370:ILE:CD1	3:C:954:LEU:HD21	2.42	0.42
1:A:1182:LEU:HD23	1:A:1182:LEU:HA	1.87	0.42
3:C:108:GLN:O	3:C:109:LEU:HD12	2.19	0.42
3:C:230:ALA:HB2	3:C:595:LEU:HD11	2.01	0.42
3:C:622:LEU:HA	3:C:622:LEU:HD23	1.86	0.42
5:E:14:U:C5	15:N:183:PHE:CD2	3.07	0.42
11:K:114:THR:O	11:K:118:ASN:CB	2.66	0.42
12:L:28:ILE:HG13	12:L:29:GLN:N	2.34	0.42
13:T:110:GLU:HA	13:T:200:ARG:HD3	2.00	0.42
15:N:127:ILE:HG22	15:N:128:GLY:H	1.83	0.42
20:S:452:GLU:H	20:S:452:GLU:CD	2.27	0.42
24:a:87:LEU:HG	24:a:92:ILE:HD11	2.00	0.42
1:A:299:LYS:O	1:A:300:LYS:HB2	2.20	0.42
1:A:429:ASN:HB3	1:A:430:PRO:HD2	2.02	0.42
1:A:762:VAL:HG13	1:A:766:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:LYS:O	1:A:913:VAL:N	2.52	0.42
1:A:1048:VAL:HA	1:A:1249:SER:O	2.20	0.42
1:A:1629:LEU:H	1:A:1629:LEU:HG	1.56	0.42
1:A:1810:PRO:O	1:A:1811:ALA:C	2.62	0.42
1:A:2046:GLU:H	1:A:2046:GLU:HG3	1.72	0.42
3:C:251:GLN:HG2	3:C:933:TRP:CD2	2.54	0.42
3:C:272:ARG:HG3	35:C:1500:GTP:N2	2.35	0.42
3:C:273:LEU:HD12	3:C:273:LEU:HA	1.80	0.42
3:C:500:ARG:HB2	3:C:578:TYR:O	2.19	0.42
4:D:56:A:O2'	4:D:57:U:O5'	2.36	0.42
8:H:669:TYR:CE2	8:H:686:ILE:HG13	2.43	0.42
9:I:219:ARG:O	9:I:222:TYR:HB2	2.19	0.42
13:T:377:PHE:CD1	13:T:377:PHE:N	2.84	0.42
14:M:74:CYS:HG	37:M:400:ZN:ZN	1.29	0.42
15:N:98:ASP:O	15:N:101:LYS:N	2.43	0.42
15:N:185:LYS:C	15:N:186:PHE:CD1	2.97	0.42
1:A:185:GLN:OE1	12:L:6:THR:HB	2.18	0.42
1:A:314:LEU:O	1:A:316:THR:N	2.52	0.42
1:A:929:LEU:CD2	1:A:937:LEU:HD12	2.50	0.42
1:A:1988:LEU:H	21:U:181:GLN:HG3	1.77	0.42
3:C:107:THR:OG1	3:C:549:TYR:HB3	2.19	0.42
3:C:246:THR:O	3:C:247:PHE:C	2.62	0.42
3:C:431:GLN:H	3:C:431:GLN:CD	2.27	0.42
3:C:787:LEU:HA	3:C:790:LYS:HE3	2.01	0.42
3:C:840:PRO:O	3:C:843:LYS:N	2.53	0.42
6:F:1096:C:H2'	6:F:1097:G:H8	1.85	0.42
13:T:60:ARG:O	13:T:63:ARG:HG2	2.20	0.42
14:M:240:LEU:HD12	14:M:250:GLY:O	2.19	0.42
15:N:124:MET:HE3	15:N:227:ASN:HD21	1.82	0.42
16:O:379:LYS:CD	18:Q:47:ARG:HH21	2.33	0.42
1:A:255:ILE:O	1:A:258:ILE:HG22	2.19	0.42
1:A:851:ARG:O	1:A:855:LEU:HG	2.19	0.42
1:A:1111:SER:OG	1:A:1112:PHE:N	2.53	0.42
1:A:1350:ILE:HG23	1:A:1356:LEU:HD22	2.02	0.42
1:A:1440:ILE:O	1:A:1442:ARG:N	2.53	0.42
1:A:1620:TYR:CD2	1:A:1621:VAL:HG13	2.54	0.42
1:A:1662:VAL:HG22	1:A:1736:VAL:HG11	2.01	0.42
2:B:43:G:OP1	2:B:43:G:N2	2.53	0.42
3:C:105:ILE:O	3:C:106:PHE:HB2	2.20	0.42
3:C:137:GLY:N	3:C:232:SER:OG	2.52	0.42
6:F:112:A:N7	30:n:63:ARG:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:182:TRP:CH2	9:I:212:HIS:NE2	2.87	0.42
10:J:90:MET:HE3	10:J:90:MET:HB3	1.92	0.42
11:K:183:MET:O	11:K:187:LYS:HG2	2.19	0.42
12:L:88:ASP:OD2	12:L:90:LEU:HB2	2.19	0.42
14:M:17:LEU:O	14:M:17:LEU:HD23	2.20	0.42
14:M:39:LEU:CD1	14:M:111:ARG:HG3	2.50	0.42
15:N:4:TRP:CE2	15:N:92:HIS:CD2	3.08	0.42
15:N:9:ALA:HB2	15:N:60:GLY:C	2.43	0.42
15:N:257:ASN:O	15:N:261:ALA:N	2.52	0.42
17:P:8:GLN:NE2	17:P:10:GLU:O	2.53	0.42
18:Q:216:ARG:O	18:Q:219:ILE:HB	2.20	0.42
1:A:133:GLU:HG3	1:A:560:THR:HA	2.01	0.42
1:A:193:TYR:CE1	1:A:558:GLN:HB2	2.54	0.42
1:A:217:TRP:HZ3	1:A:703:PHE:HA	1.84	0.42
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.93	0.42
1:A:377:VAL:HG13	1:A:378:PRO:HD2	2.02	0.42
1:A:488:ARG:O	1:A:489:THR:OG1	2.31	0.42
1:A:1031:GLY:O	1:A:1032:ILE:C	2.63	0.42
1:A:1392:LYS:HA	1:A:1396:GLY:O	2.19	0.42
1:A:1400:ILE:HG21	1:A:1400:ILE:HD13	1.85	0.42
1:A:1645:LEU:O	1:A:1648:ILE:N	2.52	0.42
3:C:101:GLN:O	3:C:101:GLN:HG2	2.19	0.42
7:G:109:SER:O	7:G:110:GLU:CB	2.67	0.42
16:O:248:ILE:HB	16:O:262:LEU:HB2	2.02	0.42
20:S:299:LEU:HD21	20:S:343:TYR:HE1	1.84	0.42
22:V:305:PHE:O	22:V:306:ALA:C	2.62	0.42
1:A:569:LEU:HD23	1:A:569:LEU:HA	1.73	0.42
1:A:655:TYR:CE1	1:A:659:HIS:CD2	3.08	0.42
1:A:712:LEU:HD23	1:A:712:LEU:C	2.43	0.42
1:A:750:LEU:O	1:A:751:ASP:C	2.63	0.42
1:A:1562:PHE:CZ	1:A:1570:TRP:HA	2.54	0.42
1:A:1682:THR:HG1	1:A:1702:THR:HG1	1.53	0.42
1:A:1698:ALA:HB1	1:A:1766:MET:HB2	2.02	0.42
1:A:1995:TRP:CE3	1:A:2004:ALA:HB1	2.53	0.42
6:F:16:U:H5'	6:F:18:U:C5	2.54	0.42
12:L:44:LYS:HD3	12:L:44:LYS:HA	1.79	0.42
12:L:126:ARG:C	12:L:128:GLN:H	2.26	0.42
15:N:1:MET:HA	15:N:5:ARG:HB3	2.01	0.42
15:N:245:GLU:HG3	15:N:249:MET:CE	2.47	0.42
16:O:303:VAL:HG12	16:O:304:LEU:N	2.33	0.42
16:O:364:LEU:HA	16:O:364:LEU:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:82:GLN:HG2	21:U:152:ARG:O	2.20	0.42
21:U:220:ILE:HG22	21:U:221:MET:H	1.84	0.42
23:W:457:TRP:CD1	23:W:522:GLU:HB3	2.54	0.42
28:e:6:ILE:N	28:e:7:PRO:CD	2.82	0.42
1:A:400:ILE:HG23	1:A:400:ILE:HD12	1.83	0.42
1:A:569:LEU:O	1:A:570:GLN:C	2.62	0.42
1:A:1058:ALA:O	1:A:1060:LYS:N	2.53	0.42
1:A:1143:GLU:H	1:A:1146:GLN:CD	2.28	0.42
1:A:1592:HIS:CE1	5:E:353:A:N7	2.85	0.42
1:A:1748:ILE:O	1:A:1751:TYR:HB3	2.20	0.42
1:A:1757:LEU:O	1:A:1760:THR:OG1	2.33	0.42
3:C:360:ARG:C	3:C:362:LYS:N	2.78	0.42
3:C:735:LEU:HD21	3:C:742:ASP:OD2	2.20	0.42
4:D:70:U:H2'	4:D:71:G:O4'	2.20	0.42
14:M:34:CYS:SG	14:M:61:CYS:N	2.79	0.42
31:o:62:ASN:HB2	31:o:84:ASN:OD1	2.20	0.42
1:A:141:LYS:HG2	12:L:49:LEU:CD2	2.50	0.42
1:A:284:ARG:HD2	1:A:287:GLU:OE2	2.20	0.42
1:A:548:LEU:O	1:A:549:LYS:C	2.63	0.42
1:A:1151:GLU:O	1:A:1154:LYS:N	2.53	0.42
1:A:1493:THR:HG1	23:W:301:GLN:CD	2.27	0.42
1:A:1656:LYS:NZ	1:A:1946:VAL:O	2.53	0.42
1:A:1669:LEU:HD23	1:A:1672:GLU:HG3	2.01	0.42
1:A:1693:LYS:HE3	1:A:1695:ASN:HB2	2.02	0.42
1:A:1699:ALA:HB1	1:A:1733:TRP:CB	2.50	0.42
2:B:76:U:OP1	3:C:173:LYS:HD3	2.20	0.42
3:C:132:ARG:O	3:C:208:ARG:HB3	2.20	0.42
3:C:454:ALA:HB1	3:C:459:PRO:HA	2.02	0.42
3:C:681:CYS:O	3:C:714:PRO:HG3	2.20	0.42
4:D:11:U:C2	4:D:12:A:H1'	2.55	0.42
5:E:345:A:N3	5:E:345:A:C2'	2.83	0.42
6:F:1116:A:C2'	6:F:1117:G:C8	2.85	0.42
12:L:14:ASP:C	12:L:16:PHE:H	2.28	0.42
14:M:111:ARG:O	14:M:114:SER:OG	2.32	0.42
15:N:153:PRO:O	15:N:156:ILE:HB	2.20	0.42
16:O:173:LYS:HA	16:O:173:LYS:HD3	1.87	0.42
16:O:285:SER:C	16:O:287:ASP:N	2.77	0.42
16:O:302:LYS:NZ	16:O:338:GLU:O	2.53	0.42
18:Q:57:LEU:C	18:Q:57:LEU:HD12	2.45	0.42
18:Q:105:LEU:O	18:Q:108:ASN:N	2.49	0.42
25:i:88:THR:HG22	25:i:89:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:O	1:A:306:PRO:C	2.62	0.41
1:A:1048:VAL:HG22	1:A:1250:VAL:HG22	2.02	0.41
1:A:1357:LEU:H	1:A:1357:LEU:HG	1.72	0.41
1:A:1491:ILE:HD12	1:A:1491:ILE:HG23	1.83	0.41
1:A:1935:VAL:O	1:A:1959:THR:HG23	2.19	0.41
2:B:121:U:H2'	2:B:122:C:C6	2.55	0.41
3:C:198:LEU:HD12	3:C:198:LEU:O	2.19	0.41
4:D:88:U:O2'	6:F:17:U:OP2	2.30	0.41
8:H:708:LEU:O	8:H:712:CYS:SG	2.70	0.41
11:K:145:LYS:HG2	11:K:152:ILE:HG13	2.02	0.41
13:T:156:ARG:O	13:T:451:ILE:O	2.38	0.41
15:N:119:ASP:N	15:N:119:ASP:OD1	2.49	0.41
16:O:148:ASP:OD2	16:O:151:ASP:N	2.40	0.41
16:O:155:PHE:CE1	16:O:415:ILE:HG12	2.55	0.41
16:O:191:SER:O	17:P:40:ARG:NH2	2.53	0.41
16:O:277:VAL:HG23	16:O:278:ASP:O	2.19	0.41
16:O:387:LEU:HA	16:O:387:LEU:HD23	1.80	0.41
18:Q:37:ASN:ND2	18:Q:145:PRO:HD3	2.35	0.41
1:A:984:VAL:HG12	1:A:985:ASP:N	2.33	0.41
1:A:2048:TRP:O	1:A:2052:GLU:HG3	2.20	0.41
3:C:758:ASP:HB3	3:C:761:ALA:HB3	2.00	0.41
4:D:53:A:C4'	4:D:54:U:OP2	2.68	0.41
9:I:115:ILE:HG23	9:I:116:ASN:N	2.35	0.41
10:J:533:LEU:O	10:J:536:GLN:CG	2.68	0.41
14:M:240:LEU:CD1	14:M:251:LEU:HD13	2.49	0.41
16:O:111:ILE:HB	16:O:114:ARG:NH2	2.34	0.41
16:O:333:SER:O	16:O:334:TRP:CG	2.73	0.41
16:O:414:LEU:HD12	16:O:415:ILE:N	2.34	0.41
17:P:15:ALA:O	17:P:18:ALA:N	2.53	0.41
18:Q:103:ASN:HB2	18:Q:112:ILE:HG21	2.02	0.41
22:V:336:TYR:O	22:V:337:GLU:C	2.62	0.41
1:A:300:LYS:HB2	1:A:300:LYS:HE3	1.86	0.41
1:A:1066:LEU:O	1:A:1069:LEU:N	2.53	0.41
1:A:1852:VAL:HB	1:A:1935:VAL:CG2	2.46	0.41
1:A:2050:THR:O	1:A:2054:GLN:HG3	2.20	0.41
1:A:2056:ARG:HH22	22:V:332:ASN:HA	1.85	0.41
3:C:69:PRO:O	16:O:390:ARG:NH1	2.53	0.41
3:C:149:LEU:O	3:C:150:MET:C	2.62	0.41
3:C:252:LEU:HD23	3:C:252:LEU:HA	1.81	0.41
3:C:707:SER:O	3:C:708:ILE:HD13	2.19	0.41
3:C:915:GLU:HG2	3:C:928:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:A:H4'	4:D:54:U:OP2	2.20	0.41
6:F:1102:C:H2'	6:F:1103:C:H5	1.69	0.41
9:I:55:GLU:O	9:I:59:LYS:HB2	2.20	0.41
12:L:47:GLU:O	12:L:48:GLN:C	2.63	0.41
12:L:90:LEU:O	12:L:91:LEU:C	2.63	0.41
13:T:65:GLY:C	13:T:66:ASP:CG	2.89	0.41
15:N:33:TRP:CD1	15:N:33:TRP:C	2.99	0.41
15:N:184:VAL:HG12	15:N:186:PHE:HE1	1.85	0.41
16:O:148:ASP:HB2	16:O:154:TRP:CE2	2.55	0.41
1:A:215:ALA:O	1:A:218:SER:N	2.53	0.41
1:A:304:ASP:OD1	1:A:306:PRO:HD2	2.21	0.41
1:A:900:PHE:HA	1:A:1078:ILE:HD11	2.03	0.41
1:A:1604:ARG:NH2	1:A:1643:ILE:HD13	2.35	0.41
1:A:1634:LEU:HA	1:A:1634:LEU:HD23	1.83	0.41
1:A:1811:ALA:O	1:A:1814:VAL:HB	2.20	0.41
3:C:775:ILE:HG22	3:C:776:ASN:N	2.35	0.41
3:C:933:TRP:O	3:C:935:LYS:HG3	2.19	0.41
6:F:1115:G:C6	6:F:1116:A:N6	2.89	0.41
8:H:648:PHE:CD1	8:H:669:TYR:HB2	2.55	0.41
10:J:64:GLU:HG2	10:J:65:PHE:N	2.33	0.41
10:J:66:SER:H	10:J:69:GLU:HB2	1.86	0.41
11:K:203:PHE:O	11:K:206:LYS:N	2.53	0.41
12:L:55:LEU:O	12:L:58:GLN:N	2.53	0.41
13:T:270:SER:HA	13:T:294:SER:O	2.21	0.41
13:T:376:ILE:HG22	13:T:377:PHE:N	2.35	0.41
14:M:290:ILE:HG22	14:M:292:PRO:HD3	2.02	0.41
15:N:156:ILE:HG21	15:N:175:TYR:CE1	2.55	0.41
16:O:348:GLU:CG	16:O:349:LYS:H	2.33	0.41
16:O:389:THR:O	16:O:390:ARG:C	2.62	0.41
20:S:370:THR:OG1	20:S:371:GLN:N	2.53	0.41
20:S:373:ILE:CG2	20:S:415:GLN:HB3	2.50	0.41
1:A:311:LEU:O	1:A:312:TYR:C	2.62	0.41
1:A:1019:GLU:OE2	1:A:1027:LYS:NZ	2.42	0.41
1:A:1145:MET:HE1	1:A:1160:LEU:HD13	2.01	0.41
1:A:1355:PRO:O	1:A:1358:ASP:HB3	2.20	0.41
1:A:1565:THR:HG22	1:A:1819:ILE:CG2	2.51	0.41
2:B:31:G:H2'	2:B:32:G:H5'	2.03	0.41
3:C:92:GLU:HG2	3:C:93:PRO:O	2.20	0.41
3:C:115:LYS:O	3:C:116:THR:OG1	2.35	0.41
3:C:234:LEU:HD11	3:C:439:ILE:HG23	2.03	0.41
3:C:656:LEU:HA	3:C:656:LEU:HD23	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:182:TRP:HA	9:I:185:VAL:HG12	2.03	0.41
10:J:179:SER:N	13:T:337:HIS:NE2	2.69	0.41
10:J:222:ALA:O	10:J:223:PRO:C	2.64	0.41
13:T:295:SER:O	13:T:313:GLU:CB	2.68	0.41
14:M:125:ILE:HD12	14:M:126:THR:HG23	2.01	0.41
15:N:17:GLU:O	15:N:18:LEU:C	2.63	0.41
16:O:125:TRP:CD1	16:O:437:GLU:OE1	2.73	0.41
16:O:306:HIS:O	16:O:307:HIS:C	2.60	0.41
16:O:319:LYS:O	18:Q:57:LEU:HD23	2.20	0.41
20:S:456:GLU:HG3	20:S:457:HIS:H	1.85	0.41
25:i:77:LEU:HD23	25:i:78:GLY:N	2.35	0.41
1:A:452:PHE:HZ	3:C:347:ARG:HG3	1.84	0.41
1:A:529:TYR:O	1:A:530:VAL:C	2.63	0.41
1:A:1070:LEU:HD23	1:A:1070:LEU:HA	1.84	0.41
1:A:1129:GLU:O	1:A:1130:ARG:C	2.63	0.41
1:A:1281:ASN:ND2	1:A:1285:VAL:HG21	2.26	0.41
1:A:1369:ASN:HB3	1:A:1378:LYS:NZ	2.35	0.41
1:A:1403:SER:O	1:A:1405:ILE:HG12	2.19	0.41
1:A:1452:LEU:HD23	1:A:1452:LEU:HA	1.83	0.41
1:A:1597:GLY:CA	5:E:348:U:O2'	2.60	0.41
1:A:1794:LEU:O	1:A:1797:LEU:N	2.54	0.41
1:A:1902:GLN:HE21	1:A:1908:LEU:CD2	2.33	0.41
3:C:359:PHE:N	3:C:359:PHE:CD1	2.88	0.41
3:C:456:LEU:C	3:C:593:LYS:HE2	2.45	0.41
3:C:758:ASP:O	3:C:762:SER:N	2.39	0.41
3:C:876:VAL:O	3:C:877:GLU:C	2.62	0.41
5:E:-2:A:H2'	5:E:-1:G:C8	2.56	0.41
7:G:113:LEU:O	7:G:116:ILE:CG1	2.69	0.41
11:K:163:LYS:HD3	11:K:163:LYS:HA	1.81	0.41
12:L:126:ARG:N	12:L:157:ASP:OD2	2.41	0.41
13:T:392:SER:O	13:T:393:GLY:C	2.62	0.41
30:g:102:ILE:HG22	30:g:103:VAL:HG23	2.01	0.41
30:n:102:ILE:HG22	30:n:103:VAL:HG23	2.01	0.41
1:A:168:LEU:O	1:A:169:PRO:C	2.62	0.41
1:A:618:SER:O	1:A:621:LEU:N	2.53	0.41
1:A:1267:VAL:HG22	1:A:1302:LEU:CD2	2.51	0.41
1:A:1499:ARG:HB2	23:W:297:TRP:CD1	2.56	0.41
1:A:1624:LEU:HA	1:A:1624:LEU:HD23	1.80	0.41
1:A:1956:ILE:O	22:V:270:SER:HB2	2.21	0.41
3:C:394:ASP:O	3:C:397:LYS:HB3	2.20	0.41
3:C:425:LEU:HD23	3:C:425:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:470:ALA:CB	3:C:488:ILE:HA	2.50	0.41
3:C:786:GLU:O	3:C:789:SER:N	2.53	0.41
3:C:796:ILE:HG13	3:C:800:TYR:CZ	2.56	0.41
3:C:943:ASP:O	3:C:945:LEU:N	2.54	0.41
5:E:1:G:H5'	5:E:301:A:C4	2.56	0.41
13:T:198:CYS:O	13:T:198:CYS:SG	2.79	0.41
16:O:265:HIS:HD2	16:O:269:ILE:HD11	1.85	0.41
16:O:374:SER:OG	16:O:376:TYR:CE1	2.74	0.41
16:O:392:MET:HG3	16:O:393:VAL:H	1.85	0.41
21:U:225:ARG:NH1	21:U:225:ARG:CB	2.84	0.41
22:V:338:TYR:O	22:V:341:LYS:HB3	2.21	0.41
27:k:26:ALA:C	27:k:43:ALA:HB3	2.46	0.41
1:A:158:LYS:HG2	1:A:581:LEU:HD21	2.03	0.41
1:A:487:ASN:C	1:A:487:ASN:OD1	2.63	0.41
1:A:744:THR:HG23	1:A:746:THR:HG23	2.03	0.41
1:A:787:SER:O	1:A:788:GLU:C	2.61	0.41
1:A:839:HIS:O	1:A:839:HIS:CG	2.73	0.41
1:A:872:PRO:HG3	18:Q:201:PHE:HD1	1.85	0.41
1:A:1111:SER:HB3	1:A:1514:PHE:HD2	1.85	0.41
1:A:1595:ARG:NH2	5:E:353:A:H61	2.19	0.41
1:A:1687:HIS:CG	1:A:1688:PRO:HD2	2.56	0.41
1:A:1926:LYS:HE2	22:V:248:LEU:CB	2.51	0.41
1:A:2011:LEU:HB3	1:A:2040:TRP:CH2	2.56	0.41
34:A:3000:IHP:P6	34:A:3000:IHP:O15	2.79	0.41
3:C:604:LYS:HE2	3:C:643:VAL:HG11	2.03	0.41
9:I:88:PHE:CD1	9:I:105:TYR:HB2	2.55	0.41
11:K:143:VAL:CG1	11:K:152:ILE:HD11	2.51	0.41
13:T:72:TRP:O	13:T:73:SER:OG	2.30	0.41
15:N:184:VAL:CG1	15:N:186:PHE:HE1	2.34	0.41
20:S:403:LYS:HD3	20:S:445:LEU:HA	2.03	0.41
25:b:77:LEU:HD23	25:b:78:GLY:N	2.35	0.41
33:q:59:GLN:O	33:q:60:ALA:HB3	2.20	0.41
33:r:112:VAL:O	33:r:115:GLU:CG	2.68	0.41
1:A:141:LYS:O	1:A:142:ILE:C	2.63	0.41
1:A:274:GLU:C	1:A:274:GLU:CD	2.89	0.41
1:A:425:ASP:HA	1:A:426:PRO:HD2	1.92	0.41
1:A:643:ASN:OD1	1:A:643:ASN:N	2.54	0.41
1:A:705:GLN:HE21	1:A:709:ARG:HG3	1.86	0.41
1:A:806:ALA:N	1:A:807:PRO:HD2	2.36	0.41
1:A:1058:ALA:O	1:A:1061:ILE:N	2.24	0.41
1:A:1214:ARG:HH12	1:A:1256:PRO:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:O	1:A:1227:PHE:C	2.64	0.41
1:A:1270:LEU:HD23	1:A:1270:LEU:HA	1.84	0.41
1:A:1328:PHE:O	1:A:1331:VAL:N	2.54	0.41
1:A:1460:GLU:O	1:A:1463:THR:OG1	2.31	0.41
1:A:1523:SER:O	1:A:1525:PHE:N	2.53	0.41
1:A:1654:TRP:O	1:A:1657:ILE:HB	2.20	0.41
1:A:1987:VAL:CG1	21:U:181:GLN:HG2	2.51	0.41
34:A:3000:IHP:O14	34:A:3000:IHP:P5	2.79	0.41
2:B:43:G:O2'	2:B:45:A:H5'	2.21	0.41
3:C:962:LEU:O	3:C:965:ASP:HB3	2.21	0.41
5:E:9:U:O4'	5:E:10:U:OP2	2.38	0.41
5:E:13:U:O2	15:N:226:ALA:HA	2.20	0.41
6:F:5:A:H5'	11:K:114:THR:HG21	2.02	0.41
6:F:25:A:C2	10:J:31:HIS:O	2.74	0.41
9:I:86:SER:O	9:I:89:GLU:N	2.54	0.41
12:L:65:THR:O	12:L:69:LYS:HB2	2.21	0.41
13:T:51:PHE:HE1	13:T:55:GLU:CG	2.32	0.41
13:T:68:PRO:HD2	13:T:69:TRP:CZ3	2.53	0.41
13:T:216:GLU:CG	13:T:257:PRO:O	2.69	0.41
13:T:245:HIS:O	13:T:246:LEU:CB	2.69	0.41
14:M:68:ARG:HH21	14:M:103:GLU:CD	2.29	0.41
14:M:69:ASN:C	14:M:70:ILE:HG23	2.46	0.41
14:M:216:GLU:O	14:M:219:ILE:N	2.53	0.41
14:M:290:ILE:HG22	14:M:292:PRO:CD	2.51	0.41
15:N:169:ASP:OD2	15:N:187:LYS:HD2	2.21	0.41
16:O:232:ILE:O	16:O:233:HIS:C	2.63	0.41
16:O:246:SER:HG	16:O:267:GLY:C	2.28	0.41
16:O:263:VAL:CG1	16:O:264:GLY:N	2.81	0.41
20:S:354:HIS:HD2	20:S:356:SER:OG	2.03	0.41
20:S:374:GLU:C	20:S:415:GLN:HE22	2.29	0.41
20:S:455:ALA:HA	20:S:458:ILE:HD12	2.01	0.41
20:S:455:ALA:HB2	20:S:484:ILE:HD13	2.03	0.41
23:W:489:ARG:HE	23:W:493:ILE:HG13	1.85	0.41
23:W:620:LYS:NZ	23:W:646:TYR:CE1	2.89	0.41
23:W:725:LEU:HD23	23:W:725:LEU:C	2.45	0.41
33:q:101:THR:O	33:q:105:LEU:CG	2.69	0.41
1:A:571:LEU:HD23	1:A:629:MET:SD	2.61	0.41
1:A:687:ILE:HG22	1:A:687:ILE:O	2.21	0.41
1:A:740:GLU:CG	1:A:741:ILE:H	2.30	0.41
1:A:900:PHE:CZ	1:A:959:LEU:HD12	2.56	0.41
1:A:1208:PRO:HB2	1:A:1417:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:LEU:HD23	1:A:1258:LEU:C	2.46	0.41
1:A:1335:TRP:HD1	1:A:1367:ILE:CD1	2.25	0.41
1:A:1478:GLU:C	1:A:1480:LEU:N	2.78	0.41
3:C:121:ASP:O	3:C:124:LEU:HB2	2.20	0.41
8:H:616:PRO:O	8:H:618:GLU:N	2.54	0.41
9:I:220:SER:O	9:I:223:SER:HB3	2.21	0.41
9:I:264:SER:HA	9:I:267:TYR:HB3	2.03	0.41
10:J:160:LEU:HA	11:K:196:ILE:HG23	2.03	0.41
12:L:55:LEU:HD23	12:L:55:LEU:HA	1.88	0.41
13:T:200:ARG:O	13:T:202:PHE:CE1	2.73	0.41
14:M:61:CYS:HB3	14:M:63:ARG:H	1.86	0.41
16:O:223:HIS:CD2	16:O:227:VAL:CG2	3.03	0.41
16:O:355:THR:O	16:O:356:LEU:HD23	2.21	0.41
20:S:422:PHE:O	20:S:425:GLN:N	2.54	0.41
1:A:194:HIS:CD2	1:A:557:PHE:HE1	2.40	0.40
1:A:660:ILE:C	1:A:662:GLN:N	2.79	0.40
1:A:756:LEU:HD11	4:D:63:G:H4'	2.03	0.40
1:A:786:LEU:O	1:A:787:SER:C	2.62	0.40
1:A:1082:ILE:HG23	1:A:1109:PHE:CE1	2.56	0.40
1:A:1653:LEU:O	1:A:1657:ILE:HG13	2.20	0.40
1:A:1905:LEU:HD12	1:A:1905:LEU:N	2.37	0.40
1:A:1959:THR:HG21	1:A:1963:LEU:HD12	2.02	0.40
1:A:2017:THR:HG21	1:A:2059:ILE:HG12	2.03	0.40
2:B:75:A:H61	3:C:101:GLN:NE2	2.19	0.40
3:C:114:PRO:O	3:C:116:THR:HG23	2.21	0.40
9:I:105:TYR:CE2	9:I:121:LEU:HD13	2.56	0.40
10:J:110:ASP:OD1	10:J:111:SER:N	2.54	0.40
11:K:200:ASN:O	11:K:204:ASN:CB	2.68	0.40
13:T:136:ASP:C	13:T:137:VAL:CG1	2.94	0.40
13:T:358:ASN:OD1	13:T:381:SER:HA	2.21	0.40
14:M:108:MET:HA	14:M:111:ARG:HB3	2.02	0.40
15:N:132:LYS:HG2	15:N:133:LYS:O	2.21	0.40
16:O:190:VAL:HG22	16:O:197:LEU:HD13	2.03	0.40
18:Q:240:LYS:O	18:Q:240:LYS:HG2	2.21	0.40
27:d:26:ALA:C	27:d:43:ALA:HB3	2.46	0.40
1:A:475:ASP:O	1:A:476:ALA:C	2.62	0.40
1:A:713:ASN:O	1:A:714:PHE:C	2.65	0.40
1:A:872:PRO:HG3	18:Q:201:PHE:CD1	2.56	0.40
1:A:1128:GLN:O	1:A:1129:GLU:C	2.64	0.40
1:A:1570:TRP:CD2	1:A:1570:TRP:C	2.96	0.40
1:A:1716:LEU:HB2	1:A:1719:GLU:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1852:VAL:HG22	1:A:1881:THR:HG22	2.02	0.40
5:E:301:A:H4'	5:E:301:A:OP2	2.22	0.40
7:G:89:GLU:CG	7:G:90:GLU:N	2.84	0.40
11:K:159:LYS:C	11:K:161:VAL:H	2.29	0.40
11:K:195:PHE:CD1	11:K:201:LYS:HA	2.57	0.40
12:L:126:ARG:HG3	13:T:72:TRP:CE2	2.56	0.40
15:N:222:LEU:HA	15:N:222:LEU:HD23	1.82	0.40
15:N:246:SER:O	15:N:250:MET:HG3	2.21	0.40
16:O:233:HIS:CE1	16:O:236:LEU:HB2	2.56	0.40
17:P:165:TYR:O	17:P:168:GLU:N	2.54	0.40
20:S:297:LEU:O	20:S:300:LYS:N	2.54	0.40
21:U:131:TYR:O	21:U:132:HIS:C	2.64	0.40
1:A:177:GLU:HB3	1:A:712:LEU:HD11	2.04	0.40
1:A:322:VAL:HG12	1:A:508:GLN:HE21	1.85	0.40
1:A:697:LYS:O	34:A:3000:IHP:O36	2.38	0.40
1:A:936:GLU:O	1:A:940:ILE:HD12	2.22	0.40
1:A:1042:SER:OG	1:A:1043:ARG:HG3	2.21	0.40
1:A:1493:THR:O	1:A:1494:LEU:C	2.63	0.40
1:A:1743:TYR:O	1:A:1743:TYR:CG	2.74	0.40
1:A:1974:LEU:O	1:A:1978:VAL:HG23	2.21	0.40
3:C:709:SER:OG	3:C:821:LEU:HD12	2.21	0.40
4:D:91:A:C5	9:I:99:ILE:HD11	2.43	0.40
9:I:153:ARG:HB2	9:I:153:ARG:CZ	2.52	0.40
9:I:173:VAL:HG12	9:I:188:ILE:HG21	2.04	0.40
16:O:358:ILE:HA	16:O:364:LEU:HD12	2.04	0.40
1:A:143:ILE:HD13	1:A:570:GLN:HG2	2.03	0.40
1:A:854:ARG:HD3	1:A:1095:MET:CE	2.52	0.40
1:A:1001:TYR:OH	1:A:1005:GLN:NE2	2.53	0.40
1:A:1399:MET:HE3	1:A:1399:MET:HB2	1.94	0.40
1:A:1491:ILE:O	1:A:1492:SER:C	2.65	0.40
1:A:1813:TYR:O	1:A:1817:GLU:HG3	2.21	0.40
2:B:43:G:C4	3:C:97:ARG:HD3	2.57	0.40
3:C:139:ILE:HD12	3:C:252:LEU:HD22	2.04	0.40
3:C:678:SER:HB2	3:C:858:LEU:HB2	2.04	0.40
5:E:2:U:H6	5:E:2:U:H3'	1.87	0.40
6:F:15:C:H2'	6:F:16:U:H5''	2.04	0.40
9:I:38:LEU:O	10:J:252:GLY:HA2	2.22	0.40
9:I:187:GLU:O	9:I:190:SER:HB3	2.21	0.40
11:K:143:VAL:HG13	11:K:152:ILE:HD11	2.03	0.40
19:R:25:ALA:HB1	20:S:306:ASP:OD1	2.22	0.40
21:U:146:LEU:HD22	21:U:229:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:225:ARG:CB	21:U:225:ARG:HH11	2.35	0.40
28:l:33:LEU:C	28:l:33:LEU:HD23	2.47	0.40
1:A:310:ASN:HA	1:A:313:ARG:NH2	2.37	0.40
1:A:607:THR:O	1:A:608:LYS:C	2.65	0.40
1:A:683:LEU:HD13	1:A:706:PRO:CB	2.52	0.40
1:A:782:ILE:O	1:A:785:HIS:HB2	2.21	0.40
1:A:1581:PHE:HB2	5:E:347:A:H2	1.87	0.40
1:A:1739:ARG:HG3	1:A:1778:ASP:OD1	2.22	0.40
1:A:1979:MET:HB3	13:T:324:ILE:HG23	2.02	0.40
3:C:90:LEU:HD22	16:O:211:LEU:HD22	2.04	0.40
3:C:839:ILE:O	3:C:842:MET:HB3	2.21	0.40
4:D:90:U:C5	9:I:104:ARG:NH1	2.90	0.40
20:S:305:GLY:HA2	20:S:342:PHE:CD1	2.57	0.40
20:S:465:PHE:CD1	20:S:468:ILE:HD12	2.56	0.40
24:h:19:LYS:HZ3	31:o:34:LEU:CB	2.32	0.40
31:o:11:ALA:O	31:o:12:PRO:C	2.65	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	1925/2413 (80%)	1558 (81%)	328 (17%)	39 (2%)	6	32
3	C	872/1008 (86%)	735 (84%)	121 (14%)	16 (2%)	6	34
7	G	150/175 (86%)	134 (89%)	13 (9%)	3 (2%)	6	32
8	H	496/859 (58%)	474 (96%)	16 (3%)	6 (1%)	10	41
9	I	481/687 (70%)	433 (90%)	45 (9%)	3 (1%)	21	54
10	J	414/590 (70%)	368 (89%)	35 (8%)	11 (3%)	4	27
11	K	92/215 (43%)	84 (91%)	7 (8%)	1 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	155/157 (99%)	118 (76%)	34 (22%)	3 (2%)	6	33
13	T	326/455 (72%)	283 (87%)	21 (6%)	22 (7%)	1	11
14	M	177/364 (49%)	137 (77%)	36 (20%)	4 (2%)	5	30
15	N	259/339 (76%)	219 (85%)	35 (14%)	5 (2%)	6	33
16	O	335/451 (74%)	268 (80%)	58 (17%)	9 (3%)	4	27
17	P	63/175 (36%)	50 (79%)	10 (16%)	3 (5%)	2	16
18	Q	193/379 (51%)	156 (81%)	29 (15%)	8 (4%)	2	19
19	R	25/135 (18%)	20 (80%)	5 (20%)	0	100	100
20	S	205/577 (36%)	166 (81%)	36 (18%)	3 (2%)	8	37
21	U	144/251 (57%)	140 (97%)	4 (3%)	0	100	100
22	V	82/382 (22%)	71 (87%)	9 (11%)	2 (2%)	4	29
23	W	697/1145 (61%)	600 (86%)	72 (10%)	25 (4%)	2	22
24	a	76/196 (39%)	69 (91%)	7 (9%)	0	100	100
24	h	74/196 (38%)	67 (90%)	7 (10%)	0	100	100
25	b	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
25	i	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
26	c	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	8	37
26	j	66/86 (77%)	61 (92%)	4 (6%)	1 (2%)	8	37
27	d	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	k	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
28	e	80/101 (79%)	70 (88%)	9 (11%)	1 (1%)	9	39
28	l	79/101 (78%)	69 (87%)	9 (11%)	1 (1%)	9	39
29	f	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
29	m	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
30	g	92/110 (84%)	85 (92%)	6 (6%)	1 (1%)	11	43
30	n	63/110 (57%)	58 (92%)	4 (6%)	1 (2%)	7	36
31	o	125/238 (52%)	111 (89%)	12 (10%)	2 (2%)	7	36
32	p	77/111 (69%)	75 (97%)	2 (3%)	0	100	100
33	q	125/503 (25%)	115 (92%)	6 (5%)	4 (3%)	3	24
33	r	119/503 (24%)	111 (93%)	5 (4%)	3 (2%)	4	28
33	s	120/503 (24%)	115 (96%)	4 (3%)	1 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	t	122/503 (24%)	116 (95%)	6 (5%)	0	100	100
All	All	8803/14738 (60%)	7603 (86%)	1021 (12%)	179 (2%)	8	32

All (179) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	ASN
1	A	645	ASP
1	A	1404	HIS
1	A	1405	ILE
1	A	1540	ASN
3	C	364	PHE
7	G	77	PRO
8	H	616	PRO
8	H	797	TYR
9	I	315	ASN
10	J	417	PRO
10	J	418	PRO
13	T	112	VAL
13	T	131	PRO
13	T	133	ASN
13	T	137	VAL
13	T	141	GLU
13	T	153	LYS
13	T	158	TYR
13	T	159	PRO
13	T	173	LYS
13	T	218	CYS
13	T	246	LEU
13	T	303	PRO
13	T	424	PRO
14	M	99	VAL
16	O	279	PRO
18	Q	36	LYS
18	Q	112	ILE
23	W	475	PRO
23	W	507	GLU
23	W	526	SER
23	W	640	SER
23	W	773	VAL
23	W	774	ASP
23	W	912	LEU

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Mol	Chain	Res	Type
23	W	1082	GLN
31	o	68	PRO
33	q	53	ILE
33	q	77	ILE
33	r	64	GLU
1	A	410	ILE
1	A	480	TYR
1	A	741	ILE
1	A	1033	ASN
1	A	1419	ASP
1	A	1964	PRO
3	C	363	PRO
7	G	110	GLU
8	H	601	VAL
8	H	618	GLU
10	J	82	ASN
10	J	230	THR
10	J	415	ILE
12	L	119	THR
13	T	61	LYS
13	T	199	LEU
13	T	357	ASP
15	N	151	LEU
16	O	435	GLU
17	P	8	GLN
18	Q	49	SER
20	S	398	PRO
23	W	448	LEU
23	W	566	PHE
23	W	605	ALA
23	W	724	GLU
23	W	729	PRO
23	W	788	GLY
23	W	913	SER
23	W	975	TYR
23	W	1061	GLY
23	W	1076	SER
1	A	240	PRO
1	A	543	ASN
1	A	618	SER
1	A	1347	ARG
1	A	1628	ASP

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Mol	Chain	Res	Type
1	A	2002	TYR
3	C	106	PHE
3	C	109	LEU
3	C	655	LEU
3	C	704	PRO
7	G	80	ASN
8	H	634	HIS
8	H	752	GLU
13	T	294	SER
14	M	61	CYS
15	N	92	HIS
16	O	124	GLU
16	O	244	ARG
17	P	159	ASP
18	Q	102	ALA
18	Q	109	SER
20	S	286	THR
23	W	292	THR
23	W	435	THR
23	W	1040	VAL
33	r	20	ARG
33	s	17	PRO
1	A	128	TYR
1	A	230	ASP
1	A	259	GLU
1	A	701	CYS
1	A	1077	ASN
1	A	1866	PHE
3	C	117	ARG
3	C	829	VAL
9	I	529	LYS
10	J	231	SER
12	L	127	ALA
13	T	405	SER
13	T	429	ILE
14	M	17	LEU
16	O	278	ASP
16	O	340	SER
17	P	9	LEU
18	Q	86	ASN
18	Q	166	PRO
22	V	263	GLU

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Mol	Chain	Res	Type
28	e	82	PRO
30	g	82	LYS
28	l	82	PRO
30	n	82	LYS
1	A	779	ALA
1	A	1233	ARG
1	A	1411	ASP
1	A	1491	ILE
1	A	1941	LEU
1	A	1972	ASP
3	C	274	ILE
3	C	365	GLU
3	C	801	TRP
10	J	16	VAL
10	J	203	PRO
10	J	218	VAL
11	K	210	GLU
12	L	122	CYS
13	T	204	GLY
15	N	110	ASP
15	N	205	LEU
16	O	265	HIS
22	V	333	PRO
23	W	641	ALA
23	W	941	ASP
23	W	1062	LYS
33	q	60	ALA
1	A	377	VAL
1	A	1015	PRO
1	A	1165	LEU
1	A	1377	SER
3	C	416	ASP
3	C	440	THR
10	J	419	SER
13	T	146	PHE
13	T	250	PRO
14	M	93	LEU
16	O	393	VAL
20	S	415	GLN
1	A	407	VAL
1	A	644	VAL
3	C	417	PRO

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Mol	Chain	Res	Type
3	C	434	GLY
9	I	151	ILE
26	c	15	PRO
26	j	15	PRO
31	o	52	LYS
33	q	36	GLY
1	A	379	ILE
3	C	831	ILE
23	W	723	GLY
10	J	225	PRO
18	Q	219	ILE
1	A	266	LEU
1	A	696	GLY
1	A	1199	ILE
16	O	277	VAL
15	N	163	VAL
33	r	36	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1751/2182 (80%)	1701 (97%)	50 (3%)	37	60
3	C	794/910 (87%)	776 (98%)	18 (2%)	44	64
7	G	36/165 (22%)	25 (69%)	11 (31%)	0	2
8	H	57/786 (7%)	46 (81%)	11 (19%)	1	9
9	I	219/633 (35%)	218 (100%)	1 (0%)	81	80
10	J	212/525 (40%)	204 (96%)	8 (4%)	29	55
11	K	88/193 (46%)	86 (98%)	2 (2%)	44	64
12	L	141/141 (100%)	140 (99%)	1 (1%)	76	78
13	T	177/413 (43%)	128 (72%)	49 (28%)	0	3
14	M	171/332 (52%)	168 (98%)	3 (2%)	51	68
15	N	224/296 (76%)	219 (98%)	5 (2%)	45	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	O	295/397 (74%)	288 (98%)	7 (2%)	43	63
17	P	56/151 (37%)	54 (96%)	2 (4%)	31	56
18	Q	173/328 (53%)	169 (98%)	4 (2%)	44	64
19	R	21/121 (17%)	20 (95%)	1 (5%)	23	50
20	S	192/538 (36%)	189 (98%)	3 (2%)	55	69
21	U	134/225 (60%)	131 (98%)	3 (2%)	45	65
22	V	24/346 (7%)	22 (92%)	2 (8%)	10	35
23	W	613/1029 (60%)	556 (91%)	57 (9%)	8	32
24	a	70/176 (40%)	69 (99%)	1 (1%)	59	71
24	h	67/176 (38%)	66 (98%)	1 (2%)	57	70
25	b	65/83 (78%)	60 (92%)	5 (8%)	12	38
25	i	65/83 (78%)	60 (92%)	5 (8%)	12	38
26	c	61/77 (79%)	60 (98%)	1 (2%)	55	69
26	j	61/77 (79%)	60 (98%)	1 (2%)	55	69
27	d	58/66 (88%)	56 (97%)	2 (3%)	32	57
27	k	58/66 (88%)	56 (97%)	2 (3%)	32	57
28	e	69/89 (78%)	68 (99%)	1 (1%)	59	71
28	l	68/89 (76%)	67 (98%)	1 (2%)	57	70
29	f	77/129 (60%)	74 (96%)	3 (4%)	28	54
29	m	77/129 (60%)	74 (96%)	3 (4%)	28	54
30	g	79/103 (77%)	73 (92%)	6 (8%)	12	39
30	n	59/103 (57%)	54 (92%)	5 (8%)	10	35
31	o	45/219 (20%)	42 (93%)	3 (7%)	15	42
32	p	26/100 (26%)	26 (100%)	0	100	100
33	q	63/451 (14%)	55 (87%)	8 (13%)	4	22
33	r	60/451 (13%)	55 (92%)	5 (8%)	10	35
33	s	59/451 (13%)	53 (90%)	6 (10%)	7	30
33	t	62/451 (14%)	54 (87%)	8 (13%)	4	22
All	All	6627/13280 (50%)	6322 (95%)	305 (5%)	25	51

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	PRO
1	A	305	LEU
1	A	419	THR
1	A	461	LEU
1	A	513	GLU
1	A	514	TYR
1	A	518	VAL
1	A	549	LYS
1	A	565	VAL
1	A	622	MET
1	A	643	ASN
1	A	653	ILE
1	A	660	ILE
1	A	712	LEU
1	A	716	ARG
1	A	740	GLU
1	A	757	GLU
1	A	762	VAL
1	A	772	GLU
1	A	786	LEU
1	A	816	ILE
1	A	928	ARG
1	A	929	LEU
1	A	1094	ASP
1	A	1113	ILE
1	A	1319	ILE
1	A	1326	THR
1	A	1339	LEU
1	A	1342	LEU
1	A	1367	ILE
1	A	1437	ILE
1	A	1510	ILE
1	A	1576	GLU
1	A	1579	SER
1	A	1584	SER
1	A	1588	LYS
1	A	1589	LYS
1	A	1591	THR
1	A	1592	HIS
1	A	1595	ARG
1	A	1598	LEU
1	A	1604	ARG
1	A	1629	LEU

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Mol	Chain	Res	Type
1	A	1819	ILE
1	A	1825	ILE
1	A	1950	ASP
1	A	1988	LEU
1	A	1999	ILE
1	A	2046	GLU
1	A	2079	ILE
3	C	104	THR
3	C	109	LEU
3	C	134	ILE
3	C	136	VAL
3	C	163	ASP
3	C	164	MET
3	C	193	LEU
3	C	234	LEU
3	C	253	ILE
3	C	269	LYS
3	C	379	ILE
3	C	415	TYR
3	C	419	PRO
3	C	429	PHE
3	C	497	ASP
3	C	501	ILE
3	C	503	ASP
3	C	625	ILE
7	G	5	SER
7	G	7	VAL
7	G	13	PRO
7	G	77	PRO
7	G	96	PRO
7	G	100	THR
7	G	105	PRO
7	G	108	SER
7	G	133	PRO
7	G	150	THR
7	G	152	THR
8	H	616	PRO
8	H	617	PRO
8	H	641	PRO
8	H	681	SER
8	H	706	LEU
8	H	712	CYS

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Mol	Chain	Res	Type
8	H	722	PRO
8	H	723	SER
8	H	725	THR
8	H	726	ARG
8	H	733	ILE
9	I	62	ARG
10	J	20	ILE
10	J	504	PRO
10	J	505	PRO
10	J	506	THR
10	J	517	VAL
10	J	523	LEU
10	J	532	PRO
10	J	550	PRO
11	K	98	ASP
11	K	145	LYS
12	L	120	CYS
13	T	51	PHE
13	T	52	THR
13	T	55	GLU
13	T	58	ARG
13	T	61	LYS
13	T	62	THR
13	T	66	ASP
13	T	126	ARG
13	T	128	TYR
13	T	131	PRO
13	T	134	ASP
13	T	135	VAL
13	T	137	VAL
13	T	139	LEU
13	T	140	ARG
13	T	145	SER
13	T	150	LEU
13	T	152	LYS
13	T	153	LYS
13	T	155	ILE
13	T	159	PRO
13	T	199	LEU
13	T	202	PHE
13	T	228	ARG
13	T	292	HIS

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Mol	Chain	Res	Type
13	T	293	LEU
13	T	303	PRO
13	T	308	PHE
13	T	315	LYS
13	T	318	ARG
13	T	320	TRP
13	T	327	PRO
13	T	329	LYS
13	T	331	ILE
13	T	337	HIS
13	T	338	SER
13	T	356	MET
13	T	367	PRO
13	T	373	PRO
13	T	374	LYS
13	T	378	LYS
13	T	380	HIS
13	T	391	PHE
13	T	392	SER
13	T	402	ASP
13	T	411	ASP
13	T	424	PRO
13	T	429	ILE
13	T	441	LYS
14	M	34	CYS
14	M	55	ILE
14	M	99	VAL
15	N	104	LEU
15	N	146	LEU
15	N	169	ASP
15	N	184	VAL
15	N	231	ASP
16	O	173	LYS
16	O	182	VAL
16	O	261	THR
16	O	319	LYS
16	O	323	VAL
16	O	343	THR
16	O	348	GLU
17	P	35	THR
17	P	36	THR
18	Q	43	PHE

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Mol	Chain	Res	Type
18	Q	47	ARG
18	Q	81	LYS
18	Q	112	ILE
19	R	24	LEU
20	S	303	LEU
20	S	398	PRO
20	S	420	ILE
21	U	81	ILE
21	U	134	GLU
21	U	184	MET
22	V	261	SER
22	V	277	THR
23	W	292	THR
23	W	293	SER
23	W	295	GLU
23	W	301	GLN
23	W	429	GLN
23	W	439	LYS
23	W	448	LEU
23	W	475	PRO
23	W	480	ARG
23	W	482	THR
23	W	489	ARG
23	W	507	GLU
23	W	513	THR
23	W	517	THR
23	W	521	ASP
23	W	522	GLU
23	W	555	LYS
23	W	556	VAL
23	W	559	ASP
23	W	587	GLU
23	W	596	LYS
23	W	613	ASP
23	W	649	ASN
23	W	696	VAL
23	W	699	THR
23	W	716	LYS
23	W	730	VAL
23	W	740	SER
23	W	742	ILE
23	W	758	ASN

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Mol	Chain	Res	Type
23	W	765	THR
23	W	767	ASP
23	W	811	ARG
23	W	812	THR
23	W	821	TYR
23	W	835	VAL
23	W	845	HIS
23	W	864	MET
23	W	870	ASN
23	W	883	GLN
23	W	894	LEU
23	W	913	SER
23	W	980	CYS
23	W	1006	LYS
23	W	1009	LEU
23	W	1010	LYS
23	W	1040	VAL
23	W	1062	LYS
23	W	1065	GLU
23	W	1067	VAL
23	W	1072	ILE
23	W	1077	ARG
23	W	1081	SER
23	W	1082	GLN
23	W	1085	SER
23	W	1087	GLU
23	W	1100	LYS
24	a	47	GLU
25	b	16	CYS
25	b	18	PHE
25	b	25	THR
25	b	79	LYS
25	b	81	LEU
26	c	79	LEU
27	d	18	ASN
27	d	71	LEU
28	e	10	LEU
29	f	20	LYS
29	f	30	GLN
29	f	77	ASP
30	g	24	PHE
30	g	48	LEU

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Mol	Chain	Res	Type
30	g	49	ARG
30	g	77	THR
30	g	99	ASP
30	g	100	SER
24	h	47	GLU
25	i	16	CYS
25	i	18	PHE
25	i	25	THR
25	i	79	LYS
25	i	81	LEU
26	j	79	LEU
27	k	18	ASN
27	k	71	LEU
28	l	10	LEU
29	m	20	LYS
29	m	30	GLN
29	m	77	ASP
30	n	48	LEU
30	n	49	ARG
30	n	77	THR
30	n	99	ASP
30	n	100	SER
31	o	4	THR
31	o	44	PRO
31	o	71	SER
33	q	14	VAL
33	q	17	PRO
33	q	44	PRO
33	q	55	PRO
33	q	56	SER
33	q	61	SER
33	q	102	LEU
33	q	126	LEU
33	r	17	PRO
33	r	44	PRO
33	r	63	THR
33	r	93	LEU
33	r	109	LEU
33	s	17	PRO
33	s	26	SER
33	s	44	PRO
33	s	63	THR

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Mol	Chain	Res	Type
33	s	109	LEU
33	s	134	SER
33	t	17	PRO
33	t	44	PRO
33	t	63	THR
33	t	80	LEU
33	t	85	GLN
33	t	93	LEU
33	t	98	LEU
33	t	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	170	HIS
1	A	181	HIS
1	A	265	ASN
1	A	405	ASN
1	A	429	ASN
1	A	541	ASN
1	A	558	GLN
1	A	574	GLN
1	A	658	ASN
1	A	659	HIS
1	A	685	HIS
1	A	705	GLN
1	A	733	GLN
1	A	739	ASN
1	A	784	GLN
1	A	785	HIS
1	A	864	GLN
1	A	952	ASN
1	A	976	GLN
1	A	1005	GLN
1	A	1011	ASN
1	A	1086	ASN
1	A	1097	HIS
1	A	1156	HIS
1	A	1231	GLN
1	A	1281	ASN
1	A	1376	ASN

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Mol	Chain	Res	Type
1	A	1470	GLN
1	A	1500	HIS
1	A	1529	ASN
1	A	1532	HIS
1	A	1592	HIS
1	A	1594	GLN
1	A	1626	GLN
1	A	1718	HIS
1	A	1782	ASN
1	A	1856	ASN
1	A	1888	HIS
3	C	84	GLN
3	C	101	GLN
3	C	158	HIS
3	C	251	GLN
3	C	289	ASN
3	C	310	ASN
3	C	588	GLN
3	C	776	ASN
3	C	794	GLN
3	C	817	GLN
3	C	830	ASN
3	C	869	HIS
9	I	67	GLN
9	I	79	HIS
10	J	31	HIS
10	J	72	GLN
10	J	163	GLN
10	J	214	ASN
11	K	184	GLN
11	K	202	GLN
12	L	34	GLN
13	T	161	HIS
13	T	292	HIS
13	T	337	HIS
13	T	358	ASN
14	M	45	HIS
14	M	72	GLN
14	M	209	ASN
15	N	25	GLN
15	N	91	HIS
15	N	191	ASN

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Mol	Chain	Res	Type
15	N	202	GLN
15	N	227	ASN
15	N	252	HIS
16	O	138	HIS
16	O	181	HIS
16	O	223	HIS
16	O	265	HIS
16	O	382	HIS
16	O	428	GLN
16	O	445	ASN
17	P	5	HIS
17	P	173	HIS
18	Q	87	ASN
18	Q	171	ASN
19	R	4	ASN
19	R	19	HIS
20	S	354	HIS
20	S	358	GLN
20	S	457	HIS
20	S	463	ASN
21	U	87	GLN
21	U	149	GLN
21	U	169	HIS
21	U	171	GLN
21	U	177	ASN
23	W	429	GLN
23	W	437	ASN
23	W	606	HIS
23	W	701	GLN
23	W	989	HIS
23	W	1015	HIS
24	a	8	HIS
24	a	91	GLN
25	b	34	GLN
25	b	86	ASN
26	c	25	HIS
26	c	52	GLN
27	d	66	ASN
28	e	41	ASN
29	f	30	GLN
29	f	86	ASN
24	h	8	HIS

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Mol	Chain	Res	Type
24	h	91	GLN
25	i	34	GLN
25	i	86	ASN
26	j	25	HIS
26	j	52	GLN
27	k	66	ASN
28	l	17	HIS
28	l	41	ASN
29	m	30	GLN
29	m	86	ASN
30	n	71	ASN
31	o	62	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	114/214 (53%)	27 (23%)	3 (2%)
4	D	102/112 (91%)	31 (30%)	5 (4%)
5	E	58/369 (15%)	35 (60%)	6 (10%)
6	F	88/1175 (7%)	30 (34%)	8 (9%)
All	All	362/1870 (19%)	123 (33%)	22 (6%)

All (123) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	32	G
2	B	33	U
2	B	42	A
2	B	44	A
2	B	74	U
2	B	75	A
2	B	76	U
2	B	77	A
2	B	79	C
2	B	80	G
2	B	81	A
2	B	82	A
2	B	84	A
2	B	90	C
2	B	94	C
2	B	101	C

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Mol	Chain	Res	Type
2	B	104	G
2	B	127	U
2	B	164	C
2	B	165	A
2	B	166	U
2	B	170	U
2	B	171	U
2	B	172	U
2	B	173	U
2	B	174	G
2	B	175	G
4	D	12	A
4	D	13	A
4	D	14	C
4	D	15	C
4	D	16	C
4	D	33	C
4	D	34	A
4	D	36	U
4	D	39	G
4	D	43	C
4	D	49	A
4	D	50	G
4	D	51	A
4	D	54	U
4	D	57	U
4	D	60	G
4	D	62	A
4	D	65	U
4	D	66	C
4	D	67	C
4	D	68	C
4	D	73	A
4	D	74	U
4	D	80	U
4	D	85	C
4	D	86	G
4	D	87	U
4	D	90	U
4	D	91	A
4	D	92	C
4	D	93	A

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Mol	Chain	Res	Type
5	E	-12	U
5	E	-11	A
5	E	-10	A
5	E	-7	U
5	E	-6	U
5	E	-2	A
5	E	2	U
5	E	3	A
5	E	9	U
5	E	10	U
5	E	11	A
5	E	13	U
5	E	284	U
5	E	285	U
5	E	286	A
5	E	287	A
5	E	292	U
5	E	294	G
5	E	295	A
5	E	296	U
5	E	297	A
5	E	300	A
5	E	301	A
5	E	302	C
5	E	303	A
5	E	304	C
5	E	346	A
5	E	347	A
5	E	348	U
5	E	349	A
5	E	350	G
5	E	351	U
5	E	353	A
5	E	354	A
5	E	355	U
6	F	15	C
6	F	16	U
6	F	17	U
6	F	19	U
6	F	23	U
6	F	25	A
6	F	26	G

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Mol	Chain	Res	Type
6	F	30	A
6	F	31	A
6	F	32	G
6	F	34	G
6	F	40	U
6	F	41	C
6	F	42	U
6	F	49	U
6	F	50	U
6	F	111	C
6	F	115	U
6	F	116	U
6	F	117	U
6	F	118	U
6	F	119	G
6	F	120	G
6	F	1099	G
6	F	1107	C
6	F	1108	A
6	F	1111	U
6	F	1112	G
6	F	1114	G
6	F	1120	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	78	A
2	B	83	C
2	B	172	U
4	D	14	C
4	D	42	A
4	D	53	A
4	D	56	A
4	D	64	U
5	E	9	U
5	E	283	U
5	E	294	G
5	E	299	U
5	E	301	A
5	E	352	A
6	F	29	C

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Mol	Chain	Res	Type
6	F	30	A
6	F	31	A
6	F	40	U
6	F	41	C
6	F	117	U
6	F	1107	C
6	F	1111	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
34	IHP	A	3000	-	36,36,36	0.70	0	60,60,60	1.00	0
35	GTP	C	1500	36	33,34,34	1.45	4 (12%)	50,54,54	2.26	18 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	IHP	A	3000	-	-	10/30/54/54	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	GTP	C	1500	36	-	5/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	1500	GTP	C5-N7	-3.65	1.31	1.39
35	C	1500	GTP	C6-N1	-3.32	1.32	1.38
35	C	1500	GTP	C4-N9	-2.84	1.30	1.38
35	C	1500	GTP	PB-O1B	-2.81	1.41	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	1500	GTP	C5-C4-N3	-5.61	119.47	128.39
35	C	1500	GTP	O2B-PB-O3A	-4.99	93.79	107.27
35	C	1500	GTP	N9-C4-N3	4.78	135.51	125.95
35	C	1500	GTP	C2-N3-C4	4.43	119.93	112.30
35	C	1500	GTP	O6-C6-C5	-4.17	115.51	126.53
35	C	1500	GTP	O4'-C4'-C3'	3.39	111.88	105.15
35	C	1500	GTP	O6-C6-N1	3.38	126.47	120.11
35	C	1500	GTP	O3A-PA-O1A	-2.98	101.73	110.70
35	C	1500	GTP	C2'-C1'-N9	-2.97	104.98	113.25
35	C	1500	GTP	C2-N1-C6	-2.62	120.36	125.11
35	C	1500	GTP	O4'-C1'-C2'	2.61	112.19	106.62
35	C	1500	GTP	O2A-PA-O1A	2.59	124.48	112.44
35	C	1500	GTP	O3B-PG-O1G	-2.51	97.84	111.04
35	C	1500	GTP	N9-C8-N7	-2.44	108.87	113.40
35	C	1500	GTP	O3A-PB-O1B	2.39	117.91	110.70
35	C	1500	GTP	C8-N9-C4	2.30	110.33	106.03
35	C	1500	GTP	C4'-O4'-C1'	-2.13	104.76	109.47
35	C	1500	GTP	PA-O5'-C5'	-2.00	109.89	121.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	3000	IHP	C1-C6-O16-P6
34	A	3000	IHP	C5-C6-O16-P6
35	C	1500	GTP	C5'-O5'-PA-O1A
35	C	1500	GTP	O4'-C4'-C5'-O5'
35	C	1500	GTP	C3'-C4'-C5'-O5'

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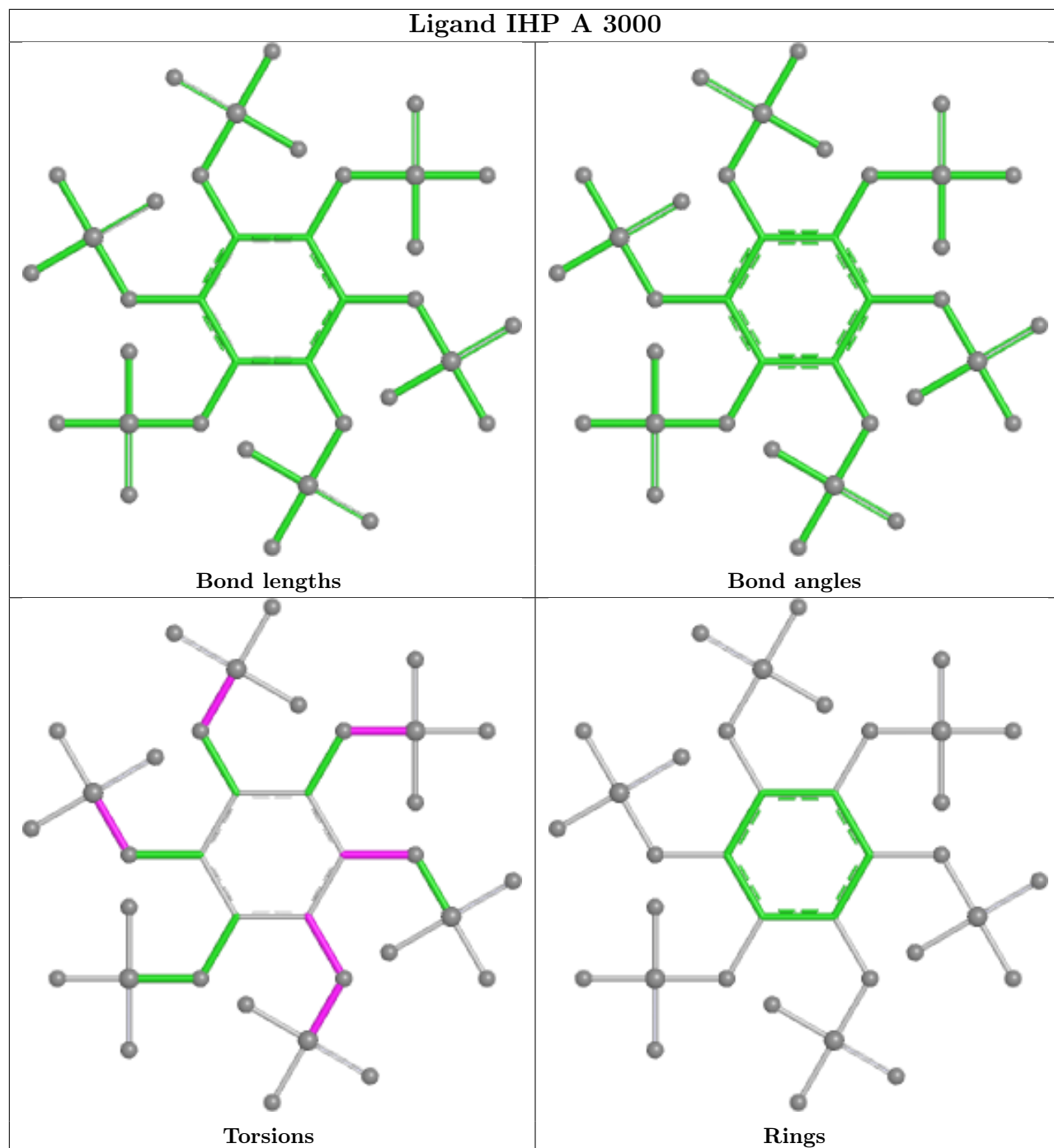
Mol	Chain	Res	Type	Atoms
34	A	3000	IHP	C4-C5-O15-P5
34	A	3000	IHP	C6-C5-O15-P5
34	A	3000	IHP	C4-O14-P4-O24
35	C	1500	GTP	C5'-O5'-PA-O3A
35	C	1500	GTP	C5'-O5'-PA-O2A
34	A	3000	IHP	C3-O13-P3-O43
34	A	3000	IHP	C2-O12-P2-O22
34	A	3000	IHP	C6-O16-P6-O26
34	A	3000	IHP	C6-O16-P6-O36
34	A	3000	IHP	C6-O16-P6-O46

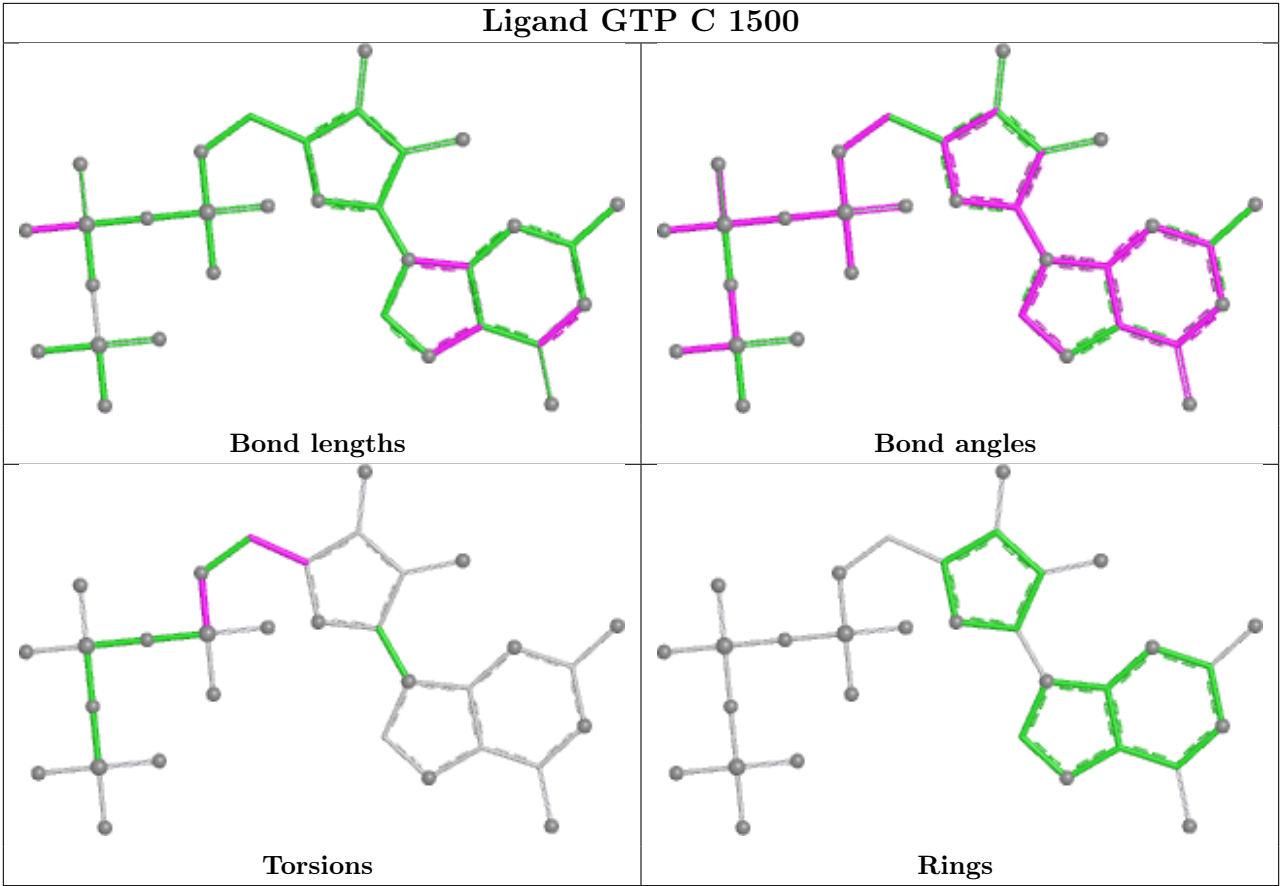
There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	3000	IHP	9	0
35	C	1500	GTP	6	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	350:G	O3'	351:U	P	3.39

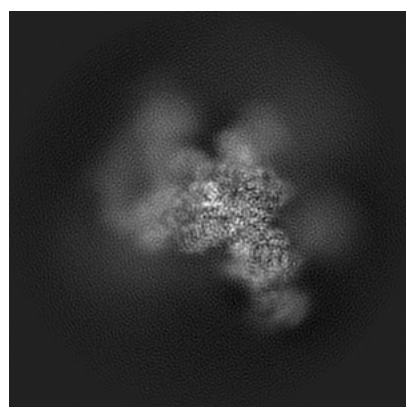
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6839. These allow visual inspection of the internal detail of the map and identification of artifacts.

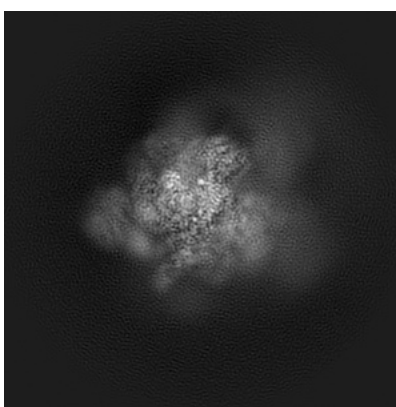
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

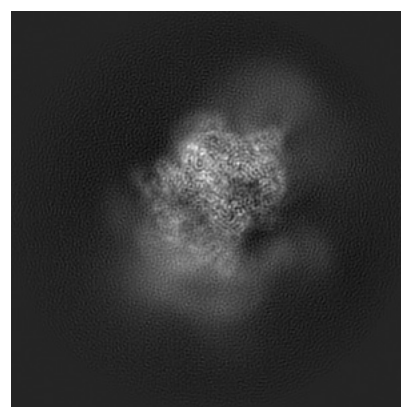
6.1.1 Primary map



X



Y

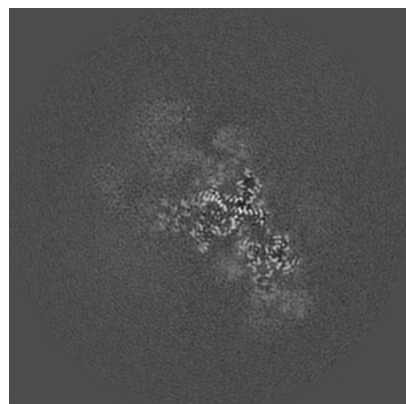


Z

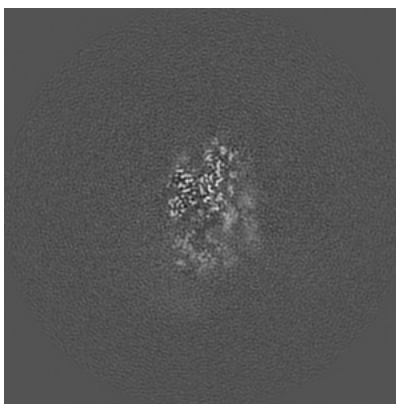
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

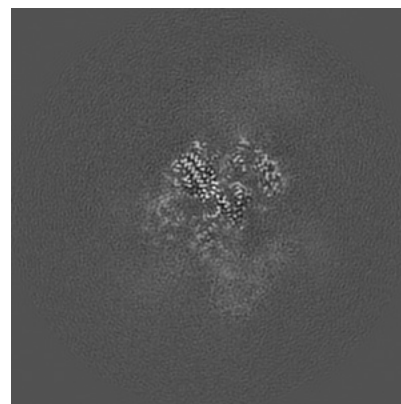
6.2.1 Primary map



X Index: 200



Y Index: 200

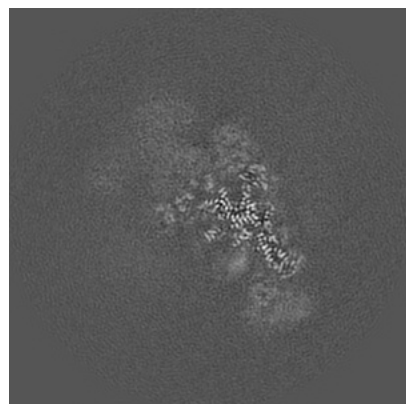


Z Index: 200

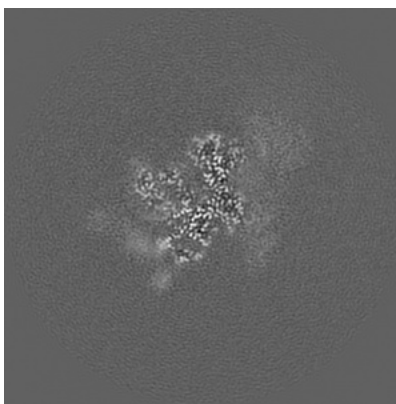
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

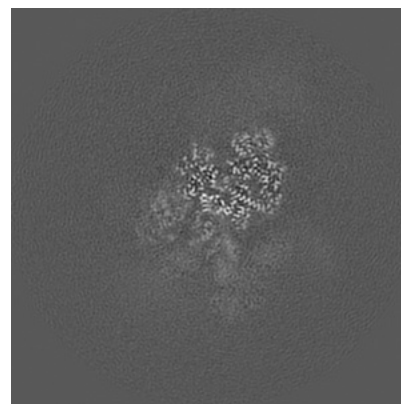
6.3.1 Primary map



X Index: 192



Y Index: 238

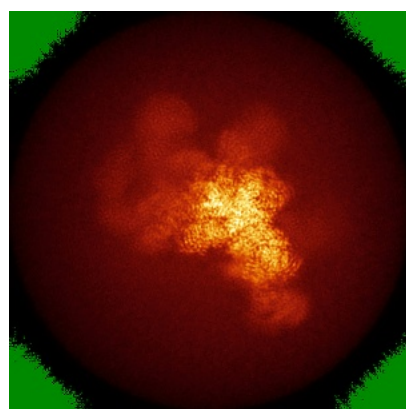


Z Index: 206

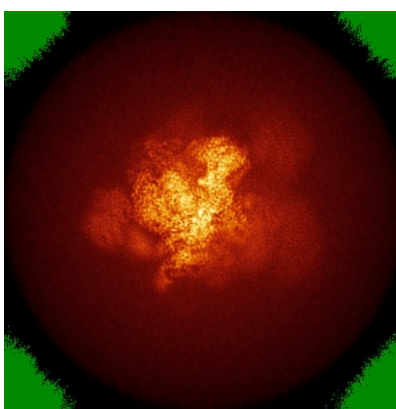
The images above show the largest variance slices of the map in three orthogonal directions.

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

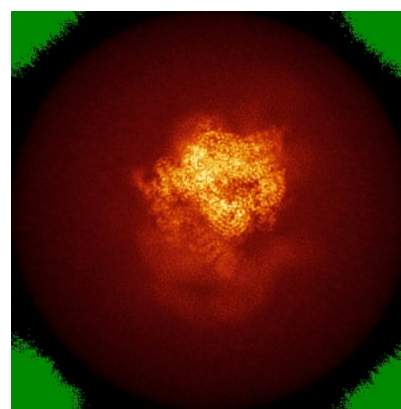
6.4.1 Primary map



X



Y

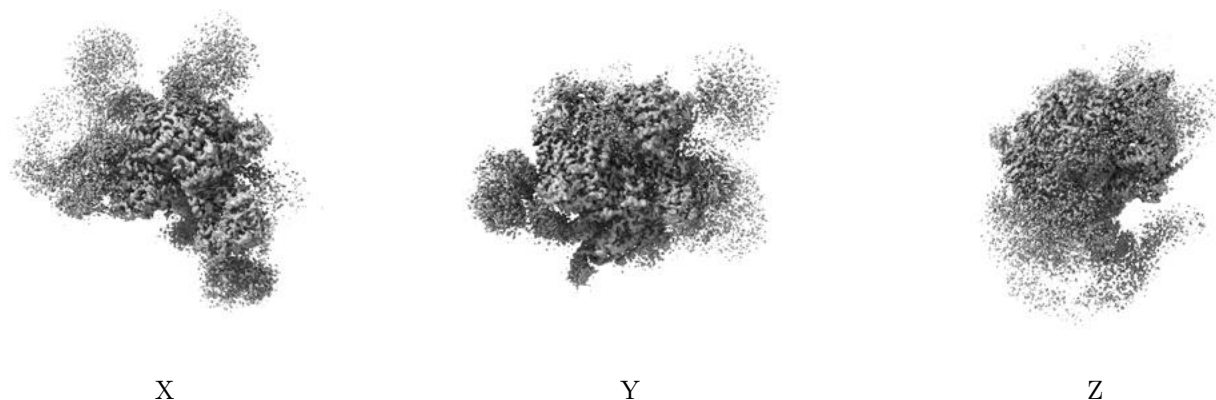


Z

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

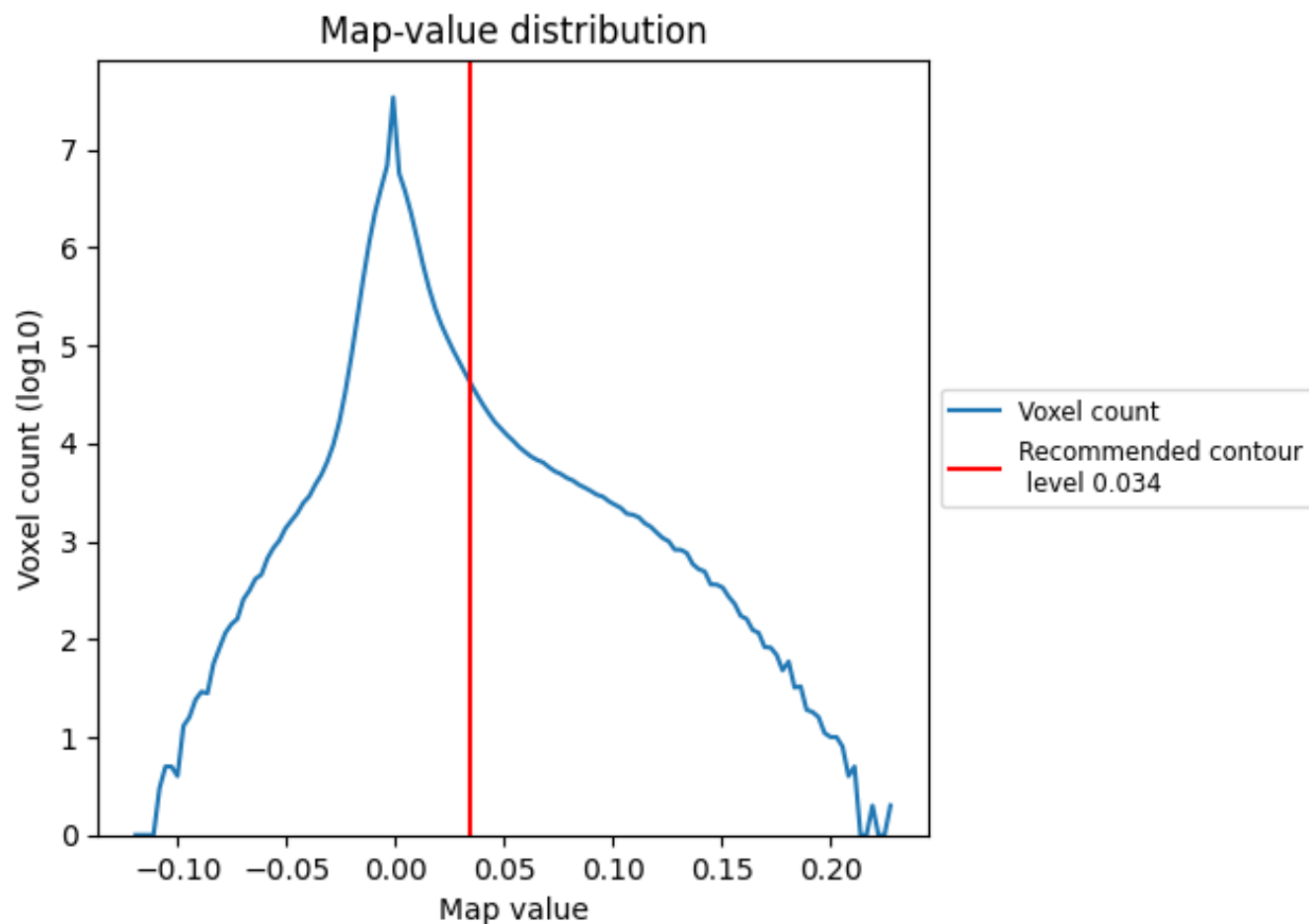
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

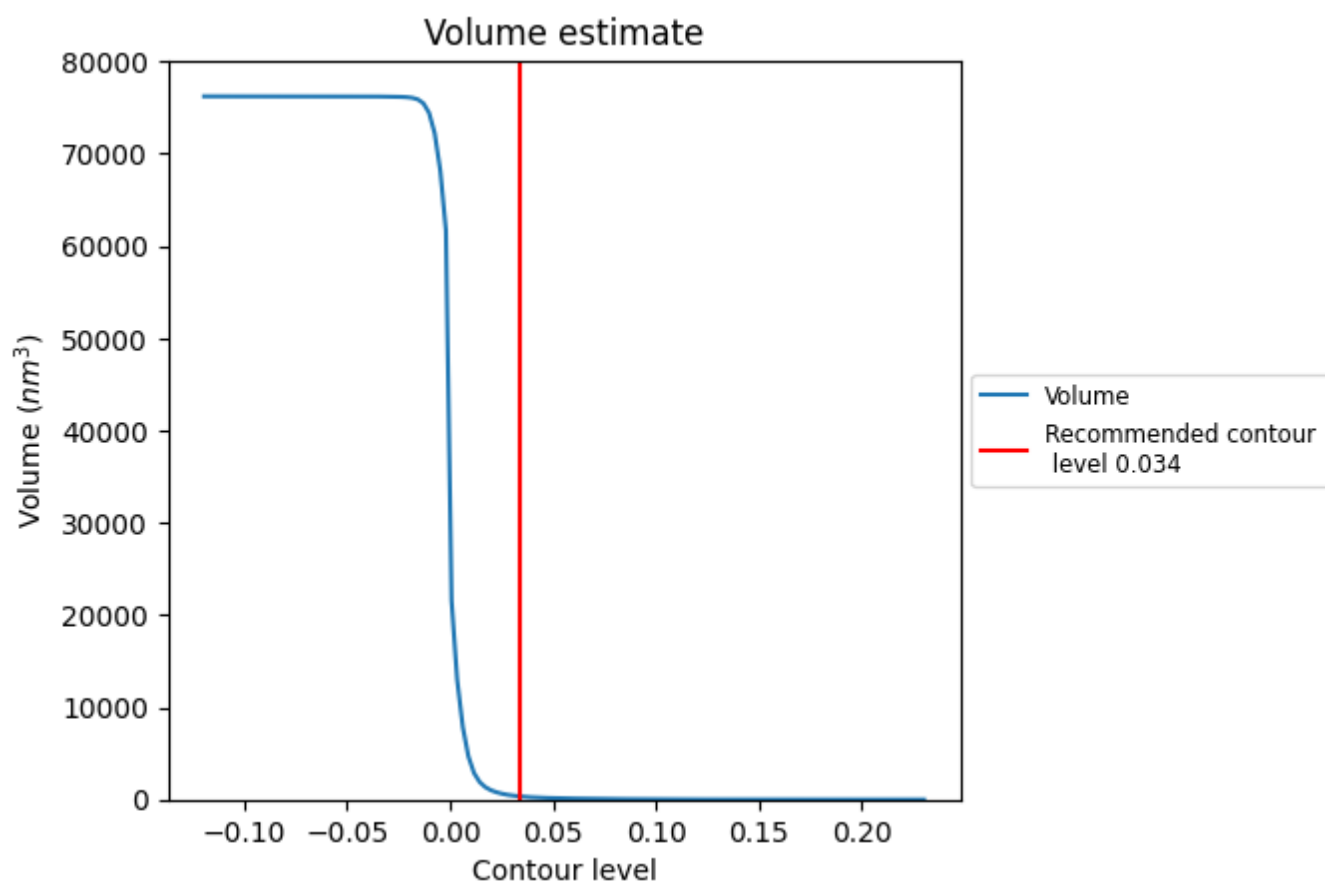
This section contains the results of statistical analysis of the map.

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.

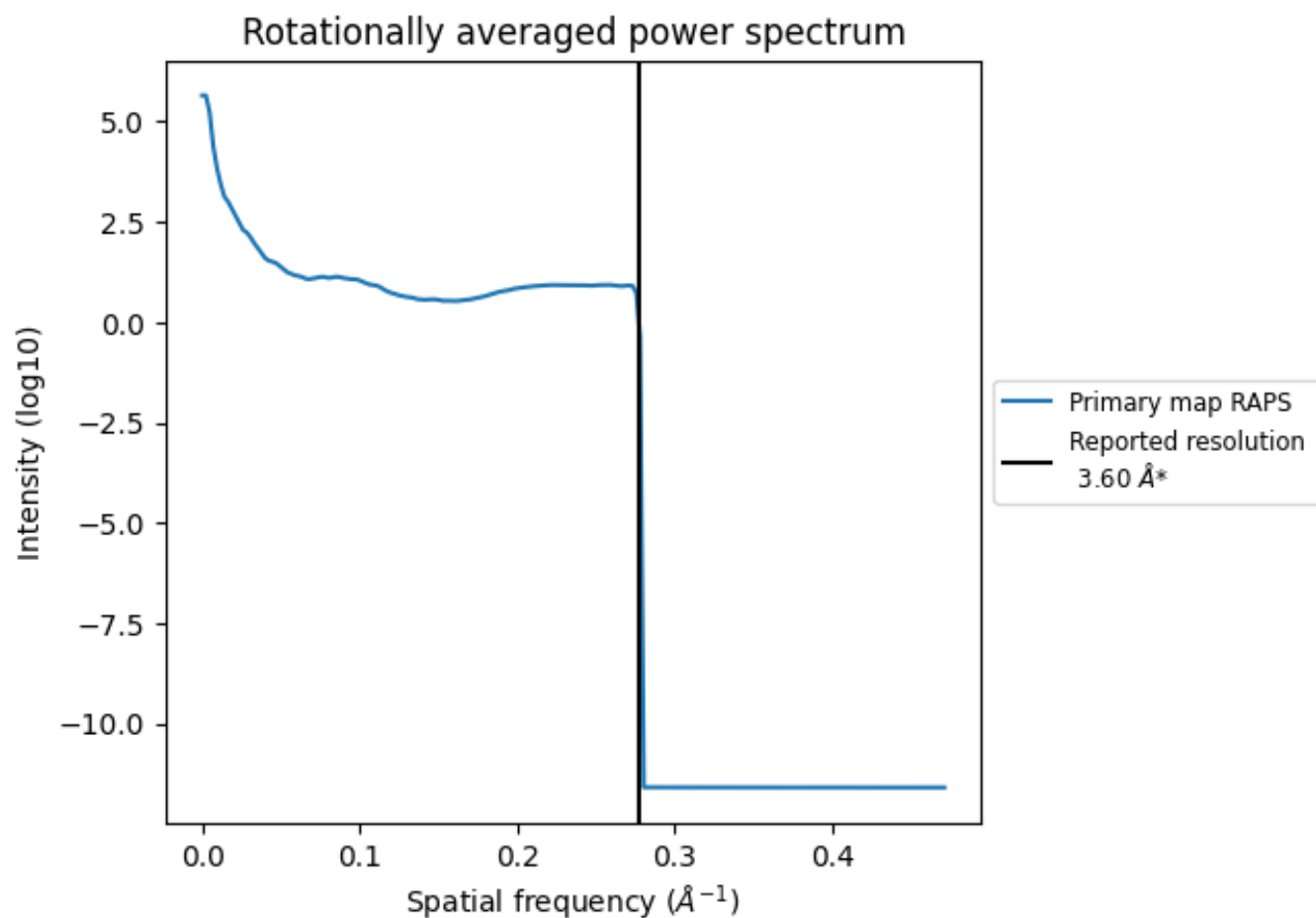
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 343 nm³; this corresponds to an approximate mass of 309 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 0.278 Å⁻¹

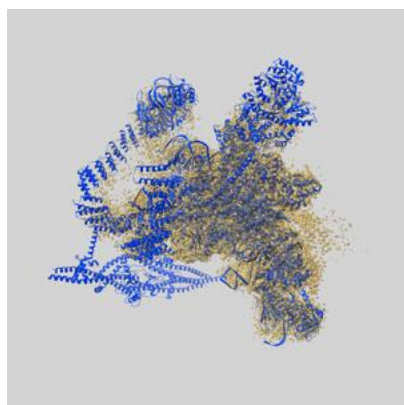
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

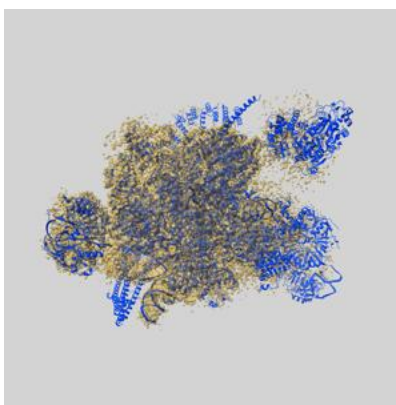
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6839 and PDB model 5YLZ. Per-residue inclusion information can be found in section 3 on page 12.

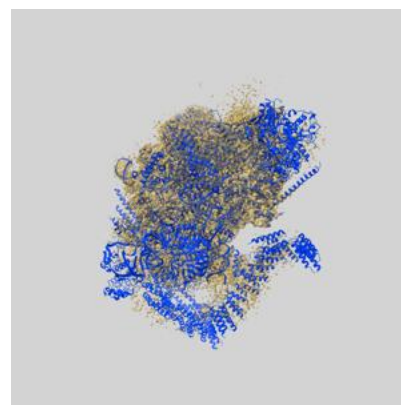
9.1 Map-model overlay [i](#)



X



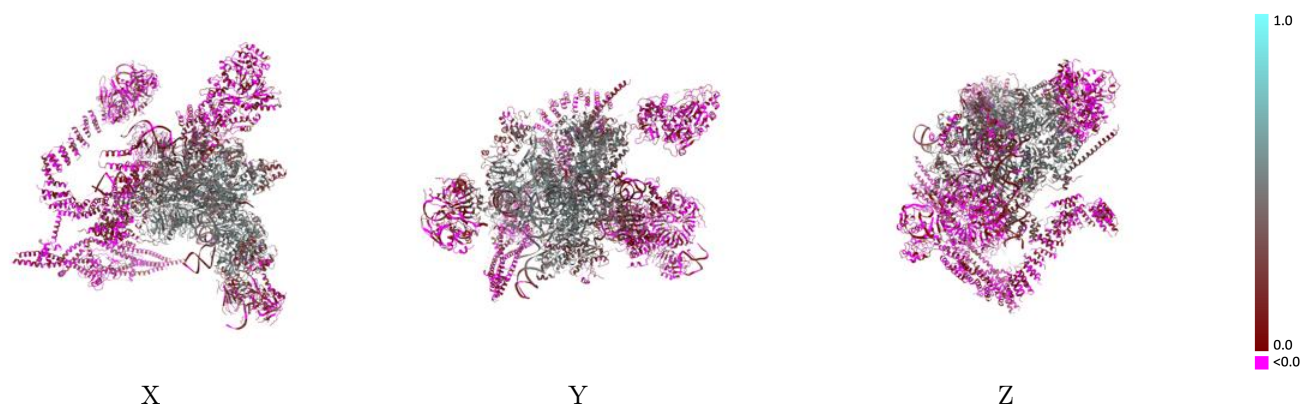
Y



Z

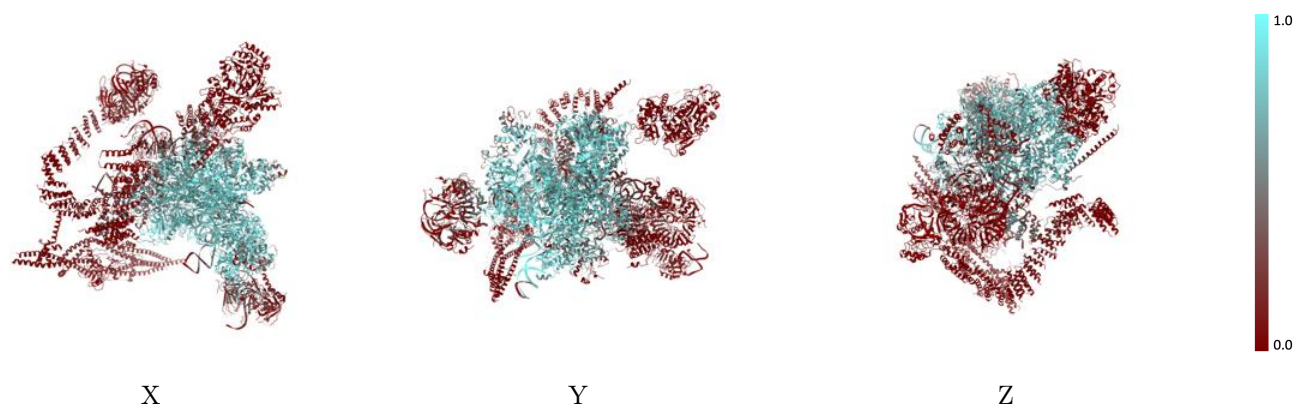
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



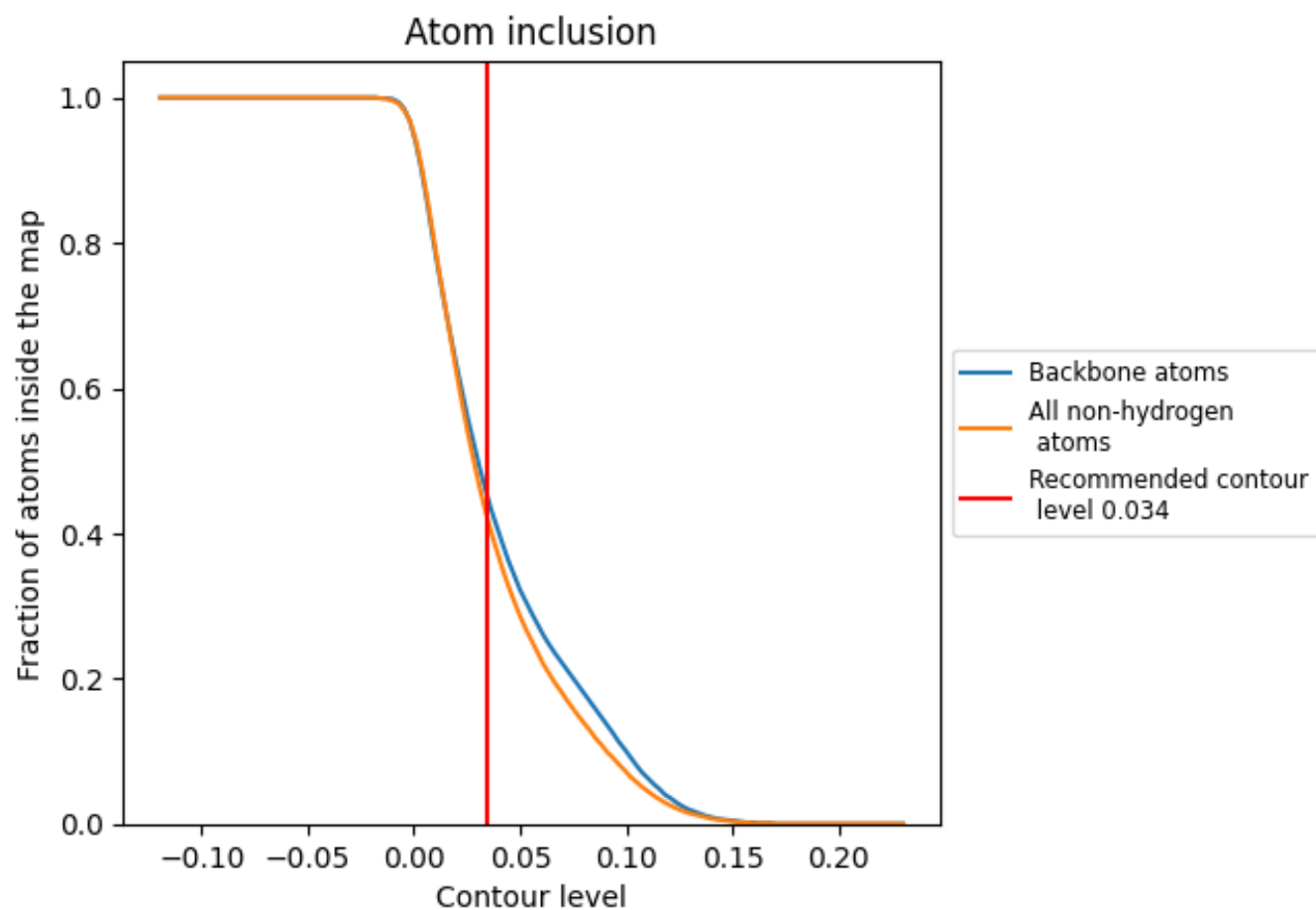
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 43% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4270	0.2510
A	0.7290	0.4270
B	0.7080	0.3360
C	0.7330	0.4230
D	0.7560	0.3550
E	0.4950	0.2470
F	0.2530	0.1240
G	0.0000	0.0080
H	0.0190	0.0080
I	0.3310	0.2120
J	0.3030	0.1980
K	0.3330	0.2530
L	0.7890	0.4380
M	0.4130	0.3100
N	0.5740	0.3440
O	0.8110	0.4820
P	0.6780	0.4730
Q	0.4650	0.3650
R	0.5400	0.4360
S	0.6810	0.3860
T	0.1840	0.1280
U	0.0200	0.0470
V	0.0240	0.0620
W	0.0310	0.0290
a	0.2710	0.1470
b	0.1140	0.0690
c	0.1160	0.0480
d	0.1860	0.1130
e	0.4260	0.2570
f	0.2310	0.0990
g	0.1260	0.0380
h	0.0070	0.0070
i	0.0050	-0.0350
j	0.0130	-0.0110
k	0.0040	-0.0070



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Chain	Atom inclusion	Q-score
l	 0.0050	 0.0330
m	 0.0270	 -0.0240
n	 0.0190	 0.0030
o	 0.0020	 0.0180
p	 0.0000	 0.0110
q	 0.0000	 -0.0150
r	 0.0000	 0.0230
s	 0.0000	 -0.0180
t	 0.0000	 0.0140