



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 03:55 AM UTC

PDB ID : 8I0W / pdb_00008i0w
EMDB ID : EMD-35113
Title : The cryo-EM structure of human C complex
Authors : Zhan, X.; Lu, Y.; Shi, Y.
Deposited on : 2023-01-11
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 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

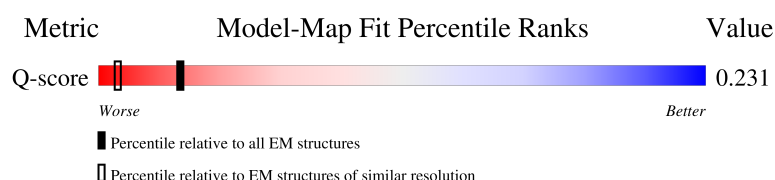
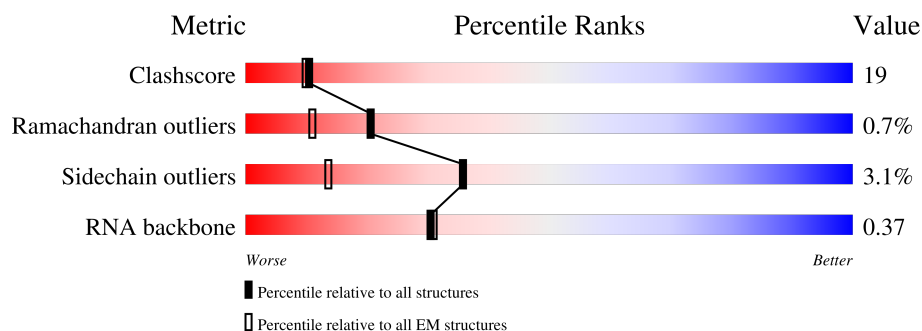
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	2335	5% 64% 31% • •
2	B	117	7% 16% 53% 15% 16%
3	C	972	• 44% 41% • 11%

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Mol	Chain	Length	Quality of chain
4	D	2136	
5	E	357	
6	F	107	
7	G	46	
8	6	174	
9	H	188	
10	I	855	
11	J	848	
12	K	225	
13	L	802	
14	M	243	
15	N	144	
16	O	420	
17	P	229	
18	R	536	
19	S	166	
20	T	514	
21	Q	1485	
22	U	2752	
23	V	908	
24	W	579	
25	X	425	
26	Y	323	
27	Z	1227	
28	q	504	

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Mol	Chain	Length	Quality of chain
28	r	504	
28	s	504	
28	t	504	
29	u	411	
30	v	146	
31	w	174	
32	x	703	
33	g	126	
33	h	126	
34	a	240	
34	i	240	
35	b	119	
35	j	119	
36	c	118	
36	k	118	
37	d	86	
37	m	86	
38	e	92	
38	l	92	
39	f	76	
39	n	76	
40	o	255	
41	p	225	
42	y	301	
43	z	285	

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Mol	Chain	Length	Quality of chain
44	3	646	29%69%29%
45	4	450	97%
46	1	654	8%42%18%40%
47	2	258	28%45%21%34%
48	5	37	27%89%8%

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 106256 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-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2253	Total	C	N	O	S	0	0
			17519	11136	3147	3166	70		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2066	925	347	696	98		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	862	Total	C	N	O	S	0	0
			6795	4344	1138	1281	32		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	1908	Total	C	N	O	0	0
			7632	3816	1908	1908		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	299	Total	C	N	O	S	0	0
			2338	1470	410	445	13		

- Molecule 6 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 7 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	18	Total	C	N	O	P	0	0
			383	172	73	121	17		

- Molecule 8 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	70	Total	C	N	O	P	0	0
			1256	554	163	469	70		

- Molecule 9 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	139	Total	C	N	O	P	0	0
			2946	1317	507	983	139		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	I	672	Total	C	N	O	0	0
			3387	2043	672	672		

- Molecule 11 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	571	Total	C	N	O	S	0	0
			3829	2385	720	718	6		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	152	Total	C	N	O	S	0	0
			979	611	177	189	2		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	419	Total	C	N	O	S	0	0
			2885	1809	534	537	5		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	91	Total	C	N	O	S	0	0
			775	482	146	145	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	283	Total	C	N	O	S	0	0
			2277	1430	403	424	20		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	96	Total	C	N	O	S	0	0
			829	508	162	157	2		

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	245	Total	C	N	O	P	S	0	0
			1962	1231	353	364	2	12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	313	Total	C	N	O	S	0	0
			2461	1554	447	452	8		

- Molecule 21 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Q	1322	Total	C	N	O	0	0
			5288	2644	1322	1322		

- Molecule 22 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	452	Total	C	N	O	S	0	0
			3410	2194	590	611	15		

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	440	Total	C	N	O	S	0	0
			2615	1601	487	523	4		

- Molecule 25 is a protein called Pre-mRNA-splicing factor CWC25 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	71	Total	C	N	O	0	0
			480	297	95	88		

- Molecule 26 is a protein called Coiled-coil domain-containing protein 94.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	204	Total	C	N	O	S	0	0
			1426	898	259	261	8		

- Molecule 27 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	754	Total	C	N	O	0	0
			3727	2219	754	754		

- Molecule 28 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	q	132	Total	C	N	O	S	0	0
			918	581	156	178	3		
28	r	131	Total	C	N	O	S	0	0
			901	572	149	177	3		
28	s	67	Total	C	N	O		0	0
			268	134	67	67			
28	t	67	Total	C	N	O	S	0	0
			476	300	83	92	1		

- Molecule 29 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	u	390	Total	C	N	O	S	0	0
			3126	1974	545	588	19		

- Molecule 30 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	v	144	Total	C	N	O	S	0	0
			1196	772	200	221	3		

- Molecule 31 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	w	91	Total	C	N	O	S	0	0
			730	463	122	142	3		

- Molecule 32 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	x	25	Total	C	N	O	0	0
			216	136	39	41		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	80	Total	C	N	O	S	0	0
			621	388	110	117	6		
33	g	81	Total	C	N	O		0	0
			324	162	81	81			

- Molecule 34 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	86	Total	C	N	O	S	0	0
			690	434	126	123	7		
34	a	86	Total	C	N	O		0	0
			344	172	86	86			

- Molecule 35 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	82	Total	C	N	O	S	0	0
			649	413	113	119	4		
35	b	82	Total	C	N	O		0	0
			328	164	82	82			

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	85	Total	C	N	O	S	0	0
			688	432	125	126	5		
36	c	97	Total	C	N	O		0	0
			388	194	97	97			

- Molecule 37 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	74	Total	C	N	O	S	0	0
			576	373	95	103	5		
37	d	74	Total	C	N	O		0	0
			296	148	74	74			

- Molecule 38 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	75	Total	C	N	O	S	0	0
			621	392	111	114	4		
38	e	79	Total	C	N	O		0	0
			316	158	79	79			

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	68	Total	C	N	O	S	0	0
			533	339	95	93	6		

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Mol	Chain	Residues	Atoms				AltConf	Trace
39	f	73	Total	C	N	O	0	0
			292	146	73	73		

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	162	Total	C	N	O	S	0	0
			1277	817	219	238	3		

- Molecule 41 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	94	Total	C	N	O	S	0	0
			760	488	135	132	5		

- Molecule 42 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	y	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 43 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	z	80	Total	C	N	O	S	0	0
			546	346	98	101	1		

- Molecule 44 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	3	460	Total	C	N	O	0	0
			2301	1381	460	460		

- Molecule 45 is a protein called Corepressor interacting with RBPJ 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4	14	Total	C	N	O	S	0	0
			112	68	21	22	1		

- Molecule 46 is a protein called WD repeat-containing protein 70.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	393	Total	C	N	O	S	0	0
			2705	1690	489	510	16		

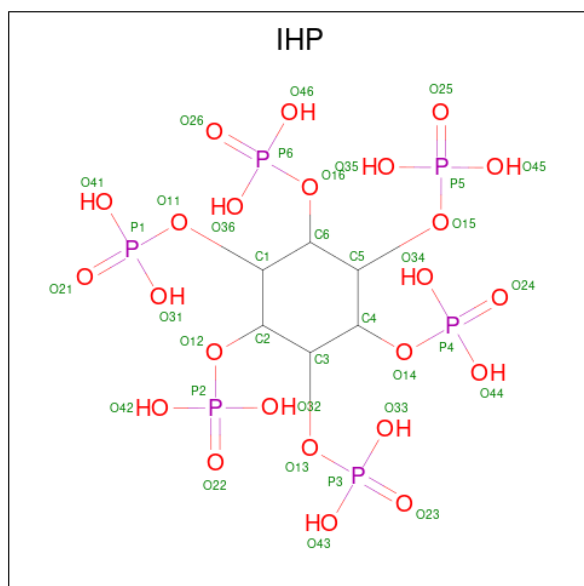
- Molecule 47 is a protein called Protein FRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	169	Total	C	N	O	S	0	0
			1296	814	228	247	7		

- Molecule 48 is a protein called UNK.

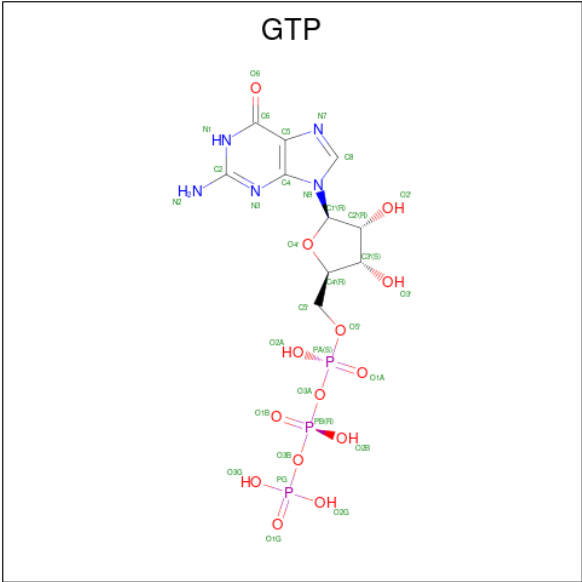
Mol	Chain	Residues	Atoms				AltConf	Trace
48	5	37	Total	C	N	O	0	0
			184	110	37	37		

- Molecule 49 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	C	1	Total	Mg	0
			1	1	
51	F	4	Total	Mg	0
			4	4	

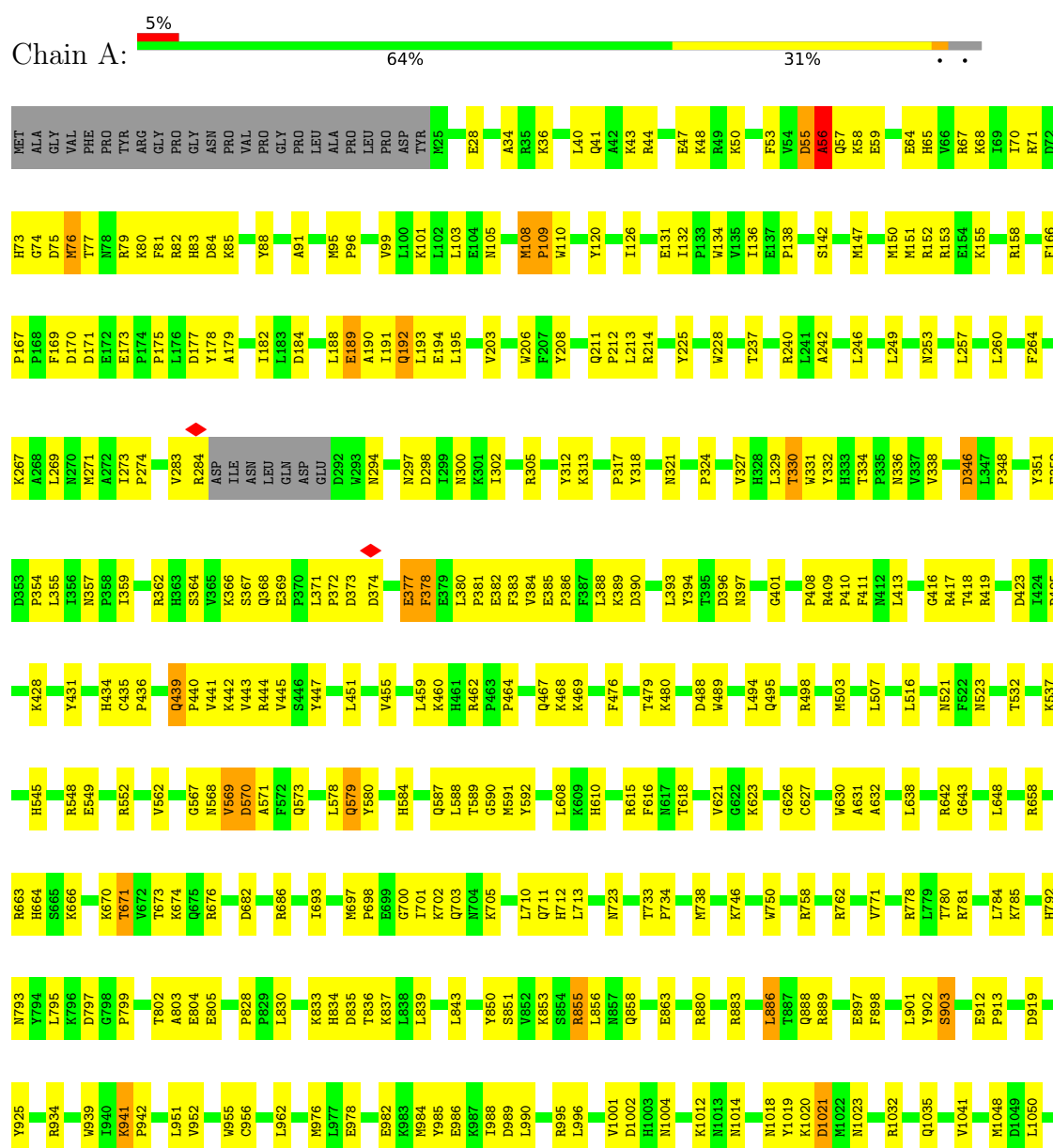
- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	N	3	Total	Zn	0
			3	3	
52	O	3	Total	Zn	0
			3	3	
52	Y	1	Total	Zn	0
			1	1	

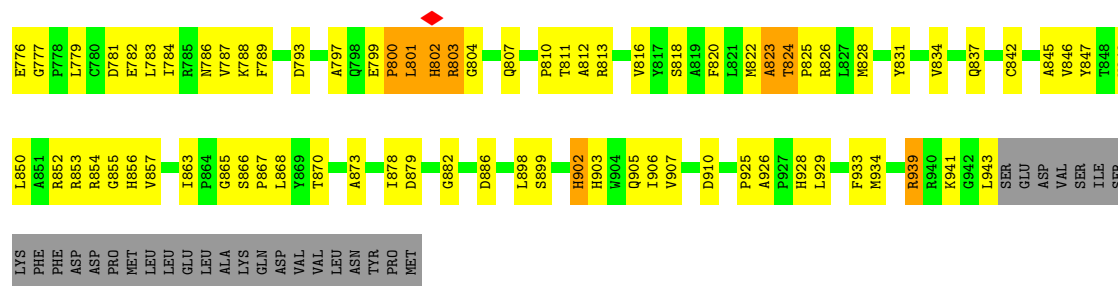
3 Residue-property plots

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

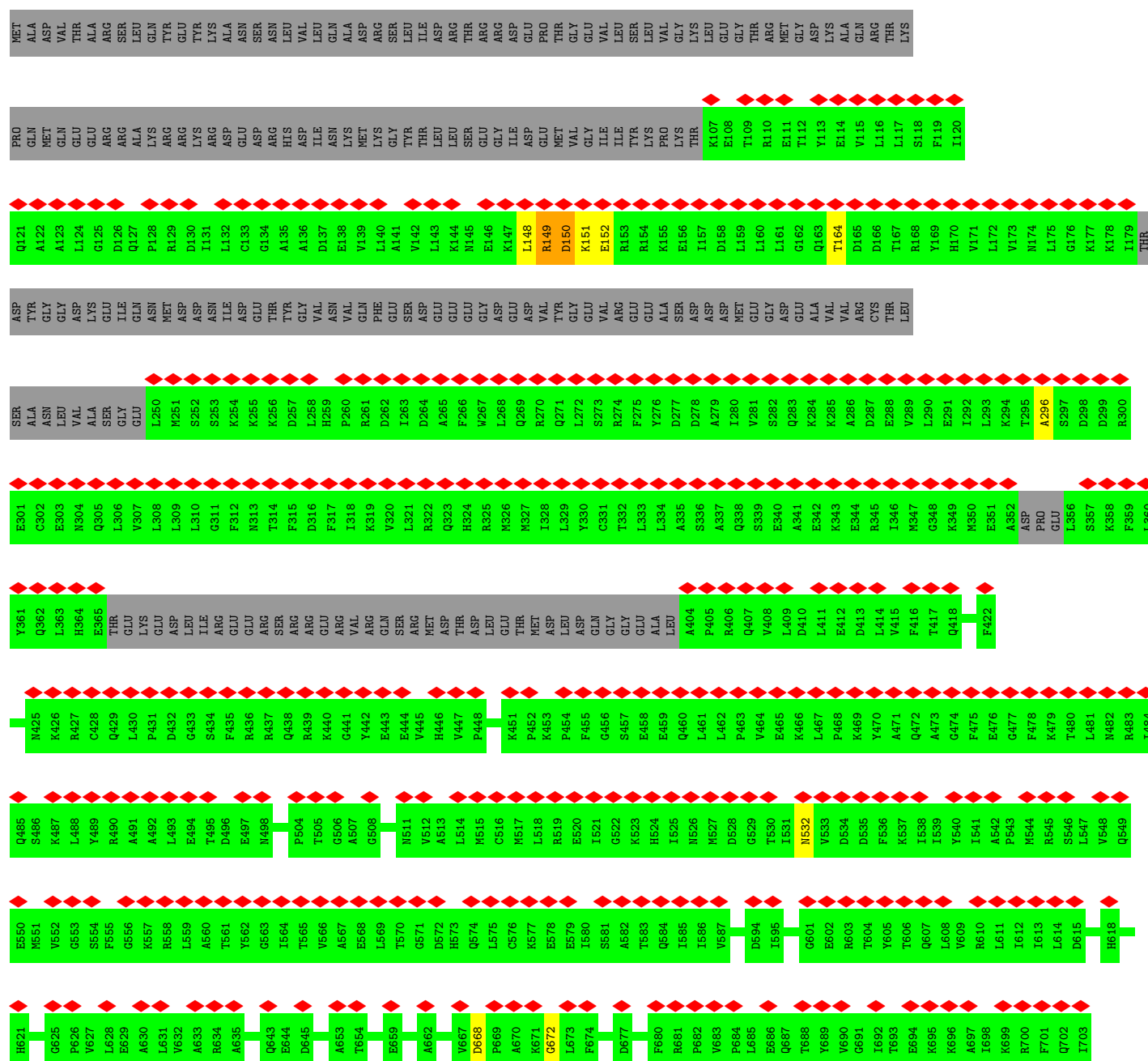
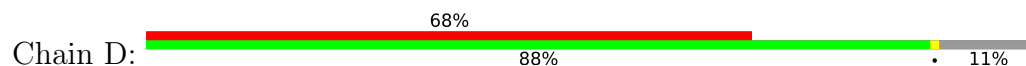
- Molecule 1: Pre-mRNA-processing-splicing factor 8

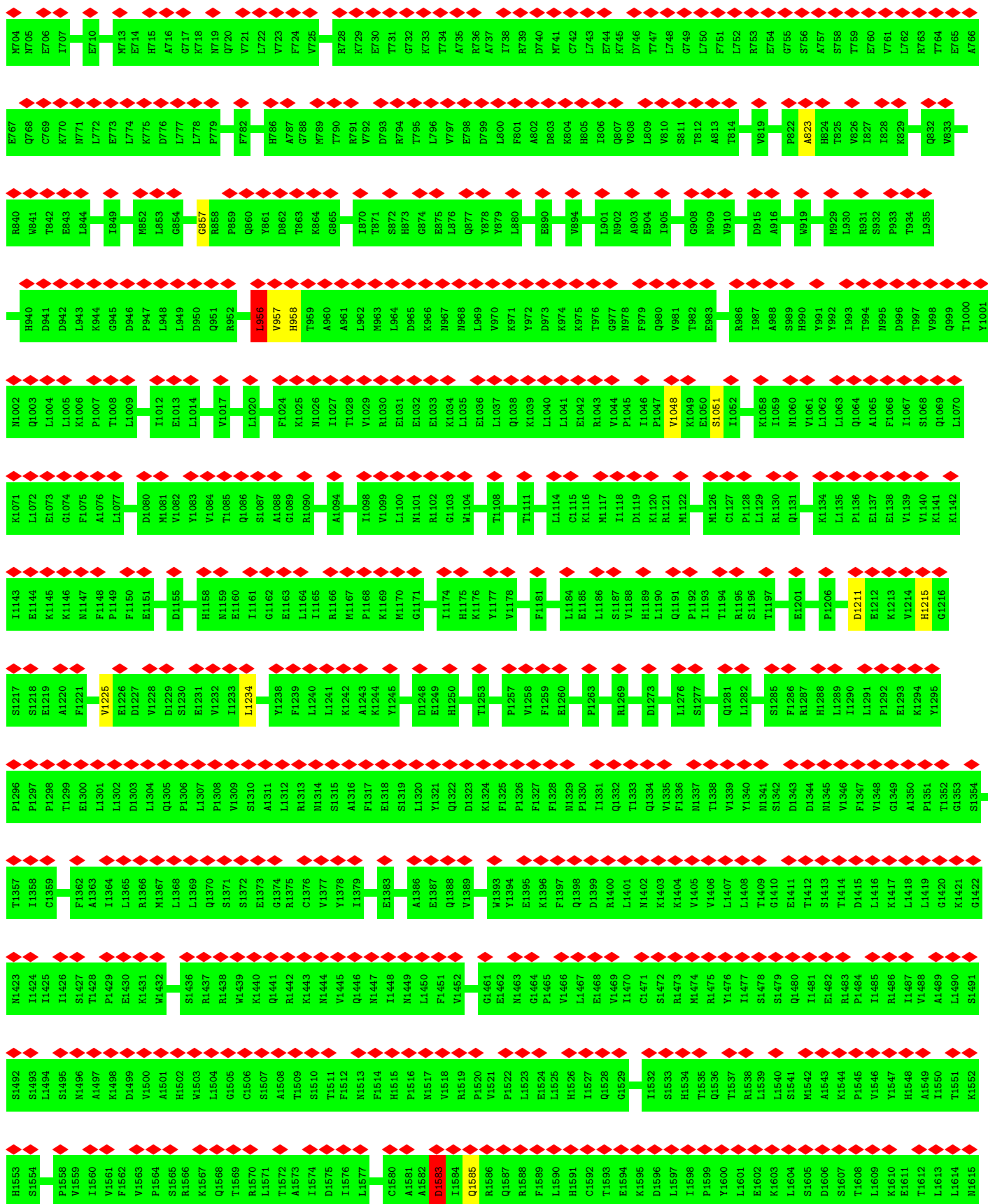


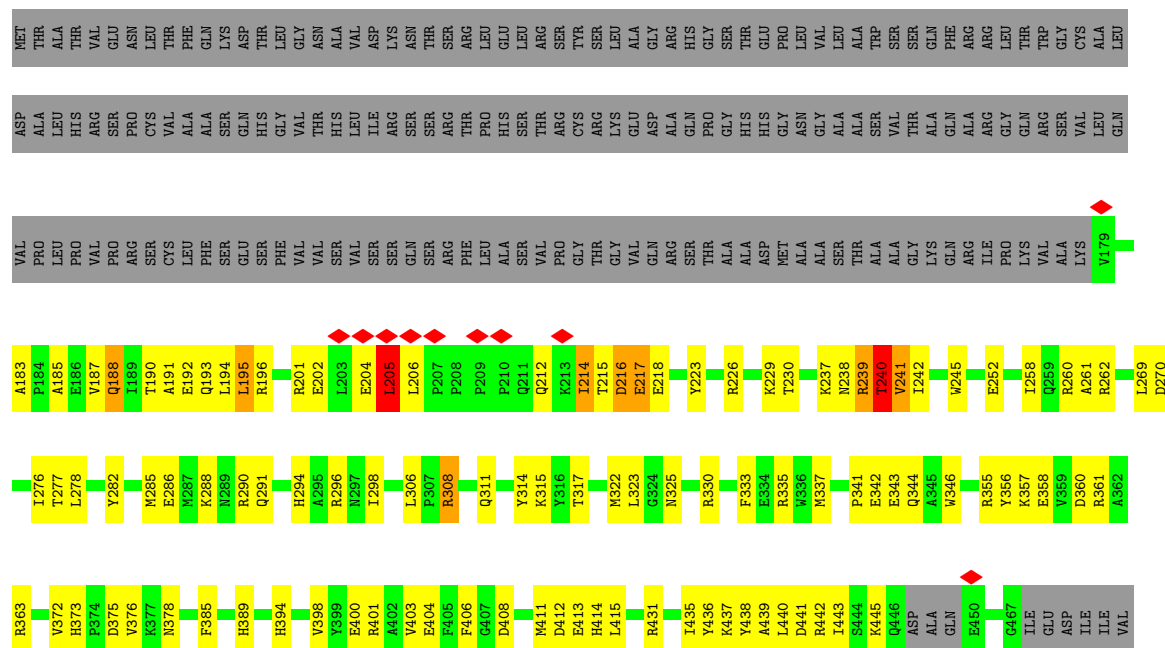


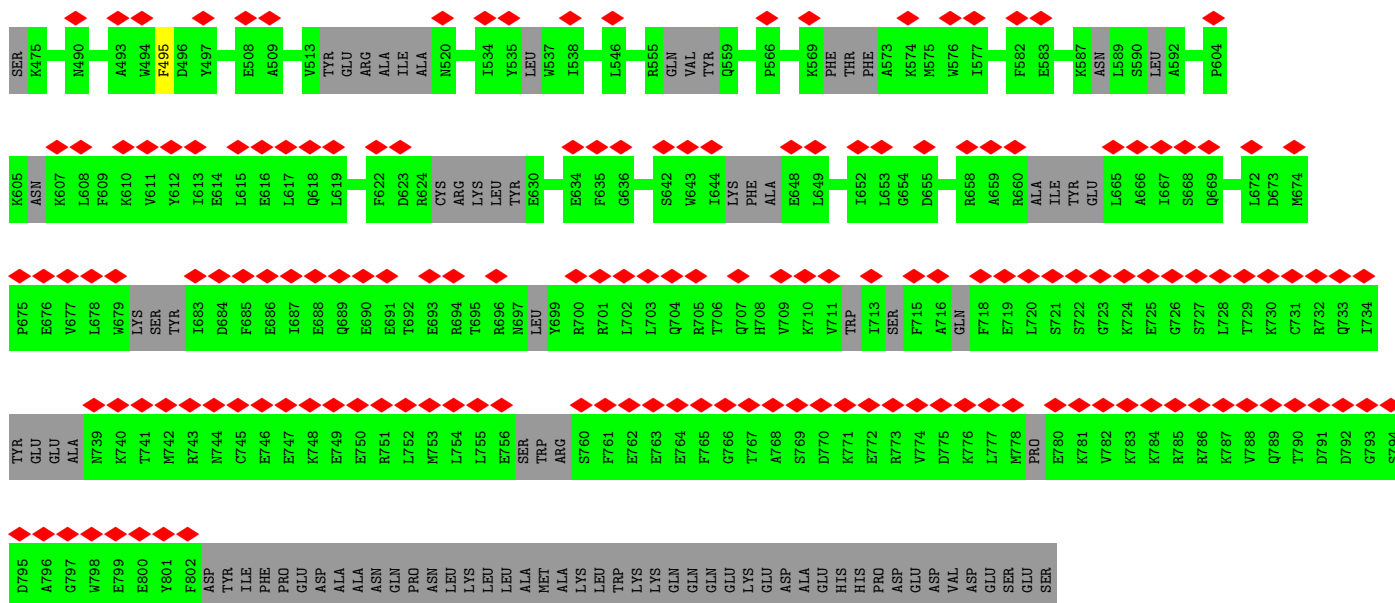


- Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

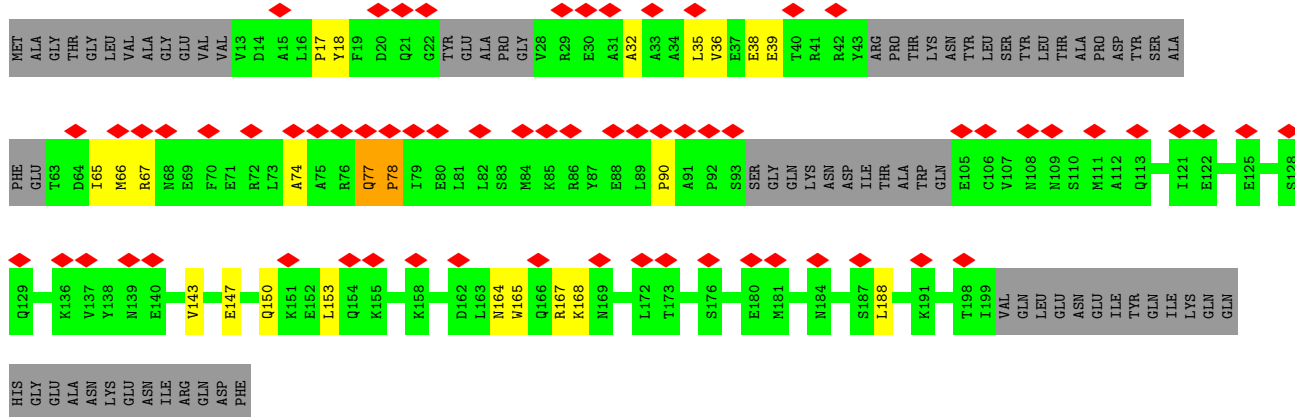




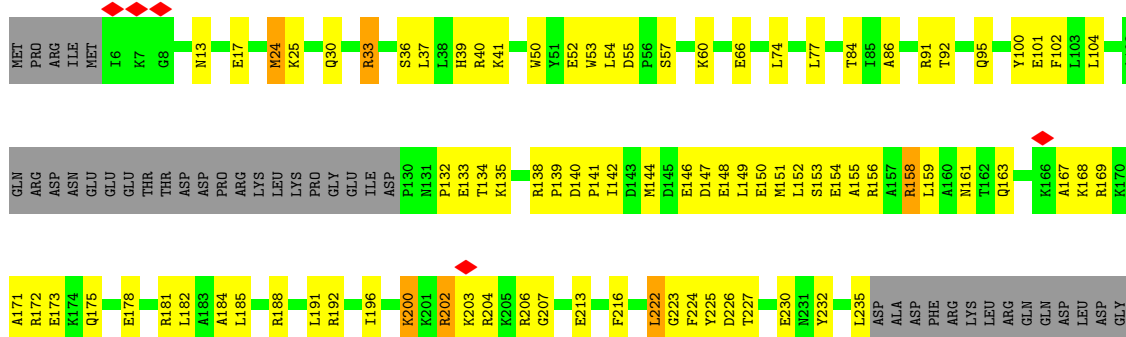
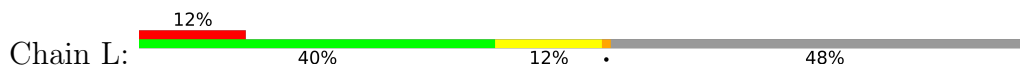


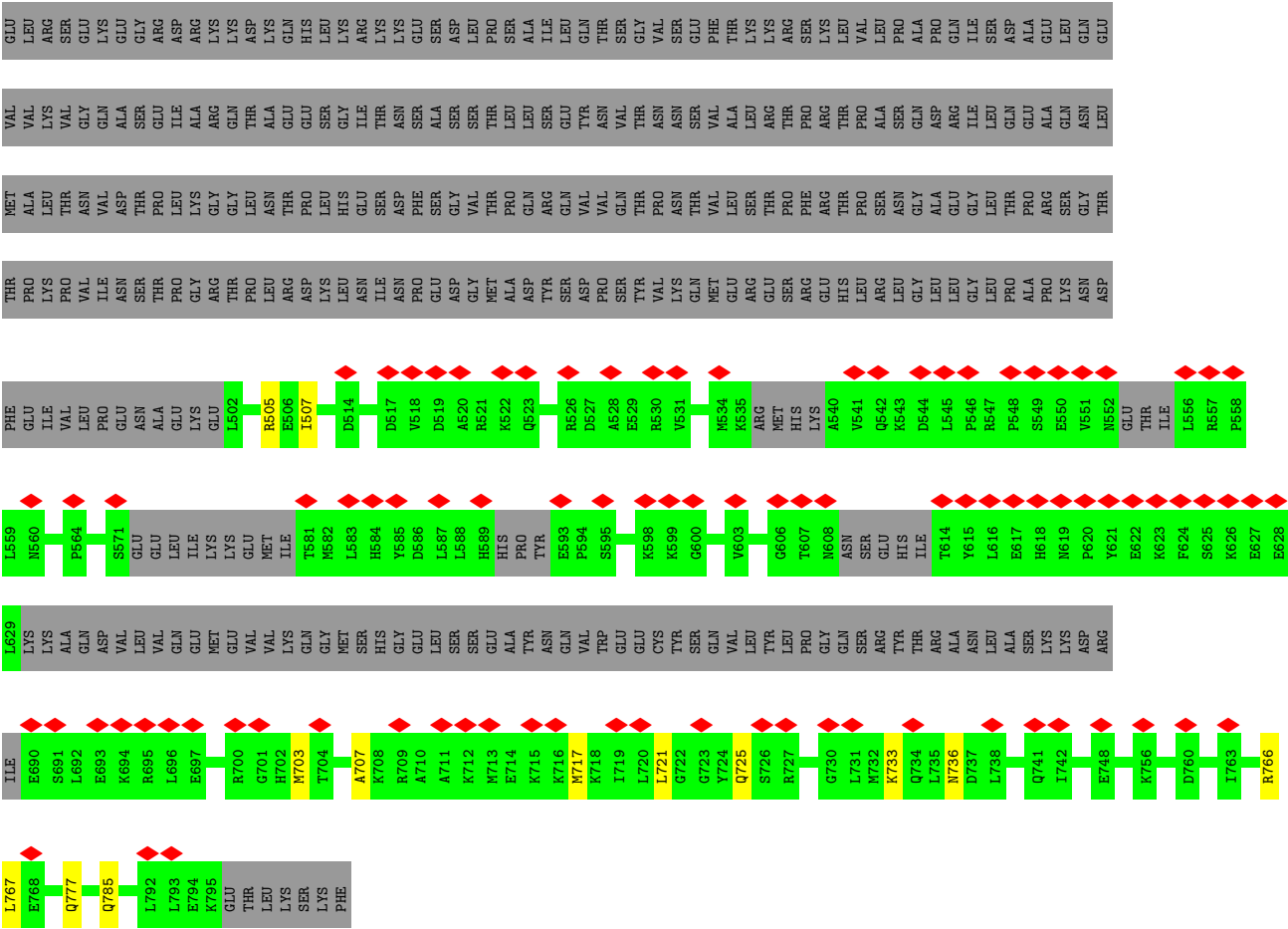


- Molecule 12: Pre-mRNA-splicing factor SPF27

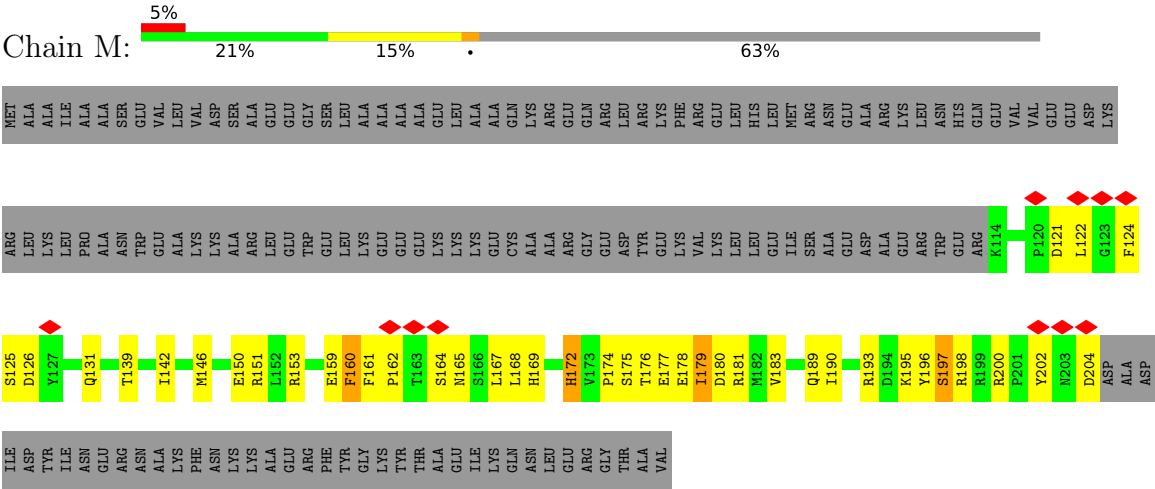


- Molecule 13: Cell division cycle 5-like protein

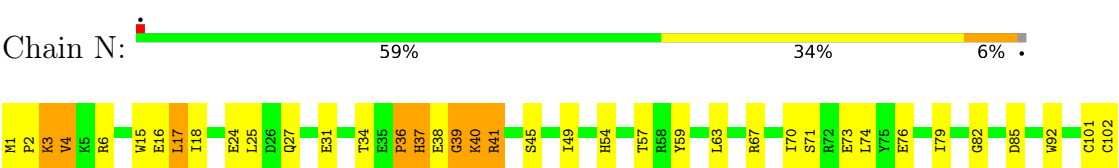




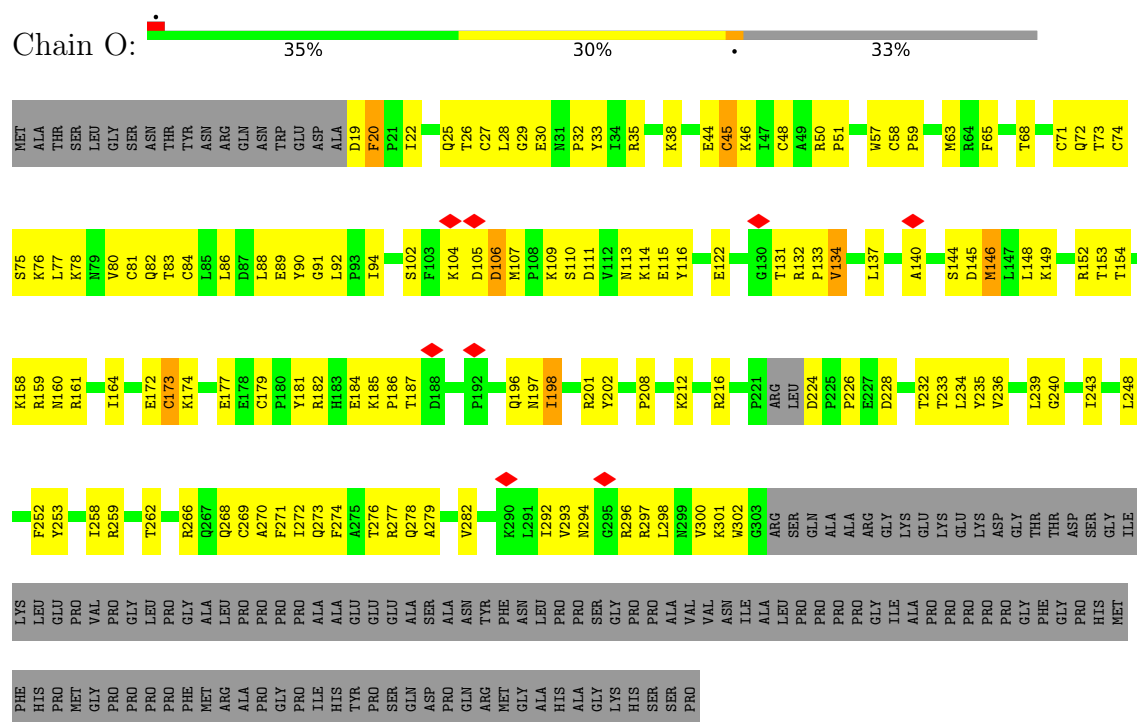
• Molecule 14: Pre-mRNA-splicing factor SYF2



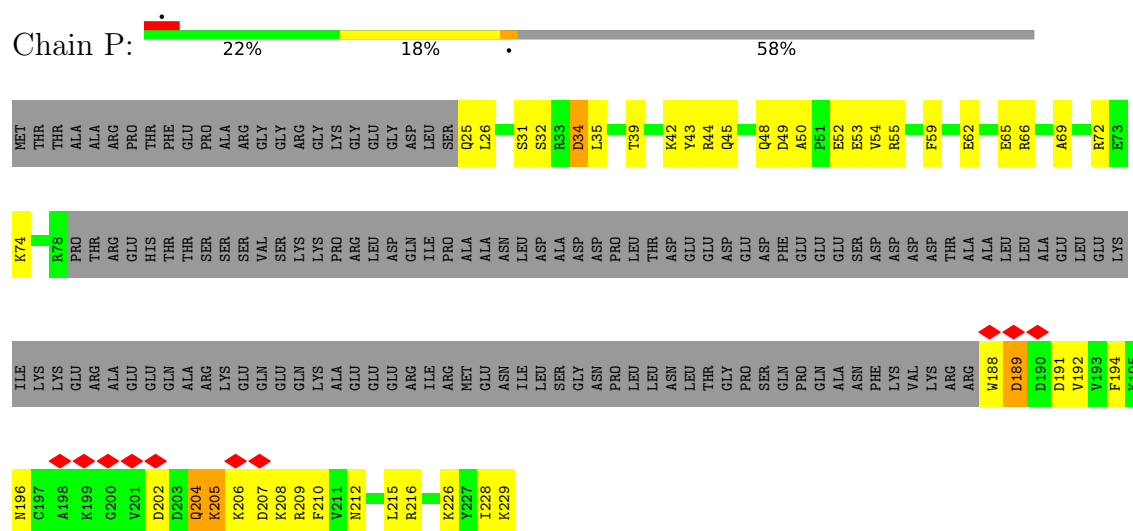
• Molecule 15: Protein BUD31 homolog



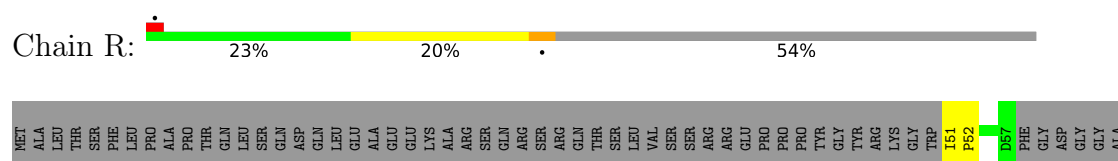
- Molecule 16: Pre-mRNA-splicing factor RBM22

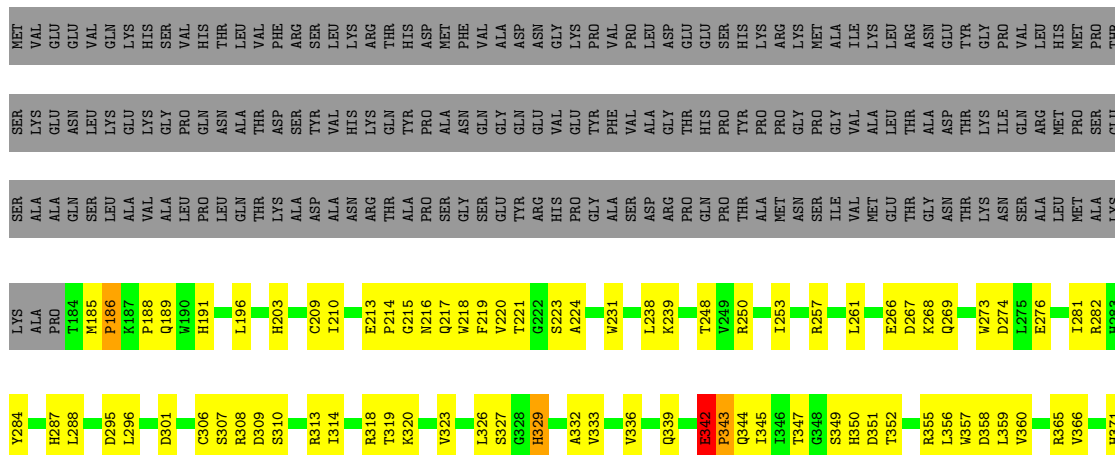


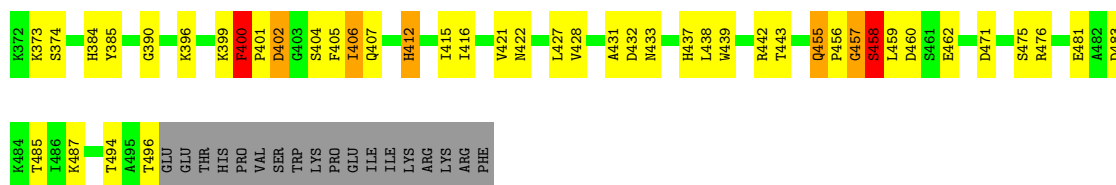
- Molecule 17: Spliceosome-associated protein CWC15 homolog



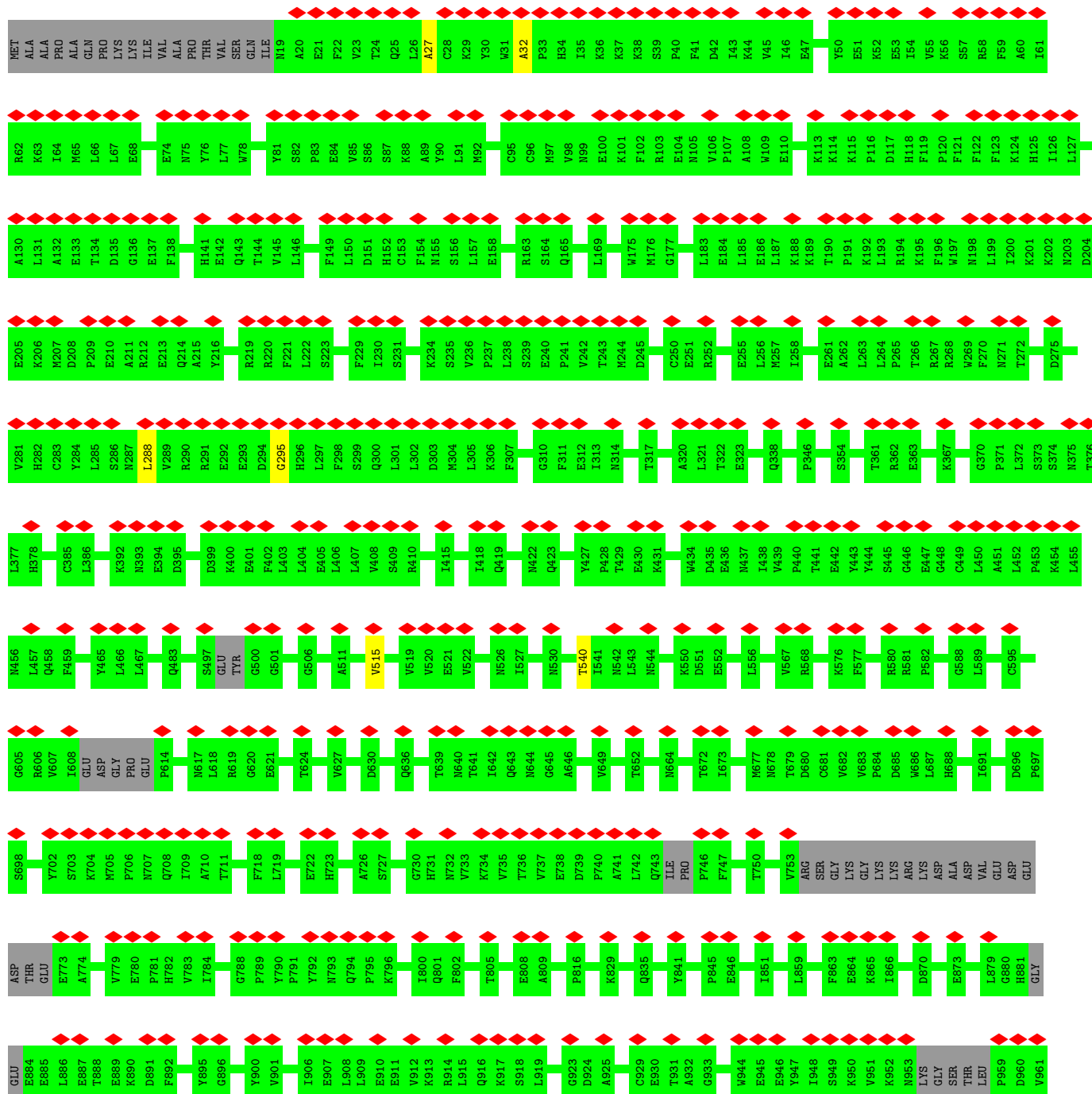
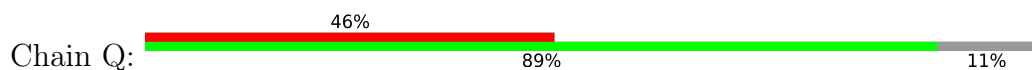
- Molecule 18: SNW domain-containing protein 1

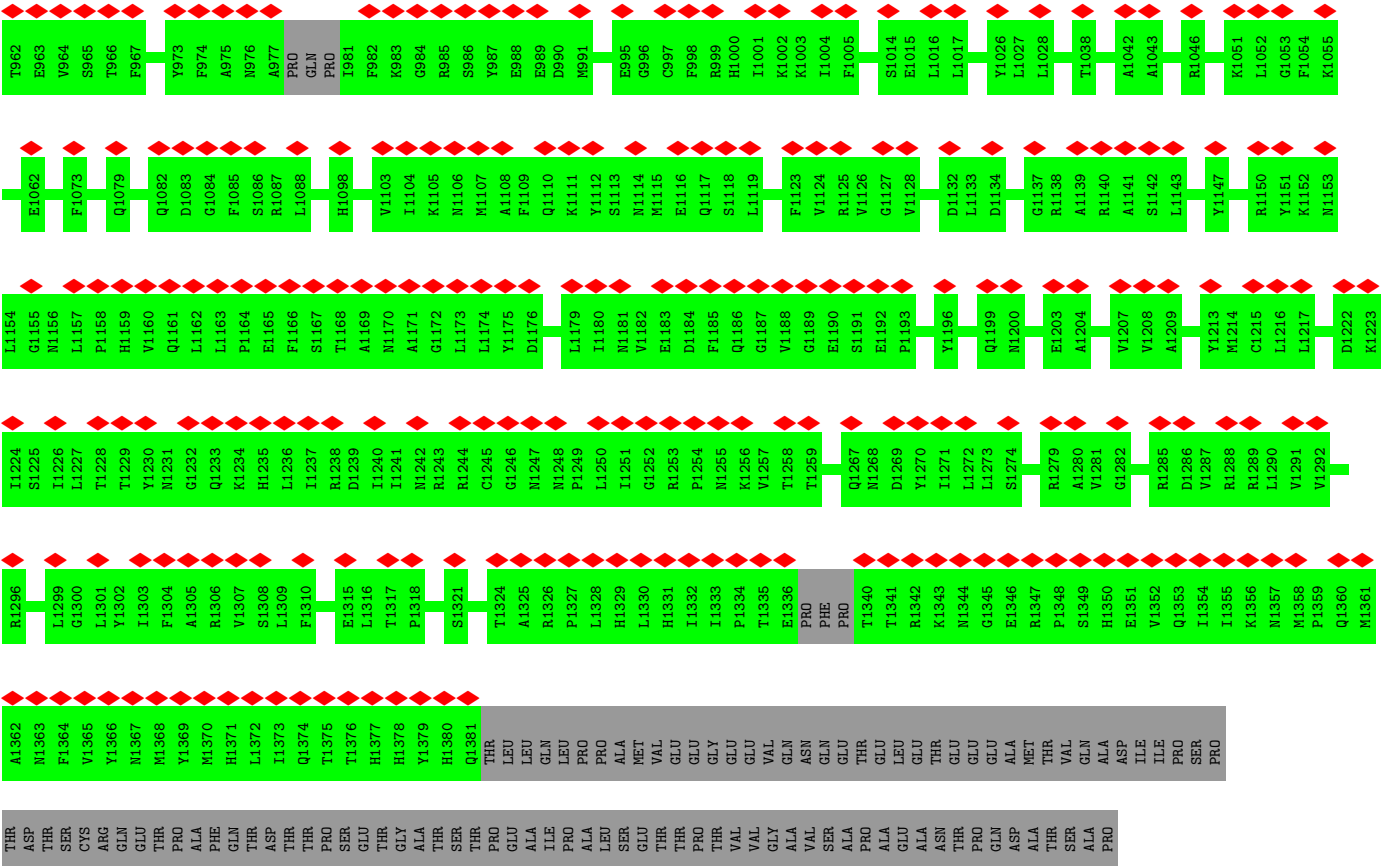




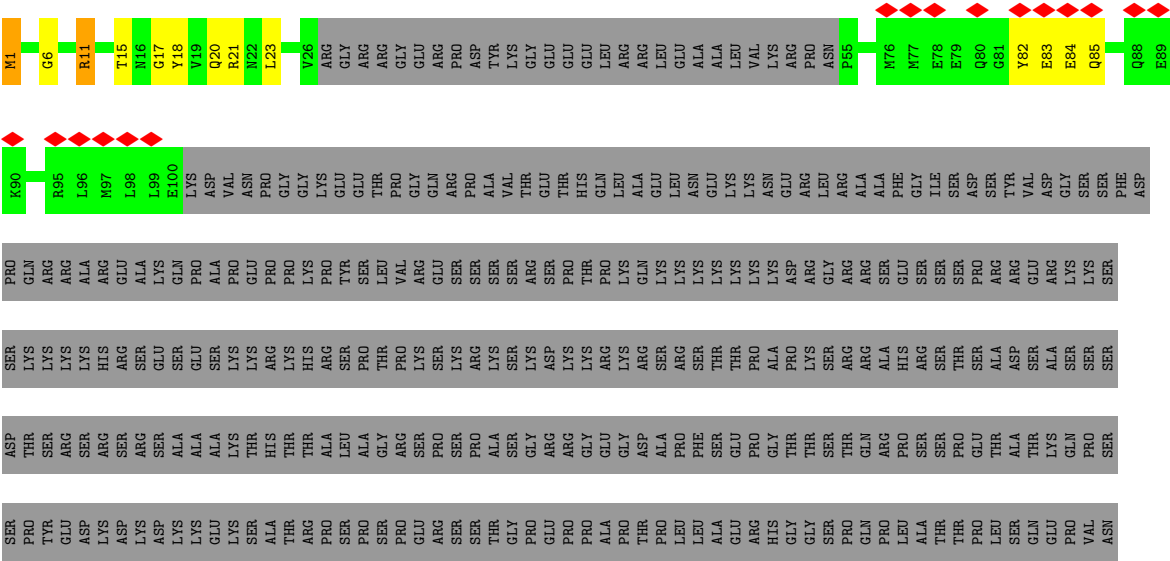


• Molecule 21: RNA helicase aquarius





● Molecule 22: Serine/arginine repetitive matrix protein 2

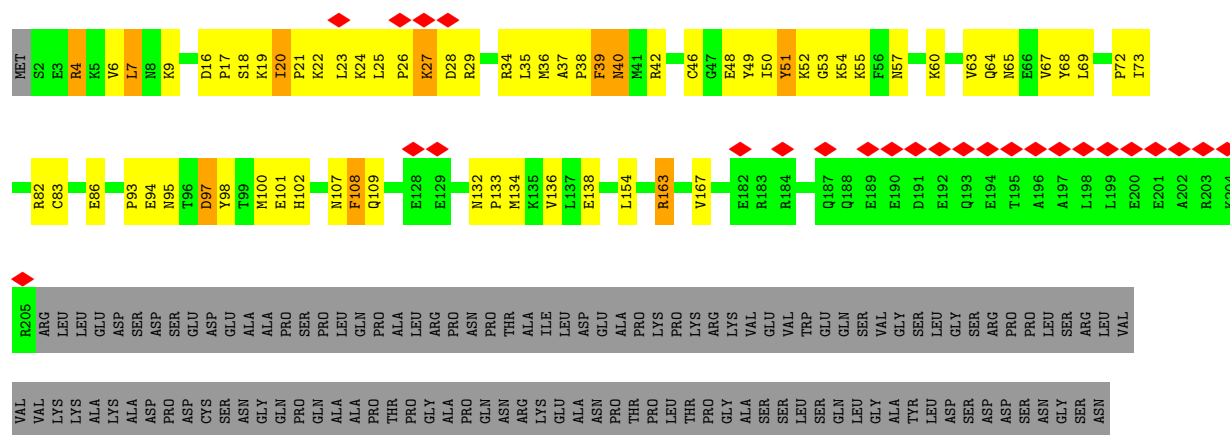




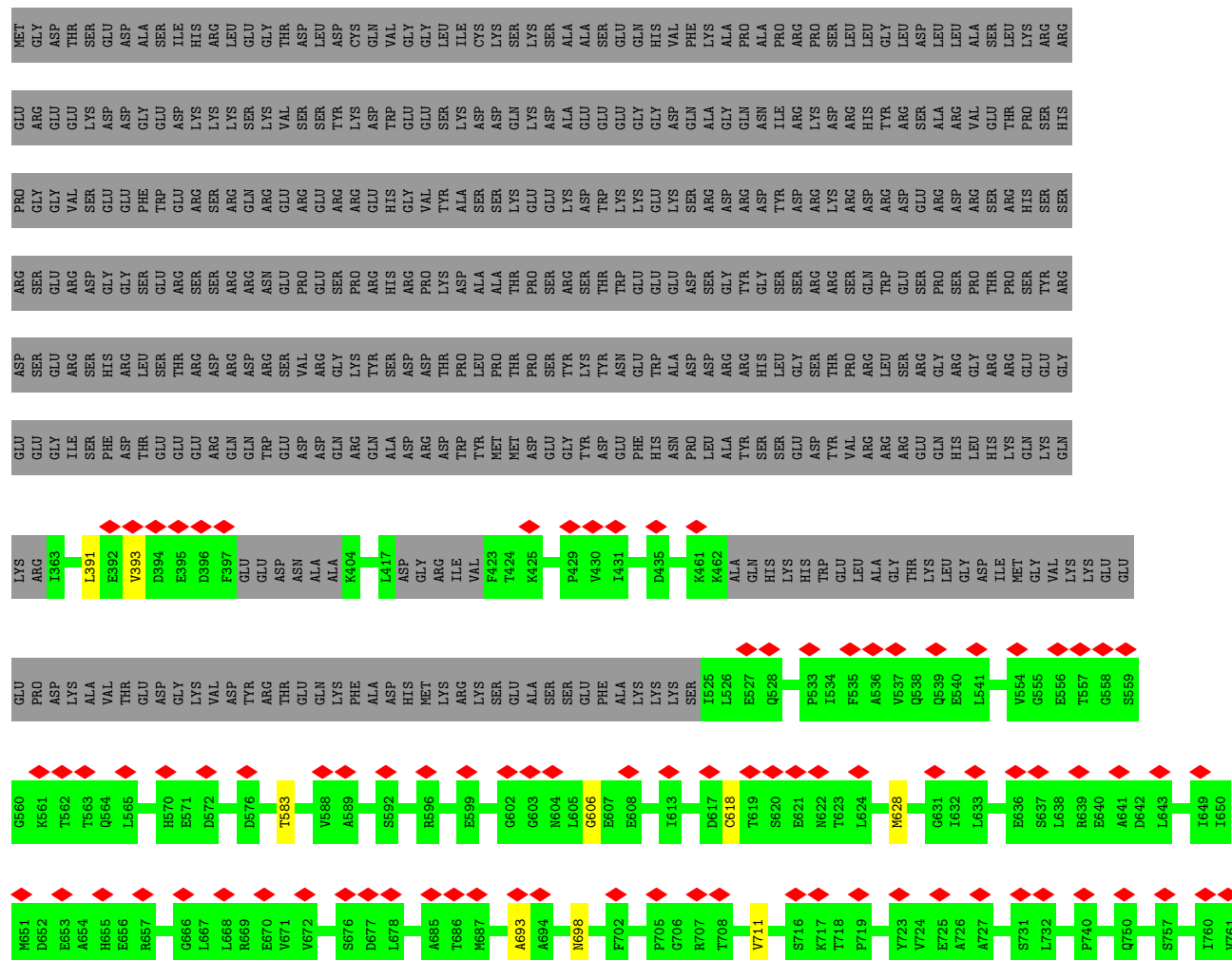
- Molecule 23: Pre-mRNA-splicing factor CWC22 homolog

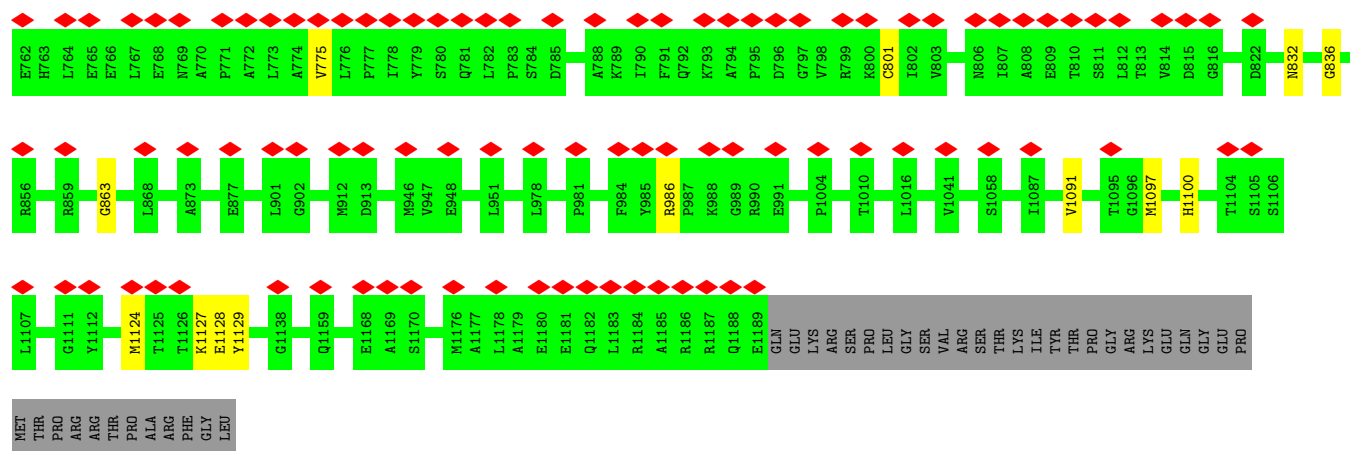


Chain Y:

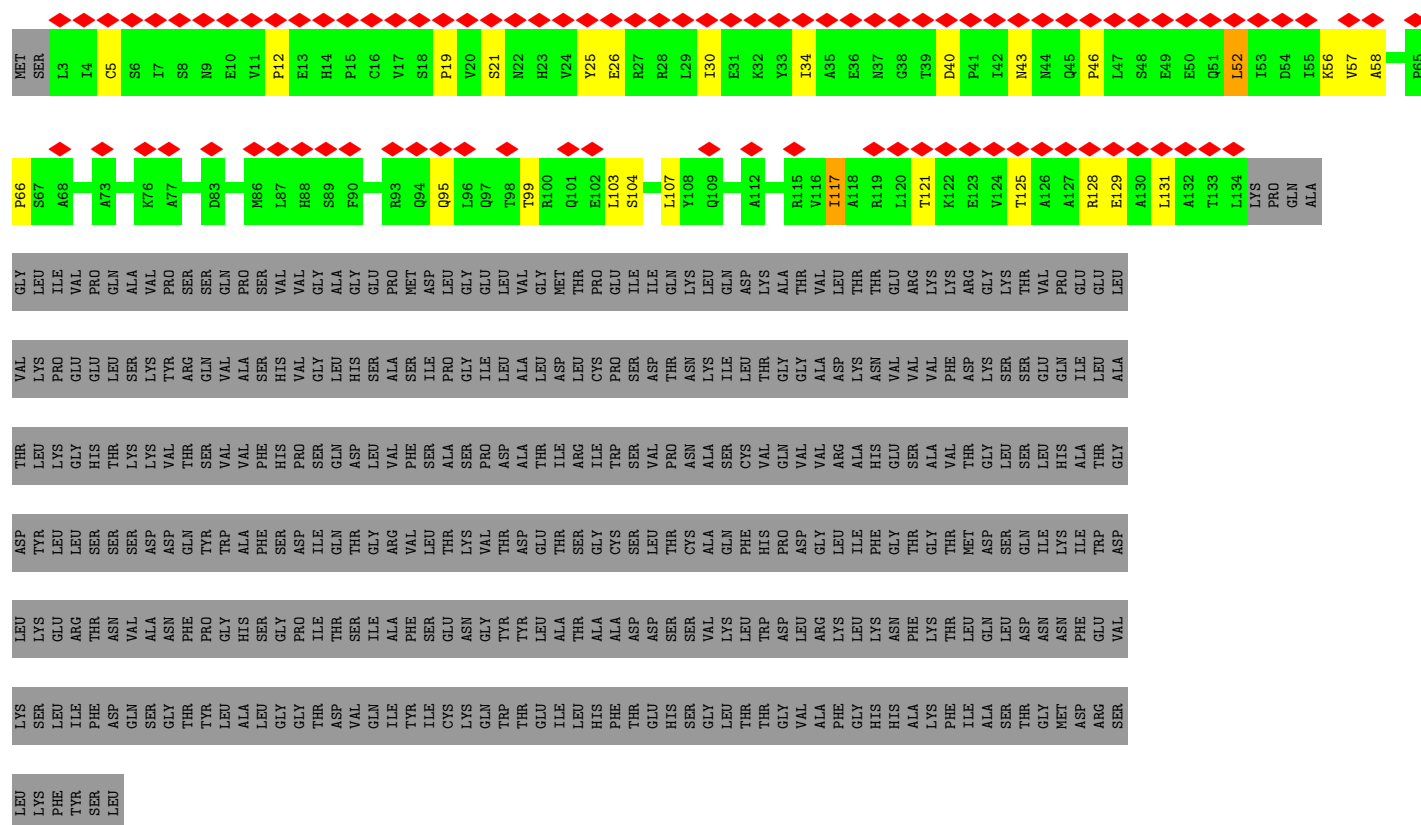


Chain Z: 15% 60% 25%

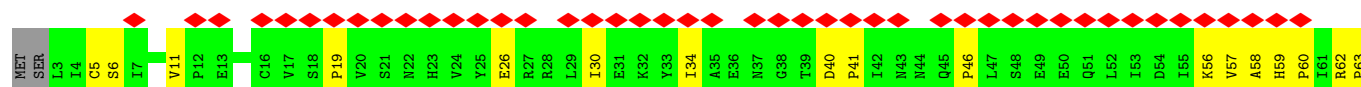




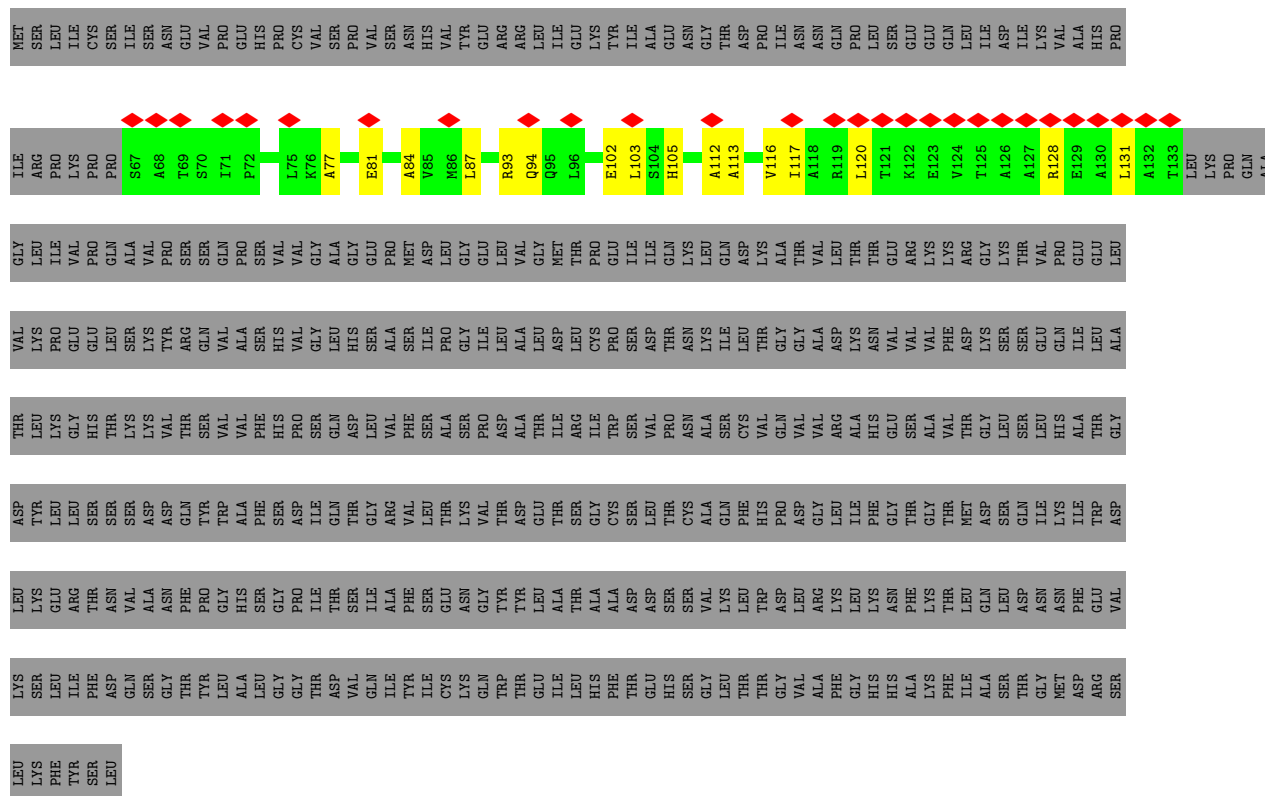
• Molecule 28: Pre-mRNA-processing factor 19



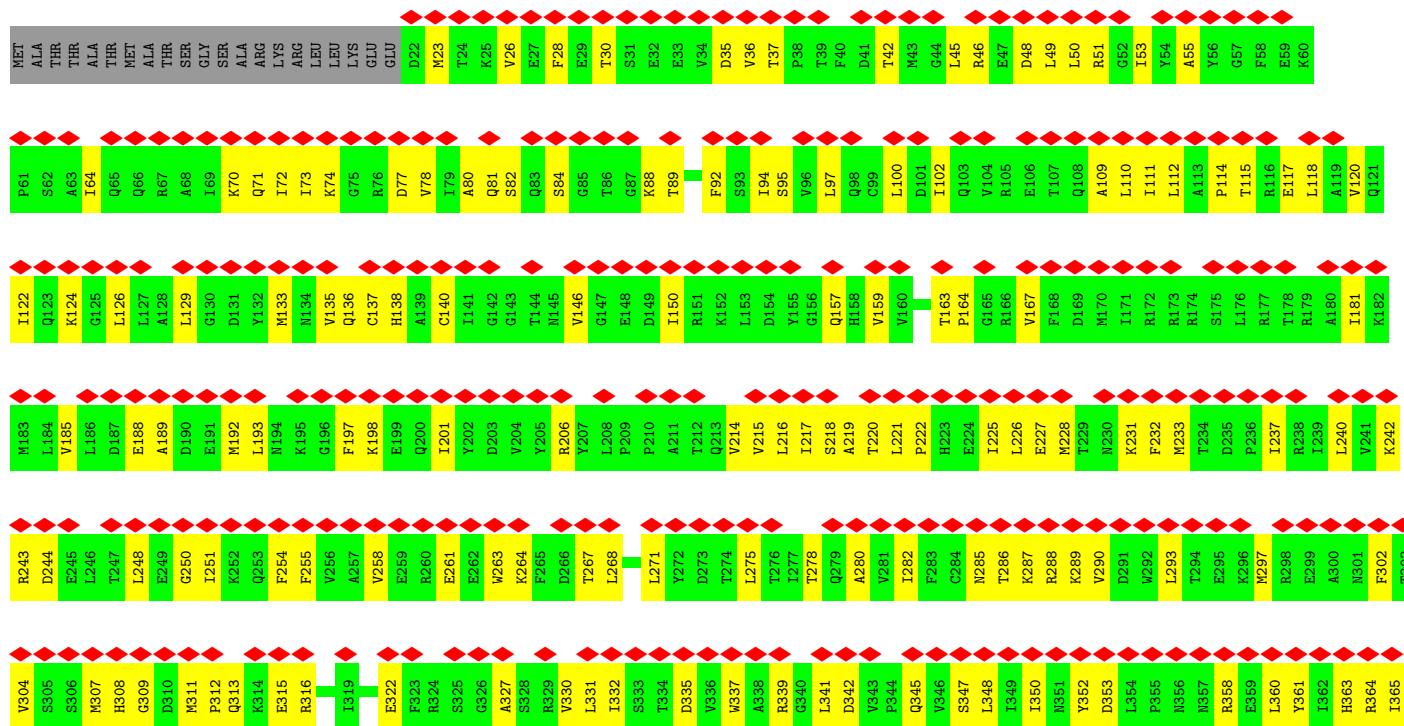
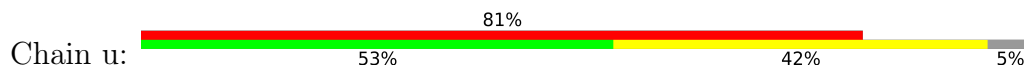
• Molecule 28: Pre-mRNA-processing factor 19





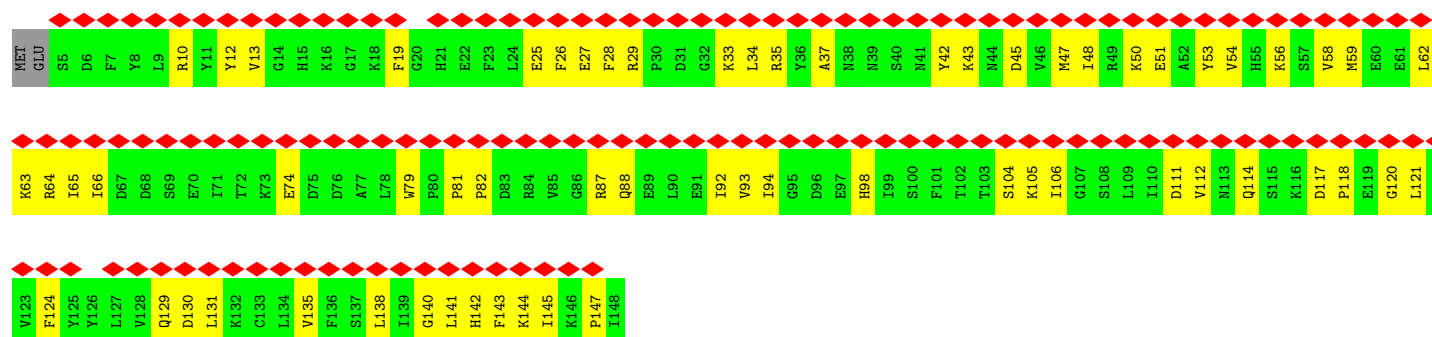


• Molecule 29: Eukaryotic initiation factor 4A-III

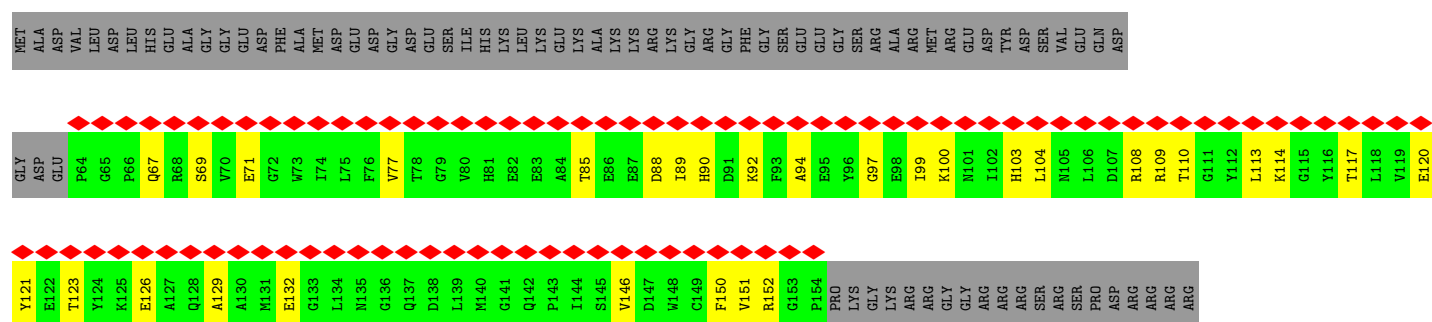
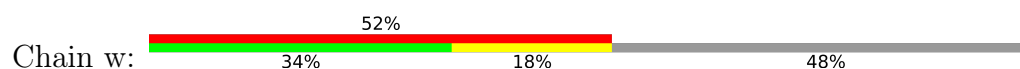




• Molecule 30: Protein mago nashi homolog



• Molecule 31: RNA-binding protein 8A

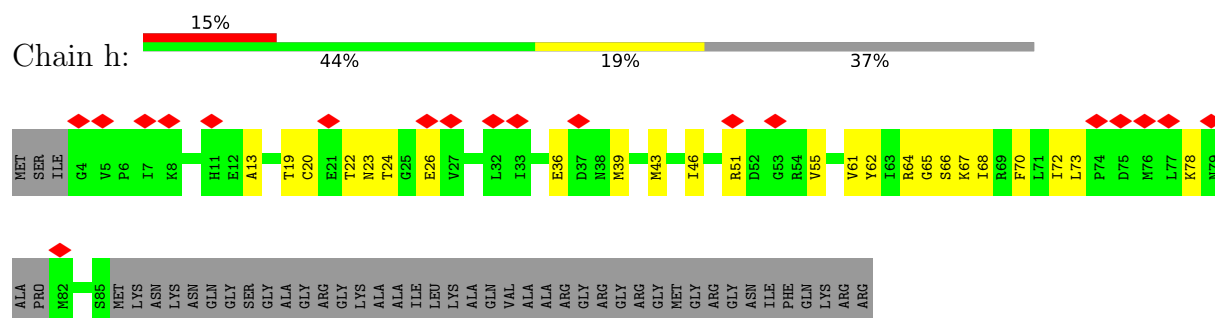


• Molecule 32: Protein CASC3



[illegible]

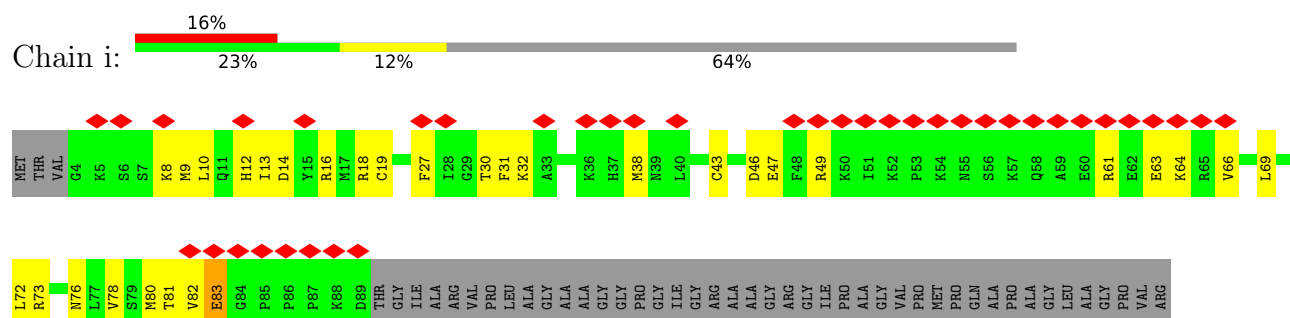
- Molecule 33: Small nuclear ribonucleoprotein Sm D3



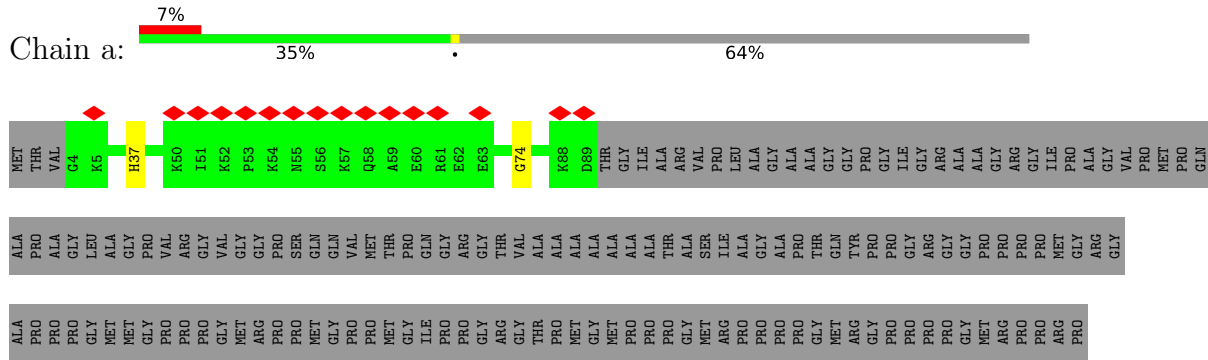
- Molecule 33: Small nuclear ribonucleoprotein Sm D3



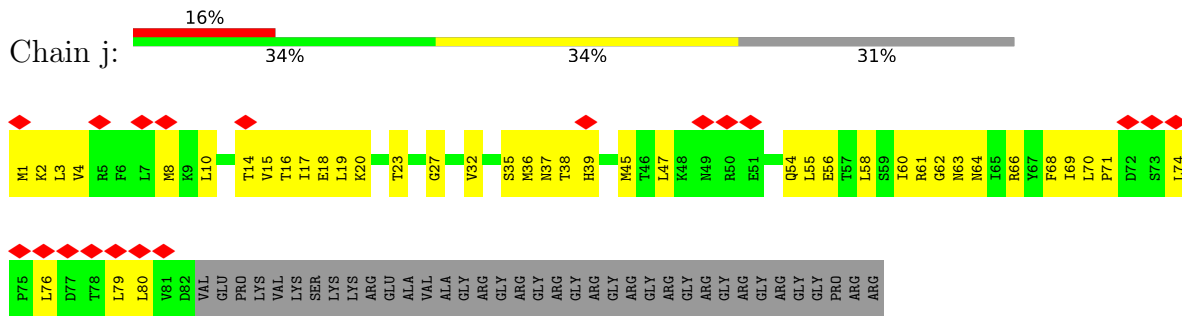
- Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'



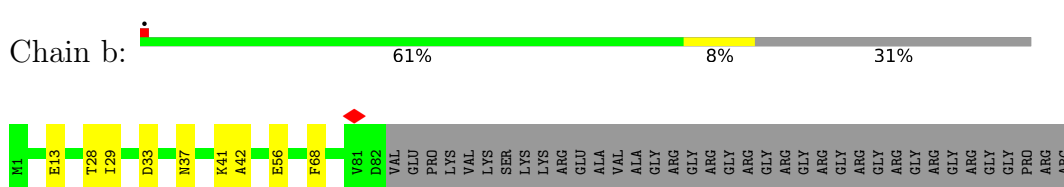
- Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'



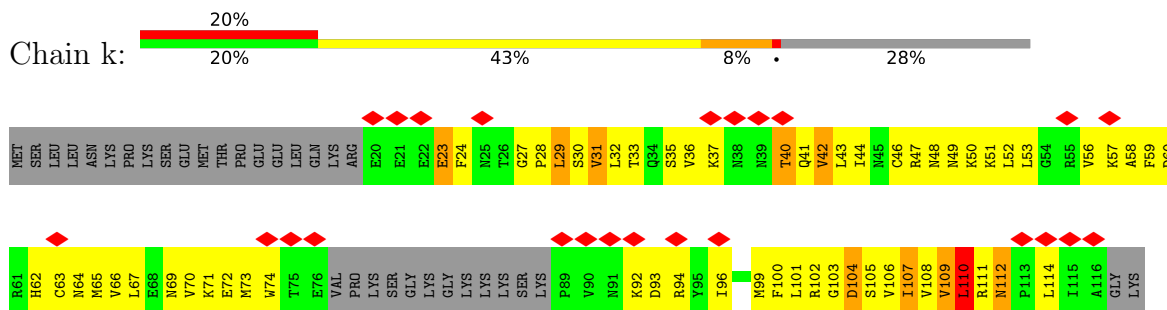
- Molecule 35: Small nuclear ribonucleoprotein Sm D1



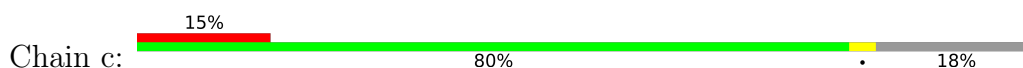
- Molecule 35: Small nuclear ribonucleoprotein Sm D1

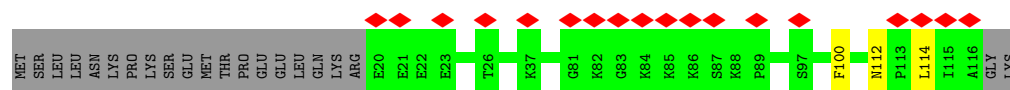


- Molecule 36: Small nuclear ribonucleoprotein Sm D2

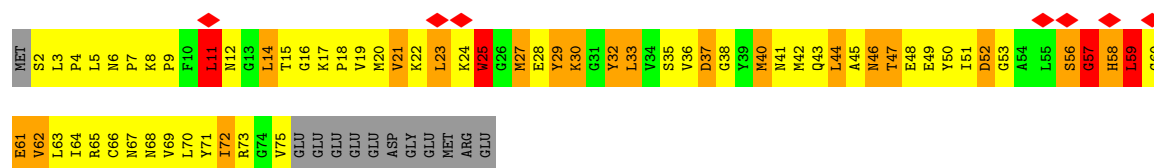


- Molecule 36: Small nuclear ribonucleoprotein Sm D2

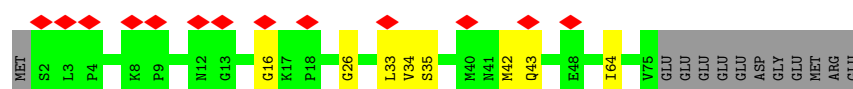
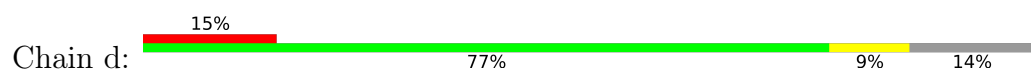




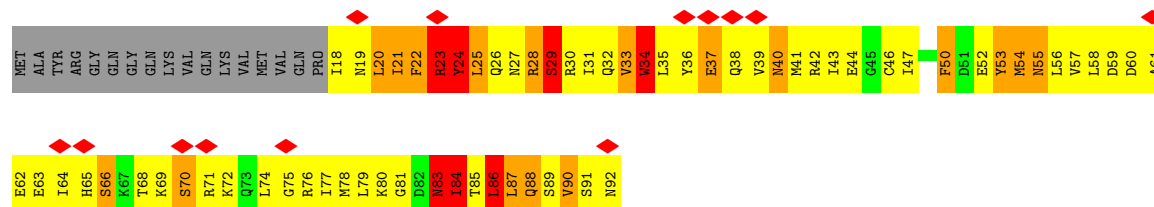
• Molecule 37: Small nuclear ribonucleoprotein F



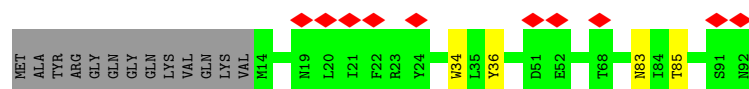
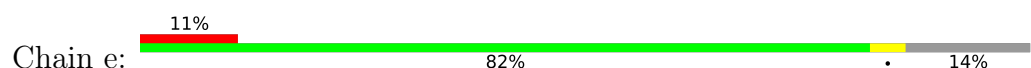
• Molecule 37: Small nuclear ribonucleoprotein F



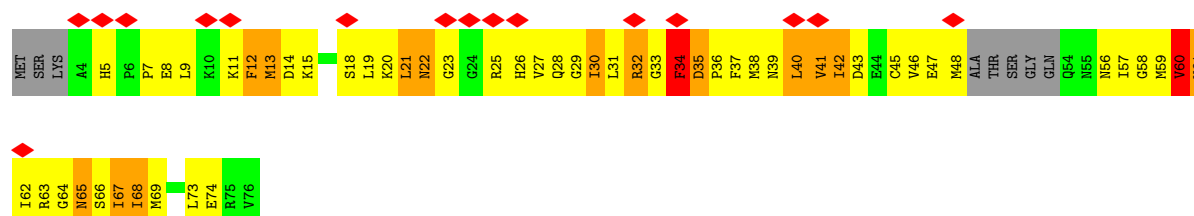
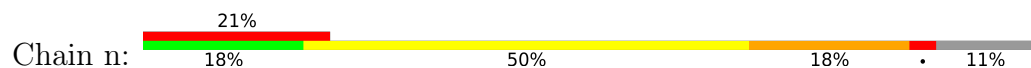
• Molecule 38: Small nuclear ribonucleoprotein E

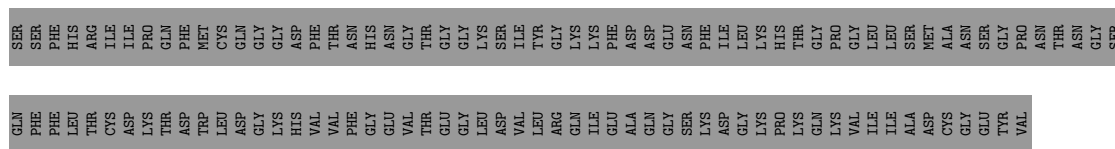


• Molecule 38: Small nuclear ribonucleoprotein E

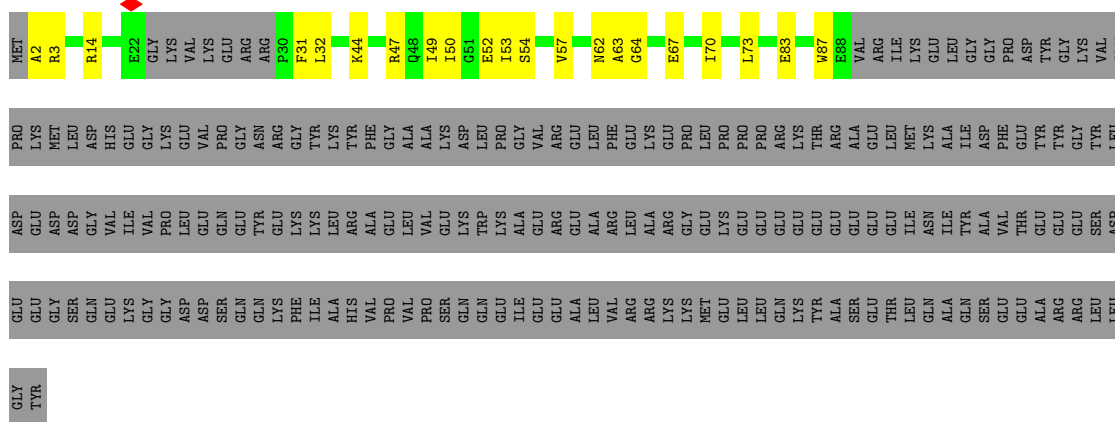


• Molecule 39: Small nuclear ribonucleoprotein G

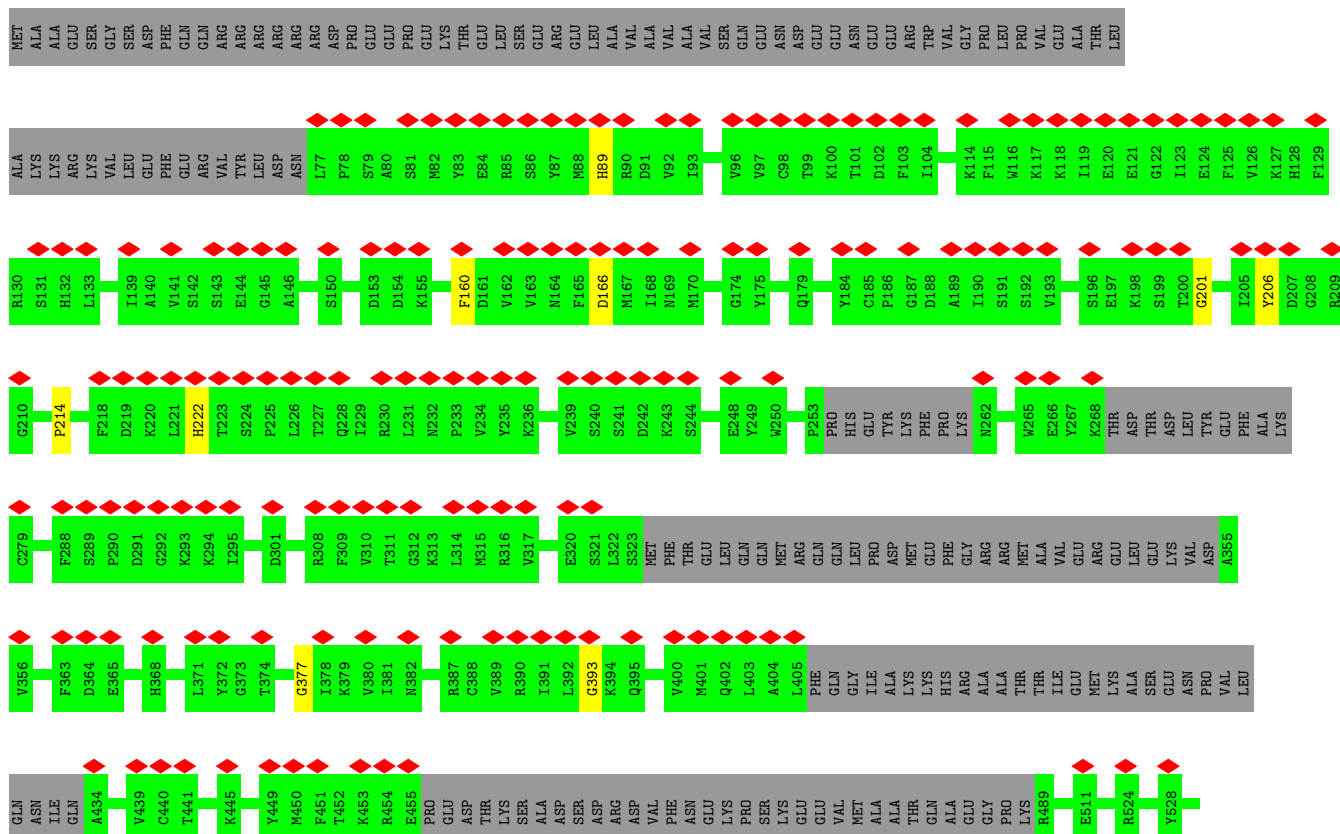


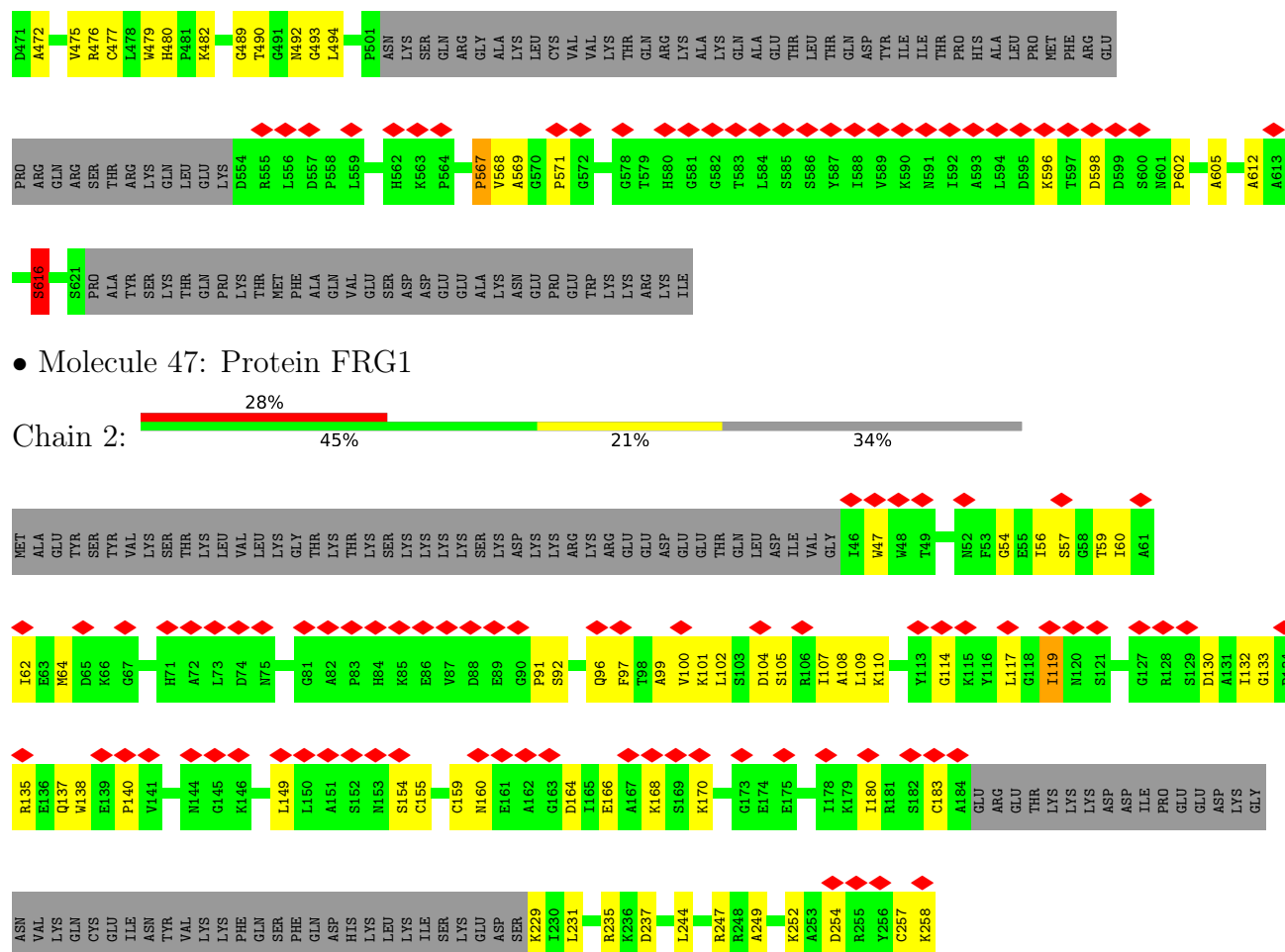


- Molecule 43: Pre-mRNA-splicing factor ISY1 homolog



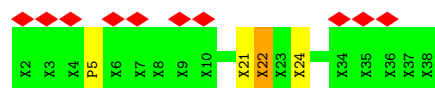
- Molecule 44: Peptidylprolyl isomerase domain and WD repeat-containing protein 1





- Molecule 48: UNK

Chain 5: 27% (red), 89% (green), 8% (yellow)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18223	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)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.121	Depositor
Minimum map value	-0.899	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.077, 1.077, 1.077	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	0/17966	0.74	11/24251 (0.0%)
2	B	0.55	0/2303	0.50	0/3579
3	C	0.48	0/6946	0.68	2/9436 (0.0%)
4	D	0.16	0/7628	0.44	0/9528
5	E	0.35	0/2392	0.59	0/3242
6	F	0.61	0/2323	0.63	1/3619 (0.0%)
7	G	0.63	1/427 (0.2%)	0.45	0/662
8	6	0.44	0/1390	0.71	1/2152 (0.0%)
9	H	0.34	0/3283	0.43	0/5096
10	I	0.19	0/3406	0.45	0/4767
11	J	0.53	0/3870	0.66	2/5252 (0.0%)
12	K	0.23	0/981	0.56	0/1317
13	L	0.50	0/2914	0.61	0/3929
14	M	0.38	0/791	0.60	0/1058
15	N	0.58	0/1210	0.77	2/1622 (0.1%)
16	O	0.47	0/2324	0.66	1/3135 (0.0%)
17	P	0.60	0/841	0.70	0/1117
18	R	0.54	0/1976	0.78	3/2651 (0.1%)
19	S	0.36	0/1268	0.58	0/1714
20	T	0.89	0/2526	0.83	0/3443
21	Q	0.16	0/5279	0.38	0/6583
22	U	0.39	0/424	0.56	0/582
23	V	0.28	0/3453	0.51	0/4640
24	W	0.30	0/2651	0.57	2/3647 (0.1%)
25	X	0.43	0/486	0.59	0/658
26	Y	0.57	0/1450	0.77	3/1975 (0.2%)
27	Z	0.18	0/3723	0.37	0/5180
28	q	0.21	0/929	0.51	0/1260
28	r	0.23	0/912	0.47	0/1239
28	s	0.22	0/267	0.60	0/332
28	t	0.23	0/480	0.51	0/650
29	u	0.22	0/3175	0.50	0/4286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	v	0.22	0/1225	0.47	0/1648
31	w	0.20	0/748	0.43	0/1012
32	x	0.18	0/221	0.41	0/296
33	g	0.18	0/322	0.48	0/399
33	h	0.25	0/627	0.54	0/842
34	a	0.19	0/343	0.53	0/427
34	i	0.22	0/700	0.54	0/933
35	b	0.19	0/327	0.47	0/407
35	j	0.25	0/657	0.51	0/888
36	c	0.18	0/387	0.52	0/482
36	k	0.76	2/696 (0.3%)	1.22	7/935 (0.7%)
37	d	0.18	0/295	0.49	0/367
37	m	0.91	1/588 (0.2%)	1.63	14/795 (1.8%)
38	e	0.17	0/315	0.50	0/392
38	l	1.90	17/628 (2.7%)	1.74	22/842 (2.6%)
39	f	0.17	0/291	0.45	0/362
39	n	1.51	13/539 (2.4%)	1.89	21/718 (2.9%)
40	o	0.21	0/1294	0.52	0/1754
41	p	0.20	0/774	0.44	0/1035
42	y	0.16	0/315	0.30	0/392
43	z	0.30	0/550	0.55	0/736
44	3	0.20	0/2313	0.45	0/3222
45	4	0.56	0/113	0.84	0/148
46	1	0.27	0/2756	0.59	1/3754 (0.0%)
47	2	0.28	0/1318	0.50	0/1773
48	5	0.64	0/7	0.92	0/8
All	All	0.50	34/108343 (0.0%)	0.64	93/147169 (0.1%)

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	11
3	C	0	11
4	D	0	6
5	E	0	1
10	I	0	4
11	J	0	3
12	K	0	1
13	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	M	0	1
15	N	0	2
17	P	0	1
18	R	0	5
20	T	0	5
24	W	0	1
25	X	0	1
26	Y	0	3
36	k	0	2
37	m	0	5
38	l	0	3
39	n	0	3
44	3	0	1
46	1	0	2
48	5	0	1
All	All	0	75

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	l	53	TYR	CD2-CE2	17.04	1.89	1.38
38	l	53	TYR	CD1-CE1	15.81	1.86	1.38
38	l	53	TYR	CE2-CZ	13.97	1.71	1.38
38	l	53	TYR	CE1-CZ	13.62	1.71	1.38
38	l	53	TYR	CG-CD1	13.43	1.67	1.39
38	l	53	TYR	CG-CD2	11.08	1.62	1.39
39	n	34	PHE	C-N	10.10	1.54	1.33
39	n	32	ARG	CA-C	9.79	1.65	1.53
39	n	32	ARG	N-CA	8.00	1.53	1.46
38	l	23	ARG	CA-C	7.74	1.62	1.52
38	l	22	PHE	C-N	7.49	1.43	1.33
38	l	21	ILE	N-CA	7.30	1.55	1.46
38	l	23	ARG	N-CA	7.17	1.55	1.46
37	m	62	VAL	CB-CG1	-7.16	1.28	1.52
38	l	22	PHE	N-CA	7.03	1.55	1.46
39	n	34	PHE	N-CA	6.85	1.55	1.46
39	n	32	ARG	CB-CG	6.73	1.72	1.52
38	l	22	PHE	CA-C	6.64	1.61	1.52
36	k	110	LEU	CG-CD2	-6.52	1.31	1.52
38	l	24	TYR	CA-C	6.51	1.61	1.52
39	n	34	PHE	CA-C	6.27	1.60	1.53
7	G	-19	C	CI'-N1	6.19	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	33	GLY	C-N	6.18	1.40	1.33
39	n	31	LEU	C-N	5.91	1.44	1.34
39	n	33	GLY	N-CA	5.81	1.53	1.45
38	l	20	LEU	C-N	5.78	1.41	1.33
38	l	21	ILE	CA-C	5.71	1.60	1.52
38	l	24	TYR	N-CA	5.59	1.53	1.46
39	n	35	ASP	N-CA	5.59	1.54	1.46
38	l	25	LEU	CB-CG	5.44	1.64	1.53
39	n	31	LEU	N-CA	5.43	1.52	1.45
39	n	34	PHE	CA-CB	5.36	1.60	1.53
39	n	60	VAL	CB-CG1	-5.32	1.34	1.52
36	k	110	LEU	C-O	5.02	1.30	1.23

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	34	PHE	N-CA-C	15.39	128.55	108.24
36	k	110	LEU	CB-CG-CD2	-14.13	68.30	110.70
18	R	94	GLY	N-CA-C	11.64	120.81	110.21
39	n	60	VAL	N-CA-C	11.53	125.51	108.45
39	n	34	PHE	CA-C-N	10.14	146.54	121.80
39	n	34	PHE	C-N-CA	10.14	146.54	121.80
37	m	59	LEU	CA-CB-CG	10.01	151.33	116.30
39	n	34	PHE	CA-CB-CG	9.44	123.24	113.80
37	m	59	LEU	CB-CA-C	-9.39	97.95	111.76
39	n	40	LEU	CA-CB-CG	9.07	148.05	116.30
6	F	26	U	C4'-C3'-O3'	8.98	122.87	109.40
38	l	22	PHE	CA-C-N	8.90	132.21	120.28
38	l	22	PHE	C-N-CA	8.90	132.21	120.28
38	l	86	LEU	CA-CB-CG	8.88	147.40	116.30
36	k	110	LEU	CD1-CG-CD2	-8.84	91.35	110.80
37	m	62	VAL	CG1-CB-CG2	-8.62	91.84	110.80
37	m	59	LEU	CD1-CG-CD2	-8.09	93.00	110.80
37	m	57	GLY	N-CA-C	8.02	122.69	110.18
37	m	29	TYR	CA-CB-CG	8.02	128.33	113.90
1	A	1091	TYR	N-CA-C	-7.86	96.58	109.40
39	n	32	ARG	N-CA-C	7.73	125.43	112.99
38	l	26	GLN	CA-C-N	-7.66	107.66	120.68
38	l	26	GLN	C-N-CA	-7.66	107.66	120.68
36	k	109	VAL	N-CA-C	-7.58	98.89	108.89
37	m	59	LEU	N-CA-C	7.54	122.03	107.71
39	n	41	VAL	CA-CB-CG2	7.21	122.65	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	40	LYS	CA-C-N	7.18	135.25	121.54
15	N	40	LYS	C-N-CA	7.18	135.25	121.54
36	k	110	LEU	CA-CB-CG	7.16	141.37	116.30
38	l	23	ARG	N-CA-C	7.16	119.08	111.28
38	l	24	TYR	N-CA-C	6.93	118.63	111.14
38	l	86	LEU	CD1-CG-CD2	-6.91	95.60	110.80
38	l	86	LEU	CB-CG-CD1	-6.80	90.29	110.70
39	n	60	VAL	CA-CB-CG1	-6.75	98.92	110.40
38	l	22	PHE	N-CA-C	6.72	121.22	112.89
39	n	41	VAL	CG1-CB-CG2	-6.71	96.04	110.80
39	n	32	ARG	O-C-N	-6.63	114.43	122.05
39	n	60	VAL	CB-CA-C	-6.57	99.35	110.71
37	m	11	LEU	CA-CB-CG	6.51	139.09	116.30
26	Y	39	PHE	N-CA-C	6.34	117.89	110.41
36	k	110	LEU	CA-C-N	6.16	132.26	122.59
36	k	110	LEU	C-N-CA	6.16	132.26	122.59
39	n	35	ASP	N-CA-C	6.16	123.41	109.81
38	l	86	LEU	CB-CG-CD2	6.14	129.13	110.70
1	A	903	SER	N-CA-C	-6.11	106.42	114.31
39	n	35	ASP	CB-CA-C	-6.10	98.16	110.17
39	n	34	PHE	CB-CA-C	-6.04	99.62	112.78
38	l	34	TRP	CA-CB-CG	6.00	125.00	113.60
37	m	46	ASN	N-CA-C	5.98	123.54	110.80
38	l	84	ILE	CA-C-N	-5.79	110.86	121.52
38	l	84	ILE	C-N-CA	-5.79	110.86	121.52
1	A	1019	TYR	N-CA-C	-5.75	100.56	109.24
1	A	434	HIS	CA-C-N	-5.72	116.67	122.74
1	A	434	HIS	C-N-CA	-5.72	116.67	122.74
3	C	822	MET	CA-C-N	-5.68	112.20	122.54
3	C	822	MET	C-N-CA	-5.68	112.20	122.54
18	R	124	VAL	CA-C-N	5.66	132.35	121.54
18	R	124	VAL	C-N-CA	5.66	132.35	121.54
39	n	40	LEU	N-CA-CB	5.59	119.03	110.70
38	l	25	LEU	CA-C-N	-5.58	111.39	120.72
38	l	25	LEU	C-N-CA	-5.58	111.39	120.72
1	A	568	ASN	CA-C-N	-5.51	112.06	121.97
1	A	568	ASN	C-N-CA	-5.51	112.06	121.97
16	O	146	MET	N-CA-C	-5.51	106.49	113.43
38	l	50	PHE	CA-C-N	5.48	132.01	121.54
38	l	50	PHE	C-N-CA	5.48	132.01	121.54
8	6	82	G	P-O3'-C3'	5.48	128.41	120.20
36	k	109	VAL	CA-CB-CG1	5.48	119.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	13	MET	N-CA-C	5.47	117.66	108.96
24	W	155	SER	CA-C-N	5.43	131.75	121.97
24	W	155	SER	C-N-CA	5.43	131.75	121.97
1	A	886	LEU	CA-C-N	-5.42	114.43	122.56
1	A	886	LEU	C-N-CA	-5.42	114.43	122.56
38	l	28	ARG	CA-CB-CG	5.40	124.89	114.10
11	J	239	ARG	CA-C-N	5.34	131.74	121.54
11	J	239	ARG	C-N-CA	5.34	131.74	121.54
46	1	616	SER	N-CA-C	5.28	121.47	109.81
39	n	68	ILE	CA-C-N	-5.23	111.58	121.63
39	n	68	ILE	C-N-CA	-5.23	111.58	121.63
1	A	1363	GLN	N-CA-C	5.20	117.62	110.35
37	m	30	LYS	N-CA-C	5.16	116.82	108.41
37	m	33	LEU	CA-C-N	-5.15	117.88	123.08
37	m	33	LEU	C-N-CA	-5.15	117.88	123.08
38	l	21	ILE	N-CA-C	5.13	116.59	111.00
38	l	23	ARG	O-C-N	-5.13	116.68	122.12
1	A	1285	LEU	CA-CB-CG	-5.12	98.39	116.30
37	m	58	HIS	CA-C-N	-5.09	115.03	123.37
37	m	58	HIS	C-N-CA	-5.09	115.03	123.37
38	l	20	LEU	CB-CG-CD1	5.09	125.97	110.70
39	n	30	ILE	CA-C-N	5.05	131.80	122.92
39	n	30	ILE	C-N-CA	5.05	131.80	122.92
26	Y	51	TYR	CA-C-N	-5.04	111.91	121.54
26	Y	51	TYR	C-N-CA	-5.04	111.91	121.54

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	1	567	PRO	Peptide
46	1	598	ASP	Peptide
44	3	89	HIS	Peptide
48	5	22	UNK	Peptide
1	A	1091	TYR	Peptide
1	A	1189	MET	Peptide
1	A	1520	ASN	Peptide
1	A	166	PHE	Peptide
1	A	1763	LEU	Peptide
1	A	1920	TYR	Peptide
1	A	346	ASP	Peptide
1	A	377	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	55	ASP	Peptide
1	A	56	ALA	Peptide
1	A	941	LYS	Peptide
3	C	359	LYS	Peptide
3	C	360	ALA	Peptide
3	C	387	ASP	Peptide
3	C	456	GLY	Peptide
3	C	560	VAL	Peptide
3	C	800	PRO	Peptide
3	C	82	GLN	Peptide
3	C	823	ALA	Peptide
3	C	902	HIS	Peptide
3	C	92	PRO	Peptide
3	C	93	ILE	Peptide
4	D	149	ARG	Peptide
4	D	1583	ASP	Peptide
4	D	164	THR	Peptide
4	D	2098	ALA	Peptide
4	D	296	ALA	Peptide
4	D	956	LEU	Peptide
5	E	163	GLY	Peptide
10	I	386	ASP	Peptide
10	I	47	GLY	Peptide
10	I	532	LYS	Peptide
10	I	85	ARG	Peptide
11	J	202	GLU	Peptide
11	J	205	LEU	Peptide
11	J	240	THR	Peptide
12	K	77	GLN	Peptide
13	L	200	LYS	Peptide
13	L	202	ARG	Peptide
14	M	124	PHE	Peptide
15	N	3	LYS	Peptide
15	N	36	PRO	Peptide
17	P	204	GLN	Peptide
18	R	126	ASN	Peptide
18	R	183	GLN	Peptide
18	R	185	GLY	Peptide
18	R	91	ASP	Peptide
18	R	94	GLY	Peptide
20	T	342	GLU	Peptide
20	T	400	PHE	Peptide

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Mol	Chain	Res	Type	Group
20	T	457	GLY	Peptide
20	T	458	SER	Peptide
20	T	494	THR	Peptide
24	W	154	GLY	Peptide
25	X	61	GLY	Peptide
26	Y	19	LYS	Peptide
26	Y	27	LYS	Peptide
26	Y	40	ASN	Peptide
36	k	110	LEU	Peptide
36	k	112	ASN	Peptide
38	l	23	ARG	Peptide
38	l	29	SER	Peptide
38	l	55	ASN	Peptide
37	m	25	TRP	Peptide
37	m	56	SER	Peptide
37	m	57	GLY	Peptide
37	m	59	LEU	Peptide
37	m	61	GLU	Peptide
39	n	12	PHE	Peptide
39	n	21	LEU	Peptide
39	n	60	VAL	Mainchain

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	17519	0	16645	698	0
2	B	2066	0	1047	89	0
3	C	6795	0	6807	366	0
4	D	7632	0	1995	15	0
5	E	2338	0	2275	104	0
6	F	2075	0	1048	113	0
7	G	383	0	200	19	0
8	6	1256	0	637	86	0
9	H	2946	0	1494	157	0
10	I	3387	0	1651	20	0
11	J	3829	0	2907	105	0
12	K	979	0	741	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	2885	0	2427	110	0
14	M	775	0	767	49	0
15	N	1184	0	1189	53	0
16	O	2277	0	2259	137	0
17	P	829	0	814	47	0
18	R	1962	0	2012	128	0
19	S	1236	0	1210	67	0
20	T	2461	0	2420	102	0
21	Q	5288	0	1361	3	0
22	U	422	0	291	12	0
23	V	3410	0	3287	132	0
24	W	2615	0	1751	93	0
25	X	480	0	401	24	0
26	Y	1426	0	1210	72	0
27	Z	3727	0	1676	13	0
28	q	918	0	801	18	0
28	r	901	0	777	21	0
28	s	268	0	65	0	0
28	t	476	0	434	9	0
29	u	3126	0	3167	145	0
30	v	1196	0	1182	55	0
31	w	730	0	690	25	0
32	x	216	0	202	18	0
33	g	324	0	89	4	0
33	h	621	0	623	39	0
34	a	344	0	93	1	0
34	i	690	0	712	29	0
35	b	328	0	89	5	0
35	j	649	0	693	41	0
36	c	388	0	102	2	0
36	k	688	0	709	176	0
37	d	296	0	87	5	0
37	m	576	0	589	175	0
38	e	316	0	85	3	0
38	l	621	0	635	179	0
39	f	292	0	83	3	0
39	n	533	0	555	146	0
40	o	1277	0	1297	29	0
41	p	760	0	783	19	0
42	y	316	0	86	0	0
43	z	546	0	454	16	0
44	3	2301	0	1090	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	4	112	0	109	18	0
46	1	2705	0	2362	97	0
47	2	1296	0	1287	44	0
48	5	184	0	42	4	0
49	A	36	0	6	8	0
50	C	32	0	12	6	0
51	C	1	0	0	0	0
51	F	4	0	0	0	0
52	N	3	0	0	0	0
52	O	3	0	0	0	0
52	Y	1	0	0	0	0
All	All	106256	0	80512	3517	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 19.

All (3517) 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)
38:l:86:LEU:HG	39:n:62:ILE:CG2	1.16	1.62
38:l:53:TYR:CD1	38:l:53:TYR:CE1	1.86	1.59
38:l:86:LEU:CG	39:n:62:ILE:HG23	1.27	1.57
38:l:53:TYR:CD2	38:l:53:TYR:CE2	1.89	1.55
38:l:39:VAL:HG22	39:n:23:GLY:CA	1.50	1.40
36:k:23:GLU:O	36:k:27:GLY:HA3	1.22	1.31
38:l:39:VAL:CG1	39:n:23:GLY:O	1.79	1.28
38:l:39:VAL:CG2	39:n:23:GLY:HA2	1.67	1.23
1:A:584:HIS:HE1	49:A:3000:IHP:O26	1.22	1.21
38:l:88:GLN:CA	39:n:60:VAL:HG11	1.68	1.21
10:I:528:LEU:O	10:I:532:LYS:HA	1.37	1.20
38:l:86:LEU:HA	39:n:63:ARG:N	1.57	1.18
38:l:39:VAL:HG13	39:n:23:GLY:C	1.67	1.18
38:l:33:VAL:HB	38:l:43:ILE:HB	1.25	1.13
38:l:87:LEU:H	39:n:62:ILE:HA	1.13	1.12
6:F:52:U:HO2'	25:X:2:GLY:N	1.48	1.11
38:l:31:ILE:O	38:l:44:GLU:HA	1.50	1.10
38:l:39:VAL:HG22	39:n:23:GLY:HA2	1.22	1.10
38:l:86:LEU:CA	39:n:63:ARG:H	1.64	1.09
38:l:39:VAL:CA	39:n:23:GLY:HA2	1.85	1.07
1:A:584:HIS:CE1	49:A:3000:IHP:O26	2.09	1.06
38:l:88:GLN:HE21	39:n:57:ILE:HD12	1.15	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:28:PRO:HG3	37:m:36:VAL:HA	1.34	1.05
39:n:30:ILE:O	39:n:43:ASP:N	1.89	1.05
37:m:42:MET:HB2	37:m:64:ILE:HD12	1.37	1.04
36:k:23:GLU:O	36:k:27:GLY:CA	2.04	1.04
36:k:31:VAL:HG23	37:m:43:GLN:HE21	1.16	1.03
3:C:483:SER:HA	3:C:490:PHE:HB3	1.36	1.03
36:k:28:PRO:O	36:k:30:SER:N	1.90	1.03
38:l:85:THR:O	39:n:63:ARG:HB3	1.59	1.02
38:l:86:LEU:HD11	39:n:67:ILE:HG12	1.37	1.02
38:l:88:GLN:HA	39:n:60:VAL:HG11	1.02	1.01
36:k:111:ARG:HD3	37:m:45:ALA:HA	1.38	1.01
9:H:99:A:N3	38:l:80:LYS:NZ	2.09	1.01
9:H:98:G:N2	37:m:66:CYS:SG	2.34	1.00
38:l:39:VAL:CG2	39:n:23:GLY:CA	2.30	1.00
1:A:1215:ASN:HB3	1:A:1224:ARG:HD2	1.37	1.00
38:l:85:THR:C	39:n:63:ARG:HB3	1.87	1.00
38:l:39:VAL:HG13	39:n:23:GLY:O	0.83	0.99
38:l:88:GLN:HA	39:n:60:VAL:CG1	1.91	0.99
8:6:85:G:H1	9:H:44:U:H3	1.00	0.98
38:l:39:VAL:CB	39:n:23:GLY:HA2	1.93	0.98
38:l:39:VAL:HG22	39:n:23:GLY:C	1.89	0.97
36:k:110:LEU:CD2	37:m:59:LEU:HD12	1.94	0.97
1:A:1463:LYS:NZ	8:6:105:C:OP2	1.98	0.96
10:I:528:LEU:O	10:I:532:LYS:CA	2.14	0.96
38:l:39:VAL:HA	39:n:23:GLY:CA	1.96	0.96
6:F:39:A:H61	8:6:8:C:H42	1.12	0.95
14:M:153:ARG:HA	14:M:160:PHE:HE2	1.30	0.95
29:u:220:THR:HG1	29:u:363:HIS:HE2	1.15	0.93
9:H:104:U:O2'	37:m:65:ARG:NH2	2.02	0.93
36:k:111:ARG:HA	37:m:60:GLY:C	1.93	0.93
6:F:38:G:H2'	6:F:39:A:C8	2.04	0.93
3:C:300:LEU:HA	3:C:306:ASN:HD22	1.31	0.93
14:M:165:ASN:HB2	18:R:95:LYS:HA	1.47	0.93
18:R:126:ASN:HD22	18:R:128:ASP:H	0.98	0.92
38:l:89:SER:N	39:n:60:VAL:CG1	2.33	0.92
16:O:26:THR:OG1	16:O:159:ARG:NH2	2.03	0.92
8:6:21:A:N6	16:O:91:GLY:O	2.02	0.92
9:H:99:A:HO2'	38:l:53:TYR:HE1	0.94	0.92
38:l:85:THR:O	39:n:63:ARG:CB	2.18	0.92
9:H:150:U:H3	9:H:181:G:H1	1.19	0.91
18:R:106:GLN:HE22	18:R:225:PRO:HD2	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:39:VAL:HA	39:n:23:GLY:HA2	1.50	0.91
38:l:34:TRP:CE3	39:n:21:LEU:HD12	2.05	0.90
15:N:40:LYS:O	15:N:41:ARG:HG3	1.70	0.90
38:l:89:SER:H	39:n:60:VAL:CG1	1.84	0.90
16:O:84:CYS:SG	16:O:159:ARG:NH2	2.45	0.90
38:l:88:GLN:C	39:n:60:VAL:HG11	1.97	0.90
38:l:61:ALA:HB3	38:l:74:LEU:HB2	1.51	0.90
1:A:329:LEU:HD23	3:C:177:ARG:HE	1.37	0.90
3:C:387:ASP:O	3:C:389:ASP:N	2.05	0.89
37:m:20:MET:SD	37:m:73:ARG:NH1	2.45	0.89
6:F:17:C:H2'	6:F:18:A:H8	1.36	0.89
36:k:109:VAL:HB	37:m:63:LEU:N	1.87	0.89
37:m:44:LEU:H	37:m:62:VAL:HG11	1.34	0.89
5:E:72:CYS:N	5:E:332:GLU:OE1	2.05	0.89
36:k:110:LEU:O	37:m:61:GLU:N	2.05	0.89
39:n:34:PHE:HD1	39:n:35:ASP:N	1.71	0.89
3:C:130:ARG:HD3	3:C:438:ILE:HB	1.55	0.88
9:H:100:U:H1'	39:n:65:ASN:HA	1.56	0.88
36:k:23:GLU:HG2	37:m:37:ASP:HB2	1.55	0.88
31:w:94:ALA:HA	31:w:99:ILE:HD11	1.54	0.88
38:l:88:GLN:NE2	39:n:57:ILE:HD12	1.86	0.88
20:T:399:LYS:HG3	20:T:406:ILE:HD11	1.56	0.88
38:l:86:LEU:CB	39:n:62:ILE:HG23	2.04	0.88
6:F:26:U:C5	16:O:65:PHE:HD2	1.92	0.88
1:A:1503:TRP:HZ3	1:A:1533:ARG:HE	1.18	0.87
19:S:84:ASP:OD1	19:S:108:ASN:ND2	2.07	0.87
16:O:71:CYS:SG	16:O:73:THR:OG1	2.32	0.87
2:B:64:G:H2'	2:B:65:G:C8	2.09	0.87
3:C:452:THR:HB	3:C:577:PHE:HD2	1.40	0.87
9:H:99:A:C2	38:l:80:LYS:NZ	2.41	0.87
38:l:87:LEU:N	39:n:62:ILE:HA	1.88	0.87
1:A:1253:SER:HG	9:H:34:U:HO2'	1.09	0.87
38:l:85:THR:O	39:n:63:ARG:O	1.92	0.87
1:A:778:ARG:NH1	9:H:23:A:OP1	2.08	0.86
1:A:1749:LYS:NZ	8:6:91:A:OP1	2.07	0.86
3:C:673:LYS:HG3	3:C:686:THR:HG23	1.56	0.86
39:n:39:ASN:HA	39:n:64:GLY:H	1.39	0.86
3:C:856:HIS:NE2	29:u:102:ILE:O	2.08	0.86
38:l:86:LEU:CG	39:n:62:ILE:CG2	2.09	0.86
13:L:191:LEU:HD22	13:L:196:ILE:HD11	1.57	0.86
38:l:39:VAL:HG22	39:n:23:GLY:N	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:111:ARG:HA	37:m:61:GLU:HA	1.57	0.85
29:u:278:THR:HG21	29:u:347:SER:HB3	1.58	0.85
38:l:86:LEU:HA	39:n:63:ARG:H	0.75	0.85
2:B:64:G:H2'	2:B:65:G:H8	1.42	0.85
7:G:-2:C:H3'	7:G:-1:G:H5''	1.56	0.85
39:n:41:VAL:HG22	39:n:61:VAL:HA	1.59	0.85
1:A:1963:GLU:HB3	1:A:1965:HIS:HD2	1.41	0.85
8:6:87:U:O2	9:H:42:G:N2	2.09	0.84
38:l:89:SER:H	39:n:60:VAL:HG13	1.39	0.84
36:k:111:ARG:HA	37:m:60:GLY:O	1.75	0.84
38:l:89:SER:N	39:n:60:VAL:HG13	1.91	0.84
48:5:22:UNK:O	48:5:24:UNK:N	2.11	0.84
36:k:42:VAL:HA	37:m:61:GLU:CB	2.08	0.84
1:A:1258:LYS:HG3	1:A:1527:ASN:HD21	1.43	0.84
5:E:260:ARG:NH1	5:E:273:CYS:SG	2.51	0.84
1:A:211:GLN:OE1	1:A:214:ARG:NH1	2.11	0.84
3:C:772:TRP:NE1	3:C:776:GLU:OE2	2.11	0.84
13:L:191:LEU:HD21	43:z:57:VAL:HG21	1.60	0.83
38:l:31:ILE:HA	38:l:89:SER:HA	1.60	0.83
38:l:32:GLN:HA	38:l:43:ILE:O	1.78	0.83
8:6:7:G:H2'	8:6:8:C:H6	1.43	0.83
1:A:1776:ILE:HB	1:A:1858:PRO:HA	1.59	0.83
29:u:97:LEU:HB3	29:u:133:MET:HE1	1.59	0.83
20:T:250:ARG:NH1	20:T:266:GLU:OE1	2.12	0.83
37:m:18:PRO:HA	37:m:32:TYR:HA	1.60	0.83
38:l:19:ASN:O	38:l:23:ARG:HB2	1.78	0.83
8:6:7:G:H2'	8:6:8:C:C6	2.14	0.83
12:K:165:TRP:HA	12:K:168:LYS:HD2	1.59	0.83
16:O:236:VAL:HG22	16:O:300:VAL:HG22	1.61	0.83
20:T:213:GLU:CD	20:T:215:GLY:H	1.86	0.82
38:l:39:VAL:CG1	39:n:23:GLY:C	2.40	0.82
36:k:33:THR:HG22	36:k:37:LYS:HE2	1.60	0.82
6:F:26:U:H5	16:O:65:PHE:CD2	1.97	0.82
16:O:234:LEU:O	16:O:271:PHE:HA	1.80	0.82
3:C:76:GLU:OE1	3:C:76:GLU:N	2.10	0.82
37:m:41:ASN:HB3	37:m:64:ILE:O	1.79	0.82
38:l:32:GLN:HB2	38:l:90:VAL:HG13	1.61	0.82
36:k:31:VAL:O	36:k:35:SER:OG	1.97	0.82
37:m:20:MET:HE2	37:m:30:LYS:HB2	1.60	0.82
3:C:114:TYR:HE1	33:g:79:ASN:O	1.63	0.82
47:2:160:ASN:HD21	47:2:164:ASP:HB2	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:161:ASN:ND2	13:L:163:GLN:O	2.13	0.81
14:M:153:ARG:HA	14:M:160:PHE:CE2	2.13	0.81
38:l:86:LEU:HG	39:n:62:ILE:HG21	1.56	0.81
16:O:30:GLU:O	18:R:190:SER:OG	1.98	0.81
36:k:28:PRO:HB3	37:m:42:MET:HA	1.63	0.81
5:E:155:ASN:ND2	5:E:196:VAL:O	2.13	0.81
1:A:663:ARG:NH1	6:F:64:U:OP2	2.12	0.81
1:A:1993:LYS:HG3	1:A:1994:LYS:HD2	1.61	0.81
3:C:448:LYS:O	3:C:452:THR:OG1	1.99	0.81
13:L:172:ARG:HA	13:L:175:GLN:HE21	1.44	0.81
38:l:32:GLN:HB3	38:l:88:GLN:HG2	1.63	0.81
1:A:1180:LYS:HA	1:A:1201:ARG:HH12	1.46	0.81
16:O:133:PRO:HG2	16:O:137:LEU:HB2	1.63	0.81
41:p:41:VAL:HG12	41:p:53:PHE:HB2	1.63	0.81
39:n:40:LEU:HG	39:n:67:ILE:HD11	1.60	0.81
1:A:1183:PRO:HB3	1:A:1201:ARG:HE	1.44	0.80
10:I:621:ARG:O	10:I:625:PRO:HD2	1.82	0.80
15:N:139:CYS:SG	15:N:140:ARG:N	2.55	0.80
36:k:44:ILE:HG12	36:k:109:VAL:HG13	1.63	0.80
19:S:13:ASN:HA	19:S:25:LEU:O	1.82	0.80
33:h:39:MET:SD	34:i:73:ARG:NH1	2.52	0.80
1:A:1211:ASP:OD2	1:A:1369:TYR:OH	1.99	0.80
13:L:149:LEU:HA	13:L:152:LEU:HD12	1.64	0.80
39:n:27:VAL:HG12	39:n:47:GLU:HA	1.63	0.80
1:A:1330:MET:HG3	1:A:1367:ASN:HD21	1.47	0.80
1:A:1887:SER:OG	1:A:1889:LEU:O	1.99	0.80
6:F:26:U:H5	16:O:65:PHE:HD2	1.25	0.80
16:O:262:THR:HB	16:O:271:PHE:HB2	1.64	0.80
17:P:52:GLU:OE1	17:P:55:ARG:NH2	2.13	0.80
39:n:21:LEU:HD22	39:n:22:ASN:OD1	1.82	0.80
39:n:37:PHE:O	39:n:64:GLY:HA3	1.81	0.80
9:H:13:C:H41	14:M:200:ARG:HH12	1.30	0.79
36:k:109:VAL:HG12	37:m:61:GLU:O	1.82	0.79
1:A:150:MET:SD	1:A:153:ARG:NH2	2.56	0.79
1:A:1678:ARG:HH21	47:2:249:ALA:HA	1.47	0.79
11:J:360:ASP:HA	11:J:363:ARG:HE	1.47	0.79
3:C:87:GLN:HE22	20:T:239:LYS:HD3	1.46	0.79
36:k:44:ILE:HG23	36:k:109:VAL:HG22	1.62	0.79
3:C:224:GLY:HA3	3:C:438:ILE:HD12	1.64	0.79
1:A:79:ARG:HH11	1:A:82:ARG:HE	1.30	0.79
23:V:169:LEU:HD11	23:V:184:GLU:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.18	0.79
1:A:79:ARG:NH1	1:A:82:ARG:HE	1.81	0.79
26:Y:68:TYR:HE2	26:Y:94:GLU:HB2	1.48	0.79
1:A:1783:THR:HA	45:4:106:LYS:HE2	1.65	0.78
3:C:114:TYR:CE1	33:g:79:ASN:O	2.37	0.78
36:k:63:CYS:SG	37:m:41:ASN:ND2	2.56	0.78
36:k:43:LEU:H	37:m:61:GLU:H	1.31	0.78
37:m:11:LEU:HD21	37:m:36:VAL:HB	1.63	0.78
3:C:507:VAL:HG11	3:C:565:ILE:HG23	1.65	0.78
24:W:162:ASN:HB3	24:W:165:LEU:HD23	1.64	0.78
37:m:41:ASN:OD1	37:m:66:CYS:N	2.15	0.78
44:3:201:GLY:HA3	44:3:222:HIS:HA	1.65	0.78
20:T:267:ASP:HB3	20:T:269:GLN:HG2	1.66	0.78
9:H:75:A:H61	9:H:77:C:H42	1.32	0.78
1:A:1533:ARG:NH1	1:A:1752:GLN:OE1	2.17	0.78
6:F:39:A:H61	8:6:8:C:N4	1.82	0.78
46:1:490:THR:HG23	46:1:492:ASN:H	1.48	0.77
2:B:46:U:O4	2:B:47:A:N6	2.17	0.77
39:n:38:MET:HE2	39:n:67:ILE:HD12	1.64	0.77
1:A:1160:ARG:NH1	17:P:189:ASP:OD2	2.16	0.77
38:l:44:GLU:OE2	38:l:71:ARG:NH2	2.18	0.77
37:m:50:TYR:HB3	37:m:53:GLY:HA2	1.66	0.77
23:V:631:PHE:HA	23:V:634:ILE:HG22	1.67	0.77
1:A:663:ARG:NH2	6:F:65:G:N7	2.32	0.77
16:O:243:ILE:HG12	16:O:294:ASN:HD22	1.48	0.77
38:l:63:GLU:O	38:l:71:ARG:HA	1.85	0.77
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.65	0.77
36:k:111:ARG:HG3	37:m:61:GLU:CG	2.15	0.77
1:A:1310:ARG:NH2	1:A:1563:HIS:O	2.17	0.77
3:C:183:SER:N	3:C:214:GLU:OE1	2.11	0.77
36:k:110:LEU:HD21	37:m:59:LEU:HD12	1.66	0.77
1:A:2005:SER:OG	1:A:2006:GLU:OE2	2.01	0.77
39:n:34:PHE:CD1	39:n:35:ASP:N	2.51	0.77
28:r:62:ARG:HD2	28:r:63:PRO:HD2	1.68	0.76
1:A:1831:LYS:HE2	1:A:1832:ARG:HG3	1.66	0.76
8:6:87:U:H3	9:H:42:G:H1	1.24	0.76
19:S:75:ALA:O	19:S:110:SER:OG	2.04	0.76
1:A:1890:GLN:O	45:4:104:ARG:NH2	2.19	0.76
1:A:623:LYS:O	49:A:3000:IHP:O44	2.01	0.76
23:V:294:ILE:HD13	23:V:335:MET:HB3	1.67	0.76
3:C:715:GLY:HA2	3:C:729:ALA:HB1	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1863:VAL:HG21	1:A:1868:MET:HB2	1.68	0.76
2:B:12:U:H3	2:B:65:G:H1	1.34	0.76
16:O:276:THR:HG23	16:O:279:ALA:H	1.50	0.76
38:l:80:LYS:O	38:l:83:ASN:ND2	2.18	0.76
39:n:42:ILE:O	39:n:60:VAL:N	2.15	0.76
38:l:34:TRP:HB2	38:l:86:LEU:O	1.86	0.76
1:A:300:ASN:O	3:C:939:ARG:NH2	2.19	0.75
9:H:98:G:N2	37:m:41:ASN:OD1	2.19	0.75
39:n:60:VAL:HG12	39:n:61:VAL:N	2.01	0.75
1:A:570:ASP:OD1	1:A:571:ALA:N	2.18	0.75
1:A:978:GLU:OE1	1:A:1096:HIS:ND1	2.20	0.75
36:k:111:ARG:HG3	37:m:61:GLU:HG3	1.68	0.75
13:L:36:SER:OG	13:L:158:ARG:NH2	2.19	0.75
23:V:297:LEU:HB3	23:V:339:MET:HE3	1.68	0.75
19:S:102:ASN:ND2	19:S:104:GLY:O	2.19	0.75
29:u:353:ASP:O	29:u:364:ARG:NH2	2.19	0.75
30:v:112:VAL:HA	30:v:121:LEU:HD23	1.69	0.75
44:3:377:GLY:HA2	44:3:393:GLY:HA2	1.69	0.75
3:C:677:GLU:HA	3:C:683:ASN:O	1.86	0.75
38:l:89:SER:N	39:n:60:VAL:HG11	1.98	0.75
39:n:23:GLY:O	39:n:25:ARG:HG3	1.86	0.75
6:F:29:A:N6	8:6:16:G:O2'	2.20	0.75
6:F:58:G:H2'	6:F:59:G:C8	2.20	0.75
9:H:3:C:H2'	9:H:4:G:H8	1.51	0.75
3:C:619:THR:HG22	3:C:629:ILE:HG12	1.69	0.75
37:m:21:VAL:HG22	37:m:72:ILE:HA	1.69	0.75
38:l:86:LEU:CD2	39:n:62:ILE:CG2	2.63	0.75
3:C:680:ASN:HB3	3:C:807:GLN:HG3	1.68	0.74
3:C:69:ALA:HA	20:T:456:PRO:HG3	1.68	0.74
44:3:206:TYR:HA	44:3:214:PRO:HD2	1.69	0.74
38:l:34:TRP:CZ2	39:n:27:VAL:HG22	2.22	0.74
1:A:41:GLN:NE2	1:A:44:ARG:HD3	2.03	0.74
1:A:312:TYR:OH	3:C:886:ASP:OD2	2.05	0.74
1:A:318:TYR:O	3:C:645:ARG:NH1	2.21	0.74
3:C:678:THR:OG1	3:C:680:ASN:O	2.05	0.74
11:J:325:ASN:HB2	14:M:172:HIS:HD2	1.51	0.74
19:S:15:TYR:HB2	19:S:163:TYR:HB2	1.69	0.74
8:6:8:C:H2'	8:6:9:C:C6	2.23	0.74
11:J:411:MET:HE1	11:J:415:LEU:HB3	1.70	0.74
23:V:221:ILE:HB	23:V:359:LEU:HD11	1.69	0.74
38:l:44:GLU:HB3	38:l:62:GLU:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:OD1	15:N:1:MET:N	2.19	0.74
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.69	0.74
3:C:707:ILE:HD11	3:C:735:PHE:HB2	1.69	0.74
9:H:84:C:H2'	9:H:85:A:H8	1.52	0.74
11:J:188:GLN:HE22	13:L:140:ASP:H	1.33	0.73
23:V:236:ARG:NH2	23:V:379:GLU:O	2.20	0.73
25:X:34:ARG:HA	25:X:37:ILE:HD12	1.71	0.73
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.21	0.73
38:l:39:VAL:CG2	39:n:23:GLY:C	2.55	0.73
3:C:779:LEU:HD11	3:C:825:PRO:HB2	1.69	0.73
11:J:185:ALA:HA	13:L:142:ILE:HD13	1.70	0.73
19:S:57:ILE:HD13	24:W:97:ASN:HB3	1.69	0.73
3:C:700:ILE:O	3:C:740:THR:OG1	2.06	0.73
1:A:1076:ASP:OD1	1:A:1077:ILE:N	2.22	0.73
38:l:86:LEU:CD2	39:n:62:ILE:HG21	2.19	0.73
29:u:72:ILE:HG12	29:u:78:VAL:HG21	1.70	0.73
1:A:396:ASP:OD1	1:A:397:ASN:N	2.22	0.73
3:C:133:THR:HG23	3:C:225:VAL:HG23	1.71	0.73
36:k:52:LEU:HD11	36:k:67:LEU:HD13	1.71	0.73
36:k:111:ARG:HB2	37:m:62:VAL:HG23	1.71	0.73
37:m:70:LEU:HD22	37:m:71:TYR:HD2	1.54	0.73
2:B:97:G:H1	2:B:116:U:H3	1.37	0.73
37:m:15:THR:HG22	37:m:35:SER:HA	1.71	0.73
23:V:189:ASN:ND2	23:V:395:GLU:OE2	2.22	0.72
36:k:32:LEU:HD11	37:m:63:LEU:HD22	1.71	0.72
37:m:12:ASN:O	37:m:15:THR:OG1	2.06	0.72
11:J:188:GLN:HE21	13:L:13:ASN:HD22	1.37	0.72
23:V:503:TYR:HB2	23:V:546:ASN:HA	1.71	0.72
36:k:110:LEU:HD23	37:m:59:LEU:HD12	1.69	0.72
11:J:192:GLU:CD	11:J:192:GLU:H	1.97	0.72
36:k:23:GLU:OE2	37:m:8:LYS:NZ	2.17	0.72
6:F:49:G:N7	13:L:33:ARG:HG3	2.04	0.72
16:O:45:CYS:SG	16:O:48:CYS:N	2.61	0.72
38:l:86:LEU:CD1	39:n:67:ILE:HG12	2.16	0.72
1:A:1588:SER:OG	1:A:1737:ASN:ND2	2.19	0.72
36:k:42:VAL:HA	37:m:61:GLU:HB3	1.71	0.72
38:l:85:THR:HG22	38:l:86:LEU:HD12	1.71	0.72
46:1:469:ILE:HG12	46:1:470:THR:HG23	1.72	0.72
1:A:1434:LYS:O	1:A:1439:ARG:NH2	2.13	0.72
13:L:52:GLU:OE2	13:L:134:THR:OG1	2.07	0.72
20:T:188:PRO:HG3	20:T:443:THR:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:62:HIS:O	37:m:65:ARG:NH1	2.22	0.72
1:A:417:ARG:NH2	2:B:58:U:O3'	2.20	0.72
26:Y:39:PHE:HE2	26:Y:98:TYR:HB2	1.54	0.72
30:v:35:ARG:HD3	30:v:51:GLU:HG2	1.70	0.72
36:k:64:ASN:HB3	36:k:100:PHE:CZ	2.25	0.72
37:m:65:ARG:HB3	37:m:68:ASN:HD22	1.53	0.72
23:V:637:GLY:O	23:V:644:ARG:NH2	2.23	0.71
13:L:134:THR:HB	13:L:135:LYS:NZ	2.04	0.71
16:O:131:THR:HG22	24:W:108:ARG:HH21	1.55	0.71
16:O:240:GLY:HA3	16:O:296:ARG:HH22	1.56	0.71
6:F:39:A:N6	8:6:8:C:H42	1.85	0.71
29:u:313:GLN:HA	29:u:316:ARG:HD3	1.71	0.71
36:k:110:LEU:C	37:m:59:LEU:O	2.32	0.71
38:l:56:LEU:HD12	38:l:79:LEU:HB3	1.70	0.71
1:A:1998:ASN:O	1:A:2001:SER:OG	2.09	0.71
9:H:99:A:C2	38:l:55:ASN:ND2	2.57	0.71
40:o:72:ASN:O	40:o:74:ASN:ND2	2.24	0.71
37:m:24:LYS:HB2	37:m:25:TRP:CE3	2.25	0.71
1:A:676:ARG:NH2	6:F:70:A:OP2	2.23	0.71
1:A:1972:THR:N	1:A:1975:GLU:OE1	2.17	0.71
3:C:774:THR:HA	3:C:784:ILE:HD12	1.71	0.71
5:E:219:VAL:HB	5:E:229:TYR:HB2	1.72	0.71
26:Y:68:TYR:HD1	26:Y:69:LEU:H	1.37	0.71
1:A:1831:LYS:HZ3	1:A:1832:ARG:H	1.38	0.71
9:H:33:G:N7	25:X:9:LYS:NZ	2.39	0.71
18:R:126:ASN:ND2	18:R:128:ASP:H	1.82	0.71
38:l:34:TRP:HZ2	39:n:27:VAL:CG2	2.03	0.71
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.06	0.71
4:D:668:ASP:O	4:D:672:GLY:N	2.23	0.71
18:R:311:LYS:HG2	18:R:315:LYS:HE2	1.72	0.70
29:u:81:GLN:HA	29:u:218:SER:O	1.92	0.70
34:i:14:ASP:N	34:i:31:PHE:O	2.22	0.70
38:l:39:VAL:CB	39:n:23:GLY:CA	2.66	0.70
1:A:158:ARG:NH2	1:A:570:ASP:OD2	2.24	0.70
9:H:99:A:O2'	38:l:53:TYR:HE1	1.71	0.70
22:U:1:MET:SD	22:U:1:MET:N	2.63	0.70
29:u:118:LEU:O	29:u:122:ILE:HG12	1.91	0.70
35:j:20:LYS:O	35:j:66:ARG:NH2	2.24	0.70
35:j:76:LEU:HD11	36:k:66:VAL:HG11	1.71	0.70
46:1:196:ARG:HH21	46:1:221:PHE:HE2	1.40	0.70
3:C:471:ASP:H	3:C:499:GLY:HA2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:956:LEU:O	4:D:958:HIS:N	2.25	0.70
23:V:166:ILE:O	23:V:170:ILE:HG12	1.92	0.70
36:k:31:VAL:HG23	37:m:43:GLN:NE2	1.99	0.70
5:E:60:MET:HB2	5:E:353:MET:HB2	1.73	0.70
23:V:341:ALA:HA	23:V:344:LYS:HE3	1.74	0.70
29:u:50:LEU:HA	29:u:53:ILE:HD12	1.74	0.70
36:k:44:ILE:CG1	36:k:109:VAL:HG13	2.22	0.70
37:m:23:LEU:HD11	37:m:68:ASN:HB3	1.72	0.70
46:1:425:PRO:HG2	46:1:475:VAL:HG12	1.73	0.70
1:A:1761:PRO:O	1:A:1885:LYS:NZ	2.25	0.70
2:B:100:C:H2'	2:B:101:U:C6	2.27	0.70
6:F:41:A:H2'	6:F:42:C:C6	2.27	0.70
35:j:15:VAL:HG12	35:j:71:PRO:HD3	1.73	0.70
37:m:20:MET:SD	37:m:28:GLU:HB3	2.32	0.70
1:A:362:ARG:HD2	23:V:333:GLN:HE22	1.57	0.69
11:J:441:ASP:OD1	11:J:445:LYS:NZ	2.25	0.69
30:v:82:PRO:HB2	30:v:87:ARG:HH11	1.56	0.69
46:1:180:HIS:HB2	46:1:207:LYS:HG3	1.72	0.69
1:A:833:LYS:HE3	1:A:834:HIS:CE1	2.27	0.69
5:E:289:LEU:HD21	5:E:304:SER:HA	1.74	0.69
16:O:27:CYS:SG	16:O:83:THR:OG1	2.50	0.69
19:S:58:LYS:HE2	19:S:144:MET:HG2	1.74	0.69
19:S:90:LEU:HB3	19:S:128:ILE:HB	1.73	0.69
31:w:77:VAL:HG22	31:w:146:VAL:HG12	1.74	0.69
46:1:602:PRO:HA	46:1:605:ALA:HB3	1.75	0.69
1:A:267:LYS:NZ	2:B:49:A:OP1	2.19	0.69
1:A:469:LYS:NZ	2:B:59:G:N7	2.37	0.69
1:A:792:HIS:HE1	18:R:279:HIS:HE1	1.39	0.69
1:A:1963:GLU:HB3	1:A:1965:HIS:CD2	2.27	0.69
11:J:356:TYR:HD1	14:M:146:MET:HE1	1.57	0.69
23:V:323:LEU:HG	23:V:324:HIS:CD2	2.27	0.69
36:k:42:VAL:HG11	36:k:56:VAL:HG23	1.73	0.69
38:l:42:ARG:NH1	39:n:47:GLU:OE2	2.26	0.69
46:1:333:VAL:HG11	46:1:353:ASN:HB2	1.73	0.69
29:u:48:ASP:OD1	29:u:51:ARG:NH1	2.25	0.69
38:l:34:TRP:HE3	39:n:21:LEU:HD12	1.54	0.69
1:A:305:ARG:HA	1:A:305:ARG:HH11	1.56	0.69
8:6:22:C:O2'	8:6:23:U:OP1	2.10	0.69
14:M:178:GLU:HA	14:M:181:ARG:HD3	1.74	0.69
39:n:13:MET:O	39:n:15:LYS:HG2	1.92	0.69
1:A:1020:LYS:NZ	9:H:26:A:OP1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1276:GLU:OE2	1:A:1375:TRP:N	2.26	0.69
2:B:98:G:H2'	2:B:99:C:C6	2.28	0.69
3:C:706:GLN:HE22	3:C:708:THR:HB	1.56	0.69
36:k:66:VAL:HG22	36:k:100:PHE:HD2	1.57	0.69
38:l:36:TYR:O	38:l:38:GLN:N	2.26	0.69
3:C:561:LYS:NZ	3:C:611:ASN:O	2.23	0.69
3:C:779:LEU:HB3	3:C:934:MET:HE1	1.74	0.69
6:F:27:A:OP1	15:N:41:ARG:NH2	2.26	0.69
18:R:306:ALA:O	18:R:310:ARG:HG3	1.92	0.69
25:X:13:HIS:NE2	25:X:15:GLN:HB2	2.08	0.69
29:u:23:MET:HB2	29:u:227:GLU:HG2	1.74	0.69
46:l:282:HIS:ND1	46:l:303:SER:OG	2.24	0.69
8:6:104:C:OP1	8:6:104:C:H4'	1.93	0.69
38:l:34:TRP:HZ2	39:n:27:VAL:HG22	1.58	0.69
38:l:56:LEU:O	38:l:78:MET:HA	1.93	0.69
3:C:852:ARG:NH2	7:G:-12:G:OP1	2.27	0.68
37:m:27:MET:SD	37:m:29:TYR:HE2	2.15	0.68
38:l:54:MET:HG2	38:l:54:MET:O	1.91	0.68
1:A:982:GLU:HG3	1:A:1169:GLN:HG3	1.75	0.68
1:A:1678:ARG:NH2	47:2:252:LYS:O	2.23	0.68
3:C:230:ASP:HB3	3:C:233:GLU:HB2	1.73	0.68
12:K:188:LEU:HG	13:L:777:GLN:HB3	1.75	0.68
38:l:88:GLN:HG3	38:l:89:SER:N	2.09	0.68
1:A:338:VAL:O	3:C:266:GLU:HG2	1.92	0.68
30:v:81:PRO:O	30:v:104:SER:OG	2.11	0.68
33:h:64:ARG:NH2	39:n:65:ASN:O	2.26	0.68
38:l:22:PHE:HD1	38:l:50:PHE:HZ	1.41	0.68
1:A:189:GLU:OE2	1:A:190:ALA:N	2.27	0.68
2:B:17:U:H3	2:B:60:G:H1	1.40	0.68
36:k:44:ILE:O	36:k:51:LYS:HA	1.94	0.68
11:J:342:GLU:OE2	11:J:344:GLN:N	2.20	0.68
38:l:55:ASN:OD1	38:l:80:LYS:HE3	1.92	0.68
38:l:87:LEU:H	39:n:62:ILE:CA	2.01	0.68
3:C:663:CYS:HB2	3:C:828:MET:HB2	1.75	0.68
29:u:110:LEU:HG	29:u:181:ILE:HD12	1.76	0.68
30:v:12:TYR:HB2	30:v:25:GLU:HG3	1.74	0.68
30:v:35:ARG:HA	30:v:51:GLU:HG3	1.76	0.68
40:o:37:LEU:O	40:o:40:THR:OG1	2.12	0.68
1:A:1382:SER:OG	1:A:1416:ILE:N	2.23	0.68
1:A:1405:LEU:HG	1:A:1423:PHE:CE2	2.29	0.68
13:L:146:GLU:OE1	13:L:146:GLU:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:146:HIS:ND1	24:W:146:HIS:O	2.27	0.68
29:u:288:ARG:NH2	32:x:177:LYS:O	2.17	0.68
1:A:419:ARG:NH2	1:A:423:ASP:O	2.26	0.67
1:A:1957:ASP:HB3	1:A:1960:THR:HG23	1.75	0.67
7:G:-11:G:OP1	22:U:21:ARG:NE	2.27	0.67
1:A:1180:LYS:NZ	1:A:1181:ASP:OD2	2.27	0.67
1:A:82:ARG:NH1	8:6:16:G:O6	2.28	0.67
1:A:283:VAL:HG22	1:A:284:ARG:HG3	1.77	0.67
3:C:236:MET:O	3:C:239:THR:OG1	2.11	0.67
3:C:452:THR:HB	3:C:577:PHE:CD2	2.28	0.67
23:V:565:LEU:HD22	23:V:608:LEU:HD13	1.77	0.67
38:l:85:THR:O	39:n:63:ARG:CA	2.42	0.67
29:u:309:GLY:HA2	29:u:316:ARG:HH12	1.59	0.67
1:A:67:ARG:HD3	1:A:179:ALA:HB2	1.76	0.67
1:A:171:ASP:OD1	1:A:521:ASN:ND2	2.25	0.67
11:J:311:GLN:HG3	14:M:131:GLN:HG2	1.77	0.67
13:L:188:ARG:HE	13:L:191:LEU:HD12	1.60	0.67
1:A:1275:ARG:NH1	1:A:1373:GLN:O	2.27	0.67
36:k:104:ASP:HA	37:m:65:ARG:HE	1.59	0.67
38:l:88:GLN:NE2	39:n:57:ILE:CD1	2.56	0.67
39:n:11:LYS:O	39:n:13:MET:N	2.28	0.67
47:2:231:LEU:HD23	47:2:247:ARG:HH21	1.59	0.67
1:A:762:ARG:HH12	17:P:226:LYS:HZ1	1.42	0.67
3:C:470:PRO:HB3	3:C:500:THR:HG23	1.77	0.67
6:F:17:C:H2'	6:F:18:A:C8	2.25	0.67
35:j:80:LEU:HD11	36:k:58:ALA:HB2	1.75	0.67
37:m:14:LEU:HB3	37:m:33:LEU:HD23	1.75	0.67
39:n:45:CYS:N	39:n:58:GLY:O	2.25	0.67
1:A:1948:ASP:HB2	1:A:1949:ARG:HH21	1.60	0.66
9:H:60:U:O2'	46:1:258:ARG:NH1	2.28	0.66
9:H:99:A:H2	38:l:55:ASN:HD21	1.42	0.66
29:u:112:LEU:HB3	29:u:192:MET:HE3	1.77	0.66
36:k:31:VAL:HG21	37:m:62:VAL:H	1.60	0.66
24:W:121:ASN:OD1	24:W:123:PHE:N	2.28	0.66
37:m:11:LEU:CD2	37:m:36:VAL:HB	2.26	0.66
3:C:68:THR:OG1	3:C:71:GLU:HB3	1.94	0.66
23:V:265:ASN:HD22	23:V:352:ILE:HG23	1.60	0.66
1:A:381:PRO:O	1:A:383:PHE:N	2.28	0.66
3:C:624:SER:HB2	3:C:626:GLU:HG2	1.77	0.66
13:L:30:GLN:OE1	13:L:33:ARG:NE	2.29	0.66
16:O:292:ILE:HG12	16:O:297:ARG:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:58:ALA:HB1	28:r:6:SER:HA	1.77	0.66
1:A:369:GLU:OE2	1:A:369:GLU:N	2.28	0.66
1:A:1407:ASP:OD2	1:A:1407:ASP:N	2.23	0.66
36:k:44:ILE:HA	36:k:109:VAL:HA	1.78	0.66
6:F:52:U:O2'	25:X:2:GLY:N	2.26	0.66
16:O:185:LYS:HD2	16:O:186:PRO:HD2	1.78	0.66
16:O:235:TYR:HD2	16:O:301:LYS:HB2	1.60	0.66
29:u:290:VAL:HG13	29:u:332:ILE:HG22	1.77	0.66
1:A:1762:TYR:HB3	1:A:1888:GLU:HB2	1.76	0.66
9:H:84:C:H2'	9:H:85:A:C8	2.31	0.66
39:n:42:ILE:N	39:n:60:VAL:O	2.26	0.66
1:A:1424:GLN:NE2	1:A:1459:ARG:O	2.24	0.66
3:C:853:ARG:NH2	3:C:886:ASP:OD2	2.24	0.66
4:D:150:ASP:C	4:D:152:GLU:H	2.04	0.66
9:H:89:U:H2'	9:H:90:A:H8	1.61	0.66
26:Y:39:PHE:CE2	26:Y:98:TYR:HB2	2.31	0.66
2:B:99:C:H2'	2:B:100:C:C6	2.31	0.66
3:C:219:LEU:HD12	3:C:245:HIS:CE1	2.30	0.66
9:H:3:C:H2'	9:H:4:G:C8	2.31	0.66
16:O:177:GLU:OE1	16:O:177:GLU:N	2.28	0.66
33:h:70:PHE:HB3	34:i:72:LEU:HD12	1.77	0.66
39:n:40:LEU:O	39:n:62:ILE:N	2.28	0.66
1:A:460:LYS:NZ	2:B:49:A:OP2	2.29	0.66
18:R:126:ASN:HD22	18:R:128:ASP:N	1.83	0.66
36:k:111:ARG:CA	37:m:61:GLU:HA	2.26	0.66
1:A:853:LYS:HE2	8:6:101:U:C5	2.31	0.65
13:L:153:SER:HA	13:L:156:ARG:HD2	1.78	0.65
20:T:210:ILE:HG12	20:T:221:THR:HG22	1.78	0.65
4:D:149:ARG:O	4:D:151:LYS:N	2.30	0.65
1:A:1764:SER:O	1:A:1767:ASN:N	2.28	0.65
9:H:100:U:O3'	39:n:65:ASN:ND2	2.30	0.65
23:V:331:ARG:HG2	23:V:335:MET:HE2	1.78	0.65
1:A:384:VAL:HG12	3:C:331:PHE:CD2	2.31	0.65
1:A:802:THR:HB	1:A:805:GLU:HG3	1.78	0.65
29:u:307:MET:HG2	29:u:331:LEU:HD11	1.78	0.65
38:l:39:VAL:HA	39:n:23:GLY:HA3	1.76	0.65
3:C:137:HIS:HB2	3:C:239:THR:HG23	1.79	0.65
9:H:153:A:H2'	9:H:154:C:H5'	1.77	0.65
38:l:58:LEU:HB2	38:l:77:ILE:HB	1.78	0.65
1:A:1352:HIS:CE1	22:U:21:ARG:HG3	2.32	0.65
1:A:1361:GLU:HB2	1:A:1363:GLN:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ASP:OD1	1:A:746:LYS:NZ	2.27	0.65
3:C:667:VAL:H	3:C:824:THR:HG23	1.61	0.65
16:O:26:THR:HG1	16:O:159:ARG:NH2	1.94	0.65
18:R:229:VAL:HG23	18:R:230:MET:H	1.61	0.65
20:T:455:GLN:HG3	20:T:485:THR:HG21	1.78	0.65
36:k:41:GLN:O	37:m:61:GLU:HB2	1.96	0.65
40:o:132:ARG:NE	40:o:154:GLU:OE1	2.22	0.65
1:A:64:GLU:OE1	1:A:64:GLU:N	2.21	0.65
1:A:71:ARG:NH1	1:A:177:ASP:OD2	2.30	0.65
29:u:193:LEU:HD11	29:u:232:PHE:CZ	2.32	0.65
36:k:110:LEU:O	37:m:60:GLY:C	2.39	0.65
43:z:44:LYS:O	43:z:47:ARG:HG2	1.97	0.65
46:1:329:GLN:HE21	46:1:331:LYS:HD3	1.62	0.65
1:A:468:LYS:HD3	1:A:469:LYS:H	1.62	0.65
1:A:799:PRO:HD3	18:R:284:PHE:CD1	2.32	0.65
20:T:345:ILE:HB	20:T:357:TRP:HB2	1.78	0.65
25:X:30:HIS:HA	25:X:33:GLU:OE2	1.97	0.65
8:6:73:G:O2'	8:6:74:G:O5'	2.15	0.65
11:J:311:GLN:OE1	11:J:311:GLN:N	2.25	0.65
46:1:249:GLY:HA3	46:1:285:MET:HE3	1.77	0.65
47:2:108:ALA:HB2	47:2:132:ILE:HD13	1.79	0.65
13:L:188:ARG:O	13:L:192:ARG:HG2	1.97	0.64
29:u:193:LEU:HD11	29:u:232:PHE:HZ	1.62	0.64
29:u:304:VAL:HG13	29:u:330:VAL:HG13	1.79	0.64
10:I:564:PHE:O	10:I:569:GLY:N	2.29	0.64
11:J:436:TYR:HD1	11:J:437:LYS:HD2	1.61	0.64
17:P:42:LYS:NZ	20:T:276:GLU:HG3	2.12	0.64
28:r:30:ILE:O	28:r:34:ILE:HG12	1.97	0.64
31:w:104:LEU:HG	31:w:113:LEU:HD11	1.79	0.64
1:A:1853:PRO:HG2	47:2:101:LYS:NZ	2.12	0.64
3:C:241:ARG:HH21	3:C:584:THR:HG22	1.61	0.64
9:H:25:G:H2'	9:H:26:A:H8	1.63	0.64
17:P:43:TYR:O	17:P:45:GLN:NE2	2.30	0.64
17:P:204:GLN:O	17:P:206:LYS:N	2.23	0.64
46:1:472:ALA:O	46:1:490:THR:OG1	2.15	0.64
5:E:158:TYR:HB3	5:E:168:CYS:SG	2.37	0.64
18:R:241:GLU:N	18:R:241:GLU:OE1	2.30	0.64
33:h:67:LYS:HG3	39:n:68:ILE:HD13	1.80	0.64
36:k:63:CYS:HB3	37:m:63:LEU:HD21	1.78	0.64
38:l:88:GLN:C	39:n:60:VAL:CG1	2.67	0.64
11:J:322:MET:HE1	14:M:142:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:225:LYS:HG2	23:V:405:ILE:HG12	1.79	0.64
26:Y:38:PRO:HG2	26:Y:39:PHE:CD2	2.32	0.64
36:k:32:LEU:HB3	36:k:59:PHE:CG	2.31	0.64
2:B:65:G:H2'	2:B:66:A:H8	1.62	0.64
29:u:189:ALA:HB1	29:u:216:LEU:HD22	1.80	0.64
1:A:469:LYS:NZ	2:B:59:G:O6	2.27	0.64
8:6:12:G:H2'	8:6:13:C:C6	2.32	0.64
20:T:347:THR:HG22	20:T:357:TRP:HE1	1.62	0.64
29:u:71:GLN:HG3	29:u:237:ILE:HG21	1.80	0.64
46:1:567:PRO:O	46:1:569:ALA:N	2.27	0.64
3:C:396:LEU:HA	3:C:399:LEU:HD12	1.79	0.64
37:m:37:ASP:OD1	37:m:38:GLY:N	2.31	0.64
3:C:670:SER:HA	3:C:823:ALA:HB3	1.78	0.64
3:C:676:ALA:O	3:C:684:LYS:HA	1.98	0.64
8:6:73:G:O2'	8:6:74:G:O4'	2.11	0.64
30:v:28:PHE:HE2	30:v:54:VAL:HG21	1.63	0.64
1:A:1892:PRO:HB3	45:4:104:ARG:HD2	1.80	0.64
11:J:201:ARG:NH2	46:1:596:LYS:O	2.31	0.64
16:O:224:ASP:O	16:O:302:TRP:NE1	2.31	0.64
31:w:67:GLN:HE21	31:w:152:ARG:HD2	1.63	0.64
46:1:480:HIS:HD2	46:1:482:LYS:H	1.46	0.64
39:n:22:ASN:H	39:n:68:ILE:HG13	1.62	0.63
1:A:351:TYR:HA	3:C:270:PRO:HG3	1.79	0.63
1:A:462:ARG:HA	1:A:462:ARG:CZ	2.27	0.63
29:u:361:TYR:HE1	29:u:379:ASN:HD21	1.46	0.63
38:l:81:GLY:HA2	38:l:84:ILE:HD12	1.80	0.63
1:A:1234:ASP:HA	1:A:1237:MET:HE2	1.80	0.63
6:F:22:A:H5''	15:N:116:ASN:O	1.98	0.63
16:O:22:ILE:HG23	24:W:112:SER:HB2	1.80	0.63
37:m:27:MET:HG2	37:m:51:ILE:HD12	1.80	0.63
1:A:40:LEU:O	1:A:44:ARG:HG2	1.97	0.63
1:A:380:LEU:O	3:C:354:ARG:NE	2.25	0.63
16:O:133:PRO:HD2	16:O:137:LEU:HD22	1.80	0.63
29:u:89:THR:HA	29:u:92:PHE:CE2	2.34	0.63
1:A:548:ARG:NH1	1:A:549:GLU:OE2	2.32	0.63
1:A:1644:LEU:HD23	1:A:1715:TYR:HD1	1.64	0.63
9:H:114:A:H61	9:H:142:C:H42	1.47	0.63
13:L:74:LEU:HD23	13:L:77:LEU:HD12	1.78	0.63
1:A:47:GLU:O	1:A:50:LYS:HG3	1.98	0.63
6:F:22:A:C6	24:W:130:ARG:HG2	2.33	0.63
8:6:2:U:O4	26:Y:4:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:106:GLN:HG2	18:R:110:LYS:HD2	1.81	0.63
18:R:281:ASN:OD1	18:R:282:GLU:N	2.32	0.63
40:o:159:GLU:O	40:o:163:LYS:HB2	1.99	0.63
1:A:1410:ASP:O	1:A:1414:ARG:NH1	2.32	0.63
13:L:717:MET:O	13:L:721:LEU:HB3	1.99	0.63
19:S:102:ASN:OD1	19:S:108:ASN:ND2	2.32	0.63
20:T:213:GLU:OE2	20:T:215:GLY:N	2.30	0.63
1:A:1779:PHE:CE1	1:A:1891:LEU:HD12	2.34	0.63
20:T:405:PHE:CG	20:T:405:PHE:O	2.52	0.63
29:u:78:VAL:HG23	29:u:215:VAL:HG13	1.81	0.63
36:k:28:PRO:HG3	37:m:36:VAL:CA	2.21	0.63
40:o:57:LEU:HD11	40:o:95:LEU:HD21	1.81	0.63
46:l:346:LEU:HD12	46:l:358:ILE:HG22	1.81	0.63
1:A:488:ASP:OD1	1:A:489:TRP:N	2.32	0.63
5:E:242:SER:HG	5:E:293:TRP:CD1	2.17	0.63
6:F:42:C:H2'	6:F:43:A:O4'	1.98	0.63
6:F:51:U:OP1	26:Y:54:LYS:HA	1.98	0.63
20:T:339:GLN:NE2	20:T:342:GLU:O	2.31	0.63
39:n:40:LEU:N	39:n:62:ILE:O	2.31	0.63
1:A:1159:ASN:ND2	17:P:196:ASN:OD1	2.32	0.62
6:F:22:A:OP1	15:N:115:THR:OG1	2.17	0.62
18:R:73:PRO:HB3	19:S:131:ARG:HH22	1.64	0.62
20:T:351:ASP:O	20:T:352:THR:OG1	2.15	0.62
23:V:264:ILE:HG13	23:V:274:CYS:SG	2.39	0.62
38:l:32:GLN:O	38:l:88:GLN:HG2	1.99	0.62
1:A:435:CYS:HB2	7:G:-11:G:H22	1.65	0.62
6:F:85:U:H5'	6:F:86:U:C5	2.34	0.62
19:S:57:ILE:HD12	19:S:61:MET:HG3	1.81	0.62
36:k:65:MET:HG2	36:k:67:LEU:HG	1.80	0.62
39:n:14:ASP:OD1	39:n:32:ARG:NH2	2.33	0.62
33:g:21:GLU:O	33:g:69:ARG:N	2.31	0.62
1:A:912:GLU:HG3	1:A:913:PRO:HD2	1.81	0.62
3:C:489:GLN:O	3:C:489:GLN:NE2	2.32	0.62
19:S:90:LEU:C	19:S:128:ILE:HD12	2.24	0.62
24:W:137:TYR:HE2	24:W:164:GLY:HA2	1.63	0.62
36:k:109:VAL:O	37:m:63:LEU:N	2.30	0.62
19:S:44:ARG:HB2	19:S:164:PRO:HG3	1.81	0.62
20:T:432:ASP:OD1	20:T:433:ASN:N	2.33	0.62
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.09	0.62
3:C:731:SER:HB2	3:C:747:ASP:O	1.99	0.62
18:R:113:TYR:OH	20:T:402:ASP:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ARG:O	1:A:618:THR:OG1	2.13	0.62
1:A:835:ASP:OD1	1:A:836:THR:N	2.33	0.62
3:C:186:VAL:HG22	3:C:535:ALA:HA	1.82	0.62
5:E:322:LYS:NZ	24:W:147:GLN:OE1	2.32	0.62
6:F:39:A:H2'	6:F:40:U:O4'	2.00	0.62
18:R:125:MET:O	18:R:126:ASN:HB2	1.99	0.62
35:j:36:MET:SD	36:k:102:ARG:HD2	2.40	0.62
1:A:369:GLU:O	1:A:371:LEU:N	2.28	0.62
13:L:178:GLU:HA	13:L:181:ARG:HG2	1.80	0.62
36:k:29:LEU:HG	36:k:32:LEU:HD12	1.81	0.62
46:1:208:PHE:HB3	46:1:221:PHE:HD2	1.65	0.62
1:A:108:MET:O	1:A:110:TRP:N	2.32	0.62
1:A:792:HIS:CE1	18:R:279:HIS:HE1	2.16	0.62
1:A:1941:ARG:NH2	1:A:2011:ILE:O	2.32	0.62
3:C:589:LYS:HE3	3:C:628:VAL:HG11	1.81	0.62
8:6:91:A:H2'	8:6:92:U:O4'	1.99	0.62
11:J:361:ARG:HD3	14:M:161:PHE:CD2	2.35	0.62
16:O:197:ASN:OD1	16:O:198:ILE:N	2.33	0.62
22:U:18:TYR:CE2	22:U:20:GLN:HB2	2.34	0.62
25:X:5:ASP:OD1	25:X:7:ASN:N	2.27	0.62
25:X:6:LEU:HD22	26:Y:55:LYS:HE2	1.82	0.62
36:k:42:VAL:O	36:k:53:LEU:HA	2.00	0.62
39:n:41:VAL:HG13	39:n:60:VAL:C	2.25	0.62
47:2:102:LEU:HD11	47:2:132:ILE:HG12	1.81	0.62
1:A:855:ARG:HG3	9:H:29:A:C2	2.35	0.62
1:A:1018:ASN:ND2	1:A:1023:ASN:OD1	2.31	0.62
3:C:679:PRO:HD2	3:C:807:GLN:HB3	1.80	0.62
5:E:251:LEU:HD21	5:E:300:ILE:HG23	1.81	0.62
6:F:30:A:H61	8:6:16:G:H1'	1.64	0.62
15:N:2:PRO:HG2	15:N:4:VAL:HA	1.82	0.62
26:Y:108:PHE:HD1	26:Y:109:GLN:H	1.48	0.62
26:Y:63:VAL:HG22	26:Y:73:ILE:O	2.00	0.62
29:u:109:ALA:HB3	29:u:159:VAL:HG13	1.82	0.62
29:u:287:LYS:HG2	29:u:308:HIS:HB2	1.81	0.62
37:m:16:GLY:N	37:m:33:LEU:O	2.33	0.62
39:n:35:ASP:HB2	39:n:36:PRO:HD2	1.80	0.62
40:o:110:ALA:HA	40:o:139:VAL:HG12	1.81	0.62
45:4:102:ALA:H	45:4:107:TYR:HD2	1.48	0.62
45:4:112:MET:N	45:4:112:MET:SD	2.72	0.62
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.81	0.61
1:A:1455:TRP:H	1:A:1455:TRP:CD1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:265:ARG:HH11	5:E:267:PHE:H	1.46	0.61
7:G:-5:G:O2'	7:G:-4:A:H5''	1.99	0.61
11:J:216:ASP:HB3	11:J:217:GLU:OE1	2.00	0.61
13:L:13:ASN:ND2	13:L:139:PRO:HA	2.15	0.61
20:T:459:LEU:HB3	20:T:462:GLU:HG3	1.81	0.61
33:h:64:ARG:HD2	39:n:67:ILE:H	1.64	0.61
39:n:28:GLN:O	39:n:45:CYS:HA	2.00	0.61
1:A:312:TYR:HH	3:C:886:ASP:CG	2.06	0.61
1:A:1173:SER:OG	1:A:1174:PHE:N	2.31	0.61
5:E:68:GLU:CD	5:E:68:GLU:H	2.08	0.61
10:I:386:ASP:O	10:I:388:PHE:N	2.34	0.61
29:u:73:ILE:HD11	29:u:95:SER:HA	1.80	0.61
38:l:42:ARG:HB2	38:l:64:ILE:HB	1.82	0.61
39:n:63:ARG:HG3	39:n:65:ASN:H	1.65	0.61
2:B:99:C:H2'	2:B:100:C:H6	1.64	0.61
3:C:474:LEU:HD12	3:C:500:THR:O	2.00	0.61
10:I:528:LEU:C	10:I:532:LYS:HA	2.22	0.61
23:V:260:VAL:O	23:V:264:ILE:HG12	1.99	0.61
39:n:39:ASN:HA	39:n:64:GLY:N	2.11	0.61
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.36	0.61
18:R:189:ASN:HD21	18:R:195:ARG:HG3	1.65	0.61
19:S:14:VAL:HG13	19:S:25:LEU:HD13	1.81	0.61
35:j:60:ILE:HD11	35:j:64:ASN:HB2	1.80	0.61
36:k:111:ARG:HA	37:m:61:GLU:CA	2.28	0.61
37:m:70:LEU:HD22	37:m:71:TYR:CD2	2.36	0.61
46:1:300:MET:HE1	46:1:347:ILE:HG21	1.82	0.61
1:A:1233:ASP:OD1	1:A:1235:GLU:N	2.32	0.61
13:L:213:GLU:OE2	16:O:110:SER:N	2.33	0.61
1:A:1381:ASP:OD2	1:A:1384:ARG:NH2	2.33	0.61
3:C:510:LEU:HB2	3:C:564:THR:OG1	2.01	0.61
8:6:6:A:H2'	8:6:7:G:O4'	2.01	0.61
24:W:285:SER:O	24:W:287:HIS:N	2.30	0.61
38:l:64:ILE:HD12	38:l:71:ARG:HG2	1.81	0.61
1:A:1234:ASP:OD2	1:A:1234:ASP:N	2.32	0.61
1:A:1602:ASP:OD1	1:A:1603:ALA:N	2.32	0.61
3:C:799:GLU:O	3:C:801:LEU:N	2.32	0.61
9:H:101:U:C4	33:h:64:ARG:NH1	2.69	0.61
11:J:188:GLN:NE2	13:L:13:ASN:HD22	1.99	0.61
35:j:76:LEU:HD23	36:k:57:LYS:HG2	1.83	0.61
37:m:32:TYR:O	37:m:44:LEU:HG	2.00	0.61
38:l:47:ILE:HA	38:l:57:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:9:LEU:HD12	39:n:34:PHE:HE2	1.63	0.61
35:b:13:GLU:O	35:b:29:ILE:N	2.32	0.61
37:d:34:VAL:N	37:d:43:GLN:O	2.32	0.61
3:C:476:CYS:HB3	3:C:565:ILE:HB	1.82	0.61
9:H:155:C:C2	9:H:176:G:N2	2.69	0.61
38:l:85:THR:O	39:n:63:ARG:C	2.43	0.61
47:2:59:THR:HB	47:2:183:CYS:SG	2.41	0.61
3:C:842:CYS:O	3:C:846:VAL:HG23	2.01	0.61
18:R:192:ALA:HB2	24:W:153:ILE:HD13	1.82	0.61
28:q:21:SER:HB3	28:q:43:ASN:CG	2.26	0.61
35:j:32:VAL:HG22	35:j:38:THR:HG23	1.82	0.61
1:A:1410:ASP:OD2	1:A:1411:SER:N	2.34	0.61
1:A:1532:ARG:HB3	1:A:1532:ARG:CZ	2.30	0.61
5:E:206:ASP:O	5:E:222:LEU:HG	2.00	0.61
5:E:239:THR:HB	5:E:289:LEU:H	1.66	0.61
9:H:106:G:H4'	9:H:107:A:O4'	2.01	0.61
23:V:294:ILE:O	23:V:298:LYS:HG2	2.01	0.61
38:l:25:LEU:O	38:l:28:ARG:HG2	2.01	0.61
39:n:40:LEU:HB2	39:n:62:ILE:CG2	2.31	0.61
1:A:1162:PRO:HG3	17:P:194:PHE:CZ	2.35	0.60
3:C:86:THR:OG1	3:C:87:GLN:N	2.34	0.60
15:N:54:HIS:CE1	15:N:92:TRP:HZ2	2.18	0.60
18:R:185:GLY:O	18:R:187:ALA:N	2.34	0.60
23:V:449:GLU:HB3	23:V:452:LEU:HB2	1.82	0.60
35:j:68:PHE:N	36:k:100:PHE:O	2.29	0.60
1:A:985:TYR:HB2	1:A:986:GLU:OE1	2.01	0.60
1:A:1783:THR:HG21	1:A:1894:GLN:HG3	1.83	0.60
1:A:1889:LEU:HD23	1:A:1890:GLN:N	2.15	0.60
8:6:26:U:H3'	16:O:235:TYR:OH	2.01	0.60
11:J:238:ASN:C	11:J:240:THR:H	2.08	0.60
13:L:204:ARG:HE	13:L:207:GLY:HA3	1.66	0.60
16:O:259:ARG:HD2	16:O:273:GLN:HG2	1.83	0.60
26:Y:40:ASN:OD1	26:Y:107:ASN:HB2	2.00	0.60
36:k:23:GLU:C	36:k:27:GLY:HA3	2.20	0.60
1:A:1765:SER:HA	1:A:1768:TYR:HB3	1.83	0.60
12:K:150:GLN:HA	12:K:153:LEU:HD12	1.83	0.60
18:R:66:GLU:HG2	18:R:67:ILE:HD13	1.83	0.60
29:u:64:ILE:HD13	29:u:88:LYS:HG2	1.81	0.60
38:l:36:TYR:CD2	38:l:37:GLU:HB2	2.36	0.60
38:l:39:VAL:CB	39:n:23:GLY:C	2.75	0.60
12:K:35:LEU:O	12:K:38:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:277:MET:HG2	23:V:372:LEU:HD22	1.83	0.60
23:V:600:ASN:HA	23:V:639:LEU:HD21	1.83	0.60
36:k:104:ASP:N	36:k:104:ASP:OD1	2.32	0.60
37:m:24:LYS:HD2	37:m:25:TRP:CZ3	2.37	0.60
1:A:359:ILE:HB	23:V:324:HIS:CE1	2.36	0.60
1:A:1562:MET:HE1	1:A:1566:ILE:H	1.67	0.60
19:S:125:LYS:HE3	19:S:126:HIS:NE2	2.16	0.60
24:W:97:ASN:ND2	24:W:97:ASN:O	2.33	0.60
26:Y:101:GLU:HB3	26:Y:102:HIS:CD2	2.36	0.60
38:l:85:THR:HG22	38:l:86:LEU:CD1	2.32	0.60
1:A:1531:ASN:ND2	9:H:35:A:OP1	2.35	0.60
3:C:490:PHE:CZ	3:C:612:LYS:HD2	2.37	0.60
5:E:236:ASP:HB3	5:E:255:MET:HB2	1.84	0.60
16:O:88:LEU:O	18:R:183:GLN:NE2	2.34	0.60
18:R:74:LEU:HB2	19:S:136:ILE:HG12	1.82	0.60
20:T:349:SER:OG	20:T:351:ASP:OD1	2.18	0.60
37:m:20:MET:CE	37:m:30:LYS:HB2	2.30	0.60
37:d:42:MET:O	37:d:64:ILE:N	2.21	0.60
1:A:712:HIS:CD2	18:R:250:CYS:HB2	2.37	0.60
19:S:60:PHE:CD2	19:S:61:MET:HG2	2.36	0.60
38:l:39:VAL:CA	39:n:23:GLY:CA	2.61	0.60
46:l:292:HIS:HB2	46:l:340:TYR:CZ	2.37	0.60
1:A:367:SER:O	1:A:369:GLU:N	2.34	0.60
2:B:27:U:O2'	2:B:28:A:O5'	2.19	0.60
6:F:22:A:C5	24:W:130:ARG:HG2	2.35	0.60
9:H:101:U:H5''	9:H:102:U:H5'	1.84	0.60
11:J:191:ALA:O	11:J:194:LEU:N	2.35	0.60
11:J:252:GLU:OE2	11:J:260:ARG:HB3	2.01	0.60
23:V:279:THR:O	23:V:283:GLU:HG3	2.02	0.60
35:b:28:THR:O	35:b:41:LYS:N	2.24	0.60
1:A:1014:ASN:HD21	13:L:84:THR:H	1.48	0.60
3:C:446:LYS:HB3	3:C:447:PRO:HD3	1.84	0.60
16:O:106:ASP:OD1	16:O:107:MET:N	2.29	0.60
1:A:934:ARG:HH22	27:Z:393:VAL:CB	2.15	0.60
5:E:346:SER:OG	5:E:348:ASP:OD1	2.20	0.60
6:F:15:A:H2'	6:F:16:G:H8	1.65	0.60
10:I:406:GLU:HA	10:I:410:GLN:HA	1.83	0.60
36:k:28:PRO:C	36:k:30:SER:H	1.99	0.60
37:m:33:LEU:HA	37:m:44:LEU:HG	1.84	0.60
39:n:7:PRO:HB2	39:n:34:PHE:CZ	2.36	0.60
3:C:463:GLU:OE1	3:C:463:GLU:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:474:LEU:HD23	3:C:474:LEU:O	2.01	0.59
6:F:26:U:C5	16:O:65:PHE:CD2	2.77	0.59
18:R:132:LEU:HD12	20:T:384:HIS:HB3	1.83	0.59
18:R:147:THR:HG23	20:T:360:VAL:HG12	1.84	0.59
26:Y:40:ASN:HA	26:Y:50:ILE:O	2.02	0.59
29:u:390:ARG:HB3	30:v:105:LYS:HE2	1.85	0.59
35:j:55:LEU:HD12	35:j:58:LEU:HD12	1.82	0.59
37:m:24:LYS:HB2	37:m:25:TRP:CZ3	2.37	0.59
37:m:36:VAL:HG22	37:m:42:MET:HG2	1.83	0.59
1:A:41:GLN:HE22	1:A:44:ARG:HD3	1.67	0.59
3:C:250:ARG:HE	3:C:451:HIS:CD2	2.19	0.59
1:A:700:GLY:HA3	18:R:237:MET:HB2	1.84	0.59
9:H:99:A:H61	37:m:40:MET:HE3	1.67	0.59
19:S:77:ILE:HG13	19:S:78:TYR:HD1	1.67	0.59
31:w:90:HIS:CE1	31:w:99:ILE:HD13	2.38	0.59
1:A:47:GLU:OE1	1:A:47:GLU:N	2.28	0.59
1:A:428:LYS:HA	1:A:431:TYR:CE2	2.37	0.59
11:J:411:MET:HE3	11:J:412:ASP:H	1.66	0.59
19:S:11:PRO:O	19:S:29:TRP:NE1	2.35	0.59
19:S:149:SER:HB2	24:W:104:MET:HE1	1.85	0.59
27:Z:1091:VAL:HA	27:Z:1097:MET:O	2.02	0.59
28:r:89:SER:O	28:r:93:ARG:HG3	2.02	0.59
29:u:111:ILE:HD12	29:u:126:LEU:HD11	1.84	0.59
46:l:249:GLY:HA2	46:l:285:MET:HG3	1.84	0.59
2:B:29:A:H2'	2:B:30:A:H8	1.68	0.59
6:F:40:U:H3	8:6:7:G:H1	1.50	0.59
28:r:57:VAL:HG22	28:r:58:ALA:H	1.67	0.59
29:u:37:THR:OG1	29:u:42:THR:OG1	2.21	0.59
29:u:77:ASP:HB3	29:u:233:MET:HE2	1.83	0.59
1:A:385:GLU:HB3	1:A:389:LYS:HD2	1.84	0.59
8:6:12:G:H2'	8:6:13:C:C5	2.37	0.59
9:H:45:C:H2'	9:H:46:U:C6	2.38	0.59
16:O:233:THR:HA	16:O:272:ILE:O	2.02	0.59
20:T:185:MET:HB3	20:T:186:PRO:HD3	1.85	0.59
38:l:44:GLU:OE2	38:l:90:VAL:HG21	2.03	0.59
1:A:1330:MET:HG3	1:A:1367:ASN:ND2	2.15	0.59
1:A:1624:SER:OG	1:A:1625:SER:N	2.33	0.59
1:A:1649:LYS:HB2	47:2:237:ASP:O	2.02	0.59
8:6:13:C:H2'	8:6:14:A:C8	2.38	0.59
16:O:196:GLN:HE21	16:O:208:PRO:HG2	1.66	0.59
26:Y:86:GLU:CD	26:Y:86:GLU:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:365:ILE:HD12	29:u:377:ALA:HB1	1.85	0.59
36:k:29:LEU:HD23	36:k:59:PHE:CD2	2.38	0.59
36:k:111:ARG:HG2	36:k:112:ASN:H	1.66	0.59
1:A:1361:GLU:C	1:A:1363:GLN:H	2.10	0.59
3:C:241:ARG:NH2	3:C:584:THR:HG22	2.17	0.59
5:E:243:LEU:HD12	5:E:249:TYR:O	2.02	0.59
44:3:627:VAL:HA	44:3:634:PRO:HA	1.83	0.59
1:A:1212:GLY:HA3	1:A:1280:ASN:ND2	2.18	0.59
9:H:172:C:H2'	9:H:173:C:H6	1.68	0.59
20:T:257:ARG:NH1	20:T:301:ASP:OD1	2.35	0.59
26:Y:16:ASP:OD1	26:Y:18:SER:N	2.36	0.59
29:u:117:GLU:HB3	29:u:341:LEU:HD11	1.83	0.59
36:k:43:LEU:HD13	36:k:53:LEU:HB2	1.85	0.59
1:A:1762:TYR:O	1:A:1764:SER:N	2.36	0.59
1:A:1889:LEU:HD23	1:A:1890:GLN:H	1.66	0.59
5:E:75:HIS:CE1	5:E:121:GLY:HA3	2.38	0.59
13:L:134:THR:HB	13:L:135:LYS:HZ1	1.67	0.59
18:R:178:ARG:HD3	18:R:194:GLN:HE22	1.68	0.59
26:Y:35:LEU:O	26:Y:55:LYS:HA	2.03	0.59
29:u:218:SER:OG	29:u:221:LEU:HG	2.03	0.59
37:m:7:PRO:O	37:m:11:LEU:HB2	2.03	0.59
37:m:49:GLU:HG2	37:m:50:TYR:N	2.17	0.59
38:l:30:ARG:HE	38:l:44:GLU:HG2	1.68	0.59
1:A:271:MET:HE1	1:A:313:LYS:HD2	1.84	0.58
1:A:703:GLN:H	1:A:703:GLN:CD	2.10	0.58
3:C:216:THR:HG22	3:C:245:HIS:HE1	1.68	0.58
6:F:88:G:H4'	14:M:121:ASP:HB2	1.84	0.58
12:K:17:PRO:HG3	12:K:167:ARG:HH12	1.68	0.58
16:O:89:GLU:OE1	24:W:103:GLN:HB2	2.03	0.58
23:V:575:THR:O	23:V:580:ARG:NH1	2.36	0.58
29:u:248:LEU:HD12	29:u:251:ILE:HD11	1.85	0.58
36:k:24:PHE:CE1	36:k:29:LEU:HD22	2.39	0.58
37:m:22:LYS:HG3	37:m:27:MET:O	2.03	0.58
46:l:282:HIS:CE1	46:l:309:ARG:HD3	2.38	0.58
1:A:188:LEU:HD22	1:A:567:GLY:HA2	1.84	0.58
1:A:1251:SER:O	1:A:1298:ARG:NH2	2.36	0.58
6:F:45:A:H2	26:Y:57:ASN:HD21	1.50	0.58
8:6:21:A:O2'	16:O:216:ARG:NH1	2.36	0.58
11:J:323:LEU:HD13	14:M:174:PRO:HG3	1.85	0.58
14:M:179:ILE:O	14:M:183:VAL:HG23	2.03	0.58
19:S:50:GLY:N	19:S:159:ILE:O	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:404:SER:OG	20:T:405:PHE:N	2.32	0.58
29:u:271:LEU:O	29:u:275:LEU:HB2	2.03	0.58
46:1:303:SER:OG	46:1:305:ASP:OD1	2.15	0.58
1:A:246:LEU:HD22	1:A:408:PRO:HG2	1.84	0.58
1:A:435:CYS:HB2	7:G:-11:G:N2	2.18	0.58
3:C:66:TYR:HB3	20:T:456:PRO:O	2.04	0.58
3:C:556:ASP:O	3:C:559:ILE:HG13	2.03	0.58
9:H:112:G:H2'	9:H:113:G:H8	1.68	0.58
13:L:132:PRO:HD2	13:L:133:GLU:OE1	2.02	0.58
16:O:84:CYS:HB3	16:O:86:LEU:HG	1.86	0.58
39:n:43:ASP:HA	39:n:59:MET:HA	1.85	0.58
1:A:1393:ARG:HH11	1:A:1397:ILE:HD11	1.67	0.58
1:A:193:LEU:HD12	1:A:194:GLU:H	1.68	0.58
1:A:1292:GLU:OE2	1:A:1331:GLY:N	2.31	0.58
18:R:151:LEU:O	18:R:155:VAL:HG23	2.04	0.58
36:k:112:ASN:HB2	37:m:60:GLY:H	1.65	0.58
9:H:13:C:H41	14:M:200:ARG:NH1	1.98	0.58
9:H:99:A:H2	38:l:55:ASN:ND2	1.98	0.58
18:R:113:TYR:OH	20:T:402:ASP:OD1	2.22	0.58
28:q:103:LEU:HD12	28:t:103:LEU:HB2	1.84	0.58
29:u:358:ARG:NH1	32:x:191:HIS:HA	2.18	0.58
35:j:23:THR:HG23	35:j:47:LEU:HA	1.86	0.58
36:k:44:ILE:HG12	36:k:109:VAL:CG1	2.33	0.58
37:m:36:VAL:HG11	37:m:42:MET:HE2	1.86	0.58
46:1:347:ILE:O	46:1:358:ILE:HA	2.03	0.58
3:C:213:ASP:O	3:C:216:THR:OG1	2.11	0.58
16:O:144:SER:HA	16:O:148:LEU:HD13	1.85	0.58
16:O:236:VAL:O	16:O:269:CYS:HA	2.04	0.58
6:F:11:C:HO2'	6:F:12:G:H8	1.52	0.58
20:T:457:GLY:O	20:T:458:SER:HB3	2.02	0.58
36:k:111:ARG:CB	37:m:62:VAL:HG23	2.34	0.58
39:n:29:GLY:C	39:n:42:ILE:HD12	2.28	0.58
2:B:97:G:H2'	2:B:98:G:C8	2.38	0.58
7:G:-8:U:H2'	7:G:-7:C:O4'	2.04	0.58
9:H:183:G:H4'	38:l:40:ASN:HD21	1.68	0.58
36:k:107:ILE:HG22	36:k:108:VAL:HG23	1.85	0.58
40:o:68:THR:HG22	40:o:92:GLU:HB3	1.85	0.58
1:A:300:ASN:C	3:C:939:ARG:HH21	2.10	0.58
1:A:354:PRO:HG3	23:V:343:ARG:CZ	2.34	0.58
5:E:67:GLY:H	5:E:87:ASP:CG	2.11	0.58
5:E:233:GLY:O	5:E:260:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:229:LYS:O	17:P:229:LYS:NZ	2.32	0.58
29:u:80:ALA:HB3	29:u:217:ILE:HD13	1.84	0.58
36:k:31:VAL:HG21	37:m:61:GLU:HG2	1.85	0.58
1:A:1633:ALA:HB2	1:A:1637:TRP:CE3	2.39	0.57
3:C:144:CYS:SG	3:C:312:SER:OG	2.60	0.57
9:H:32:U:O5'	25:X:17:LEU:HD12	2.04	0.57
9:H:172:C:H2'	9:H:173:C:C6	2.39	0.57
13:L:223:GLY:HA2	18:R:86:LEU:HD11	1.86	0.57
15:N:16:GLU:N	15:N:16:GLU:OE1	2.36	0.57
20:T:213:GLU:HG3	20:T:218:TRP:CE2	2.39	0.57
38:l:18:ILE:C	38:l:20:LEU:N	2.61	0.57
41:p:90:ILE:HG12	41:p:94:MET:HE2	1.85	0.57
1:A:476:PHE:O	1:A:479:THR:OG1	2.22	0.57
1:A:1661:TRP:CD2	1:A:1700:GLY:HA3	2.39	0.57
3:C:73:TYR:HB3	3:C:77:VAL:HG21	1.85	0.57
3:C:500:THR:HG22	3:C:545:PRO:HA	1.86	0.57
9:H:179:C:H2'	9:H:180:G:H8	1.67	0.57
29:u:342:ASP:OD1	29:u:370:ARG:NE	2.31	0.57
38:l:34:TRP:CB	38:l:86:LEU:O	2.51	0.57
46:l:432:SER:HB2	46:l:479:TRP:CD2	2.38	0.57
1:A:1450:GLN:NE2	1:A:1451:ASN:H	2.02	0.57
3:C:454:THR:OG1	3:C:575:GLN:HB3	2.04	0.57
19:S:87:HIS:HB3	19:S:90:LEU:HG	1.86	0.57
27:Z:832:ASN:O	27:Z:836:GLY:N	2.37	0.57
1:A:1283:GLU:CD	1:A:1283:GLU:H	2.09	0.57
3:C:115:GLU:O	3:C:118:PHE:N	2.36	0.57
9:H:154:C:OP1	41:p:19:LYS:HD3	2.03	0.57
20:T:287:HIS:CE1	20:T:313:ARG:HG3	2.39	0.57
1:A:65:HIS:ND1	1:A:120:TYR:OH	2.33	0.57
1:A:1218:ASN:OD1	1:A:1220:VAL:N	2.37	0.57
3:C:850:LEU:O	3:C:855:GLY:N	2.37	0.57
9:H:101:U:C6	33:h:64:ARG:NH2	2.71	0.57
13:L:175:GLN:O	13:L:178:GLU:HG3	2.04	0.57
38:l:59:ASP:OD1	38:l:76:ARG:NE	2.29	0.57
38:l:89:SER:OG	39:n:59:MET:O	2.21	0.57
2:B:40:U:H3	7:G:-1:G:H1	1.52	0.57
3:C:62:ASP:OD1	3:C:62:ASP:N	2.36	0.57
3:C:506:PRO:HB2	3:C:569:ARG:NH1	2.20	0.57
19:S:138:MET:O	19:S:142:VAL:HG23	2.04	0.57
22:U:23:LEU:H	23:V:474:HIS:CD2	2.22	0.57
26:Y:46:CYS:SG	26:Y:83:CYS:HB3	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:HIS:HD2	1:A:81:PHE:CE2	2.22	0.57
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.87	0.57
1:A:805:GLU:OE1	1:A:1162:PRO:HB3	2.04	0.57
7:G:-5:G:HO2'	7:G:-4:A:H5''	1.69	0.57
18:R:151:LEU:HD22	20:T:323:VAL:HG11	1.84	0.57
29:u:322:GLU:HG3	29:u:327:ALA:HB3	1.87	0.57
29:u:386:ILE:HG23	29:u:387:ARG:HD2	1.87	0.57
30:v:10:ARG:HG3	30:v:27:GLU:HB3	1.87	0.57
36:k:60:ASP:OD2	36:k:64:ASN:HB2	2.04	0.57
1:A:312:TYR:OH	3:C:853:ARG:NH2	2.37	0.57
1:A:1171:GLU:OE1	1:A:1171:GLU:N	2.33	0.57
5:E:75:HIS:HB2	5:E:80:THR:HG22	1.86	0.57
9:H:41:U:H2'	9:H:42:G:H8	1.69	0.57
10:I:394:PRO:HG2	10:I:429:VAL:HA	1.87	0.57
29:u:133:MET:HB2	29:u:135:VAL:HG13	1.85	0.57
37:m:36:VAL:CG2	37:m:42:MET:HG2	2.34	0.57
1:A:1625:SER:OG	1:A:1626:CYS:O	2.23	0.57
1:A:1810:PHE:CE1	1:A:1815:GLY:HA2	2.39	0.57
3:C:233:GLU:CD	3:C:837:GLN:HE22	2.12	0.57
3:C:686:THR:HB	3:C:793:ASP:HB3	1.87	0.57
3:C:925:PRO:HD2	3:C:928:HIS:HE2	1.69	0.57
5:E:284:PHE:HZ	24:W:120:ILE:HD13	1.70	0.57
6:F:33:G:O2'	6:F:34:G:OP1	2.21	0.57
11:J:346:TRP:CZ2	11:J:372:VAL:HG11	2.40	0.57
46:1:424:PHE:HB2	46:1:425:PRO:HD3	1.86	0.57
47:2:119:ILE:O	47:2:135:ARG:HD2	2.04	0.57
1:A:532:THR:OG1	8:6:2:U:H3'	2.05	0.57
1:A:1719:PHE:O	1:A:1722:SER:OG	2.19	0.57
1:A:2014:MET:HE3	1:A:2015:GLU:H	1.70	0.57
3:C:692:LEU:HD11	3:C:744:ILE:HG13	1.87	0.57
18:R:124:VAL:HG13	18:R:125:MET:H	1.70	0.57
36:k:110:LEU:HD11	37:m:47:THR:HG21	1.87	0.57
36:k:111:ARG:CD	37:m:45:ALA:HA	2.26	0.57
1:A:1500:GLY:O	1:A:1756:SER:OG	2.10	0.56
1:A:1894:GLN:HE21	1:A:1898:LYS:NZ	2.03	0.56
3:C:801:LEU:O	3:C:803:ARG:N	2.38	0.56
5:E:202:ASN:ND2	5:E:204:THR:OG1	2.38	0.56
9:H:100:U:C2	39:n:37:PHE:HB3	2.40	0.56
9:H:100:U:N3	39:n:37:PHE:HB3	2.20	0.56
11:J:394:HIS:O	11:J:398:VAL:HG23	2.04	0.56
16:O:38:LYS:HB2	18:R:199:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:112:LEU:HD11	29:u:167:VAL:HG21	1.86	0.56
36:k:32:LEU:HA	36:k:56:VAL:HG11	1.87	0.56
36:k:71:LYS:O	36:k:73:MET:HE2	2.05	0.56
46:1:188:LEU:HD23	46:1:197:LEU:HD21	1.86	0.56
1:A:670:LYS:O	20:T:268:LYS:NZ	2.36	0.56
3:C:138:LEU:HG	3:C:139:HIS:CD2	2.39	0.56
3:C:313:GLN:HB2	50:C:1500:GTP:C6	2.41	0.56
8:6:22:C:H5''	16:O:216:ARG:HD2	1.86	0.56
16:O:248:LEU:O	16:O:252:PHE:HD2	1.87	0.56
20:T:189:GLN:OE1	20:T:191:HIS:NE2	2.35	0.56
20:T:459:LEU:HD12	20:T:460:ASP:H	1.68	0.56
30:v:111:ASP:HA	30:v:114:GLN:HG2	1.86	0.56
33:h:67:LYS:HE3	39:n:66:SER:HB2	1.86	0.56
36:k:111:ARG:HB2	37:m:62:VAL:CG2	2.34	0.56
1:A:76:MET:HE1	1:A:88:TYR:CG	2.39	0.56
1:A:264:PHE:CE1	1:A:459:LEU:HD13	2.40	0.56
1:A:587:GLN:O	1:A:587:GLN:HG2	2.05	0.56
1:A:1136:ARG:HD2	1:A:1139:ARG:HH21	1.70	0.56
1:A:1567:PRO:HB2	9:H:36:G:OP1	2.05	0.56
3:C:196:LYS:HD3	3:C:198:TYR:OH	2.05	0.56
3:C:221:ILE:HG23	3:C:495:ARG:HB3	1.88	0.56
3:C:320:LEU:HD21	3:C:343:LEU:HB2	1.87	0.56
3:C:379:LYS:O	3:C:383:GLN:HG2	2.04	0.56
3:C:692:LEU:HD21	3:C:788:LYS:HB2	1.87	0.56
9:H:171:U:H2'	9:H:172:C:C6	2.40	0.56
11:J:196:ARG:HH12	46:1:616:SER:CB	2.19	0.56
11:J:308:ARG:HG3	18:R:232:SEP:O	2.05	0.56
13:L:172:ARG:HA	13:L:175:GLN:NE2	2.18	0.56
23:V:515:CYS:HA	23:V:521:TYR:HB2	1.88	0.56
24:W:130:ARG:HH11	24:W:168:PHE:HE1	1.53	0.56
28:q:30:ILE:O	28:q:34:ILE:HG12	2.05	0.56
28:r:5:CYS:SG	28:r:26:GLU:N	2.74	0.56
28:r:88:HIS:O	28:r:92:LEU:HG	2.05	0.56
31:w:99:ILE:HD12	31:w:99:ILE:H	1.70	0.56
33:h:24:THR:OG1	33:h:26:GLU:OE1	2.20	0.56
36:k:92:LYS:NZ	36:k:93:ASP:O	2.32	0.56
1:A:173:GLU:HG2	46:1:273:ILE:HB	1.87	0.56
1:A:324:PRO:HB2	1:A:327:VAL:HG21	1.86	0.56
3:C:245:HIS:O	3:C:249:GLU:HG2	2.05	0.56
6:F:92:A:H2'	6:F:93:G:H8	1.70	0.56
8:6:13:C:H2'	8:6:14:A:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:240:THR:OG1	11:J:241:VAL:N	2.38	0.56
11:J:372:VAL:HG13	11:J:373:HIS:CD2	2.41	0.56
15:N:38:GLU:C	15:N:40:LYS:H	2.12	0.56
29:u:222:PRO:CB	30:v:43:LYS:HD2	2.35	0.56
1:A:401:GLY:HA3	3:C:386:GLY:HA2	1.88	0.56
1:A:1179:SER:OG	1:A:1180:LYS:N	2.38	0.56
1:A:1279:VAL:HG12	23:V:467:LEU:HD11	1.86	0.56
3:C:902:HIS:ND1	3:C:903:HIS:HB2	2.19	0.56
9:H:101:U:O4'	33:h:66:SER:HB2	2.05	0.56
16:O:293:VAL:HB	16:O:298:LEU:HD11	1.87	0.56
1:A:1639:VAL:HG13	1:A:1717:ASN:HB3	1.86	0.56
3:C:606:GLY:O	3:C:610:VAL:HG23	2.05	0.56
6:F:34:G:H1	8:6:12:G:C1'	2.18	0.56
6:F:48:A:O2'	6:F:49:G:OP1	2.18	0.56
13:L:222:LEU:H	13:L:222:LEU:HD22	1.71	0.56
18:R:292:TYR:CZ	26:Y:167:VAL:HG11	2.41	0.56
46:1:300:MET:HE2	46:1:338:CYS:SG	2.46	0.56
8:6:2:U:H4'	8:6:3:A:O5'	2.05	0.56
8:6:20:A:H2	16:O:187:THR:HG21	1.71	0.56
29:u:112:LEU:HD12	29:u:164:PRO:HG3	1.88	0.56
29:u:115:THR:HG23	29:u:118:LEU:H	1.71	0.56
35:j:3:LEU:HD23	36:k:100:PHE:CE2	2.41	0.56
1:A:56:ALA:HB3	15:N:109:ARG:HH12	1.71	0.56
1:A:1813:ARG:HB3	1:A:1813:ARG:CZ	2.35	0.56
9:H:60:U:H1'	46:1:258:ARG:HH12	1.69	0.56
10:I:177:PRO:HB3	10:I:211:SER:HA	1.87	0.56
23:V:455:PHE:O	23:V:459:ILE:HG12	2.06	0.56
36:k:66:VAL:HG22	36:k:100:PHE:CD2	2.39	0.56
36:k:109:VAL:C	37:m:62:VAL:HA	2.30	0.56
39:n:9:LEU:HD12	39:n:34:PHE:CE2	2.41	0.56
2:B:31:U:H2'	2:B:32:C:H6	1.71	0.56
8:6:94:C:OP1	26:Y:60:LYS:NZ	2.37	0.56
38:l:60:ASP:HA	38:l:75:GLY:HA2	1.88	0.56
1:A:1166:THR:OG1	1:A:1167:THR:N	2.39	0.56
1:A:1283:GLU:OE2	1:A:1283:GLU:N	2.28	0.56
1:A:1953:ILE:HG22	1:A:1979:VAL:HG13	1.86	0.56
1:A:1968:TRP:HA	1:A:1968:TRP:CE3	2.41	0.56
5:E:62:LEU:HB2	5:E:351:LEU:HB2	1.88	0.56
36:k:64:ASN:HB3	36:k:100:PHE:HZ	1.69	0.56
38:l:24:TYR:N	38:l:24:TYR:HD1	2.04	0.56
40:o:133:LEU:HD12	40:o:158:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HD3	15:N:49:ILE:HD11	1.88	0.55
1:A:228:TRP:H	1:A:228:TRP:CD1	2.23	0.55
1:A:357:ASN:O	3:C:865:GLY:N	2.33	0.55
1:A:1338:SER:OG	1:A:1351:THR:N	2.33	0.55
1:A:1436:TRP:CD1	1:A:1436:TRP:H	2.23	0.55
2:B:23:C:H5	2:B:26:A:N7	2.03	0.55
3:C:131:ASN:ND2	3:C:495:ARG:HH12	2.04	0.55
3:C:510:LEU:HD22	3:C:514:TYR:CE2	2.41	0.55
4:D:1225:VAL:O	4:D:1234:LEU:N	2.39	0.55
24:W:122:ASP:OD2	24:W:123:PHE:N	2.40	0.55
30:v:56:LYS:HA	30:v:59:MET:HE2	1.88	0.55
38:l:36:TYR:HD2	38:l:37:GLU:HB2	1.69	0.55
40:o:43:GLN:O	40:o:65:ARG:NH1	2.39	0.55
43:z:83:GLU:O	43:z:87:TRP:HD1	1.89	0.55
46:1:253:ALA:H	46:1:266:CYS:HB2	1.71	0.55
1:A:750:TRP:CZ2	1:A:778:ARG:HG2	2.42	0.55
1:A:1731:ALA:O	1:A:1735:LYS:HG2	2.06	0.55
8:6:8:C:H2'	8:6:9:C:H6	1.70	0.55
11:J:401:ARG:HA	11:J:404:GLU:OE2	2.06	0.55
16:O:228:ASP:O	16:O:277:ARG:NH2	2.39	0.55
20:T:261:LEU:HB2	20:T:273:TRP:HB2	1.88	0.55
20:T:267:ASP:O	20:T:268:LYS:HB2	2.06	0.55
24:W:439:ASP:O	24:W:441:SER:N	2.39	0.55
28:q:95:GLN:O	28:q:99:THR:HG23	2.05	0.55
33:h:36:GLU:OE2	33:h:62:TYR:OH	2.20	0.55
36:k:31:VAL:CG2	37:m:61:GLU:HG2	2.37	0.55
1:A:702:LYS:HB2	1:A:705:LYS:HZ2	1.71	0.55
3:C:770:PHE:HE1	3:C:789:PHE:CD1	2.23	0.55
3:C:803:ARG:O	3:C:807:GLN:HG2	2.06	0.55
5:E:259:VAL:HB	5:E:277:PHE:HB2	1.88	0.55
6:F:59:G:H1	6:F:76:A:H61	1.54	0.55
20:T:314:ILE:HD11	20:T:326:LEU:HD11	1.89	0.55
36:k:109:VAL:HB	37:m:63:LEU:H	1.69	0.55
40:o:13:ALA:HB3	40:o:25:ASP:HB3	1.87	0.55
1:A:1941:ARG:NH1	1:A:2010:ILE:O	2.31	0.55
26:Y:138:GLU:CB	27:Z:1097:MET:HA	2.37	0.55
29:u:214:VAL:HG21	29:u:233:MET:HG2	1.87	0.55
1:A:203:VAL:HA	1:A:206:TRP:CZ2	2.42	0.55
1:A:1258:LYS:CG	1:A:1527:ASN:HD21	2.18	0.55
8:6:72:G:H5''	8:6:73:G:OP1	2.07	0.55
9:H:102:U:O2'	35:j:61:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:144:MET:CB	13:L:149:LEU:HD21	2.36	0.55
28:r:96:LEU:O	28:r:99:THR:HG22	2.06	0.55
36:k:107:ILE:HG22	36:k:108:VAL:N	2.21	0.55
38:l:83:ASN:O	38:l:84:ILE:C	2.50	0.55
39:n:40:LEU:HB2	39:n:62:ILE:HG22	1.88	0.55
1:A:36:LYS:HA	24:W:169:GLU:OE1	2.07	0.55
3:C:183:SER:OG	3:C:203:MET:SD	2.65	0.55
3:C:481:MET:SD	3:C:492:ALA:HA	2.47	0.55
3:C:856:HIS:CE1	29:u:102:ILE:HG22	2.41	0.55
11:J:214:ILE:H	11:J:214:ILE:HD12	1.72	0.55
11:J:406:PHE:HB3	11:J:411:MET:HG2	1.88	0.55
15:N:2:PRO:O	15:N:4:VAL:N	2.39	0.55
16:O:84:CYS:SG	16:O:159:ARG:CZ	2.95	0.55
23:V:290:VAL:HG21	23:V:332:VAL:HG22	1.88	0.55
24:W:335:VAL:HA	24:W:351:ALA:HB2	1.89	0.55
37:m:23:LEU:HD21	37:m:68:ASN:HB3	1.89	0.55
38:l:35:LEU:HD12	38:l:41:MET:HE3	1.88	0.55
37:d:35:SER:O	37:d:43:GLN:N	2.25	0.55
3:C:185:PRO:HB3	3:C:203:MET:HE1	1.87	0.55
3:C:357:THR:OG1	3:C:358:LYS:O	2.18	0.55
6:F:15:A:H2'	6:F:16:G:C8	2.42	0.55
24:W:290:GLY:HA3	24:W:571:TRP:HA	1.89	0.55
37:d:16:GLY:N	37:d:33:LEU:O	2.38	0.55
1:A:723:ASN:HB2	1:A:785:LYS:HG2	1.88	0.55
1:A:1853:PRO:HG2	47:2:101:LYS:HZ3	1.70	0.55
5:E:313:ASP:OD2	5:E:316:SER:OG	2.25	0.55
13:L:163:GLN:HG2	13:L:167:ALA:HB3	1.89	0.55
36:k:104:ASP:HA	37:m:65:ARG:NE	2.21	0.55
39:f:15:LYS:O	39:f:31:LEU:N	2.38	0.55
1:A:762:ARG:NH1	17:P:226:LYS:HZ1	2.05	0.55
1:A:1778:TRP:CE2	1:A:1858:PRO:HG3	2.41	0.55
3:C:220:ARG:NH1	3:C:578:ARG:O	2.39	0.55
3:C:812:ALA:O	3:C:816:VAL:HG23	2.07	0.55
9:H:43:U:H2'	9:H:44:U:H6	1.72	0.55
20:T:421:VAL:HG12	20:T:422:ASN:O	2.07	0.55
23:V:302:LEU:HD12	23:V:306:GLN:HE22	1.71	0.55
23:V:334:TYR:O	23:V:338:VAL:HG23	2.06	0.55
26:Y:95:ASN:O	26:Y:97:ASP:N	2.39	0.55
36:k:28:PRO:O	37:m:43:GLN:HB2	2.07	0.55
39:n:15:LYS:HB3	39:n:74:GLU:HB2	1.88	0.55
1:A:147:MET:HB3	1:A:151:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:OD1	1:A:334:THR:OG1	2.24	0.55
1:A:1615:HIS:CE1	46:1:271:GLN:HG2	2.42	0.55
1:A:1935:ARG:HD3	1:A:1976:TRP:CZ3	2.42	0.55
3:C:196:LYS:HD3	3:C:198:TYR:CZ	2.42	0.55
3:C:529:ARG:H	3:C:553:GLU:HB3	1.70	0.55
3:C:555:VAL:HG11	3:C:565:ILE:HD11	1.89	0.55
13:L:134:THR:HB	13:L:135:LYS:HZ2	1.72	0.55
29:u:267:THR:HG22	29:u:405:MET:HG2	1.87	0.55
36:k:43:LEU:N	37:m:61:GLU:H	2.03	0.55
38:l:32:GLN:HB3	38:l:88:GLN:CG	2.35	0.55
39:n:18:SER:HB3	39:n:73:LEU:HD21	1.88	0.55
1:A:1532:ARG:HA	1:A:1568:THR:HG21	1.89	0.54
3:C:567:GLU:OE2	3:C:570:GLY:HA3	2.07	0.54
6:F:47:A:H4'	6:F:48:A:OP1	2.07	0.54
8:6:4:A:H2'	8:6:5:G:O4'	2.07	0.54
11:J:242:ILE:HA	11:J:245:TRP:HD1	1.71	0.54
16:O:81:CYS:SG	16:O:84:CYS:N	2.70	0.54
17:P:32:SER:O	17:P:35:LEU:HD12	2.06	0.54
18:R:180:THR:HB	24:W:114:TYR:HB3	1.89	0.54
20:T:442:ARG:HB3	20:T:443:THR:HG23	1.89	0.54
37:m:23:LEU:HG	37:m:68:ASN:O	2.06	0.54
3:C:534:VAL:HB	3:C:537:TYR:HB2	1.88	0.54
3:C:781:ASP:HB3	3:C:941:LYS:NZ	2.22	0.54
5:E:344:SER:OG	5:E:352:TYR:HB2	2.07	0.54
6:F:45:A:C4	26:Y:34:ARG:NH2	2.75	0.54
16:O:89:GLU:HG3	16:O:90:TYR:CE1	2.42	0.54
27:Z:693:ALA:O	27:Z:698:ASN:N	2.41	0.54
29:u:222:PRO:HB3	30:v:43:LYS:HD2	1.89	0.54
35:j:70:LEU:HB3	35:j:74:LEU:HD12	1.89	0.54
44:3:545:GLY:HA3	44:3:591:GLN:HA	1.89	0.54
1:A:671:THR:O	1:A:676:ARG:NH1	2.41	0.54
1:A:1020:LYS:HB3	9:H:24:A:C5	2.41	0.54
6:F:22:A:OP2	24:W:130:ARG:NH2	2.35	0.54
20:T:343:PRO:HG2	20:T:356:LEU:HD23	1.89	0.54
30:v:53:TYR:HB2	31:w:151:VAL:O	2.07	0.54
1:A:853:LYS:HD2	1:A:855:ARG:O	2.08	0.54
3:C:801:LEU:C	3:C:803:ARG:N	2.63	0.54
5:E:311:VAL:HB	5:E:321:TYR:HB2	1.88	0.54
18:R:123:GLU:O	18:R:125:MET:HG3	2.07	0.54
30:v:142:HIS:CE1	31:w:69:SER:HA	2.42	0.54
37:m:65:ARG:O	37:m:68:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:62:LEU:HB2	40:o:64:ARG:HH12	1.72	0.54
1:A:1900:GLU:OE2	1:A:1951:LYS:NZ	2.24	0.54
2:B:98:G:H2'	2:B:99:C:H6	1.71	0.54
11:J:192:GLU:OE1	11:J:192:GLU:N	2.32	0.54
16:O:234:LEU:HB2	16:O:272:ILE:HB	1.89	0.54
36:k:112:ASN:HD21	37:m:58:HIS:CD2	2.25	0.54
38:l:33:VAL:HG22	38:l:87:LEU:CD2	2.38	0.54
38:l:87:LEU:HB3	39:n:61:VAL:HB	1.89	0.54
1:A:1668:TRP:CD2	1:A:1708:ALA:HB2	2.43	0.54
1:A:1790:ILE:HD11	45:4:111:ASP:CG	2.33	0.54
2:B:20:G:H4'	2:B:20:G:OP1	2.06	0.54
3:C:134:LEU:CD2	3:C:226:VAL:HB	2.37	0.54
3:C:244:LYS:HB2	3:C:292:TYR:CE2	2.43	0.54
3:C:390:THR:OG1	3:C:391:SER:N	2.41	0.54
5:E:67:GLY:N	5:E:87:ASP:OD2	2.37	0.54
6:F:40:U:H2'	6:F:41:A:H8	1.72	0.54
11:J:290:ARG:NH2	14:M:179:ILE:HD11	2.23	0.54
16:O:30:GLU:OE1	16:O:30:GLU:N	2.35	0.54
23:V:315:ILE:O	23:V:319:LEU:HG	2.07	0.54
30:v:74:GLU:OE1	30:v:120:GLY:HA2	2.07	0.54
37:m:65:ARG:CB	37:m:68:ASN:HD22	2.21	0.54
38:l:33:VAL:HG22	38:l:87:LEU:HD21	1.90	0.54
40:o:14:GLN:HG3	40:o:44:PHE:HE1	1.73	0.54
3:C:440:SER:O	3:C:442:LYS:N	2.40	0.54
3:C:528:GLY:N	3:C:553:GLU:O	2.40	0.54
5:E:61:LEU:HD23	5:E:61:LEU:H	1.72	0.54
5:E:321:TYR:OH	5:E:356:ILE:HG23	2.08	0.54
13:L:505:ARG:C	13:L:507:ILE:H	2.16	0.54
23:V:199:ARG:HB2	23:V:383:ASN:HD21	1.72	0.54
23:V:301:GLY:O	23:V:305:THR:HG23	2.07	0.54
26:Y:68:TYR:CE2	26:Y:94:GLU:HB2	2.38	0.54
33:h:23:ASN:ND2	33:h:67:LYS:HD3	2.23	0.54
33:h:43:MET:HE2	33:h:46:ILE:HD12	1.90	0.54
36:k:63:CYS:CB	37:m:63:LEU:HD21	2.38	0.54
46:l:446:ARG:HH12	46:l:472:ALA:HB2	1.73	0.54
3:C:605:ASP:HA	3:C:608:ARG:NH1	2.22	0.54
13:L:100:TYR:CE2	13:L:104:LEU:HD11	2.43	0.54
17:P:188:TRP:CG	17:P:189:ASP:H	2.25	0.54
19:S:57:ILE:HG21	24:W:97:ASN:HB2	1.88	0.54
38:l:46:CYS:HB3	38:l:59:ASP:HB3	1.89	0.54
38:l:47:ILE:HG12	38:l:58:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1:282:HIS:HA	46:1:309:ARG:HH12	1.72	0.54
47:2:138:TRP:HB3	47:2:149:LEU:HD22	1.90	0.54
1:A:195:LEU:HD11	1:A:208:TYR:HE2	1.73	0.54
1:A:1494:TYR:HB3	1:A:1744:ARG:HD3	1.90	0.54
8:6:9:C:H2'	8:6:10:U:C6	2.43	0.54
13:L:223:GLY:O	13:L:225:TYR:N	2.41	0.54
18:R:180:THR:N	24:W:114:TYR:O	2.38	0.54
18:R:262:ILE:HG13	18:R:263:PRO:HD2	1.90	0.54
20:T:306:CYS:SG	20:T:336:VAL:HB	2.48	0.54
35:j:3:LEU:HD23	36:k:100:PHE:HE2	1.72	0.54
1:A:142:SER:HA	1:A:242:ALA:HB2	1.89	0.54
1:A:1312:PRO:HB3	1:A:1360:GLU:CD	2.33	0.54
9:H:150:U:H4'	38:l:69:LYS:HG3	1.89	0.54
41:p:7:HIS:CE1	41:p:59:LEU:HB2	2.43	0.54
46:1:414:LEU:HG	46:1:415:PHE:H	1.73	0.54
1:A:1210:LYS:O	1:A:1212:GLY:N	2.41	0.53
1:A:1647:ASP:O	1:A:1723:LYS:NZ	2.39	0.53
3:C:847:TYR:CE1	3:C:857:VAL:HG21	2.42	0.53
5:E:322:LYS:HE2	24:W:88:MET:HE1	1.90	0.53
6:F:2:U:H2'	6:F:3:G:H8	1.73	0.53
16:O:240:GLY:HA3	16:O:296:ARG:HH12	1.71	0.53
19:S:123:ASP:OD1	19:S:123:ASP:N	2.40	0.53
23:V:301:GLY:HA2	23:V:304:LEU:HD12	1.90	0.53
1:A:1404:THR:HG23	1:A:1406:GLU:H	1.73	0.53
1:A:1456:THR:OG1	1:A:1457:HIS:N	2.33	0.53
1:A:1661:TRP:CE2	1:A:1700:GLY:HA3	2.44	0.53
3:C:222:SER:OG	3:C:223:ASP:N	2.39	0.53
3:C:801:LEU:O	3:C:804:GLY:N	2.41	0.53
5:E:171:SER:OG	5:E:173:ASP:OD1	2.25	0.53
19:S:77:ILE:HG13	19:S:78:TYR:CD1	2.41	0.53
20:T:475:SER:OG	20:T:476:ARG:NH1	2.41	0.53
24:W:185:ASP:OD2	24:W:187:SER:OG	2.26	0.53
25:X:29:LYS:O	25:X:33:GLU:HG3	2.08	0.53
29:u:146:VAL:O	29:u:150:ILE:HG13	2.09	0.53
36:k:42:VAL:HA	37:m:61:GLU:HB2	1.89	0.53
34:a:37:HIS:O	34:a:74:GLY:HA3	2.08	0.53
1:A:1359:HIS:HB3	1:A:1363:GLN:HB2	1.90	0.53
6:F:94:C:H2'	6:F:95:G:H8	1.73	0.53
9:H:98:G:H5'	9:H:104:U:OP2	2.08	0.53
20:T:350:HIS:HA	20:T:374:SER:HB3	1.90	0.53
21:Q:27:ALA:O	21:Q:32:ALA:N	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:13:HIS:CD2	25:X:15:GLN:HB2	2.44	0.53
29:u:136:GLN:HB2	29:u:157:GLN:HA	1.91	0.53
38:l:30:ARG:NH2	38:l:60:ASP:O	2.40	0.53
1:A:283:VAL:HG13	1:A:284:ARG:H	1.74	0.53
1:A:1262:LYS:HE2	8:6:102:G:OP1	2.08	0.53
1:A:1782:ASP:O	1:A:1785:VAL:HG12	2.08	0.53
12:K:17:PRO:HG3	12:K:167:ARG:NH1	2.24	0.53
1:A:354:PRO:O	23:V:344:LYS:HG2	2.09	0.53
1:A:1135:PRO:HB2	1:A:1137:ASP:OD1	2.09	0.53
3:C:650:GLU:OE1	3:C:650:GLU:N	2.27	0.53
5:E:336:HIS:CG	5:E:337:PRO:HD2	2.44	0.53
6:F:34:G:H5'	13:L:203:LYS:HE2	1.91	0.53
6:F:78:A:O3'	11:J:237:LYS:NZ	2.31	0.53
23:V:271:GLU:O	23:V:275:LEU:HG	2.09	0.53
23:V:497:CYS:HB3	23:V:507:PHE:CG	2.43	0.53
29:u:254:PHE:CD2	29:u:401:ASP:HB3	2.44	0.53
36:k:47:ARG:N	36:k:107:ILE:HG13	2.23	0.53
36:k:109:VAL:C	37:m:63:LEU:H	2.14	0.53
38:l:31:ILE:HD13	38:l:89:SER:HB2	1.91	0.53
39:n:7:PRO:HB2	39:n:34:PHE:HZ	1.73	0.53
47:2:64:MET:HG2	47:2:159:CYS:SG	2.48	0.53
2:B:65:G:H2'	2:B:66:A:C8	2.42	0.53
5:E:172:ASP:O	5:E:195:GLN:HG3	2.08	0.53
8:6:22:C:HO2'	8:6:23:U:P	2.32	0.53
9:H:165:A:N3	41:p:41:VAL:HG11	2.23	0.53
9:H:165:A:H62	41:p:86:THR:HG23	1.72	0.53
16:O:232:THR:HG22	16:O:277:ARG:HA	1.91	0.53
18:R:205:ASP:OD1	18:R:207:MET:N	2.37	0.53
24:W:154:GLY:C	24:W:156:VAL:N	2.67	0.53
24:W:155:SER:O	24:W:157:GLU:N	2.41	0.53
1:A:1870:ASP:HB2	1:A:1871:PRO:HD3	1.90	0.53
1:A:1943:LEU:HA	1:A:1947:ASN:HA	1.90	0.53
6:F:2:U:H2'	6:F:3:G:C8	2.44	0.53
9:H:34:U:C2	9:H:35:A:C8	2.96	0.53
15:N:120:ARG:HH11	15:N:142:CYS:HB2	1.74	0.53
23:V:352:ILE:HG22	23:V:353:ILE:HG13	1.89	0.53
29:u:311:MET:O	29:u:316:ARG:HD2	2.08	0.53
47:2:56:ILE:O	47:2:101:LYS:HE3	2.08	0.53
1:A:1189:MET:HG2	1:A:1190:CYS:H	1.74	0.53
14:M:160:PHE:HB3	14:M:161:PHE:CD1	2.44	0.53
18:R:208:GLU:OE2	18:R:211:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:238:ILE:HG23	23:V:372:LEU:HD12	1.90	0.53
23:V:316:PHE:CE2	23:V:343:ARG:HD3	2.44	0.53
25:X:30:HIS:ND1	25:X:33:GLU:OE2	2.41	0.53
36:k:111:ARG:HG3	37:m:61:GLU:HG2	1.91	0.53
1:A:1131:LYS:NZ	1:A:1193:GLU:OE1	2.41	0.53
1:A:1503:TRP:HZ3	1:A:1533:ARG:NE	1.98	0.53
5:E:92:LEU:HD12	5:E:103:ALA:HB3	1.91	0.53
5:E:153:PHE:HB2	5:E:172:ASP:OD2	2.08	0.53
11:J:333:PHE:O	11:J:337:MET:HG2	2.09	0.53
11:J:439:ALA:O	11:J:443:ILE:HG12	2.09	0.53
14:M:175:SER:N	14:M:178:GLU:OE2	2.42	0.53
16:O:78:LYS:HG3	16:O:202:TYR:CZ	2.43	0.53
16:O:224:ASP:OD2	16:O:224:ASP:N	2.41	0.53
20:T:412:HIS:HE1	20:T:431:ALA:HB2	1.74	0.53
23:V:332:VAL:O	23:V:336:ILE:HG13	2.08	0.53
26:Y:37:ALA:O	26:Y:52:LYS:O	2.26	0.53
33:h:43:MET:HB3	33:h:46:ILE:HD11	1.89	0.53
43:z:62:ASN:C	43:z:64:GLY:H	2.17	0.53
1:A:799:PRO:HD3	18:R:284:PHE:CE1	2.43	0.53
1:A:1413:ASP:O	1:A:1418:ARG:NH1	2.42	0.53
1:A:1763:LEU:HD22	1:A:1889:LEU:HD13	1.91	0.53
1:A:1999:VAL:HA	1:A:2002:LEU:HG	1.90	0.53
5:E:265:ARG:HG2	5:E:266:PRO:HD2	1.91	0.53
6:F:87:C:OP2	14:M:193:ARG:HA	2.09	0.53
9:H:4:G:H2'	9:H:5:C:C6	2.44	0.53
9:H:74:U:H2'	9:H:75:A:H8	1.73	0.53
13:L:101:GLU:OE1	26:Y:163:ARG:NH2	2.38	0.53
14:M:168:LEU:HG	19:S:141:ARG:HH12	1.73	0.53
18:R:185:GLY:O	18:R:188:PHE:N	2.37	0.53
22:U:23:LEU:H	23:V:474:HIS:HD2	1.55	0.53
30:v:26:PHE:CD1	30:v:135:VAL:HG11	2.44	0.53
35:j:18:GLU:O	35:j:66:ARG:HB3	2.09	0.53
39:n:43:ASP:OD1	39:n:59:MET:HG3	2.09	0.53
43:z:52:GLU:OE1	43:z:52:GLU:N	2.35	0.53
1:A:569:VAL:O	1:A:570:ASP:HB2	2.09	0.52
3:C:223:ASP:OD1	3:C:495:ARG:NH2	2.42	0.52
3:C:777:GLY:HA3	3:C:782:GLU:O	2.09	0.52
16:O:235:TYR:HD1	16:O:271:PHE:HE1	1.57	0.52
23:V:178:ILE:O	23:V:182:ILE:HG12	2.09	0.52
23:V:316:PHE:CZ	23:V:343:ARG:HD3	2.44	0.52
23:V:340:PHE:O	23:V:344:LYS:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:26:GLU:O	28:q:30:ILE:HG22	2.09	0.52
36:k:111:ARG:HD3	37:m:45:ALA:CA	2.25	0.52
1:A:57:GLN:O	1:A:59:GLU:N	2.42	0.52
1:A:1788:VAL:HG23	1:A:1801:LYS:C	2.35	0.52
1:A:1839:TRP:HH2	1:A:1874:VAL:HG21	1.73	0.52
1:A:1923:TRP:CZ3	1:A:1935:ARG:HD2	2.45	0.52
3:C:387:ASP:OD2	3:C:390:THR:OG1	2.26	0.52
3:C:588:ILE:O	3:C:630:LEU:HA	2.09	0.52
3:C:820:PHE:CE1	3:C:825:PRO:HB3	2.45	0.52
8:6:6:A:N6	8:6:7:G:O6	2.41	0.52
13:L:152:LEU:HB3	13:L:156:ARG:NH1	2.25	0.52
13:L:206:ARG:H	13:L:206:ARG:HD3	1.75	0.52
16:O:131:THR:HG23	24:W:111:LEU:H	1.75	0.52
29:u:280:ALA:HA	29:u:348:LEU:O	2.09	0.52
1:A:79:ARG:HH11	1:A:82:ARG:NE	2.04	0.52
1:A:362:ARG:HA	1:A:362:ARG:NE	2.25	0.52
8:6:5:G:H3'	8:6:6:A:H2	1.74	0.52
8:6:19:G:C6	8:6:20:A:N6	2.77	0.52
13:L:55:ASP:OD1	13:L:57:SER:OG	2.18	0.52
15:N:143:SER:O	15:N:143:SER:OG	2.27	0.52
43:z:50:ILE:O	43:z:53:ILE:HB	2.09	0.52
1:A:976:MET:HG2	1:A:1187:PHE:HB3	1.91	0.52
1:A:1094:ARG:NH1	1:A:1094:ARG:HB2	2.24	0.52
1:A:1411:SER:HA	1:A:1414:ARG:HE	1.74	0.52
1:A:1902:PHE:O	1:A:1906:ILE:HG12	2.10	0.52
4:D:2098:ALA:O	4:D:2100:GLY:N	2.42	0.52
15:N:38:GLU:O	15:N:40:LYS:N	2.43	0.52
16:O:19:ASP:OD1	16:O:20:PHE:N	2.42	0.52
23:V:312:ILE:HA	23:V:315:ILE:HD12	1.91	0.52
24:W:153:ILE:O	24:W:153:ILE:HG13	2.09	0.52
26:Y:46:CYS:C	26:Y:48:GLU:H	2.17	0.52
30:v:142:HIS:HB2	31:w:150:PHE:CZ	2.45	0.52
34:i:61:ARG:HD2	34:i:64:LYS:HD3	1.91	0.52
44:3:582:ASN:O	44:3:584:GLY:N	2.41	0.52
1:A:64:GLU:H	1:A:64:GLU:CD	2.07	0.52
1:A:1189:MET:CG	1:A:1190:CYS:H	2.22	0.52
1:A:1790:ILE:CG2	1:A:1798:LEU:HB3	2.40	0.52
2:B:117:A:C2	37:d:26:GLY:HA3	2.43	0.52
3:C:929:LEU:HB3	3:C:933:PHE:CZ	2.44	0.52
4:D:668:ASP:O	4:D:672:GLY:CA	2.57	0.52
10:I:533:TYR:HA	13:L:505:ARG:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:146:GLU:HG2	13:L:147:ASP:N	2.23	0.52
38:l:64:ILE:HA	38:l:70:SER:O	2.10	0.52
1:A:373:ASP:OD1	1:A:374:ASP:N	2.42	0.52
1:A:1809:ILE:O	1:A:1817:LEU:HD12	2.10	0.52
1:A:1820:LYS:NZ	1:A:1844:GLU:OE1	2.37	0.52
1:A:1949:ARG:NH1	1:A:1952:VAL:HG21	2.25	0.52
3:C:679:PRO:HD3	3:C:811:THR:OG1	2.08	0.52
3:C:831:TYR:N	3:C:903:HIS:O	2.38	0.52
6:F:39:A:C6	6:F:40:U:C4	2.98	0.52
9:H:29:A:C2	9:H:31:G:C6	2.97	0.52
11:J:356:TYR:CD1	14:M:146:MET:HE1	2.41	0.52
35:j:36:MET:HE1	36:k:102:ARG:HG3	1.92	0.52
37:m:42:MET:CB	37:m:64:ILE:HD12	2.26	0.52
38:l:29:SER:HA	38:l:46:CYS:SG	2.50	0.52
39:n:64:GLY:O	39:n:66:SER:N	2.42	0.52
40:o:62:LEU:HB2	40:o:64:ARG:NH1	2.25	0.52
1:A:436:PRO:HB2	1:A:439:GLN:HG3	1.91	0.52
1:A:1783:THR:HA	45:4:106:LYS:CE	2.37	0.52
3:C:132:VAL:HA	3:C:224:GLY:O	2.10	0.52
3:C:254:THR:HB	3:C:433:MET:HE3	1.90	0.52
6:F:26:U:O2	6:F:26:U:H2'	2.09	0.52
8:6:104:C:O2'	8:6:105:C:O5'	2.27	0.52
9:H:43:U:H2'	9:H:44:U:C6	2.45	0.52
13:L:178:GLU:HA	13:L:181:ARG:CG	2.40	0.52
23:V:219:VAL:HA	23:V:222:ILE:HG12	1.90	0.52
23:V:250:LYS:HD3	23:V:288:ASP:CG	2.35	0.52
36:k:50:LYS:HG2	36:k:74:TRP:HB3	1.92	0.52
38:l:46:CYS:O	38:l:59:ASP:N	2.41	0.52
46:1:252:GLN:HG2	46:1:266:CYS:O	2.09	0.52
5:E:197:LEU:HG	5:E:212:GLY:HA2	1.91	0.52
6:F:59:G:H1	6:F:76:A:N6	2.07	0.52
16:O:29:GLY:O	18:R:195:ARG:NH1	2.43	0.52
18:R:263:PRO:HB2	18:R:266:LYS:HG2	1.90	0.52
23:V:577:SER:HA	23:V:580:ARG:HD2	1.91	0.52
24:W:204:ASP:CG	24:W:205:VAL:N	2.68	0.52
29:u:242:LYS:HD2	30:v:50:LYS:NZ	2.25	0.52
36:k:42:VAL:CA	37:m:61:GLU:HB3	2.37	0.52
38:e:36:TYR:N	38:e:83:ASN:O	2.42	0.52
1:A:941:LYS:HG3	1:A:1071:PHE:CE1	2.45	0.52
1:A:1772:PHE:CD2	1:A:1813:ARG:HG2	2.44	0.52
1:A:1780:VAL:HG22	1:A:1809:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:G:N2	2:B:117:A:H62	2.08	0.52
9:H:81:G:H2'	9:H:82:G:H8	1.74	0.52
15:N:15:TRP:CE3	15:N:18:ILE:HD11	2.45	0.52
19:S:55:ARG:HB2	19:S:63:GLN:HB3	1.91	0.52
19:S:150:GLN:O	19:S:152:ARG:HG3	2.10	0.52
29:u:358:ARG:HH22	32:x:192:ASP:H	1.58	0.52
36:k:42:VAL:HG12	37:m:61:GLU:OE1	2.10	0.52
38:l:35:LEU:HA	38:l:84:ILE:HA	1.91	0.52
39:n:29:GLY:O	39:n:42:ILE:HD12	2.09	0.52
1:A:1292:GLU:OE2	1:A:1330:MET:N	2.39	0.52
5:E:94:ASN:OD1	5:E:96:TYR:N	2.41	0.52
5:E:241:LEU:HA	5:E:251:LEU:O	2.10	0.52
9:H:25:G:C2	9:H:26:A:C8	2.98	0.52
9:H:105:G:C2	35:j:20:LYS:HD3	2.45	0.52
19:S:57:ILE:HD12	19:S:61:MET:CG	2.40	0.52
24:W:188:ASN:ND2	24:W:191:GLY:HA3	2.25	0.52
28:r:97:GLN:O	28:r:101:GLN:HG3	2.10	0.52
29:u:282:ILE:HG12	29:u:350:ILE:HD13	1.91	0.52
29:u:311:MET:SD	29:u:315:GLU:HG2	2.50	0.52
33:h:78:LYS:HZ3	34:i:32:LYS:HG3	1.74	0.52
36:k:32:LEU:HD22	36:k:65:MET:HE1	1.92	0.52
38:l:24:TYR:O	38:l:27:ASN:N	2.42	0.52
40:o:95:LEU:C	40:o:98:ASN:HD22	2.16	0.52
46:1:396:ARG:NH2	46:1:440:THR:OG1	2.43	0.52
4:D:1048:VAL:O	4:D:1051:SER:N	2.24	0.51
14:M:126:ASP:OD2	14:M:126:ASP:N	2.40	0.51
26:Y:132:ASN:O	26:Y:136:VAL:HG23	2.10	0.51
28:q:128:ARG:HD2	28:q:131:LEU:HD21	1.92	0.51
36:k:44:ILE:HG12	36:k:109:VAL:HG22	1.92	0.51
38:l:29:SER:O	38:l:31:ILE:HG12	2.10	0.51
1:A:136:ILE:HG22	1:A:138:PRO:HD2	1.91	0.51
1:A:712:HIS:CG	18:R:250:CYS:HB2	2.44	0.51
1:A:758:ARG:HH11	1:A:902:TYR:HA	1.75	0.51
1:A:1607:GLU:OE2	1:A:1634:SER:HA	2.10	0.51
2:B:31:U:H2'	2:B:32:C:C6	2.44	0.51
13:L:92:THR:HB	13:L:95:GLN:HG3	1.93	0.51
18:R:132:LEU:HD23	18:R:132:LEU:H	1.76	0.51
23:V:182:ILE:HG13	23:V:221:ILE:HG21	1.91	0.51
24:W:199:TYR:HB3	24:W:202:GLU:HG2	1.91	0.51
29:u:164:PRO:HA	29:u:167:VAL:HG22	1.91	0.51
36:k:44:ILE:HD12	36:k:52:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:62:HIS:C	37:m:65:ARG:HH12	2.17	0.51
37:m:22:LYS:HB3	37:m:71:TYR:CZ	2.44	0.51
47:2:155:CYS:SG	47:2:170:LYS:HD3	2.50	0.51
1:A:385:GLU:OE1	1:A:386:PRO:HD2	2.10	0.51
1:A:1002:ASP:OD1	1:A:1004:ASN:N	2.33	0.51
1:A:1286:ASP:OD1	1:A:1286:ASP:N	2.38	0.51
1:A:1668:TRP:CE2	1:A:1708:ALA:HB2	2.45	0.51
1:A:1790:ILE:HA	1:A:1799:THR:O	2.10	0.51
2:B:40:U:H6	2:B:40:U:O5'	1.93	0.51
3:C:176:GLU:OE1	3:C:176:GLU:N	2.37	0.51
3:C:323:PHE:CD1	3:C:373:ILE:HG12	2.44	0.51
3:C:623:GLU:C	3:C:625:GLY:H	2.18	0.51
3:C:863:ILE:HD12	3:C:868:LEU:HB2	1.93	0.51
8:6:24:G:O2'	8:6:25:G:OP1	2.20	0.51
15:N:36:PRO:O	15:N:38:GLU:N	2.43	0.51
16:O:20:PHE:CD1	18:R:177:ILE:HD11	2.45	0.51
24:W:391:PHE:O	24:W:402:GLN:HA	2.11	0.51
28:q:5:CYS:SG	28:q:26:GLU:N	2.82	0.51
30:v:145:ILE:HG22	31:w:71:GLU:OE2	2.09	0.51
35:j:56:GLU:CD	35:j:56:GLU:H	2.19	0.51
36:k:29:LEU:HD23	36:k:59:PHE:HD2	1.75	0.51
1:A:79:ARG:O	1:A:82:ARG:HG3	2.10	0.51
1:A:1655:THR:OG1	1:A:1656:THR:N	2.43	0.51
1:A:1820:LYS:HD3	1:A:1914:MET:HE2	1.93	0.51
5:E:295:PRO:HD3	5:E:335:PHE:HB3	1.91	0.51
6:F:10:U:H2'	6:F:11:C:O4'	2.09	0.51
6:F:41:A:H61	8:6:6:A:N6	2.08	0.51
9:H:7:U:H2'	9:H:8:C:C6	2.46	0.51
11:J:357:LYS:N	11:J:357:LYS:HD2	2.24	0.51
13:L:224:PHE:H	18:R:86:LEU:HD12	1.75	0.51
20:T:295:ASP:OD1	20:T:296:LEU:N	2.42	0.51
23:V:515:CYS:SG	23:V:525:PHE:CG	3.03	0.51
34:i:27:PHE:CE1	34:i:47:GLU:HG3	2.46	0.51
38:l:30:ARG:NH1	38:l:60:ASP:O	2.43	0.51
47:2:62:ILE:HD12	47:2:180:ILE:HG12	1.93	0.51
1:A:348:PRO:HB3	1:A:394:TYR:CZ	2.46	0.51
1:A:1337:GLN:OE1	1:A:1354:ARG:NH1	2.43	0.51
1:A:2013:GLY:HA2	45:4:104:ARG:HH21	1.74	0.51
8:6:93:A:C6	9:H:38:A:N1	2.79	0.51
10:I:374:ILE:O	10:I:376:ASN:N	2.43	0.51
15:N:57:THR:HG22	15:N:85:ASP:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:196:GLN:OE1	16:O:201:ARG:HD2	2.11	0.51
19:S:9:TRP:C	19:S:11:PRO:HD3	2.36	0.51
28:q:125:THR:O	28:q:129:GLU:HG2	2.10	0.51
29:u:94:ILE:HG12	29:u:129:LEU:HD21	1.93	0.51
30:v:28:PHE:CZ	30:v:62:LEU:HD11	2.45	0.51
1:A:698:PRO:HG2	1:A:701:ILE:HD11	1.92	0.51
1:A:1810:PHE:CE1	1:A:1919:LEU:HD12	2.46	0.51
3:C:478:THR:OG1	3:C:563:ALA:HB3	2.11	0.51
3:C:673:LYS:HG3	3:C:686:THR:CG2	2.34	0.51
8:6:87:U:N3	9:H:42:G:N1	2.37	0.51
11:J:205:LEU:HG	11:J:206:LEU:H	1.76	0.51
23:V:305:THR:HG22	23:V:312:ILE:HD13	1.92	0.51
1:A:1084:PRO:HG2	17:P:188:TRP:CE3	2.46	0.51
1:A:1778:TRP:HB2	1:A:1861:ILE:HD12	1.91	0.51
3:C:471:ASP:OD1	3:C:472:GLY:N	2.43	0.51
9:H:168:A:H5'	9:H:169:C:OP2	2.11	0.51
18:R:117:THR:O	18:R:120:VAL:HG12	2.09	0.51
24:W:318:VAL:C	24:W:320:GLY:H	2.18	0.51
24:W:465:PRO:HD2	24:W:479:GLN:O	2.10	0.51
26:Y:68:TYR:CD2	26:Y:93:PRO:HG2	2.46	0.51
31:w:109:ARG:HG3	31:w:110:THR:N	2.26	0.51
35:j:2:LYS:HZ2	35:j:4:VAL:CG2	2.24	0.51
36:k:47:ARG:C	36:k:49:ASN:H	2.18	0.51
36:k:72:GLU:HG2	36:k:74:TRP:CE3	2.46	0.51
38:l:33:VAL:HG13	38:l:84:ILE:HG23	1.93	0.51
3:C:507:VAL:CG1	3:C:565:ILE:HG23	2.40	0.51
6:F:94:C:H2'	6:F:95:G:C8	2.45	0.51
8:6:21:A:O2'	8:6:22:C:O5'	2.28	0.51
9:H:104:U:O4	36:k:64:ASN:ND2	2.41	0.51
13:L:66:GLU:H	13:L:66:GLU:CD	2.19	0.51
36:k:31:VAL:O	36:k:32:LEU:C	2.53	0.51
36:k:110:LEU:HA	37:m:62:VAL:CG2	2.41	0.51
38:l:43:ILE:HG22	38:l:44:GLU:N	2.25	0.51
38:l:54:MET:O	38:l:54:MET:CG	2.58	0.51
1:A:919:ASP:HB3	1:A:1035:GLN:HB2	1.93	0.51
1:A:1809:ILE:HB	1:A:1818:PHE:HB2	1.92	0.51
2:B:46:U:C4	2:B:47:A:N7	2.79	0.51
2:B:115:C:H2'	2:B:116:U:O4'	2.11	0.51
3:C:470:PRO:HB3	3:C:500:THR:CG2	2.40	0.51
3:C:564:THR:HG21	3:C:577:PHE:H	1.76	0.51
3:C:572:GLU:HG3	3:C:573:GLU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:168:LYS:O	13:L:172:ARG:HG3	2.10	0.51
17:P:42:LYS:HZ2	20:T:276:GLU:HG3	1.75	0.51
26:Y:23:LEU:O	26:Y:25:LEU:N	2.44	0.51
1:A:1160:ARG:HD3	17:P:192:VAL:HG11	1.92	0.51
3:C:83:GLU:OE1	3:C:83:GLU:N	2.42	0.51
3:C:434:CYS:HA	3:C:438:ILE:HG12	1.93	0.51
5:E:94:ASN:O	5:E:99:CYS:HA	2.10	0.51
9:H:174:A:H2'	9:H:175:G:C8	2.46	0.51
17:P:50:ALA:HB3	17:P:53:GLU:HG2	1.92	0.51
24:W:156:VAL:HG12	24:W:160:GLU:OE1	2.11	0.51
29:u:403:MET:HE3	29:u:411:ILE:HB	1.92	0.51
35:j:8:MET:HG2	35:j:32:VAL:O	2.11	0.51
45:4:102:ALA:N	45:4:107:TYR:HD2	2.08	0.51
1:A:781:ARG:HH22	1:A:1021:ASP:HB2	1.75	0.50
1:A:1258:LYS:HG3	1:A:1527:ASN:ND2	2.20	0.50
1:A:1337:GLN:NE2	22:U:6:GLY:H	2.09	0.50
1:A:1649:LYS:HD2	47:2:237:ASP:HB2	1.93	0.50
3:C:742:PRO:HB2	3:C:786:ASN:H	1.76	0.50
6:F:92:A:H2'	6:F:93:G:C8	2.46	0.50
8:6:88:G:H22	9:H:41:U:H3	1.59	0.50
17:P:69:ALA:HA	17:P:72:ARG:NH1	2.26	0.50
18:R:220:ARG:HB3	18:R:220:ARG:CZ	2.41	0.50
23:V:240:ASN:HA	23:V:243:LYS:HD3	1.92	0.50
27:Z:711:VAL:HA	27:Z:863:GLY:O	2.11	0.50
28:t:113:ALA:O	28:t:117:ILE:HG23	2.11	0.50
28:t:116:VAL:O	28:t:120:LEU:HG	2.10	0.50
33:h:19:THR:HB	33:h:72:ILE:HB	1.92	0.50
34:i:49:ARG:HB2	34:i:63:GLU:HG2	1.92	0.50
1:A:36:LYS:O	1:A:40:LEU:HG	2.11	0.50
1:A:1503:TRP:O	1:A:1504:GLU:HG3	2.11	0.50
1:A:1979:VAL:O	1:A:1983:LEU:HG	2.11	0.50
8:6:104:C:HO2'	8:6:105:C:P	2.33	0.50
9:H:13:C:N3	14:M:197:SER:OG	2.39	0.50
9:H:147:G:H2'	9:H:148:C:C6	2.46	0.50
15:N:79:ILE:O	15:N:82:GLY:N	2.34	0.50
16:O:32:PRO:HG3	24:W:153:ILE:HD11	1.93	0.50
19:S:57:ILE:HB	19:S:60:PHE:HB3	1.94	0.50
23:V:273:LEU:O	23:V:277:MET:HG3	2.11	0.50
25:X:16:THR:HG23	25:X:19:ASN:H	1.76	0.50
36:k:111:ARG:CA	37:m:60:GLY:O	2.54	0.50
1:A:425:PRO:HG3	2:B:26:A:H5'	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:ASP:OD1	1:A:1664:ILE:N	2.44	0.50
11:J:188:GLN:OE1	11:J:188:GLN:HA	2.10	0.50
11:J:238:ASN:O	11:J:240:THR:N	2.32	0.50
17:P:206:LYS:O	17:P:209:ARG:HB2	2.11	0.50
38:l:42:ARG:NH1	38:l:66:SER:OG	2.44	0.50
46:1:284:ALA:HB1	46:1:304:ASN:HB3	1.93	0.50
1:A:298:ASP:O	1:A:302:ILE:HG12	2.11	0.50
1:A:380:LEU:HD23	1:A:384:VAL:HG23	1.93	0.50
1:A:984:MET:O	1:A:988:ILE:HG13	2.12	0.50
1:A:1352:HIS:ND1	22:U:21:ARG:HA	2.26	0.50
2:B:61:A:H2'	2:B:62:G:H8	1.77	0.50
6:F:67:G:H8	6:F:67:G:OP2	1.94	0.50
8:6:17:U:O2	16:O:46:LYS:NZ	2.43	0.50
9:H:103:U:O4	34:i:38:MET:HG2	2.12	0.50
11:J:438:TYR:HE2	11:J:442:ARG:NH1	2.09	0.50
19:S:36:CYS:HA	19:S:129:PHE:CZ	2.47	0.50
23:V:173:VAL:HG21	23:V:218:LEU:HD12	1.92	0.50
24:W:204:ASP:CG	24:W:205:VAL:H	2.18	0.50
29:u:221:LEU:HB3	29:u:226:LEU:HD21	1.92	0.50
29:u:289:LYS:HG3	32:x:180:ALA:HA	1.94	0.50
30:v:92:ILE:HG22	30:v:94:ILE:HG23	1.93	0.50
35:j:61:ARG:HB3	35:j:64:ASN:HD22	1.76	0.50
46:1:246:VAL:HG23	46:1:254:LYS:HB3	1.94	0.50
1:A:58:LYS:HA	15:N:107:GLN:NE2	2.26	0.50
1:A:1821:ILE:HG12	1:A:1906:ILE:HG22	1.92	0.50
3:C:670:SER:HA	3:C:823:ALA:CB	2.41	0.50
11:J:217:GLU:HG2	11:J:218:GLU:OE1	2.11	0.50
14:M:153:ARG:CA	14:M:160:PHE:HE2	2.15	0.50
18:R:79:LYS:HG3	18:R:81:LYS:NZ	2.27	0.50
18:R:154:SER:O	18:R:158:LYS:HD3	2.12	0.50
47:2:100:VAL:CG2	47:2:108:ALA:HB3	2.42	0.50
1:A:537:LYS:HD2	6:F:37:C:N4	2.27	0.50
2:B:107:U:H2'	2:B:108:G:O4'	2.11	0.50
3:C:719:GLN:OE1	3:C:726:LEU:HD13	2.12	0.50
9:H:25:G:N3	9:H:26:A:C8	2.80	0.50
12:K:32:ALA:O	12:K:36:VAL:HG23	2.12	0.50
13:L:172:ARG:NH1	26:Y:82:ARG:HA	2.25	0.50
31:w:77:VAL:HB	31:w:117:THR:HG22	1.92	0.50
37:m:36:VAL:HG13	37:m:41:ASN:O	2.11	0.50
38:l:18:ILE:O	38:l:19:ASN:C	2.54	0.50
39:n:34:PHE:CD1	39:n:34:PHE:C	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1608:THR:HG22	1:A:1632:PHE:HB2	1.93	0.50
1:A:1667:ARG:HD2	1:A:1679:TYR:CE2	2.47	0.50
3:C:275:TYR:HD1	3:C:369:PHE:CD2	2.30	0.50
3:C:800:PRO:O	3:C:801:LEU:O	2.29	0.50
4:D:148:LEU:O	4:D:150:ASP:N	2.42	0.50
5:E:73:LYS:O	5:E:81:LEU:HD13	2.12	0.50
18:R:74:LEU:HD13	19:S:136:ILE:HB	1.94	0.50
18:R:154:SER:OG	18:R:158:LYS:NZ	2.31	0.50
19:S:11:PRO:HB3	19:S:166:GLY:HA3	1.92	0.50
20:T:352:THR:HG22	20:T:373:LYS:C	2.37	0.50
29:u:185:VAL:HG22	29:u:215:VAL:HB	1.94	0.50
45:4:106:LYS:HZ2	45:4:108:ALA:CA	2.25	0.50
35:b:68:PHE:N	36:c:100:PHE:O	2.35	0.50
1:A:58:LYS:HE2	15:N:110:ASP:OD1	2.12	0.50
1:A:436:PRO:HB2	1:A:439:GLN:CG	2.42	0.50
1:A:1870:ASP:O	1:A:1874:VAL:HG23	2.12	0.50
3:C:514:TYR:HB3	3:C:576:ILE:HD11	1.94	0.50
5:E:206:ASP:C	5:E:222:LEU:HG	2.37	0.50
6:F:43:A:O2'	6:F:44:G:H5'	2.12	0.50
13:L:39:HIS:H	13:L:151:MET:HE3	1.76	0.50
13:L:153:SER:O	13:L:156:ARG:HB2	2.11	0.50
16:O:145:ASP:OD2	16:O:146:MET:N	2.42	0.50
16:O:185:LYS:NZ	16:O:186:PRO:O	2.44	0.50
18:R:125:MET:HE1	20:T:399:LYS:HE2	1.94	0.50
19:S:81:GLN:HA	19:S:108:ASN:O	2.12	0.50
20:T:481:GLU:OE2	20:T:487:LYS:HD2	2.11	0.50
24:W:181:PHE:HD1	24:W:200:VAL:HG12	1.76	0.50
24:W:212:GLU:OE2	24:W:216:LEU:HD11	2.11	0.50
47:2:154:SER:O	47:2:154:SER:OG	2.28	0.50
1:A:84:ASP:OD1	1:A:84:ASP:N	2.42	0.50
1:A:834:HIS:O	1:A:837:LYS:N	2.44	0.50
2:B:17:U:H2'	2:B:18:C:H6	1.77	0.50
6:F:4:C:H2'	6:F:5:U:H6	1.77	0.50
6:F:58:G:O2'	6:F:59:G:OP1	2.26	0.50
7:G:-12:G:O2'	7:G:-11:G:O5'	2.25	0.50
9:H:5:C:H2'	9:H:6:U:H6	1.77	0.50
16:O:68:THR:HA	16:O:83:THR:HG22	1.94	0.50
23:V:297:LEU:HB3	23:V:339:MET:CE	2.40	0.50
24:W:172:GLN:HE21	24:W:173:LYS:NZ	2.09	0.50
30:v:19:PHE:HE2	32:x:192:ASP:HB2	1.77	0.50
33:h:67:LYS:CG	39:n:68:ILE:HD13	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:78:LYS:HD3	34:i:69:LEU:HD13	1.92	0.50
36:k:31:VAL:HB	37:m:62:VAL:O	2.12	0.50
36:k:32:LEU:HD23	36:k:32:LEU:N	2.27	0.50
37:m:43:GLN:O	37:m:44:LEU:HD12	2.12	0.50
40:o:14:GLN:HG3	40:o:44:PHE:CE1	2.47	0.50
40:o:55:ARG:HA	40:o:75:ARG:O	2.12	0.50
46:l:281:GLY:O	46:l:309:ARG:NH1	2.44	0.50
46:l:480:HIS:HD2	46:l:482:LYS:N	2.09	0.50
47:2:229:LYS:NZ	47:2:235:ARG:HH22	2.09	0.50
1:A:780:THR:HG22	1:A:898:PHE:CD1	2.47	0.49
2:B:17:U:H2'	2:B:18:C:C6	2.47	0.49
3:C:370:VAL:HA	3:C:374:LEU:HB2	1.94	0.49
11:J:431:ARG:O	11:J:435:ILE:HG12	2.12	0.49
17:P:210:PHE:HD2	20:T:455:GLN:HE22	1.60	0.49
18:R:65:PRO:HB2	19:S:90:LEU:HA	1.94	0.49
35:j:14:THR:HA	35:j:27:GLY:O	2.12	0.49
36:k:63:CYS:SG	37:m:63:LEU:HD21	2.52	0.49
38:l:32:GLN:HG3	38:l:43:ILE:O	2.12	0.49
38:l:32:GLN:CB	38:l:90:VAL:HG13	2.36	0.49
46:l:428:ASP:OD1	46:l:429:CYS:N	2.45	0.49
1:A:269:LEU:HD22	1:A:321:ASN:HD21	1.77	0.49
3:C:490:PHE:CE1	3:C:612:LYS:HD2	2.47	0.49
6:F:59:G:N2	6:F:76:A:N1	2.55	0.49
9:H:174:A:H2'	9:H:175:G:H8	1.77	0.49
11:J:286:GLU:HG3	11:J:298:ILE:HD12	1.95	0.49
13:L:37:LEU:HD11	13:L:158:ARG:HG3	1.93	0.49
17:P:188:TRP:CE3	17:P:189:ASP:HB2	2.46	0.49
20:T:248:THR:HB	20:T:266:GLU:HG2	1.93	0.49
29:u:286:THR:HG23	29:u:289:LYS:H	1.76	0.49
30:v:19:PHE:CE2	32:x:192:ASP:HB2	2.47	0.49
38:l:24:TYR:N	38:l:24:TYR:CD1	2.79	0.49
1:A:1892:PRO:O	1:A:1940:LEU:HD23	2.12	0.49
5:E:280:ASN:ND2	5:E:303:GLY:O	2.45	0.49
14:M:165:ASN:HB2	18:R:95:LYS:CA	2.32	0.49
16:O:131:THR:HG22	24:W:108:ARG:NH2	2.26	0.49
19:S:39:PHE:HB3	19:S:129:PHE:HZ	1.77	0.49
19:S:42:LEU:HD22	19:S:47:TYR:CG	2.48	0.49
23:V:189:ASN:HA	23:V:398:TYR:CE2	2.47	0.49
23:V:258:LYS:HG3	23:V:299:GLU:HG3	1.93	0.49
24:W:189:ILE:C	24:W:191:GLY:H	2.20	0.49
30:v:58:VAL:HG11	30:v:138:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:42:VAL:HG12	37:m:61:GLU:HB3	1.94	0.49
36:k:112:ASN:N	37:m:60:GLY:O	2.45	0.49
38:l:30:ARG:NE	38:l:44:GLU:HG2	2.28	0.49
1:A:1537:TRP:CE3	1:A:1751:LEU:HD13	2.47	0.49
1:A:1949:ARG:HH12	1:A:1952:VAL:HG21	1.78	0.49
3:C:349:PHE:HB2	3:C:356:PHE:CD1	2.47	0.49
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.27	0.49
5:E:193:THR:HG23	5:E:194:TYR:CG	2.48	0.49
9:H:4:G:H2'	9:H:5:C:H6	1.77	0.49
13:L:172:ARG:CA	13:L:175:GLN:HE21	2.20	0.49
35:j:16:THR:HB	35:j:69:ILE:HB	1.94	0.49
38:l:34:TRP:H	38:l:87:LEU:HA	1.78	0.49
41:p:66:LEU:HD22	41:p:83:TYR:CZ	2.47	0.49
1:A:1625:SER:OG	1:A:1663:ASP:OD2	2.19	0.49
1:A:1766:GLN:CD	1:A:1766:GLN:H	2.20	0.49
1:A:1831:LYS:HG3	1:A:1832:ARG:H	1.77	0.49
3:C:878:ILE:HG13	3:C:879:ASP:H	1.77	0.49
13:L:721:LEU:O	13:L:725:GLN:N	2.39	0.49
18:R:79:LYS:HG3	18:R:81:LYS:HZ3	1.77	0.49
20:T:219:PHE:CE2	20:T:231:TRP:HB2	2.47	0.49
27:Z:1100:HIS:O	27:Z:1129:TYR:HA	2.13	0.49
46:1:285:MET:O	46:1:304:ASN:N	2.35	0.49
46:1:287:HIS:HB2	46:1:302:CYS:SG	2.53	0.49
1:A:109:PRO:HD3	1:A:630:TRP:CZ2	2.48	0.49
1:A:579:GLN:HG3	1:A:580:TYR:N	2.23	0.49
1:A:658:ARG:NH2	6:F:65:G:OP2	2.45	0.49
1:A:1334:LEU:HB2	23:V:471:GLU:OE2	2.13	0.49
3:C:453:TYR:CE2	3:C:575:GLN:HB2	2.46	0.49
8:6:103:U:H2'	8:6:104:C:O4'	2.11	0.49
9:H:100:U:O4'	39:n:63:ARG:NH2	2.45	0.49
23:V:177:ASN:O	23:V:181:ILE:HG12	2.13	0.49
23:V:234:LEU:HD22	23:V:269:ALA:HB2	1.95	0.49
41:p:45:THR:HG23	41:p:48:MET:H	1.77	0.49
1:A:1217:GLN:HB2	1:A:1224:ARG:CZ	2.42	0.49
1:A:1615:HIS:CG	46:1:271:GLN:HE21	2.30	0.49
3:C:349:PHE:HB2	3:C:356:PHE:CE1	2.48	0.49
3:C:350:ASN:HB3	3:C:353:THR:HG23	1.94	0.49
3:C:745:LEU:HD23	3:C:767:VAL:HG22	1.93	0.49
11:J:270:ASP:OD2	18:R:223:PRO:HD2	2.13	0.49
13:L:149:LEU:HD23	13:L:152:LEU:HD12	1.95	0.49
16:O:76:LYS:HA	24:W:111:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:240:GLY:HA3	16:O:296:ARG:NH2	2.23	0.49
20:T:329:HIS:CE1	20:T:355:ARG:HG3	2.48	0.49
24:W:156:VAL:O	24:W:160:GLU:HG2	2.12	0.49
36:k:31:VAL:HG12	36:k:32:LEU:HD23	1.94	0.49
36:k:32:LEU:HD21	37:m:63:LEU:HD22	1.93	0.49
39:n:35:ASP:HB2	39:n:36:PRO:CD	2.39	0.49
46:1:352:GLN:O	46:1:377:SER:HA	2.12	0.49
1:A:1199:LYS:NZ	1:A:1206:GLU:OE2	2.28	0.49
1:A:1580:HIS:CE1	26:Y:17:PRO:HG3	2.48	0.49
1:A:1892:PRO:HB3	45:4:104:ARG:CD	2.42	0.49
1:A:2013:GLY:HA2	45:4:104:ARG:NH2	2.28	0.49
5:E:127:ALA:HB2	5:E:157:CYS:HB3	1.95	0.49
11:J:258:ILE:HG23	13:L:232:TYR:CD2	2.47	0.49
11:J:408:ASP:OD2	11:J:408:ASP:N	2.44	0.49
26:Y:27:LYS:O	26:Y:28:ASP:HB2	2.12	0.49
34:i:30:THR:OG1	34:i:43:CYS:HB3	2.12	0.49
46:1:396:ARG:HB2	46:1:429:CYS:SG	2.53	0.49
1:A:134:TRP:HB3	1:A:418:THR:HG21	1.93	0.49
1:A:283:VAL:HG13	1:A:284:ARG:N	2.28	0.49
1:A:673:THR:HG22	1:A:674:LYS:H	1.77	0.49
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.38	0.49
1:A:1276:GLU:O	1:A:1279:VAL:HG22	2.13	0.49
1:A:1762:TYR:HB3	1:A:1888:GLU:CB	2.42	0.49
1:A:1860:GLN:O	1:A:1861:ILE:HD13	2.13	0.49
2:B:101:U:H2'	2:B:102:U:C6	2.48	0.49
5:E:79:SER:O	5:E:95:VAL:HG22	2.13	0.49
10:I:528:LEU:O	10:I:532:LYS:CB	2.61	0.49
14:M:160:PHE:C	14:M:161:PHE:HD1	2.21	0.49
15:N:37:HIS:CG	15:N:37:HIS:O	2.65	0.49
16:O:240:GLY:H	16:O:268:GLN:HB3	1.78	0.49
19:S:39:PHE:HB3	19:S:129:PHE:CZ	2.47	0.49
23:V:457:ARG:HH21	23:V:457:ARG:HG3	1.77	0.49
29:u:302:PHE:O	29:u:304:VAL:HG23	2.13	0.49
30:v:59:MET:HB3	30:v:63:LYS:HE3	1.94	0.49
38:l:47:ILE:CD1	38:l:56:LEU:HD22	2.43	0.49
3:C:845:ALA:O	3:C:849:VAL:HG23	2.13	0.49
9:H:101:U:O2	33:h:64:ARG:HG2	2.13	0.49
12:K:18:TYR:CD2	12:K:168:LYS:HA	2.48	0.49
13:L:101:GLU:CD	26:Y:163:ARG:HH21	2.20	0.49
16:O:172:GLU:O	16:O:174:LYS:HG3	2.12	0.49
20:T:213:GLU:HG2	20:T:214:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:466:SER:HB2	23:V:471:GLU:HB3	1.95	0.49
24:W:212:GLU:HG2	24:W:216:LEU:HG	1.94	0.49
40:o:102:GLU:CD	40:o:104:GLY:H	2.21	0.49
1:A:68:LYS:NZ	15:N:45:SER:OG	2.46	0.48
3:C:135:CYS:HB2	3:C:242:LEU:HD13	1.94	0.48
3:C:507:VAL:HG13	3:C:566:THR:O	2.13	0.48
3:C:705:VAL:HG22	3:C:705:VAL:O	2.12	0.48
8:6:2:U:HO2'	43:z:2:ALA:N	2.10	0.48
11:J:195:LEU:HD12	11:J:195:LEU:H	1.78	0.48
17:P:50:ALA:O	17:P:54:VAL:HG23	2.13	0.48
23:V:169:LEU:HD13	23:V:185:LEU:HG	1.95	0.48
23:V:187:GLN:HA	23:V:402:LYS:HD2	1.95	0.48
29:u:81:GLN:HB2	29:u:221:LEU:HD12	1.94	0.48
34:i:73:ARG:HB3	34:i:76:ASN:ND2	2.28	0.48
36:k:114:LEU:HD12	37:m:60:GLY:HA2	1.95	0.48
37:m:22:LYS:HB3	37:m:71:TYR:CE2	2.48	0.48
39:n:26:HIS:HB3	39:n:48:MET:HB2	1.95	0.48
1:A:73:HIS:O	1:A:74:GLY:C	2.55	0.48
1:A:1209:HIS:CD2	1:A:1210:LYS:HG2	2.48	0.48
1:A:1303:LEU:HD12	1:A:1311:PHE:CZ	2.48	0.48
1:A:1615:HIS:CD2	46:1:271:GLN:HE21	2.31	0.48
3:C:461:LEU:O	3:C:465:MET:HG2	2.13	0.48
5:E:283:ASN:ND2	5:E:305:ALA:HB1	2.28	0.48
9:H:34:U:H2'	9:H:35:A:H8	1.78	0.48
14:M:168:LEU:HB3	18:R:96:ILE:HD11	1.95	0.48
16:O:81:CYS:SG	16:O:83:THR:N	2.79	0.48
16:O:131:THR:HG22	24:W:108:ARG:HE	1.79	0.48
17:P:39:THR:O	20:T:318:ARG:HD3	2.13	0.48
17:P:59:PHE:HB3	20:T:216:ASN:HD22	1.78	0.48
17:P:202:ASP:OD2	17:P:202:ASP:N	2.44	0.48
24:W:181:PHE:CD1	24:W:200:VAL:HG12	2.48	0.48
47:2:110:LYS:HE2	47:2:114:GLY:HA2	1.95	0.48
1:A:70:ILE:HD13	1:A:495:GLN:HG3	1.96	0.48
1:A:1758:PRO:O	48:5:5:PRO:HG2	2.13	0.48
3:C:775:ARG:HA	3:C:783:LEU:HD13	1.95	0.48
5:E:234:HIS:CE1	5:E:260:ARG:HG3	2.47	0.48
18:R:73:PRO:HB2	18:R:74:LEU:HD12	1.93	0.48
18:R:282:GLU:O	18:R:285:ALA:N	2.36	0.48
24:W:189:ILE:HG22	24:W:190:ASP:OD1	2.13	0.48
25:X:12:TRP:CZ2	26:Y:35:LEU:HD21	2.49	0.48
26:Y:42:ARG:HG3	26:Y:49:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:30:ILE:HD13	28:q:52:LEU:HD12	1.95	0.48
29:u:35:ASP:OD2	29:u:36:VAL:N	2.46	0.48
29:u:231:LYS:HG3	29:u:232:PHE:HD2	1.79	0.48
35:j:15:VAL:HG21	35:j:68:PHE:CE1	2.47	0.48
37:m:48:GLU:HA	37:m:57:GLY:O	2.14	0.48
38:l:22:PHE:HD1	38:l:50:PHE:CZ	2.27	0.48
46:1:332:LYS:HB3	46:1:332:LYS:HE2	1.64	0.48
47:2:54:GLY:C	47:2:101:LYS:HZ1	2.21	0.48
1:A:468:LYS:HD3	1:A:469:LYS:N	2.25	0.48
1:A:1775:GLN:HG2	1:A:1859:LYS:CB	2.43	0.48
1:A:1838:LYS:HA	1:A:1868:MET:HE1	1.94	0.48
1:A:1904:ASP:O	1:A:1908:LYS:HG2	2.13	0.48
3:C:508:LYS:HB3	3:C:566:THR:HG23	1.94	0.48
3:C:651:ILE:O	3:C:653:ILE:HG13	2.13	0.48
29:u:271:LEU:HD21	29:u:378:ILE:HD12	1.95	0.48
46:1:292:HIS:CE1	46:1:295:ILE:HD12	2.47	0.48
2:B:62:G:H2'	2:B:63:A:H8	1.79	0.48
3:C:174:GLU:OE2	3:C:182:LYS:N	2.46	0.48
3:C:205:THR:HB	3:C:215:VAL:HG22	1.96	0.48
7:G:-20:A:O3'	29:u:163:THR:HB	2.13	0.48
8:6:21:A:H4'	8:6:22:C:OP1	2.12	0.48
9:H:10:C:H2'	9:H:11:G:H8	1.79	0.48
14:M:160:PHE:C	14:M:162:PRO:HD3	2.38	0.48
15:N:54:HIS:CE1	15:N:92:TRP:CZ2	3.00	0.48
18:R:238:THR:HG22	18:R:240:LYS:H	1.78	0.48
23:V:173:VAL:HB	23:V:181:ILE:HG21	1.96	0.48
24:W:279:LYS:O	24:W:578:TRP:HA	2.13	0.48
28:q:66:PRO:HD3	28:r:11:VAL:HG11	1.95	0.48
3:C:309:PHE:HB2	3:C:318:PHE:CZ	2.48	0.48
3:C:570:GLY:O	3:C:572:GLU:N	2.38	0.48
4:D:148:LEU:C	4:D:150:ASP:N	2.72	0.48
5:E:155:ASN:N	5:E:170:GLY:O	2.47	0.48
9:H:167:U:C2	41:p:43:LEU:HG	2.49	0.48
13:L:146:GLU:O	13:L:149:LEU:N	2.46	0.48
16:O:158:LYS:HG3	16:O:161:ARG:HD2	1.95	0.48
17:P:52:GLU:CD	17:P:55:ARG:HH22	2.15	0.48
17:P:204:GLN:C	17:P:206:LYS:H	2.18	0.48
19:S:100:MET:HE3	19:S:109:GLY:O	2.13	0.48
23:V:338:VAL:O	23:V:342:VAL:HG23	2.13	0.48
24:W:183:GLU:HG2	24:W:188:ASN:HD21	1.79	0.48
26:Y:97:ASP:C	26:Y:97:ASP:OD2	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:6:ASN:OD1	41:p:7:HIS:N	2.47	0.48
46:1:302:CYS:HB3	46:1:338:CYS:SG	2.53	0.48
47:2:108:ALA:CB	47:2:132:ILE:HD13	2.42	0.48
1:A:355:LEU:O	3:C:867:PRO:HB3	2.13	0.48
1:A:803:ALA:HB2	18:R:287:LEU:HA	1.94	0.48
1:A:1167:THR:OG1	1:A:1168:VAL:N	2.46	0.48
1:A:1787:ARG:HB3	45:4:112:MET:CE	2.44	0.48
3:C:348:TYR:CD1	3:C:359:LYS:HB3	2.48	0.48
3:C:824:THR:HG23	3:C:824:THR:O	2.13	0.48
8:6:79:C:O2'	8:6:80:U:OP1	2.28	0.48
31:w:88:ASP:O	31:w:92:LYS:HG2	2.13	0.48
36:k:48:ASN:ND2	36:k:50:LYS:HD2	2.28	0.48
36:k:111:ARG:HB3	37:m:45:ALA:HA	1.96	0.48
37:m:43:GLN:HG2	37:m:44:LEU:N	2.29	0.48
1:A:152:ARG:NH1	1:A:616:PHE:O	2.47	0.48
1:A:155:LYS:HD2	1:A:626:GLY:O	2.14	0.48
1:A:828:PRO:HG3	1:A:925:TYR:CE2	2.49	0.48
3:C:929:LEU:HB3	3:C:933:PHE:CE2	2.48	0.48
5:E:284:PHE:HB3	24:W:139:LEU:HD13	1.95	0.48
9:H:168:A:H3'	9:H:169:C:H6	1.79	0.48
9:H:179:C:H2'	9:H:180:G:C8	2.48	0.48
16:O:33:TYR:HD1	24:W:125:PHE:CE1	2.32	0.48
16:O:236:VAL:HB	16:O:270:ALA:HB3	1.96	0.48
19:S:15:TYR:O	19:S:162:ALA:HA	2.14	0.48
23:V:215:TYR:O	23:V:219:VAL:HG23	2.14	0.48
28:q:25:TYR:CD2	28:q:30:ILE:HD12	2.49	0.48
33:h:43:MET:HB2	33:h:61:VAL:HG22	1.96	0.48
33:h:64:ARG:NH1	39:n:64:GLY:O	2.47	0.48
34:i:8:LYS:O	34:i:12:HIS:ND1	2.45	0.48
34:i:18:ARG:HB2	34:i:83:GLU:HG2	1.95	0.48
36:k:52:LEU:HB2	36:k:70:VAL:HG13	1.96	0.48
46:1:273:ILE:HD11	46:1:279:THR:HB	1.95	0.48
46:1:432:SER:OG	46:1:433:PRO:HD3	2.14	0.48
47:2:54:GLY:O	47:2:101:LYS:NZ	2.46	0.48
2:B:101:U:H2'	2:B:102:U:H6	1.78	0.48
9:H:105:G:C8	36:k:104:ASP:HB2	2.49	0.48
9:H:156:U:N3	9:H:157:G:N7	2.62	0.48
11:J:229:LYS:HG3	11:J:230:THR:N	2.28	0.48
12:K:143:VAL:O	12:K:147:GLU:HG2	2.14	0.48
16:O:72:GLN:O	16:O:75:SER:OG	2.28	0.48
18:R:88:ILE:H	18:R:88:ILE:HD12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:42:LEU:HD22	19:S:47:TYR:CD1	2.49	0.48
24:W:154:GLY:C	24:W:156:VAL:H	2.22	0.48
26:Y:20:ILE:HG23	26:Y:21:PRO:HD2	1.95	0.48
35:j:2:LYS:HZ2	35:j:4:VAL:HG23	1.78	0.48
36:k:111:ARG:HB2	37:m:62:VAL:CB	2.44	0.48
37:m:65:ARG:HG3	37:m:65:ARG:HH11	1.79	0.48
43:z:67:GLU:HA	43:z:70:ILE:HG12	1.96	0.48
1:A:56:ALA:HB3	15:N:109:ARG:NH1	2.29	0.48
1:A:386:PRO:HA	3:C:327:TYR:OH	2.14	0.48
1:A:439:GLN:HB3	1:A:443:VAL:CG2	2.44	0.48
1:A:462:ARG:HA	1:A:462:ARG:NE	2.29	0.48
1:A:1775:GLN:HG2	1:A:1859:LYS:HB2	1.95	0.48
1:A:1831:LYS:HZ3	1:A:1832:ARG:N	2.08	0.48
1:A:1931:THR:O	1:A:1934:SER:OG	2.30	0.48
3:C:201:ASN:HB3	3:C:549:TRP:CE3	2.48	0.48
3:C:925:PRO:HD2	3:C:928:HIS:NE2	2.28	0.48
16:O:81:CYS:SG	16:O:83:THR:OG1	2.71	0.48
18:R:66:GLU:CD	18:R:66:GLU:H	2.20	0.48
24:W:145:ASN:OD1	24:W:146:HIS:N	2.43	0.48
25:X:12:TRP:HZ2	26:Y:35:LEU:HD21	1.78	0.48
26:Y:39:PHE:O	26:Y:40:ASN:ND2	2.47	0.48
26:Y:163:ARG:HA	26:Y:163:ARG:HD3	1.60	0.48
28:r:57:VAL:HG13	28:r:59:HIS:H	1.79	0.48
34:i:49:ARG:HD2	34:i:63:GLU:HG2	1.95	0.48
35:j:23:THR:HG21	35:j:45:MET:HE3	1.95	0.48
46:1:199:THR:OG1	46:1:207:LYS:HB2	2.13	0.48
1:A:1067:MET:HE1	27:Z:391:LEU:O	2.14	0.47
1:A:1241:HIS:ND1	1:A:1287:LEU:HD11	2.29	0.47
1:A:1667:ARG:HD2	1:A:1679:TYR:CD2	2.49	0.47
1:A:1763:LEU:O	1:A:1763:LEU:HD23	2.14	0.47
9:H:158:G:O6	41:p:17:LYS:NZ	2.46	0.47
11:J:190:THR:O	11:J:193:GLN:HB2	2.14	0.47
13:L:37:LEU:HA	13:L:37:LEU:HD12	1.57	0.47
16:O:258:ILE:HG12	16:O:274:PHE:CE1	2.49	0.47
17:P:212:ASN:HB2	20:T:455:GLN:OE1	2.13	0.47
18:R:91:ASP:OD2	18:R:91:ASP:N	2.36	0.47
25:X:28:GLN:HA	25:X:28:GLN:OE1	2.14	0.47
28:r:112:ALA:O	28:r:116:VAL:HG23	2.14	0.47
30:v:54:VAL:HG11	30:v:138:LEU:HD23	1.95	0.47
36:k:53:LEU:HD11	36:k:114:LEU:HD13	1.96	0.47
36:k:108:VAL:HB	37:m:29:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:40:LEU:HG	39:n:67:ILE:CD1	2.40	0.47
47:2:92:SER:O	47:2:96:GLN:HG3	2.14	0.47
47:2:160:ASN:ND2	47:2:164:ASP:HB2	2.21	0.47
1:A:260:LEU:HD23	1:A:455:VAL:HG22	1.96	0.47
1:A:332:TYR:C	1:A:332:TYR:CD1	2.91	0.47
2:B:110:C:H2'	2:B:111:A:C8	2.49	0.47
3:C:529:ARG:HB3	3:C:540:GLU:OE1	2.15	0.47
3:C:593:GLU:HG3	3:C:594:PRO:HD2	1.95	0.47
11:J:330:ARG:HG2	11:J:361:ARG:HH21	1.78	0.47
18:R:134:ARG:O	18:R:135:PRO:C	2.57	0.47
23:V:152:LEU:H	23:V:152:LEU:HD12	1.77	0.47
26:Y:68:TYR:O	26:Y:69:LEU:C	2.56	0.47
29:u:404:PRO:HB2	29:u:407:VAL:HG12	1.95	0.47
31:w:85:THR:O	31:w:89:ILE:HG12	2.14	0.47
36:k:46:CYS:C	36:k:107:ILE:HG13	2.38	0.47
37:m:6:ASN:CB	37:m:9:PRO:HD2	2.44	0.47
1:A:578:LEU:HD23	1:A:578:LEU:HA	1.53	0.47
1:A:1203:SER:C	1:A:1205:GLU:H	2.21	0.47
1:A:1965:HIS:C	1:A:1966:HIS:HD1	2.21	0.47
3:C:749:THR:O	3:C:753:GLU:N	2.43	0.47
3:C:834:VAL:HG22	3:C:899:SER:HB3	1.97	0.47
5:E:147:LEU:HD22	5:E:179:TRP:CE3	2.49	0.47
5:E:215:ASN:ND2	5:E:235:ALA:O	2.47	0.47
9:H:168:A:H5''	9:H:169:C:H5	1.80	0.47
15:N:113:PHE:CZ	16:O:35:ARG:HB3	2.49	0.47
22:U:15:THR:OG1	22:U:17:GLY:N	2.40	0.47
28:t:112:ALA:O	28:t:116:VAL:HG23	2.14	0.47
37:m:67:ASN:OD1	37:m:68:ASN:N	2.47	0.47
38:l:44:GLU:O	38:l:61:ALA:HA	2.14	0.47
1:A:1332:HIS:ND1	1:A:1359:HIS:CE1	2.82	0.47
1:A:1537:TRP:HE3	1:A:1751:LEU:HD13	1.80	0.47
2:B:27:U:HO2'	2:B:28:A:P	2.37	0.47
2:B:61:A:H2'	2:B:62:G:C8	2.50	0.47
3:C:65:TYR:CD2	17:P:216:ARG:HD3	2.50	0.47
3:C:348:TYR:CE1	3:C:359:LYS:HB3	2.49	0.47
3:C:534:VAL:HG12	3:C:535:ALA:H	1.79	0.47
9:H:156:U:C2	9:H:157:G:C8	3.03	0.47
15:N:70:ILE:HG23	15:N:74:LEU:HD23	1.96	0.47
16:O:73:THR:OG1	16:O:74:CYS:N	2.47	0.47
20:T:318:ARG:HE	20:T:319:THR:CG2	2.28	0.47
24:W:467:VAL:HA	24:W:477:ALA:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:38:PRO:HG2	26:Y:39:PHE:CE2	2.50	0.47
33:h:65:GLY:HA2	33:h:68:ILE:HD12	1.96	0.47
37:m:33:LEU:HD11	37:m:36:VAL:HG23	1.97	0.47
1:A:384:VAL:HA	3:C:331:PHE:CE2	2.49	0.47
1:A:888:GLN:O	1:A:889:ARG:HD3	2.15	0.47
1:A:1553:VAL:HG11	26:Y:7:LEU:HD12	1.97	0.47
1:A:1777:ILE:HG12	1:A:1860:GLN:HB2	1.96	0.47
1:A:1863:VAL:HG22	1:A:1865:ARG:H	1.79	0.47
1:A:1943:LEU:O	1:A:1947:ASN:HB2	2.14	0.47
3:C:59:LEU:HB3	3:C:61:GLU:HG2	1.97	0.47
3:C:693:GLU:H	3:C:696:LEU:HD12	1.78	0.47
6:F:48:A:HI'	13:L:33:ARG:CZ	2.44	0.47
11:J:215:THR:O	11:J:216:ASP:HB2	2.14	0.47
11:J:436:TYR:CD1	11:J:437:LYS:HD2	2.46	0.47
18:R:123:GLU:OE2	18:R:123:GLU:N	2.42	0.47
18:R:138:GLU:O	18:R:142:GLU:HG2	2.13	0.47
20:T:405:PHE:O	20:T:406:ILE:C	2.56	0.47
28:q:117:ILE:O	28:q:121:THR:HG23	2.14	0.47
35:j:19:LEU:HD12	35:j:23:THR:HB	1.97	0.47
46:l:235:LEU:HA	46:l:245:LEU:O	2.14	0.47
1:A:1137:ASP:OD1	1:A:1137:ASP:N	2.44	0.47
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.96	0.47
3:C:126:SER:O	3:C:126:SER:OG	2.30	0.47
3:C:561:LYS:HD3	3:C:615:PRO:O	2.15	0.47
9:H:25:G:C2	9:H:26:A:N7	2.83	0.47
11:J:294:HIS:HE1	13:L:230:GLU:HB2	1.79	0.47
16:O:50:ARG:NH1	16:O:122:GLU:OE1	2.47	0.47
16:O:72:GLN:C	16:O:75:SER:HG	2.20	0.47
18:R:76:MET:HG2	19:S:95:ALA:CB	2.44	0.47
23:V:550:MET:O	23:V:554:LEU:HG	2.15	0.47
29:u:120:VAL:O	29:u:124:LYS:HG2	2.14	0.47
29:u:293:LEU:HD11	29:u:352:TYR:CE2	2.49	0.47
37:m:23:LEU:HG	37:m:68:ASN:C	2.39	0.47
38:e:34:TRP:O	38:e:85:THR:CA	2.63	0.47
1:A:312:TYR:CZ	3:C:882:GLY:HA3	2.49	0.47
1:A:982:GLU:OE1	1:A:1172:ASN:HB2	2.15	0.47
1:A:1134:TRP:O	1:A:1139:ARG:NH1	2.48	0.47
1:A:1787:ARG:HB3	45:4:112:MET:HE1	1.96	0.47
1:A:1870:ASP:OD2	1:A:1870:ASP:N	2.48	0.47
1:A:1941:ARG:O	1:A:1945:VAL:HG22	2.14	0.47
3:C:225:VAL:HG12	3:C:252:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:323:PHE:CE2	3:C:424:PHE:HE1	2.33	0.47
3:C:325:LYS:HG2	3:C:329:ASP:OD1	2.14	0.47
3:C:343:LEU:HA	3:C:368:SER:OG	2.15	0.47
5:E:260:ARG:HD3	5:E:276:ILE:HG12	1.96	0.47
9:H:6:U:H2'	9:H:7:U:H6	1.80	0.47
9:H:101:U:O4	39:n:38:MET:HB2	2.14	0.47
9:H:156:U:C4	9:H:157:G:N7	2.83	0.47
9:H:160:A:H2'	9:H:161:U:C6	2.50	0.47
16:O:35:ARG:HD3	24:W:129:ARG:NE	2.29	0.47
18:R:134:ARG:NH2	20:T:339:GLN:OE1	2.48	0.47
19:S:14:VAL:HA	19:S:163:TYR:O	2.15	0.47
23:V:515:CYS:SG	23:V:522:MET:HA	2.54	0.47
29:u:228:MET:O	29:u:231:LYS:HG2	2.15	0.47
29:u:231:LYS:HG3	29:u:232:PHE:CD2	2.49	0.47
29:u:255:PHE:HD2	29:u:400:ILE:HG22	1.79	0.47
29:u:388:ILE:O	29:u:392:ILE:HG13	2.14	0.47
30:v:33:LYS:HD3	30:v:53:TYR:CD1	2.50	0.47
33:h:20:CYS:SG	33:h:68:ILE:HG12	2.55	0.47
34:i:78:VAL:O	35:j:60:ILE:HD12	2.15	0.47
36:k:111:ARG:CB	37:m:61:GLU:HA	2.45	0.47
36:k:114:LEU:CD1	37:m:60:GLY:HA2	2.44	0.47
1:A:75:ASP:C	1:A:77:THR:H	2.21	0.47
1:A:839:LEU:O	1:A:843:LEU:HG	2.14	0.47
1:A:1404:THR:C	1:A:1406:GLU:H	2.22	0.47
1:A:1638:ASN:HB3	1:A:1652:MET:O	2.15	0.47
1:A:1819:LEU:HB3	1:A:1915:VAL:HG13	1.97	0.47
1:A:1823:HIS:HB3	1:A:1912:PRO:HG3	1.95	0.47
1:A:1826:VAL:HG23	1:A:1827:TRP:CE3	2.50	0.47
5:E:158:TYR:OH	5:E:161:ARG:NH1	2.48	0.47
6:F:38:G:H2'	6:F:39:A:H8	1.74	0.47
6:F:83:A:O2'	6:F:84:A:OP2	2.30	0.47
9:H:156:U:C2	9:H:175:G:C2	3.03	0.47
14:M:162:PRO:HB3	14:M:167:LEU:HB2	1.97	0.47
15:N:120:ARG:NH1	15:N:142:CYS:HB2	2.29	0.47
16:O:51:PRO:HB3	18:R:212:PHE:CZ	2.50	0.47
16:O:278:GLN:O	16:O:282:VAL:HG23	2.15	0.47
18:R:111:VAL:CG1	20:T:366:VAL:HG22	2.45	0.47
20:T:213:GLU:HG3	20:T:218:TRP:CZ2	2.50	0.47
26:Y:28:ASP:OD1	26:Y:29:ARG:N	2.48	0.47
26:Y:67:VAL:HG12	26:Y:72:PRO:HA	1.96	0.47
29:u:138:HIS:HB2	29:u:157:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:361:TYR:O	29:u:365:ILE:HG12	2.15	0.47
30:v:37:ALA:HA	30:v:48:ILE:O	2.15	0.47
33:h:67:LYS:HD3	33:h:67:LYS:HA	1.56	0.47
38:l:83:ASN:HD22	38:l:84:ILE:HG13	1.79	0.47
40:o:57:LEU:HG	40:o:76:ILE:HD12	1.95	0.47
1:A:43:LYS:NZ	24:W:168:PHE:HB3	2.29	0.47
1:A:372:PRO:HG3	3:C:341:LYS:O	2.15	0.47
1:A:1771:LEU:HD21	1:A:1930:TYR:HA	1.97	0.47
3:C:240:GLU:HG2	3:C:288:LEU:HD13	1.95	0.47
5:E:111:ALA:O	5:E:129:THR:HG23	2.15	0.47
9:H:98:G:N2	37:m:66:CYS:HG	2.10	0.47
9:H:162:U:O4	41:p:77:LYS:NZ	2.46	0.47
16:O:226:PRO:HG3	16:O:302:TRP:CH2	2.50	0.47
23:V:577:SER:HA	23:V:580:ARG:HH11	1.80	0.47
26:Y:94:GLU:OE2	26:Y:95:ASN:HB2	2.15	0.47
37:m:36:VAL:HG12	37:m:37:ASP:H	1.80	0.47
39:n:63:ARG:HE	39:n:65:ASN:HB2	1.80	0.47
1:A:1848:LEU:HD22	1:A:1914:MET:HE3	1.97	0.47
3:C:461:LEU:HA	3:C:461:LEU:HD23	1.61	0.47
3:C:831:TYR:CE1	3:C:905:GLN:HB3	2.50	0.47
6:F:40:U:H3	8:6:7:G:H22	1.61	0.47
8:6:7:G:C4	8:6:8:C:C5	3.03	0.47
8:6:19:G:C2	8:6:20:A:C6	3.03	0.47
8:6:19:G:H2'	8:6:20:A:C8	2.49	0.47
9:H:34:U:H2'	9:H:35:A:C8	2.50	0.47
13:L:203:LYS:HD2	13:L:203:LYS:HA	1.51	0.47
16:O:239:LEU:HG	16:O:240:GLY:O	2.16	0.47
19:S:99:ALA:HA	19:S:129:PHE:H	1.80	0.47
20:T:415:ILE:HD12	20:T:432:ASP:OD2	2.14	0.47
23:V:303:LYS:HA	23:V:303:LYS:HD2	1.79	0.47
23:V:305:THR:OG1	23:V:306:GLN:NE2	2.47	0.47
24:W:177:LYS:HE3	24:W:177:LYS:HB3	1.65	0.47
29:u:82:SER:O	29:u:219:ALA:HA	2.15	0.47
30:v:28:PHE:CZ	30:v:34:LEU:HD22	2.50	0.47
33:h:24:THR:O	33:h:51:ARG:NH1	2.47	0.47
34:i:10:LEU:HA	34:i:13:ILE:HG23	1.97	0.47
1:A:1076:ASP:O	1:A:1079:THR:OG1	2.25	0.46
1:A:1208:THR:HG21	23:V:553:HIS:CD2	2.50	0.46
1:A:1212:GLY:HA3	1:A:1280:ASN:HD21	1.80	0.46
5:E:313:ASP:HB2	5:E:320:LEU:HD21	1.96	0.46
8:6:87:U:O2	9:H:42:G:C2	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:80:VAL:HG12	16:O:94:ILE:HD11	1.97	0.46
19:S:20:MET:HE1	19:S:141:ARG:HB3	1.96	0.46
23:V:260:VAL:HG11	23:V:277:MET:HE2	1.97	0.46
24:W:180:LYS:HD3	24:W:199:TYR:CE2	2.50	0.46
29:u:197:PHE:O	29:u:201:ILE:HG12	2.14	0.46
31:w:123:THR:HB	31:w:126:GLU:HG3	1.97	0.46
36:k:33:THR:O	36:k:36:VAL:HG12	2.15	0.46
38:l:20:LEU:HA	38:l:20:LEU:HD23	1.30	0.46
1:A:1300:LYS:HB3	1:A:1305:SER:O	2.15	0.46
3:C:524:ILE:HD12	3:C:569:ARG:HH22	1.80	0.46
3:C:693:GLU:N	3:C:696:LEU:HD12	2.30	0.46
6:F:16:G:C6	6:F:17:C:C4	3.04	0.46
9:H:156:U:C2	9:H:175:G:N2	2.83	0.46
13:L:24:MET:HE2	13:L:24:MET:HB2	1.57	0.46
17:P:205:LYS:HB3	17:P:208:LYS:HG2	1.96	0.46
23:V:182:ILE:HG21	23:V:221:ILE:HG12	1.98	0.46
23:V:306:GLN:OE1	23:V:352:ILE:HD11	2.15	0.46
24:W:204:ASP:OD2	24:W:205:VAL:HG23	2.16	0.46
29:u:365:ILE:HG23	29:u:377:ALA:HB2	1.96	0.46
30:v:140:GLY:O	30:v:144:LYS:HB3	2.15	0.46
46:1:295:ILE:HG22	46:1:296:LYS:O	2.15	0.46
1:A:48:LYS:HE3	1:A:48:LYS:HB3	1.77	0.46
1:A:191:ILE:CG1	1:A:571:ALA:HB1	2.45	0.46
1:A:191:ILE:O	1:A:191:ILE:HG22	2.14	0.46
1:A:693:ILE:HG22	1:A:738:MET:HE2	1.98	0.46
1:A:951:LEU:HA	1:A:951:LEU:HD23	1.58	0.46
1:A:1891:LEU:HD23	1:A:1891:LEU:HA	1.68	0.46
2:B:55:C:H2'	2:B:56:C:H6	1.81	0.46
3:C:926:ALA:HA	3:C:929:LEU:HG	1.97	0.46
13:L:53:TRP:CE2	13:L:60:LYS:HE2	2.50	0.46
16:O:145:ASP:CG	16:O:146:MET:H	2.24	0.46
17:P:25:GLN:HG2	17:P:25:GLN:O	2.15	0.46
18:R:67:ILE:HG22	18:R:69:VAL:HG23	1.97	0.46
20:T:405:PHE:O	20:T:407:GLN:N	2.48	0.46
27:Z:1124:MET:HA	27:Z:1127:LYS:O	2.15	0.46
28:t:77:ALA:O	28:t:81:GLU:HG2	2.16	0.46
29:u:45:LEU:HD21	29:u:94:ILE:CG2	2.45	0.46
31:w:129:ALA:O	31:w:132:GLU:HG3	2.15	0.46
38:l:44:GLU:CD	38:l:90:VAL:HG21	2.41	0.46
38:l:52:GLU:HG3	38:l:53:TYR:CD2	2.50	0.46
39:n:63:ARG:HG2	39:n:65:ASN:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:OE2	1:A:132:ILE:N	2.45	0.46
1:A:388:LEU:O	3:C:379:LYS:NZ	2.38	0.46
1:A:643:GLY:HA3	2:B:28:A:O2'	2.14	0.46
2:B:88:A:H4'	2:B:94:U:O4	2.15	0.46
3:C:813:ARG:NH1	3:C:813:ARG:HB2	2.30	0.46
6:F:88:G:O6	14:M:198:ARG:HD3	2.14	0.46
9:H:29:A:H2	9:H:31:G:C6	2.33	0.46
26:Y:68:TYR:CD1	26:Y:69:LEU:HG	2.50	0.46
29:u:92:PHE:HE1	29:u:111:ILE:HD13	1.80	0.46
29:u:97:LEU:HA	29:u:100:LEU:HG	1.97	0.46
29:u:379:ASN:HD22	29:u:389:LEU:HD12	1.80	0.46
30:v:129:GLN:OE1	31:w:108:ARG:HB3	2.16	0.46
38:l:25:LEU:HD13	38:l:50:PHE:CZ	2.50	0.46
38:l:31:ILE:O	38:l:44:GLU:CA	2.42	0.46
40:o:107:ASP:CG	40:o:138:LYS:HE2	2.40	0.46
46:1:314:GLU:N	46:1:314:GLU:OE1	2.49	0.46
1:A:195:LEU:HD11	1:A:208:TYR:CE2	2.50	0.46
1:A:702:LYS:O	1:A:705:LYS:NZ	2.31	0.46
5:E:264:VAL:HA	5:E:272:ARG:HH21	1.79	0.46
9:H:101:U:C4	33:h:64:ARG:CZ	2.98	0.46
12:K:74:ALA:O	12:K:78:PRO:HA	2.16	0.46
19:S:125:LYS:HE3	19:S:126:HIS:CE1	2.50	0.46
35:j:63:ASN:HA	36:k:102:ARG:CZ	2.46	0.46
38:l:35:LEU:HD22	38:l:83:ASN:HB2	1.98	0.46
38:l:54:MET:O	38:l:56:LEU:N	2.48	0.46
38:l:88:GLN:CA	39:n:60:VAL:CG1	2.63	0.46
1:A:549:GLU:HB3	1:A:591:MET:HG2	1.98	0.46
3:C:137:HIS:HD2	3:C:238:ASN:H	1.63	0.46
5:E:281:VAL:N	5:E:304:SER:OG	2.47	0.46
6:F:41:A:H2'	6:F:42:C:H6	1.78	0.46
6:F:48:A:N3	13:L:33:ARG:NH2	2.53	0.46
8:6:6:A:C5	8:6:7:G:N7	2.83	0.46
9:H:107:A:C4'	36:k:47:ARG:HH21	2.29	0.46
11:J:223:TYR:HA	11:J:226:ARG:CZ	2.46	0.46
11:J:288:LYS:HD2	14:M:190:ILE:HD11	1.97	0.46
24:W:199:TYR:O	24:W:200:VAL:C	2.59	0.46
25:X:34:ARG:HA	25:X:37:ILE:CD1	2.43	0.46
30:v:26:PHE:CE1	30:v:135:VAL:HG11	2.50	0.46
45:4:106:LYS:HZ2	45:4:108:ALA:HB2	1.79	0.46
47:2:166:GLU:HB2	47:2:168:LYS:HD3	1.98	0.46
1:A:302:ILE:HD12	3:C:657:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:PRO:HG2	2:B:20:G:H2'	1.97	0.46
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.24	0.46
3:C:259:LYS:HG2	50:C:1500:GTP:C2	2.51	0.46
8:6:21:A:H5'	8:6:21:A:H8	1.81	0.46
9:H:161:U:O2	9:H:163:G:N2	2.47	0.46
11:J:296:ARG:HD2	13:L:225:TYR:CZ	2.51	0.46
11:J:325:ASN:CB	14:M:172:HIS:HD2	2.24	0.46
15:N:120:ARG:HD2	15:N:142:CYS:SG	2.55	0.46
17:P:26:LEU:HD12	17:P:26:LEU:HA	1.71	0.46
19:S:14:VAL:HG12	19:S:25:LEU:HB2	1.97	0.46
24:W:188:ASN:OD1	24:W:188:ASN:N	2.48	0.46
46:1:203:ASP:OD1	46:1:203:ASP:N	2.46	0.46
46:1:469:ILE:HG23	46:1:470:THR:H	1.81	0.46
1:A:1084:PRO:HG2	17:P:188:TRP:CD2	2.51	0.46
1:A:1495:PHE:CD2	1:A:1501:LEU:HD11	2.51	0.46
10:I:194:ASP:C	10:I:196:ALA:H	2.24	0.46
11:J:261:ALA:HB1	11:J:285:MET:HE2	1.98	0.46
12:K:65:ILE:O	12:K:67:ARG:N	2.48	0.46
16:O:158:LYS:HG3	16:O:161:ARG:CD	2.46	0.46
18:R:91:ASP:OD1	18:R:95:LYS:NZ	2.30	0.46
24:W:146:HIS:HB3	24:W:148:VAL:O	2.15	0.46
47:2:101:LYS:HG2	47:2:107:ILE:CD1	2.45	0.46
1:A:377:GLU:O	1:A:378:PHE:HB2	2.16	0.46
1:A:469:LYS:NZ	2:B:59:G:C6	2.84	0.46
1:A:658:ARG:NH1	6:F:67:G:OP1	2.49	0.46
3:C:724:TRP:HD1	3:C:729:ALA:HB2	1.79	0.46
5:E:266:PRO:HG2	13:L:785:GLN:HB2	1.97	0.46
18:R:178:ARG:NH1	24:W:143:LEU:HD21	2.31	0.46
25:X:16:THR:O	25:X:20:VAL:HG23	2.16	0.46
38:l:54:MET:SD	38:l:81:GLY:HA3	2.56	0.46
39:n:42:ILE:HG22	39:n:45:CYS:HB2	1.98	0.46
1:A:359:ILE:HB	23:V:324:HIS:NE2	2.31	0.46
1:A:1014:ASN:HD21	13:L:84:THR:N	2.13	0.46
1:A:1083:HIS:NE2	17:P:189:ASP:OD1	2.43	0.46
1:A:1258:LYS:HE2	8:6:102:G:C6	2.51	0.46
1:A:1334:LEU:HB2	23:V:471:GLU:CD	2.41	0.46
3:C:182:LYS:HA	3:C:214:GLU:OE2	2.16	0.46
3:C:556:ASP:OD1	3:C:556:ASP:N	2.33	0.46
3:C:567:GLU:O	3:C:567:GLU:HG3	2.16	0.46
3:C:590:ILE:HD11	3:C:637:LEU:HD13	1.98	0.46
6:F:2:U:C2	6:F:3:G:C8	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:112:G:H2'	9:H:113:G:C8	2.48	0.46
13:L:154:GLU:HG3	13:L:155:ALA:N	2.30	0.46
29:u:188:GLU:CD	29:u:339:ARG:HB3	2.40	0.46
40:o:102:GLU:HG2	40:o:128:LYS:HZ2	1.81	0.46
41:p:63:THR:O	41:p:67:ARG:HG3	2.15	0.46
1:A:705:LYS:H	1:A:705:LYS:HD2	1.80	0.45
1:A:762:ARG:HH22	17:P:226:LYS:NZ	2.13	0.45
1:A:1621:LYS:HE3	1:A:1623:ASN:HD21	1.80	0.45
1:A:1790:ILE:HG21	1:A:1798:LEU:HB3	1.98	0.45
2:B:23:C:C5	2:B:26:A:N7	2.83	0.45
3:C:415:LEU:HD12	3:C:415:LEU:HA	1.54	0.45
3:C:657:ASP:OD2	3:C:657:ASP:N	2.49	0.45
8:6:6:A:N6	8:6:7:G:C6	2.84	0.45
9:H:153:A:C5	9:H:154:C:C6	3.04	0.45
11:J:258:ILE:HG12	13:L:232:TYR:CE2	2.51	0.45
16:O:174:LYS:HA	24:W:205:VAL:HG13	1.97	0.45
24:W:549:HIS:C	24:W:551:LYS:H	2.24	0.45
32:x:173:ASP:HB2	32:x:182:ILE:HG13	1.97	0.45
36:k:111:ARG:HG2	36:k:112:ASN:N	2.31	0.45
37:m:33:LEU:HD11	37:m:36:VAL:CG2	2.46	0.45
1:A:182:ILE:HD11	1:A:562:VAL:HG13	1.98	0.45
1:A:381:PRO:HD2	3:C:334:ILE:HG22	1.98	0.45
1:A:989:ASP:OD1	1:A:990:LEU:N	2.49	0.45
1:A:1274:PHE:O	1:A:1275:ARG:HB2	2.16	0.45
2:B:30:A:O2'	2:B:31:U:H5'	2.16	0.45
3:C:732:ILE:HA	3:C:746:VAL:HG22	1.98	0.45
3:C:801:LEU:O	3:C:802:HIS:C	2.58	0.45
5:E:116:HIS:O	5:E:124:LEU:HD12	2.16	0.45
5:E:285:GLU:OE1	24:W:121:ASN:HB3	2.17	0.45
11:J:343:GLU:OE1	11:J:373:HIS:ND1	2.49	0.45
18:R:280:ILE:HD12	18:R:281:ASN:N	2.32	0.45
23:V:311:GLY:O	23:V:315:ILE:HG13	2.16	0.45
26:Y:39:PHE:HE1	26:Y:100:MET:CE	2.29	0.45
26:Y:39:PHE:HE1	26:Y:100:MET:HE3	1.81	0.45
29:u:285:ASN:HD21	32:x:182:ILE:HG12	1.80	0.45
30:v:142:HIS:ND1	31:w:69:SER:HA	2.31	0.45
36:k:72:GLU:O	36:k:93:ASP:HA	2.15	0.45
37:m:65:ARG:HB3	37:m:68:ASN:ND2	2.24	0.45
46:1:185:VAL:O	46:1:475:VAL:HG21	2.16	0.45
1:A:81:PHE:O	1:A:83:HIS:N	2.49	0.45
1:A:1808:PHE:CZ	1:A:1817:LEU:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1953:ILE:O	1:A:1956:PRO:HD3	2.15	0.45
3:C:175:GLN:NE2	3:C:536:ARG:HH12	2.14	0.45
3:C:440:SER:O	3:C:441:PRO:C	2.59	0.45
3:C:711:ARG:NH2	3:C:730:ARG:O	2.49	0.45
5:E:81:LEU:O	5:E:92:LEU:HA	2.16	0.45
5:E:167:VAL:O	5:E:178:LEU:HD12	2.16	0.45
9:H:101:U:C2	33:h:64:ARG:CZ	3.00	0.45
15:N:124:SER:O	15:N:127:GLU:HG2	2.16	0.45
17:P:229:LYS:HD2	17:P:229:LYS:HA	1.68	0.45
24:W:135:TYR:OH	24:W:165:LEU:HD11	2.15	0.45
29:u:254:PHE:HA	29:u:401:ASP:O	2.16	0.45
36:k:92:LYS:NZ	36:k:93:ASP:H	2.14	0.45
36:k:110:LEU:HD23	37:m:59:LEU:CD1	2.45	0.45
37:m:18:PRO:CA	37:m:32:TYR:HA	2.38	0.45
39:n:46:VAL:HG22	39:n:56:ASN:HA	1.97	0.45
1:A:1503:TRP:CE2	1:A:1753:LEU:HD21	2.51	0.45
2:B:32:C:O2'	2:B:33:U:H5'	2.16	0.45
2:B:100:C:H2'	2:B:101:U:C5	2.50	0.45
3:C:396:LEU:HA	3:C:396:LEU:HD12	1.83	0.45
5:E:192:ASN:OD1	5:E:218:LYS:NZ	2.45	0.45
8:6:88:G:C2	8:6:89:U:C4	3.04	0.45
9:H:6:U:H2'	9:H:7:U:C6	2.51	0.45
9:H:45:C:H2'	9:H:46:U:H6	1.80	0.45
9:H:89:U:H2'	9:H:90:A:C8	2.46	0.45
9:H:100:U:H1'	39:n:65:ASN:HD22	1.81	0.45
20:T:412:HIS:HB2	20:T:437:HIS:CE1	2.51	0.45
23:V:554:LEU:O	23:V:559:SER:N	2.49	0.45
30:v:138:LEU:O	30:v:141:LEU:HG	2.17	0.45
31:w:120:GLU:HG2	31:w:121:TYR:N	2.30	0.45
37:m:49:GLU:O	37:m:50:TYR:CD1	2.70	0.45
38:l:91:SER:O	38:l:92:ASN:C	2.58	0.45
44:3:160:PHE:HA	44:3:166:ASP:O	2.16	0.45
46:1:426:MET:HE2	46:1:426:MET:N	2.32	0.45
1:A:352:PHE:HB3	23:V:320:ARG:NH2	2.31	0.45
1:A:549:GLU:OE1	1:A:552:ARG:NH1	2.49	0.45
1:A:995:ARG:HA	1:A:995:ARG:HD2	1.87	0.45
1:A:1896:CYS:HB2	1:A:1940:LEU:HD21	1.98	0.45
49:A:3000:IHP:O24	49:A:3000:IHP:H3	2.16	0.45
2:B:24:G:O4'	2:B:57:G:N2	2.50	0.45
2:B:88:A:H2'	2:B:88:A:N3	2.32	0.45
3:C:733:TRP:CE2	3:C:763:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:LEU:HB3	5:E:102:TYR:CZ	2.52	0.45
5:E:193:THR:HG23	5:E:194:TYR:CD2	2.52	0.45
6:F:86:U:O2'	6:F:87:C:O5'	2.30	0.45
7:G:-12:G:H4'	7:G:-11:G:OP1	2.16	0.45
15:N:25:LEU:HD23	15:N:25:LEU:HA	1.81	0.45
19:S:35:THR:C	19:S:129:PHE:HE1	2.24	0.45
19:S:98:LEU:O	19:S:129:PHE:N	2.48	0.45
23:V:294:ILE:HG13	23:V:295:GLY:N	2.30	0.45
24:W:167:VAL:HG23	24:W:168:PHE:CD1	2.52	0.45
30:v:93:VAL:HG13	30:v:98:HIS:CD2	2.51	0.45
36:k:28:PRO:C	36:k:30:SER:N	2.64	0.45
37:m:22:LYS:O	37:m:70:LEU:HB3	2.16	0.45
43:z:70:ILE:HA	43:z:73:LEU:HD12	1.98	0.45
46:1:454:VAL:CG2	46:1:463:ARG:HG3	2.47	0.45
46:1:490:THR:HG22	46:1:494:LEU:HB2	1.98	0.45
1:A:1112:ARG:O	1:A:1115:THR:HB	2.16	0.45
1:A:1253:SER:O	1:A:1253:SER:OG	2.35	0.45
1:A:1285:LEU:HA	1:A:1285:LEU:HD23	1.64	0.45
1:A:1337:GLN:OE1	1:A:1354:ARG:HD3	2.16	0.45
1:A:1418:ARG:O	1:A:1420:ASN:N	2.49	0.45
1:A:1527:ASN:HD22	8:6:102:G:N2	2.15	0.45
1:A:1784:ASN:OD1	1:A:1806:ALA:HB3	2.17	0.45
1:A:2006:GLU:OE2	1:A:2006:GLU:N	2.49	0.45
2:B:62:G:C2	2:B:63:A:C4	3.05	0.45
3:C:177:ARG:NH2	3:C:638:ASP:OD2	2.45	0.45
3:C:183:SER:OG	3:C:184:THR:N	2.50	0.45
3:C:497:LEU:HD13	3:C:577:PHE:CZ	2.51	0.45
3:C:509:VAL:O	3:C:510:LEU:HD23	2.16	0.45
9:H:100:U:C1'	39:n:65:ASN:HD22	2.30	0.45
11:J:204:GLU:HG3	11:J:204:GLU:O	2.17	0.45
11:J:278:LEU:HA	11:J:278:LEU:HD12	1.74	0.45
18:R:237:MET:HE2	18:R:237:MET:HA	1.99	0.45
20:T:188:PRO:HG3	20:T:443:THR:CG2	2.43	0.45
23:V:242:ARG:NH1	23:V:372:LEU:O	2.50	0.45
25:X:13:HIS:ND1	26:Y:98:TYR:OH	2.49	0.45
29:u:72:ILE:HB	29:u:95:SER:OG	2.17	0.45
31:w:90:HIS:O	31:w:94:ALA:HB2	2.17	0.45
36:k:112:ASN:ND2	37:m:58:HIS:CD2	2.84	0.45
37:m:42:MET:HB2	37:m:64:ILE:CD1	2.28	0.45
43:z:54:SER:O	43:z:57:VAL:HG22	2.16	0.45
47:2:132:ILE:HG23	47:2:132:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2:133:GLY:O	47:2:137:GLN:HG3	2.17	0.45
1:A:386:PRO:HD3	3:C:372:PHE:CE1	2.52	0.45
1:A:1199:LYS:HZ3	1:A:1206:GLU:CD	2.16	0.45
1:A:1852:LEU:HD12	1:A:1853:PRO:HD2	1.97	0.45
3:C:847:TYR:CD1	3:C:857:VAL:HG21	2.51	0.45
4:D:823:ALA:O	4:D:857:GLY:N	2.37	0.45
6:F:17:C:C2	6:F:18:A:C8	3.04	0.45
6:F:30:A:N6	8:6:16:G:H1'	2.30	0.45
9:H:105:G:OP2	37:m:67:ASN:HB3	2.17	0.45
9:H:107:A:H4'	36:k:47:ARG:HH21	1.81	0.45
11:J:291:GLN:HA	13:L:230:GLU:OE2	2.17	0.45
13:L:213:GLU:OE1	16:O:109:LYS:N	2.44	0.45
15:N:131:ILE:O	15:N:132:ILE:HD13	2.16	0.45
37:m:32:TYR:HD1	37:m:32:TYR:H	1.63	0.45
38:l:86:LEU:HD11	39:n:67:ILE:CG1	2.27	0.45
46:1:185:VAL:HG11	46:1:489:GLY:HA3	1.99	0.45
46:1:231:GLN:HE22	46:1:233:LYS:NZ	2.15	0.45
47:2:100:VAL:HG23	47:2:108:ALA:HB3	1.99	0.45
35:b:42:ALA:N	35:b:56:GLU:O	2.50	0.45
1:A:83:HIS:C	1:A:85:LYS:N	2.73	0.45
1:A:733:THR:OG1	1:A:734:PRO:HD3	2.16	0.45
1:A:1298:ARG:HD2	1:A:1298:ARG:HA	1.68	0.45
1:A:1762:TYR:C	1:A:1764:SER:H	2.23	0.45
2:B:66:A:H2'	2:B:67:A:H8	1.82	0.45
2:B:108:G:H3'	2:B:109:G:H8	1.81	0.45
6:F:5:U:H3'	6:F:7:G:H5'	1.99	0.45
7:G:-1:G:O3'	26:Y:4:ARG:HD2	2.17	0.45
23:V:261:ALA:HB2	23:V:296:PHE:CE1	2.52	0.45
36:k:42:VAL:O	36:k:53:LEU:HD12	2.17	0.45
37:m:23:LEU:HD12	37:m:69:VAL:HA	1.99	0.45
47:2:258:LYS:HA	47:2:258:LYS:HD3	1.83	0.45
38:e:34:TRP:O	38:e:85:THR:N	2.48	0.45
1:A:441:VAL:O	1:A:445:VAL:HG23	2.16	0.45
1:A:1055:LEU:HA	1:A:1055:LEU:HD23	1.77	0.45
1:A:1061:MET:HE1	1:A:1088:PHE:HB2	1.99	0.45
2:B:59:G:C4	2:B:60:G:C8	3.05	0.45
11:J:360:ASP:O	11:J:363:ARG:HG2	2.17	0.45
15:N:63:LEU:HD23	15:N:67:ARG:HD2	1.99	0.45
19:S:99:ALA:HA	19:S:129:PHE:HB2	1.99	0.45
23:V:303:LYS:O	23:V:307:VAL:HG22	2.17	0.45
36:k:110:LEU:HA	37:m:62:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:z:31:PHE:CG	43:z:32:LEU:N	2.84	0.45
46:1:480:HIS:CD2	46:1:482:LYS:H	2.31	0.45
1:A:443:VAL:O	1:A:447:TYR:HD2	1.99	0.45
1:A:793:ASN:O	1:A:797:ASP:HB2	2.17	0.45
1:A:1201:ARG:O	1:A:1203:SER:N	2.48	0.45
3:C:449:ILE:HG22	3:C:456:GLY:O	2.17	0.45
3:C:524:ILE:HD12	3:C:569:ARG:NH2	2.32	0.45
9:H:105:G:N1	35:j:20:LYS:HD3	2.32	0.45
15:N:27:GLN:NE2	15:N:31:GLU:OE2	2.50	0.45
16:O:90:TYR:O	16:O:92:LEU:HG	2.17	0.45
18:R:214:ILE:O	18:R:216:LYS:N	2.49	0.45
26:Y:20:ILE:HG21	43:z:14:ARG:HB3	1.98	0.45
28:r:40:ASP:OD1	28:r:41:PRO:HD2	2.17	0.45
29:u:243:ARG:HD3	30:v:45:ASP:OD2	2.17	0.45
33:h:78:LYS:HG2	34:i:69:LEU:HD22	1.98	0.45
34:i:30:THR:HG23	34:i:43:CYS:O	2.17	0.45
38:l:55:ASN:HA	38:l:80:LYS:HA	1.98	0.45
39:n:21:LEU:HD23	39:n:21:LEU:HA	1.72	0.45
40:o:45:ASP:OD2	40:o:67:LYS:HB2	2.16	0.45
46:1:195:ALA:HB1	46:1:211:PHE:HD2	1.82	0.45
46:1:300:MET:SD	46:1:347:ILE:HD13	2.57	0.45
46:1:381:THR:HA	46:1:397:GLY:HA2	1.99	0.45
1:A:249:LEU:HA	1:A:249:LEU:HD13	1.83	0.44
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.74	0.44
2:B:29:A:H2'	2:B:30:A:C8	2.49	0.44
2:B:62:G:H2'	2:B:63:A:C8	2.51	0.44
3:C:233:GLU:OE2	3:C:837:GLN:NE2	2.43	0.44
3:C:474:LEU:HD13	3:C:505:GLN:HE22	1.82	0.44
3:C:668:GLU:N	3:C:824:THR:HG21	2.32	0.44
3:C:736:GLY:HA3	3:C:737:PRO:HD3	1.89	0.44
8:6:5:G:H3'	8:6:6:A:C2	2.51	0.44
11:J:191:ALA:N	13:L:17:GLU:OE1	2.50	0.44
18:R:139:ALA:O	18:R:143:ILE:HG12	2.17	0.44
18:R:229:VAL:HG23	18:R:230:MET:N	2.30	0.44
19:S:101:ALA:HB1	24:W:95:PRO:HD3	1.99	0.44
26:Y:94:GLU:OE2	26:Y:95:ASN:N	2.50	0.44
29:u:278:THR:OG1	29:u:345:GLN:O	2.35	0.44
32:x:193:LEU:HD23	32:x:193:LEU:HA	1.79	0.44
35:j:1:MET:HG3	35:j:2:LYS:H	1.82	0.44
36:k:29:LEU:O	36:k:32:LEU:HB2	2.17	0.44
36:k:42:VAL:CB	37:m:61:GLU:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:61:ALA:H	38:l:75:GLY:N	2.15	0.44
1:A:191:ILE:O	1:A:192:GLN:C	2.60	0.44
1:A:284:ARG:HD2	1:A:284:ARG:O	2.17	0.44
1:A:1295:ILE:HG13	1:A:1296:GLN:N	2.32	0.44
1:A:1922:ASP:OD2	1:A:1966:HIS:NE2	2.51	0.44
2:B:12:U:H2'	2:B:13:C:H6	1.82	0.44
5:E:124:LEU:HD12	5:E:124:LEU:HA	1.71	0.44
9:H:5:C:H2'	9:H:6:U:C6	2.52	0.44
9:H:25:G:H2'	9:H:26:A:C8	2.48	0.44
9:H:40:C:OP1	43:z:14:ARG:NH2	2.51	0.44
15:N:118:ILE:O	15:N:119:CYS:C	2.60	0.44
16:O:26:THR:OG1	16:O:27:CYS:N	2.50	0.44
24:W:121:ASN:OD1	24:W:121:ASN:C	2.60	0.44
24:W:199:TYR:O	24:W:201:ASP:N	2.49	0.44
24:W:354:ARG:HA	24:W:376:PRO:HD3	2.00	0.44
26:Y:35:LEU:HA	26:Y:35:LEU:HD23	1.51	0.44
28:t:93:ARG:HG3	28:t:94:GLN:N	2.33	0.44
37:m:18:PRO:HB2	37:m:75:VAL:O	2.17	0.44
47:2:97:PHE:CE2	47:2:117:LEU:HD21	2.52	0.44
1:A:273:ILE:O	1:A:274:PRO:C	2.60	0.44
1:A:393:LEU:HD12	1:A:393:LEU:HA	1.69	0.44
1:A:442:LYS:NZ	49:A:3000:IHP:O33	2.42	0.44
1:A:738:MET:HE3	1:A:738:MET:HB3	1.80	0.44
1:A:1284:LEU:HA	1:A:1284:LEU:HD23	1.57	0.44
1:A:1416:ILE:HD13	1:A:1416:ILE:HA	1.80	0.44
2:B:15:C:H2'	2:B:16:U:H6	1.82	0.44
3:C:259:LYS:CG	50:C:1500:GTP:C6	3.00	0.44
3:C:674:CYS:HB2	3:C:818:SER:HB3	1.99	0.44
6:F:50:A:HO2'	6:F:51:U:P	2.38	0.44
16:O:212:LYS:HE3	16:O:212:LYS:HB3	1.84	0.44
20:T:455:GLN:HG3	20:T:485:THR:CG2	2.44	0.44
29:u:388:ILE:HD12	32:x:191:HIS:HB3	1.99	0.44
34:i:30:THR:OG1	34:i:30:THR:O	2.35	0.44
38:l:86:LEU:HG	39:n:62:ILE:HG23	0.46	0.44
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.82	0.44
1:A:467:GLN:NE2	2:B:20:G:H2'	2.32	0.44
1:A:830:LEU:H	1:A:830:LEU:HG	1.34	0.44
1:A:883:ARG:HG3	1:A:883:ARG:NH1	2.32	0.44
1:A:1501:LEU:HD12	1:A:1753:LEU:HD13	1.98	0.44
3:C:878:ILE:HG13	3:C:879:ASP:N	2.33	0.44
13:L:202:ARG:O	13:L:203:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:310:ARG:O	18:R:314:GLN:HG2	2.17	0.44
20:T:471:ASP:C	20:T:471:ASP:OD1	2.59	0.44
24:W:137:TYR:CE2	24:W:164:GLY:HA2	2.50	0.44
30:v:62:LEU:O	30:v:66:ILE:HG12	2.16	0.44
36:k:110:LEU:CD1	37:m:47:THR:HG21	2.47	0.44
46:l:348:ALA:HA	46:l:358:ILE:HD13	1.98	0.44
48:5:22:UNK:C	48:5:24:UNK:N	2.78	0.44
1:A:178:TYR:HB2	1:A:494:LEU:HD12	2.00	0.44
1:A:378:PHE:HB2	3:C:342:ARG:NH1	2.33	0.44
1:A:1032:ARG:H	1:A:1032:ARG:HD2	1.82	0.44
1:A:1536:LEU:HA	1:A:1536:LEU:HD23	1.57	0.44
1:A:1560:ILE:HD13	1:A:1573:LEU:HD13	2.00	0.44
1:A:1639:VAL:CG1	1:A:1717:ASN:HB3	2.48	0.44
1:A:1923:TRP:CE3	1:A:1935:ARG:HD2	2.52	0.44
1:A:1957:ASP:O	1:A:1960:THR:OG1	2.13	0.44
3:C:323:PHE:CE1	3:C:373:ILE:HG12	2.53	0.44
3:C:934:MET:HE2	3:C:934:MET:HB2	1.75	0.44
5:E:115:LEU:HA	5:E:125:PHE:O	2.18	0.44
6:F:34:G:H22	8:6:12:G:C2'	2.31	0.44
7:G:-21:A:OP1	29:u:309:GLY:N	2.47	0.44
8:6:84:U:H2'	8:6:85:G:H8	1.82	0.44
9:H:98:G:H22	37:m:41:ASN:CG	2.26	0.44
11:J:196:ARG:NE	46:l:612:ALA:HB1	2.33	0.44
16:O:179:CYS:SG	16:O:181:TYR:HB2	2.58	0.44
20:T:287:HIS:CE1	20:T:307:SER:HG	2.36	0.44
30:v:140:GLY:O	30:v:144:LYS:CB	2.66	0.44
34:i:9:MET:HE2	35:j:39:HIS:HE1	1.82	0.44
36:k:44:ILE:HD12	36:k:52:LEU:CD1	2.48	0.44
36:k:92:LYS:HA	36:k:92:LYS:HD2	1.79	0.44
37:m:65:ARG:O	37:m:69:VAL:HG23	2.18	0.44
38:l:22:PHE:CD1	38:l:50:PHE:HZ	2.28	0.44
46:l:345:ASN:OD1	46:l:345:ASN:N	2.51	0.44
47:2:109:LEU:HD23	47:2:138:TRP:CD1	2.52	0.44
1:A:1869:LEU:HA	1:A:1869:LEU:HD23	1.72	0.44
1:A:1968:TRP:HA	1:A:1968:TRP:HE3	1.82	0.44
1:A:1971:LEU:HB3	1:A:1975:GLU:HB2	2.00	0.44
3:C:215:VAL:HG11	3:C:242:LEU:HD22	2.00	0.44
3:C:531:TRP:CZ3	3:C:540:GLU:HB2	2.53	0.44
3:C:589:LYS:HG3	3:C:628:VAL:HG13	2.00	0.44
3:C:799:GLU:HG3	3:C:801:LEU:CD2	2.47	0.44
7:G:-1:G:H8	7:G:-1:G:OP1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:146:MET:O	16:O:149:LYS:N	2.51	0.44
23:V:226:PHE:HB3	23:V:229:ILE:HG12	1.99	0.44
28:r:69:THR:HG22	28:r:70:SER:H	1.81	0.44
28:r:99:THR:HA	28:r:102:GLU:OE1	2.18	0.44
37:m:49:GLU:C	37:m:50:TYR:CD1	2.96	0.44
37:m:52:ASP:N	37:m:52:ASP:OD1	2.49	0.44
40:o:66:LEU:HD21	40:o:69:LEU:HG	1.99	0.44
1:A:331:TRP:O	1:A:331:TRP:HE3	2.01	0.44
1:A:588:LEU:HA	1:A:588:LEU:HD23	1.67	0.44
1:A:686:ARG:NH2	1:A:710:LEU:HB3	2.33	0.44
1:A:1224:ARG:HD3	1:A:1224:ARG:HA	1.63	0.44
1:A:1317:TYR:CE1	1:A:1329:SER:HB3	2.52	0.44
1:A:1790:ILE:HG23	1:A:1800:THR:HG22	2.00	0.44
2:B:106:U:H2'	2:B:107:U:C6	2.53	0.44
3:C:77:VAL:HG11	20:T:196:LEU:HD23	2.00	0.44
3:C:337:GLN:O	3:C:341:LYS:HG3	2.18	0.44
3:C:383:GLN:O	3:C:387:ASP:HB2	2.18	0.44
3:C:725:ASP:OD1	3:C:727:LEU:N	2.50	0.44
3:C:730:ARG:N	3:C:730:ARG:HD2	2.32	0.44
5:E:281:VAL:O	5:E:304:SER:OG	2.35	0.44
6:F:24:A:C5	16:O:65:PHE:HE2	2.36	0.44
9:H:150:U:H4'	38:l:69:LYS:CG	2.48	0.44
10:I:50:LYS:CB	10:I:51:PRO:HD3	2.47	0.44
13:L:703:MET:O	13:L:707:ALA:HB3	2.17	0.44
16:O:253:TYR:HB2	18:R:68:HIS:O	2.18	0.44
18:R:104:GLN:CD	18:R:105:GLY:N	2.76	0.44
18:R:132:LEU:O	18:R:133:GLN:HG2	2.16	0.44
19:S:99:ALA:HB2	19:S:128:ILE:HA	1.99	0.44
20:T:274:ASP:OD1	20:T:274:ASP:C	2.61	0.44
23:V:158:SER:O	23:V:162:LEU:HG	2.18	0.44
23:V:314:ALA:O	23:V:318:ARG:HG2	2.18	0.44
23:V:622:ARG:HA	23:V:625:ARG:HH11	1.83	0.44
28:q:12:PRO:HB3	28:q:26:GLU:HB2	1.99	0.44
28:t:128:ARG:HA	28:t:131:LEU:HG	1.99	0.44
29:u:261:GLU:CD	32:x:173:ASP:HB3	2.43	0.44
34:i:19:CYS:SG	34:i:80:MET:HG2	2.58	0.44
34:i:73:ARG:HB3	34:i:76:ASN:HD21	1.83	0.44
1:A:75:ASP:O	1:A:77:THR:N	2.41	0.44
1:A:1323:GLY:HA2	1:A:1529:ILE:HD11	2.00	0.44
1:A:1528:GLN:O	1:A:1530:PRO:HD3	2.18	0.44
1:A:1763:LEU:HB2	1:A:1887:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:LYS:HG3	3:C:65:TYR:CE1	2.53	0.44
3:C:199:LEU:HD12	3:C:199:LEU:HA	1.79	0.44
5:E:265:ARG:H	5:E:272:ARG:HH21	1.64	0.44
6:F:11:C:O2'	6:F:12:G:H8	2.00	0.44
8:6:2:U:O2	8:6:2:U:O4'	2.34	0.44
10:I:406:GLU:HA	10:I:410:GLN:CA	2.47	0.44
11:J:206:LEU:HD11	13:L:171:ALA:HB1	2.00	0.44
12:K:39:GLU:HG3	28:r:116:VAL:HG22	1.99	0.44
18:R:180:THR:HA	18:R:181:PRO:HD3	1.80	0.44
20:T:385:TYR:CE2	20:T:401:PRO:HD3	2.52	0.44
24:W:135:TYR:CZ	24:W:165:LEU:HD11	2.53	0.44
29:u:242:LYS:HB3	29:u:244:ASP:OD2	2.18	0.44
33:h:55:VAL:HG11	40:o:67:LYS:NZ	2.33	0.44
37:m:49:GLU:CG	37:m:50:TYR:N	2.80	0.44
39:n:63:ARG:NE	39:n:65:ASN:HB2	2.33	0.44
40:o:32:PRO:O	40:o:54:ILE:HA	2.18	0.44
46:1:213:GLY:C	46:1:214:MET:HE2	2.43	0.44
1:A:53:PHE:CE2	1:A:55:ASP:HB3	2.53	0.44
1:A:126:ILE:HG21	18:R:207:MET:HE2	1.99	0.44
1:A:357:ASN:HB2	3:C:863:ILE:O	2.18	0.44
1:A:642:ARG:O	1:A:642:ARG:HG2	2.12	0.44
1:A:702:LYS:HB2	1:A:705:LYS:NZ	2.33	0.44
3:C:366:GLN:OE1	3:C:370:VAL:HG21	2.17	0.44
3:C:709:TRP:HB3	3:C:713:LYS:HB2	1.98	0.44
9:H:70:C:H2'	9:H:71:C:C6	2.53	0.44
13:L:40:ARG:HG3	26:Y:109:GLN:HE22	1.82	0.44
13:L:154:GLU:HB3	26:Y:49:TYR:HE2	1.83	0.44
18:R:103:ARG:HD3	18:R:108:LYS:HA	2.00	0.44
19:S:149:SER:OG	19:S:150:GLN:NE2	2.42	0.44
28:t:84:ALA:O	28:t:87:LEU:HG	2.18	0.44
36:k:32:LEU:HD22	36:k:65:MET:CE	2.48	0.44
36:k:70:VAL:HG21	36:k:99:MET:SD	2.58	0.44
36:k:111:ARG:N	37:m:62:VAL:HG23	2.33	0.44
37:m:40:MET:C	37:m:66:CYS:HB3	2.42	0.44
41:p:86:THR:OG1	41:p:87:ASP:N	2.51	0.44
47:2:101:LYS:HG2	47:2:107:ILE:HD12	2.00	0.44
1:A:103:LEU:O	1:A:105:ASN:N	2.51	0.43
1:A:409:ARG:HD2	2:B:25:C:O2'	2.18	0.43
4:D:1583:ASP:O	4:D:1585:GLN:N	2.51	0.43
9:H:101:U:C2	33:h:64:ARG:NE	2.85	0.43
14:M:150:GLU:OE2	14:M:153:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:126:LEU:O	15:N:128:VAL:HG23	2.18	0.43
19:S:57:ILE:HG21	24:W:97:ASN:CB	2.48	0.43
19:S:66:ASP:OD1	19:S:68:THR:OG1	2.33	0.43
20:T:203:HIS:CE1	20:T:223:SER:OG	2.71	0.43
20:T:307:SER:OG	20:T:309:ASP:OD1	2.36	0.43
20:T:308:ARG:C	20:T:310:SER:H	2.25	0.43
24:W:205:VAL:HG12	24:W:207:LYS:HD2	2.00	0.43
28:q:104:SER:O	28:q:107:LEU:HG	2.18	0.43
33:h:23:ASN:HD22	33:h:67:LYS:HD3	1.82	0.43
36:k:110:LEU:O	37:m:60:GLY:CA	2.66	0.43
36:k:111:ARG:CA	37:m:60:GLY:C	2.78	0.43
37:m:23:LEU:CD1	37:m:68:ASN:HB3	2.45	0.43
38:l:38:GLN:OE1	38:l:41:MET:HE2	2.18	0.43
39:n:34:PHE:CD1	39:n:35:ASP:O	2.71	0.43
39:n:64:GLY:O	39:n:65:ASN:C	2.60	0.43
46:1:329:GLN:O	46:1:329:GLN:HG2	2.18	0.43
1:A:697:MET:HG3	1:A:701:ILE:HD12	1.99	0.43
1:A:956:CYS:HB3	1:A:1216:LEU:HD11	2.00	0.43
1:A:1898:LYS:HD3	1:A:1898:LYS:N	2.33	0.43
1:A:1919:LEU:HD23	1:A:1967:ILE:HD13	1.99	0.43
1:A:1965:HIS:O	1:A:1966:HIS:ND1	2.38	0.43
3:C:85:ASP:HB3	20:T:238:LEU:HG	1.99	0.43
3:C:267:LEU:HB3	3:C:269:LEU:HG	1.99	0.43
3:C:589:LYS:HB3	3:C:659:VAL:O	2.17	0.43
5:E:68:GLU:O	5:E:85:GLY:HA3	2.18	0.43
5:E:224:GLN:O	5:E:226:LYS:HG3	2.18	0.43
9:H:7:U:H2'	9:H:8:C:H6	1.80	0.43
9:H:169:C:H2'	9:H:170:C:C6	2.54	0.43
13:L:86:ALA:HB1	13:L:91:ARG:O	2.18	0.43
14:M:121:ASP:O	14:M:122:LEU:HD13	2.18	0.43
16:O:111:ASP:O	16:O:115:GLU:HG3	2.18	0.43
16:O:172:GLU:O	16:O:173:CYS:C	2.60	0.43
18:R:211:ARG:HB2	18:R:211:ARG:NH1	2.33	0.43
19:S:42:LEU:HB3	19:S:47:TYR:HB3	2.00	0.43
23:V:403:LYS:HD3	23:V:403:LYS:C	2.43	0.43
23:V:530:LYS:HA	23:V:533:TYR:CZ	2.53	0.43
26:Y:46:CYS:C	26:Y:48:GLU:N	2.75	0.43
28:q:21:SER:OG	28:q:40:ASP:OD1	2.36	0.43
29:u:84:SER:O	29:u:248:LEU:HD11	2.16	0.43
33:h:64:ARG:CZ	39:n:65:ASN:O	2.65	0.43
36:k:110:LEU:CD2	37:m:59:LEU:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:LYS:HE3	1:A:834:HIS:HE1	1.81	0.43
1:A:855:ARG:C	1:A:856:LEU:HD22	2.43	0.43
1:A:1249:MET:HE2	1:A:1249:MET:HB3	1.77	0.43
1:A:1418:ARG:HD3	1:A:1418:ARG:HA	1.79	0.43
1:A:1876:LEU:HA	1:A:1876:LEU:HD23	1.75	0.43
3:C:69:ALA:HA	20:T:456:PRO:CG	2.42	0.43
3:C:255:VAL:O	3:C:307:VAL:HA	2.18	0.43
3:C:512:GLU:HG2	3:C:562:THR:HB	2.01	0.43
3:C:750:LEU:HB3	3:C:751:PRO:HD3	2.01	0.43
3:C:763:LYS:HD2	3:C:764:ASP:OD1	2.18	0.43
6:F:45:A:C8	8:6:3:A:C2	3.07	0.43
8:6:99:C:H5''	8:6:100:C:OP2	2.19	0.43
9:H:40:C:H2'	9:H:41:U:C6	2.52	0.43
17:P:31:SER:N	17:P:34:ASP:OD2	2.51	0.43
17:P:44:ARG:NH1	17:P:49:ASP:HB3	2.34	0.43
25:X:19:ASN:O	25:X:23:VAL:HG23	2.19	0.43
31:w:97:GLY:HA3	31:w:126:GLU:CD	2.44	0.43
34:i:18:ARG:HB3	34:i:81:THR:CG2	2.48	0.43
36:k:56:VAL:HG22	36:k:65:MET:SD	2.59	0.43
36:k:65:MET:HE3	36:k:65:MET:HB2	1.85	0.43
37:m:23:LEU:HD21	37:m:68:ASN:OD1	2.18	0.43
38:l:24:TYR:O	38:l:25:LEU:C	2.61	0.43
41:p:9:ILE:HG23	41:p:62:SER:OG	2.19	0.43
46:1:276:MET:HE3	46:1:305:ASP:HB2	1.99	0.43
1:A:410:PRO:HG2	1:A:411:PHE:CD2	2.53	0.43
1:A:710:LEU:HD23	1:A:710:LEU:HA	1.77	0.43
1:A:797:ASP:OD1	3:C:63:LYS:HE3	2.19	0.43
1:A:1050:LEU:HA	1:A:1050:LEU:HD23	1.66	0.43
1:A:1495:PHE:CE2	1:A:1501:LEU:HD11	2.53	0.43
1:A:1868:MET:C	1:A:1871:PRO:HD2	2.44	0.43
1:A:1953:ILE:HD13	1:A:1982:GLN:HB3	1.99	0.43
2:B:66:A:H2'	2:B:67:A:C8	2.53	0.43
3:C:594:PRO:HG3	3:C:600:LEU:HA	1.99	0.43
5:E:314:THR:HG23	5:E:315:THR:HG23	1.99	0.43
6:F:34:G:C5'	13:L:203:LYS:HE2	2.48	0.43
6:F:58:G:C6	6:F:78:A:N1	2.86	0.43
6:F:89:U:C4	9:H:10:C:N3	2.86	0.43
8:6:105:C:H4'	8:6:106:C:OP1	2.16	0.43
9:H:101:U:C5	33:h:64:ARG:NH2	2.87	0.43
10:I:148:ILE:O	10:I:152:TYR:N	2.44	0.43
16:O:90:TYR:HB3	16:O:92:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:191:ASP:OD1	17:P:191:ASP:N	2.50	0.43
18:R:66:GLU:O	18:R:68:HIS:HD2	2.00	0.43
20:T:196:LEU:HD12	20:T:196:LEU:HA	1.74	0.43
23:V:620:ASN:HB3	23:V:623:ASN:HB2	2.01	0.43
26:Y:68:TYR:HD1	26:Y:69:LEU:HG	1.84	0.43
29:u:188:GLU:HB3	29:u:339:ARG:HH11	1.82	0.43
29:u:250:GLY:O	29:u:374:LYS:HA	2.18	0.43
30:v:26:PHE:HZ	30:v:131:LEU:HB3	1.83	0.43
30:v:79:TRP:CH2	30:v:124:PHE:HB2	2.54	0.43
36:k:31:VAL:O	36:k:35:SER:CB	2.66	0.43
38:l:65:HIS:HB2	38:l:70:SER:OG	2.18	0.43
39:n:61:VAL:O	39:n:62:ILE:HG13	2.18	0.43
41:p:39:ASP:HB3	41:p:55:ILE:HD12	2.00	0.43
46:1:310:THR:OG1	46:1:320:LYS:HB2	2.18	0.43
1:A:175:PRO:HG2	1:A:498:ARG:NH2	2.33	0.43
1:A:758:ARG:O	1:A:758:ARG:HG3	2.15	0.43
1:A:952:VAL:HG22	1:A:1189:MET:HB3	1.99	0.43
1:A:1146:ASP:OD2	1:A:1182:ASN:ND2	2.52	0.43
1:A:1570:LYS:NZ	26:Y:6:VAL:O	2.51	0.43
1:A:1637:TRP:O	1:A:1656:THR:HA	2.18	0.43
3:C:534:VAL:O	3:C:535:ALA:C	2.61	0.43
6:F:1:G:H2'	6:F:2:U:C6	2.54	0.43
6:F:49:G:H2'	6:F:50:A:H8	1.82	0.43
6:F:97:U:O5'	6:F:97:U:H6	2.01	0.43
10:I:565:ILE:HA	10:I:569:GLY:HA3	1.99	0.43
11:J:212:GLN:HE21	13:L:182:LEU:HD13	1.84	0.43
11:J:411:MET:HE3	11:J:412:ASP:N	2.32	0.43
17:P:207:ASP:OD2	17:P:208:LYS:HE2	2.18	0.43
19:S:57:ILE:O	19:S:116:LEU:HD12	2.19	0.43
20:T:308:ARG:HG3	20:T:332:ALA:HB2	2.01	0.43
23:V:476:LEU:HA	23:V:476:LEU:HD23	1.71	0.43
29:u:64:ILE:HD11	29:u:80:ALA:HB1	2.00	0.43
29:u:358:ARG:HD3	30:v:42:TYR:CE1	2.53	0.43
32:x:173:ASP:HA	32:x:180:ALA:O	2.18	0.43
37:m:32:TYR:O	37:m:44:LEU:CG	2.67	0.43
38:l:34:TRP:CH2	39:n:27:VAL:HG22	2.52	0.43
43:z:49:ILE:O	43:z:53:ILE:HG12	2.19	0.43
36:c:112:ASN:O	36:c:114:LEU:N	2.48	0.43
1:A:91:ALA:HA	18:R:207:MET:HE3	2.01	0.43
1:A:409:ARG:HG2	1:A:409:ARG:HH11	1.84	0.43
1:A:469:LYS:NZ	2:B:59:G:C5	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1922:ASP:OD2	1:A:1966:HIS:CE1	2.71	0.43
2:B:36:C:C2	2:B:37:G:C8	3.06	0.43
7:G:-2:C:C3'	7:G:-1:G:H5''	2.39	0.43
8:6:7:G:O2'	8:6:8:C:H5'	2.19	0.43
9:H:92:U:H2'	9:H:93:A:C8	2.54	0.43
11:J:314:TYR:O	11:J:317:THR:OG1	2.31	0.43
13:L:50:TRP:CD1	13:L:50:TRP:C	2.97	0.43
13:L:148:GLU:O	13:L:151:MET:HB2	2.19	0.43
15:N:2:PRO:C	15:N:4:VAL:N	2.76	0.43
15:N:116:ASN:OD1	15:N:116:ASN:N	2.51	0.43
16:O:32:PRO:HG2	16:O:33:TYR:CD2	2.53	0.43
18:R:279:HIS:ND1	18:R:279:HIS:N	2.66	0.43
20:T:427:LEU:O	20:T:439:TRP:HD1	2.00	0.43
23:V:199:ARG:HD3	23:V:383:ASN:ND2	2.34	0.43
23:V:228:GLN:HG2	23:V:229:ILE:HD13	1.99	0.43
23:V:302:LEU:CD1	23:V:306:GLN:HE22	2.32	0.43
28:t:102:GLU:HA	28:t:105:HIS:CG	2.53	0.43
29:u:136:GLN:CB	29:u:157:GLN:HA	2.48	0.43
33:h:36:GLU:OE1	39:n:7:PRO:HA	2.17	0.43
34:i:82:VAL:HG13	35:j:56:GLU:OE2	2.19	0.43
36:k:44:ILE:HG12	36:k:109:VAL:CG2	2.48	0.43
38:l:47:ILE:HD11	38:l:56:LEU:HD22	2.01	0.43
43:z:47:ARG:HA	43:z:50:ILE:CG1	2.48	0.43
1:A:228:TRP:CD1	1:A:416:GLY:O	2.72	0.43
1:A:488:ASP:OD1	1:A:488:ASP:C	2.62	0.43
1:A:589:THR:OG1	1:A:590:GLY:N	2.51	0.43
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.80	0.43
1:A:883:ARG:HG3	1:A:883:ARG:HH11	1.83	0.43
1:A:1386:TRP:HE1	1:A:1417:PRO:HD2	1.84	0.43
3:C:134:LEU:HD23	3:C:226:VAL:HB	2.01	0.43
3:C:733:TRP:CH2	3:C:759:LEU:HD11	2.53	0.43
8:6:84:U:H2'	8:6:85:G:C8	2.53	0.43
11:J:252:GLU:OE1	11:J:260:ARG:HD3	2.19	0.43
11:J:315:LYS:NZ	14:M:189:GLN:HE22	2.17	0.43
14:M:202:TYR:OH	14:M:204:ASP:OD1	2.31	0.43
16:O:115:GLU:HG3	16:O:115:GLU:H	1.70	0.43
17:P:66:ARG:NH1	17:P:66:ARG:HB2	2.34	0.43
18:R:189:ASN:OD1	18:R:195:ARG:NE	2.52	0.43
21:Q:515:VAL:N	21:Q:540:THR:O	2.48	0.43
29:u:70:LYS:O	29:u:74:LYS:HG3	2.18	0.43
29:u:407:VAL:HG22	29:u:410:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:w:92:LYS:N	31:w:92:LYS:HD3	2.31	0.43
38:l:86:LEU:HD21	39:n:62:ILE:HG21	1.96	0.43
41:p:66:LEU:HD12	41:p:81:ILE:HG22	2.00	0.43
46:l:238:SER:OG	46:l:241:GLY:N	2.51	0.43
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.63	0.43
1:A:1415:GLY:C	1:A:1418:ARG:H	2.27	0.43
3:C:129:ILE:HG22	3:C:199:LEU:HB3	2.01	0.43
5:E:162:ARG:NH2	5:E:203:ASP:O	2.52	0.43
6:F:42:C:H2'	6:F:43:A:C8	2.54	0.43
14:M:181:ARG:H	14:M:181:ARG:HG3	1.60	0.43
16:O:25:GLN:HE22	18:R:195:ARG:HH21	1.67	0.43
16:O:57:TRP:CD1	16:O:57:TRP:C	2.96	0.43
18:R:214:ILE:HG13	18:R:215:ASN:N	2.32	0.43
23:V:636:LEU:O	23:V:638:GLY:N	2.52	0.43
29:u:206:ARG:HD3	29:u:206:ARG:HA	1.86	0.43
29:u:311:MET:SD	29:u:312:PRO:HD2	2.59	0.43
30:v:82:PRO:HB2	30:v:87:ARG:HD3	2.01	0.43
36:k:110:LEU:HD11	37:m:47:THR:CG2	2.47	0.43
39:n:8:GLU:OE1	39:n:8:GLU:HA	2.19	0.43
41:p:19:LYS:H	41:p:19:LYS:HG3	1.70	0.43
1:A:103:LEU:C	1:A:105:ASN:H	2.26	0.43
1:A:170:ASP:OD1	1:A:1621:LYS:NZ	2.47	0.43
1:A:440:PRO:O	1:A:443:VAL:HG22	2.18	0.43
1:A:590:GLY:HA2	1:A:592:TYR:CE2	2.53	0.43
1:A:955:TRP:HE1	1:A:976:MET:HE1	1.84	0.43
1:A:962:LEU:HD23	1:A:962:LEU:HA	1.84	0.43
1:A:1361:GLU:C	1:A:1363:GLN:N	2.74	0.43
1:A:1607:GLU:HB2	1:A:1633:ALA:O	2.19	0.43
1:A:1866:LYS:HG3	1:A:1867:GLY:N	2.33	0.43
3:C:343:LEU:HA	3:C:343:LEU:HD23	1.66	0.43
3:C:366:GLN:HB3	3:C:370:VAL:HB	2.01	0.43
3:C:374:LEU:HA	3:C:374:LEU:HD23	1.68	0.43
5:E:74:PHE:CD2	5:E:337:PRO:HD3	2.53	0.43
5:E:95:VAL:HG23	5:E:96:TYR:CD2	2.53	0.43
6:F:16:G:H2'	6:F:17:C:C6	2.53	0.43
8:6:87:U:C2	9:H:42:G:N1	2.77	0.43
11:J:206:LEU:HD23	11:J:206:LEU:HA	1.75	0.43
11:J:258:ILE:HG12	13:L:232:TYR:CZ	2.54	0.43
15:N:125:LYS:N	15:N:125:LYS:HD3	2.33	0.43
16:O:102:SER:OG	16:O:105:ASP:OD1	2.37	0.43
16:O:240:GLY:HA3	16:O:296:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:182:SER:OG	24:W:113:GLY:HA2	2.19	0.43
20:T:296:LEU:HD23	20:T:296:LEU:HA	1.80	0.43
29:u:225:ILE:HD13	29:u:228:MET:HE3	2.00	0.43
29:u:282:ILE:HG12	29:u:350:ILE:HB	1.99	0.43
29:u:358:ARG:HG3	29:u:392:ILE:HG12	2.01	0.43
29:u:360:LEU:HD23	29:u:360:LEU:HA	1.86	0.43
30:v:130:ASP:HA	31:w:114:LYS:NZ	2.34	0.43
33:h:13:ALA:HB2	33:h:73:LEU:HD13	2.01	0.43
35:j:37:ASN:OD1	35:j:62:GLY:N	2.41	0.43
38:l:65:HIS:O	38:l:69:LYS:N	2.52	0.43
1:A:1454:TRP:H	1:A:1454:TRP:CD1	2.36	0.43
1:A:1740:LEU:O	1:A:1744:ARG:HG3	2.19	0.43
1:A:1771:LEU:HD12	1:A:1772:PHE:N	2.34	0.43
2:B:10:U:H2'	2:B:11:U:C6	2.54	0.43
3:C:174:GLU:OE2	3:C:181:ILE:N	2.32	0.43
11:J:183:ALA:O	13:L:141:PRO:HA	2.19	0.43
11:J:201:ARG:HD2	11:J:201:ARG:O	2.19	0.43
11:J:325:ASN:HB2	14:M:172:HIS:CD2	2.41	0.43
13:L:184:ALA:O	13:L:188:ARG:HG2	2.19	0.43
14:M:200:ARG:HD2	14:M:200:ARG:N	2.33	0.43
29:u:254:PHE:HD2	29:u:401:ASP:HB3	1.80	0.43
30:v:50:LYS:HD2	30:v:143:PHE:CD2	2.54	0.43
34:i:16:ARG:HH11	34:i:30:THR:HG22	1.84	0.43
46:1:381:THR:HB	46:1:396:ARG:O	2.19	0.43
1:A:1975:GLU:O	1:A:1979:VAL:HG23	2.19	0.42
2:B:40:U:H2'	2:B:41:U:H6	1.83	0.42
3:C:381:LEU:O	3:C:385:VAL:HG22	2.19	0.42
3:C:509:VAL:C	3:C:510:LEU:HD23	2.44	0.42
3:C:678:THR:HG21	3:C:683:ASN:HD22	1.84	0.42
3:C:726:LEU:O	3:C:730:ARG:HG2	2.19	0.42
3:C:789:PHE:CE2	3:C:816:VAL:HG13	2.54	0.42
5:E:192:ASN:CG	5:E:193:THR:H	2.27	0.42
8:6:73:G:O2'	8:6:74:G:P	2.77	0.42
11:J:262:ARG:NE	11:J:286:GLU:OE2	2.39	0.42
11:J:355:ARG:NH2	14:M:139:THR:HG23	2.34	0.42
11:J:385:PHE:CE1	11:J:389:HIS:CD2	3.07	0.42
11:J:400:GLU:O	11:J:403:VAL:HG22	2.19	0.42
13:L:224:PHE:H	18:R:86:LEU:CD1	2.30	0.42
16:O:44:GLU:HA	16:O:50:ARG:O	2.19	0.42
16:O:45:CYS:HB2	16:O:71:CYS:N	2.34	0.42
23:V:596:LEU:HD13	23:V:599:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:37:ALA:O	26:Y:53:GLY:HA2	2.18	0.42
29:u:242:LYS:HD2	30:v:50:LYS:HZ2	1.83	0.42
34:i:47:GLU:O	34:i:64:LYS:HA	2.18	0.42
37:m:25:TRP:CZ2	37:m:68:ASN:HA	2.54	0.42
38:l:64:ILE:CD1	38:l:71:ARG:HG2	2.49	0.42
46:1:214:MET:HE2	46:1:214:MET:N	2.34	0.42
46:1:455:PHE:O	46:1:463:ARG:HA	2.19	0.42
47:2:108:ALA:HB2	47:2:132:ILE:CD1	2.47	0.42
1:A:80:LYS:HZ3	15:N:37:HIS:CD2	2.36	0.42
1:A:516:LEU:HA	1:A:516:LEU:HD23	1.79	0.42
1:A:673:THR:HG22	1:A:674:LYS:N	2.34	0.42
1:A:750:TRP:CE2	1:A:778:ARG:HG2	2.54	0.42
1:A:1070:ASP:OD1	1:A:1070:ASP:C	2.62	0.42
1:A:1854:VAL:HA	1:A:1857:GLN:HB2	2.01	0.42
2:B:55:C:H2'	2:B:56:C:C6	2.54	0.42
3:C:132:VAL:HG21	3:C:226:VAL:HG23	2.02	0.42
3:C:303:LEU:HD21	3:C:344:TRP:HB3	2.00	0.42
3:C:454:THR:HG23	3:C:576:ILE:O	2.19	0.42
5:E:122:SER:HA	5:E:138:SER:OG	2.19	0.42
6:F:28:A:O2'	15:N:39:GLY:HA2	2.19	0.42
6:F:59:G:O2'	6:F:61:C:P	2.77	0.42
9:H:105:G:P	37:m:67:ASN:HB3	2.59	0.42
11:J:335:ARG:HA	14:M:164:SER:OG	2.19	0.42
13:L:163:GLN:OE1	13:L:168:LYS:N	2.53	0.42
13:L:185:LEU:HA	13:L:185:LEU:HD12	1.71	0.42
15:N:4:VAL:O	15:N:6:ARG:NH1	2.52	0.42
23:V:238:ILE:CG2	23:V:372:LEU:HD12	2.49	0.42
36:k:110:LEU:O	37:m:60:GLY:HA3	2.19	0.42
38:l:20:LEU:HD13	39:n:41:VAL:CB	2.48	0.42
40:o:102:GLU:HG2	40:o:128:LYS:NZ	2.34	0.42
1:A:1248:LEU:HA	1:A:1248:LEU:HD23	1.69	0.42
1:A:1639:VAL:O	1:A:1654:SER:HB3	2.19	0.42
1:A:1965:HIS:ND1	47:2:130:ASP:OD1	2.52	0.42
1:A:2008:ARG:O	1:A:2012:LEU:HB3	2.19	0.42
3:C:87:GLN:HG3	3:C:91:GLU:HG2	2.01	0.42
3:C:140:HIS:CE1	3:C:230:ASP:H	2.37	0.42
3:C:190:LEU:HA	3:C:190:LEU:HD23	1.70	0.42
3:C:259:LYS:HG2	50:C:1500:GTP:C6	2.54	0.42
6:F:49:G:O2'	6:F:50:A:H5'	2.18	0.42
6:F:77:C:C2'	6:F:78:A:H5'	2.49	0.42
9:H:12:G:N2	14:M:196:TYR:CZ	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:171:U:H2'	9:H:172:C:H6	1.84	0.42
13:L:149:LEU:O	13:L:152:LEU:HB2	2.19	0.42
16:O:185:LYS:HD2	16:O:185:LYS:HA	1.93	0.42
17:P:206:LYS:HA	17:P:209:ARG:HD2	2.01	0.42
18:R:232:SEP:OG	18:R:233:PRO:HD2	2.19	0.42
19:S:146:GLU:O	19:S:146:GLU:HG2	2.18	0.42
20:T:347:THR:CG2	20:T:357:TRP:HE1	2.30	0.42
23:V:486:THR:HA	23:V:489:LEU:HB3	2.01	0.42
27:Z:775:VAL:HA	27:Z:801:CYS:O	2.20	0.42
29:u:102:ILE:HD13	29:u:133:MET:O	2.19	0.42
1:A:711:GLN:OE1	9:H:18:U:H5''	2.19	0.42
1:A:858:GLN:HB2	9:H:29:A:OP1	2.19	0.42
1:A:912:GLU:HG3	1:A:913:PRO:CD	2.48	0.42
1:A:1184:ASN:OD1	1:A:1197:LEU:HD13	2.19	0.42
1:A:1627:ALA:HB2	1:A:1695:TYR:HD1	1.85	0.42
1:A:1855:GLU:OE1	47:2:57:SER:OG	2.33	0.42
2:B:47:A:C1'	22:U:11:ARG:HH21	2.33	0.42
3:C:531:TRP:HB2	3:C:551:LEU:HB2	2.01	0.42
3:C:823:ALA:O	3:C:824:THR:HG22	2.18	0.42
6:F:8:C:N4	6:F:9:U:C2	2.87	0.42
9:H:100:U:O2	39:n:65:ASN:N	2.52	0.42
18:R:282:GLU:C	18:R:284:PHE:N	2.77	0.42
24:W:276:LEU:HA	24:W:277:PRO:HD3	1.87	0.42
29:u:264:LYS:HD3	29:u:380:PHE:HB3	2.01	0.42
33:h:64:ARG:NE	39:n:66:SER:HA	2.35	0.42
36:k:106:VAL:O	37:m:68:ASN:ND2	2.46	0.42
46:l:197:LEU:HB3	46:l:209:TRP:HB2	1.99	0.42
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.87	0.42
1:A:357:ASN:ND2	3:C:866:SER:O	2.53	0.42
1:A:579:GLN:HG2	1:A:627:CYS:O	2.20	0.42
1:A:1944:HIS:CG	45:4:104:ARG:HB2	2.54	0.42
3:C:213:ASP:OD1	3:C:213:ASP:N	2.50	0.42
3:C:623:GLU:C	3:C:625:GLY:N	2.78	0.42
3:C:807:GLN:O	3:C:810:PRO:HD2	2.18	0.42
4:D:150:ASP:C	4:D:152:GLU:N	2.75	0.42
6:F:95:G:C6	9:H:4:G:C6	3.08	0.42
7:G:-20:A:H5'	29:u:114:PRO:O	2.20	0.42
7:G:-19:C:OP1	29:u:163:THR:OG1	2.35	0.42
9:H:105:G:O6	35:j:66:ARG:NH1	2.53	0.42
13:L:40:ARG:HG3	26:Y:109:GLN:NE2	2.35	0.42
15:N:59:TYR:CZ	15:N:63:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:26:THR:HG1	16:O:159:ARG:HH21	1.61	0.42
16:O:63:MET:SD	16:O:160:ASN:HB2	2.60	0.42
16:O:132:ARG:CZ	16:O:137:LEU:HD23	2.49	0.42
16:O:253:TYR:HE1	19:S:93:THR:HG1	1.62	0.42
18:R:76:MET:HG2	19:S:95:ALA:HB2	2.01	0.42
19:S:24:VAL:HB	19:S:134:GLN:HB3	2.00	0.42
20:T:215:GLY:O	20:T:217:GLN:HG2	2.19	0.42
20:T:261:LEU:HD23	20:T:261:LEU:HA	1.89	0.42
23:V:584:LYS:HA	23:V:634:ILE:HD12	2.01	0.42
29:u:286:THR:O	29:u:290:VAL:HG23	2.19	0.42
32:x:173:ASP:OD2	32:x:174:GLU:HG2	2.20	0.42
39:n:40:LEU:C	39:n:62:ILE:HB	2.44	0.42
46:l:181:GLY:O	46:l:493:GLY:HA3	2.19	0.42
1:A:237:THR:HG23	1:A:240:ARG:NH1	2.35	0.42
1:A:982:GLU:CD	1:A:1172:ASN:HD22	2.28	0.42
1:A:1391:LEU:HD12	1:A:1391:LEU:HA	1.80	0.42
1:A:1783:THR:HG21	1:A:1894:GLN:CG	2.50	0.42
2:B:30:A:H2'	2:B:31:U:H6	1.83	0.42
3:C:64:LYS:H	3:C:64:LYS:HG2	1.65	0.42
3:C:114:TYR:HE1	33:g:79:ASN:C	2.24	0.42
3:C:213:ASP:OD2	3:C:615:PRO:HD2	2.19	0.42
3:C:906:ILE:HG22	3:C:907:VAL:O	2.20	0.42
5:E:221:ASP:HB2	5:E:228:THR:OG1	2.20	0.42
10:I:393:LYS:N	10:I:394:PRO:HD3	2.34	0.42
16:O:58:CYS:HA	16:O:59:PRO:HD3	1.82	0.42
18:R:73:PRO:HB3	19:S:131:ARG:NH2	2.32	0.42
18:R:178:ARG:HD3	18:R:194:GLN:NE2	2.33	0.42
18:R:296:ARG:O	18:R:300:GLU:HG2	2.20	0.42
20:T:250:ARG:HD2	20:T:250:ARG:HA	1.78	0.42
20:T:428:VAL:HG22	20:T:438:LEU:HD22	2.01	0.42
23:V:457:ARG:HG3	23:V:457:ARG:NH2	2.35	0.42
23:V:506:PHE:CD1	23:V:506:PHE:C	2.98	0.42
28:r:84:ALA:O	28:r:88:HIS:HB2	2.20	0.42
29:u:49:LEU:HD13	29:u:133:MET:CE	2.50	0.42
29:u:214:VAL:HG23	29:u:233:MET:HE3	2.01	0.42
30:v:47:MET:HE3	30:v:47:MET:HB2	1.87	0.42
30:v:144:LYS:HZ2	30:v:147:PRO:HD3	1.84	0.42
35:j:68:PHE:HB2	36:k:100:PHE:HB3	2.02	0.42
36:k:102:ARG:NE	36:k:104:ASP:OD2	2.40	0.42
36:k:109:VAL:N	37:m:63:LEU:O	2.38	0.42
38:l:19:ASN:O	38:l:23:ARG:CB	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:63:GLU:HB2	38:l:72:LYS:HB3	2.01	0.42
1:A:385:GLU:OE1	1:A:389:LYS:HD2	2.20	0.42
1:A:507:LEU:HA	1:A:507:LEU:HD12	1.79	0.42
1:A:941:LYS:HA	1:A:941:LYS:HD2	1.77	0.42
1:A:1282:GLN:O	1:A:1285:LEU:N	2.51	0.42
3:C:501:ILE:HG22	3:C:530:LEU:HD11	2.02	0.42
3:C:679:PRO:HD3	3:C:811:THR:HG1	1.84	0.42
5:E:208:ILE:HG13	5:E:222:LEU:HD21	2.01	0.42
5:E:289:LEU:HD12	5:E:289:LEU:HA	1.70	0.42
9:H:25:G:C2	9:H:26:A:C5	3.08	0.42
9:H:157:G:O6	9:H:174:A:N6	2.53	0.42
11:J:188:GLN:HE21	13:L:13:ASN:ND2	2.13	0.42
11:J:376:VAL:HG23	11:J:415:LEU:HB2	2.00	0.42
16:O:113:ASN:O	16:O:114:LYS:C	2.61	0.42
16:O:137:LEU:HD12	16:O:140:ALA:HB3	2.02	0.42
16:O:164:ILE:HD12	16:O:182:ARG:O	2.20	0.42
18:R:124:VAL:HG13	18:R:125:MET:N	2.33	0.42
20:T:390:GLY:HA3	20:T:416:ILE:HD11	2.02	0.42
29:u:30:THR:HG22	29:u:240:LEU:H	1.85	0.42
37:m:43:GLN:C	37:m:44:LEU:HD12	2.45	0.42
39:n:20:LYS:HB3	39:n:69:MET:HE2	2.02	0.42
1:A:95:MET:N	1:A:96:PRO:HD2	2.35	0.42
1:A:1534:PHE:CE1	1:A:1538:TRP:CD1	3.08	0.42
1:A:1763:LEU:HD12	1:A:1887:SER:HB2	2.02	0.42
1:A:1816:GLN:NE2	1:A:1817:LEU:O	2.52	0.42
1:A:1920:TYR:CE1	1:A:1936:LEU:HD22	2.55	0.42
2:B:12:U:H2'	2:B:13:C:C6	2.54	0.42
3:C:154:HIS:C	3:C:156:GLU:H	2.26	0.42
3:C:154:HIS:C	3:C:156:GLU:N	2.77	0.42
3:C:259:LYS:HG2	50:C:1500:GTP:N1	2.34	0.42
3:C:621:VAL:HG22	3:C:627:HIS:ND1	2.35	0.42
3:C:641:MET:HE2	3:C:655:VAL:HG21	2.01	0.42
5:E:63:SER:OG	5:E:350:ARG:HG2	2.19	0.42
5:E:243:LEU:HD21	5:E:247:GLY:HA2	2.01	0.42
6:F:26:U:O2	6:F:26:U:C2'	2.67	0.42
6:F:75:G:N1	6:F:76:A:C5	2.88	0.42
6:F:89:U:C2	6:F:90:G:C8	3.08	0.42
11:J:194:LEU:HA	11:J:194:LEU:HD23	1.73	0.42
13:L:54:LEU:HD12	13:L:54:LEU:HA	1.73	0.42
19:S:98:LEU:CD2	19:S:129:PHE:HD2	2.33	0.42
23:V:173:VAL:HA	23:V:181:ILE:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:288:ASP:O	23:V:292:VAL:HG23	2.19	0.42
23:V:341:ALA:CA	23:V:344:LYS:HE3	2.47	0.42
23:V:533:TYR:HA	23:V:536:ILE:HG23	2.01	0.42
33:h:64:ARG:HG2	33:h:65:GLY:N	2.35	0.42
36:k:101:LEU:HD11	36:k:105:SER:HB2	2.01	0.42
38:l:35:LEU:HA	38:l:35:LEU:HD23	1.77	0.42
38:l:74:LEU:HB3	38:l:77:ILE:HD11	2.00	0.42
38:l:84:ILE:HG13	38:l:84:ILE:H	1.44	0.42
43:z:3:ARG:H	43:z:3:ARG:HG2	1.69	0.42
1:A:317:PRO:HB2	1:A:327:VAL:HG11	2.01	0.42
1:A:664:HIS:NE2	1:A:666:LYS:HD3	2.35	0.42
1:A:673:THR:O	1:A:674:LYS:C	2.63	0.42
1:A:939:TRP:CD1	1:A:939:TRP:C	2.97	0.42
1:A:1108:ASP:HA	1:A:1111:GLN:OE1	2.18	0.42
1:A:1839:TRP:CZ3	1:A:1871:PRO:HA	2.55	0.42
49:A:3000:IHP:O12	49:A:3000:IHP:P1	2.78	0.42
3:C:138:LEU:HG	3:C:139:HIS:CG	2.54	0.42
5:E:131:LYS:HD3	5:E:151:THR:C	2.45	0.42
5:E:204:THR:O	5:E:205:SER:OG	2.31	0.42
5:E:240:GLY:O	5:E:252:SER:HA	2.19	0.42
6:F:42:C:C4	6:F:43:A:C5	3.07	0.42
8:6:89:U:H2'	8:6:90:C:O4'	2.20	0.42
15:N:24:GLU:HG3	24:W:189:ILE:HG13	2.02	0.42
20:T:432:ASP:OD1	20:T:432:ASP:C	2.63	0.42
23:V:631:PHE:HB2	23:V:640:THR:HG21	2.02	0.42
28:r:62:ARG:HD2	28:r:63:PRO:CD	2.42	0.42
36:k:32:LEU:HD13	36:k:59:PHE:HB2	2.02	0.42
36:k:94:ARG:HE	36:k:96:ILE:HD11	1.85	0.42
38:l:18:ILE:O	38:l:20:LEU:N	2.52	0.42
38:l:42:ARG:O	38:l:63:GLU:HA	2.20	0.42
40:o:53:GLU:HG2	40:o:75:ARG:CZ	2.50	0.42
1:A:439:GLN:O	1:A:444:ARG:NH1	2.53	0.42
1:A:440:PRO:HG2	1:A:443:VAL:HG13	2.01	0.42
1:A:569:VAL:HG12	1:A:573:GLN:OE1	2.20	0.42
1:A:1404:THR:O	1:A:1405:LEU:HB2	2.20	0.42
1:A:1788:VAL:HG13	45:4:111:ASP:OD1	2.20	0.42
3:C:134:LEU:HD22	3:C:228:PHE:HE1	1.85	0.42
3:C:327:TYR:OH	3:C:372:PHE:HD1	2.03	0.42
3:C:863:ILE:HG12	3:C:870:THR:HG23	2.02	0.42
5:E:178:LEU:HD12	5:E:178:LEU:HA	1.86	0.42
7:G:-12:G:HO2'	7:G:-11:G:C5'	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:56:A:N1	9:H:93:A:C6	2.88	0.42
11:J:269:LEU:HD23	11:J:269:LEU:HA	1.67	0.42
13:L:133:GLU:CD	13:L:133:GLU:H	2.28	0.42
13:L:151:MET:HA	13:L:154:GLU:HG2	2.00	0.42
14:M:159:GLU:OE1	14:M:169:HIS:HB2	2.20	0.42
16:O:131:THR:CG2	24:W:108:ARG:HE	2.33	0.42
17:P:74:LYS:HE2	17:P:74:LYS:HB2	1.72	0.42
17:P:206:LYS:HA	17:P:209:ARG:CD	2.50	0.42
18:R:107:SER:OG	18:R:109:ASP:OD1	2.37	0.42
20:T:371:HIS:CE1	20:T:396:LYS:HD2	2.55	0.42
23:V:234:LEU:HD23	23:V:263:LEU:HD13	2.02	0.42
26:Y:98:TYR:CD1	26:Y:98:TYR:N	2.88	0.42
29:u:268:LEU:HG	29:u:297:MET:HE2	2.02	0.42
32:x:187:LEU:H	32:x:187:LEU:HD12	1.84	0.42
37:m:27:MET:SD	37:m:29:TYR:CE2	3.04	0.42
46:1:358:ILE:HB	46:1:368:LYS:HB2	2.01	0.42
1:A:331:TRP:CE3	1:A:331:TRP:C	2.98	0.41
1:A:1210:LYS:HE2	1:A:1280:ASN:OD1	2.20	0.41
1:A:1485:LEU:HD23	1:A:1485:LEU:HA	1.80	0.41
1:A:1635:TYR:O	1:A:1636:LYS:HG3	2.20	0.41
49:A:3000:IHP:O24	49:A:3000:IHP:P3	2.78	0.41
2:B:67:A:O2'	2:B:68:C:H5'	2.19	0.41
3:C:93:ILE:HG22	3:C:94:ILE:H	1.85	0.41
3:C:319:THR:HG23	3:C:429:GLY:HA3	2.02	0.41
3:C:389:ASP:OD1	3:C:390:THR:N	2.53	0.41
3:C:718:PHE:HB3	3:C:724:TRP:CB	2.49	0.41
10:I:621:ARG:O	10:I:624:GLU:N	2.52	0.41
15:N:17:LEU:HD12	15:N:18:ILE:HG23	2.02	0.41
16:O:25:GLN:HB2	18:R:183:GLN:OE1	2.20	0.41
18:R:248:PRO:HA	18:R:249:PRO:HD3	1.97	0.41
20:T:209:CYS:O	20:T:221:THR:HA	2.20	0.41
20:T:358:ASP:OD1	20:T:365:ARG:HD2	2.20	0.41
23:V:334:TYR:OH	29:u:55:ALA:HB2	2.19	0.41
26:Y:25:LEU:HA	26:Y:26:PRO:HD3	1.88	0.41
36:k:110:LEU:HD23	37:m:59:LEU:HB2	2.01	0.41
38:l:54:MET:SD	38:l:84:ILE:HD12	2.60	0.41
46:1:440:THR:HA	46:1:477:CYS:SG	2.60	0.41
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.61	0.41
1:A:1448:LEU:HA	1:A:1448:LEU:HD12	1.62	0.41
1:A:1634:SER:OG	1:A:1635:TYR:N	2.53	0.41
1:A:1890:GLN:HG2	45:4:105:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:C:H2'	2:B:101:U:H6	1.82	0.41
3:C:64:LYS:HE3	17:P:209:ARG:HH22	1.85	0.41
3:C:90:THR:O	3:C:92:PRO:HD3	2.20	0.41
3:C:295:ASP:OD1	3:C:297:ASN:ND2	2.53	0.41
5:E:277:PHE:N	5:E:277:PHE:CD1	2.87	0.41
8:6:19:G:N1	8:6:20:A:N6	2.68	0.41
8:6:21:A:C2	16:O:152:ARG:HB2	2.55	0.41
9:H:12:G:N7	14:M:200:ARG:NH2	2.67	0.41
17:P:228:ILE:O	17:P:229:LYS:C	2.63	0.41
22:U:83:GLU:C	22:U:85:GLN:H	2.28	0.41
23:V:300:CYS:SG	23:V:304:LEU:HD11	2.60	0.41
27:Z:583:THR:HA	27:Z:628:MET:O	2.18	0.41
30:v:29:ARG:HH11	30:v:29:ARG:HG2	1.85	0.41
37:m:25:TRP:CZ2	37:m:68:ASN:OD1	2.73	0.41
1:A:75:ASP:HB3	1:A:77:THR:HG23	2.02	0.41
1:A:294:ASN:HB2	1:A:297:ASN:HD22	1.84	0.41
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.55	0.41
1:A:1661:TRP:CD1	1:A:1699:THR:O	2.73	0.41
3:C:531:TRP:CE3	3:C:538:HIS:HB3	2.54	0.41
5:E:162:ARG:HE	5:E:162:ARG:HB2	1.54	0.41
11:J:185:ALA:HA	13:L:142:ILE:CD1	2.45	0.41
11:J:306:LEU:HD23	18:R:229:VAL:HG21	2.02	0.41
13:L:169:ARG:O	13:L:173:GLU:HG2	2.20	0.41
18:R:265:ASP:N	18:R:265:ASP:OD1	2.51	0.41
19:S:90:LEU:O	19:S:91:LYS:HD3	2.20	0.41
20:T:344:GLN:OE1	20:T:359:LEU:HB3	2.20	0.41
23:V:392:MET:HB3	23:V:392:MET:HE3	1.78	0.41
26:Y:36:MET:HG2	26:Y:53:GLY:HA3	2.02	0.41
30:v:117:ASP:N	30:v:118:PRO:HD3	2.35	0.41
32:x:172:ASP:HB3	32:x:180:ALA:HB3	2.02	0.41
38:l:37:GLU:N	39:n:22:ASN:ND2	2.68	0.41
40:o:121:LEU:HG	40:o:146:ASP:CG	2.45	0.41
47:2:244:LEU:HD23	47:2:244:LEU:HA	1.86	0.41
48:5:21:UNK:O	48:5:22:UNK:C	2.68	0.41
1:A:59:GLU:HA	1:A:59:GLU:OE2	2.21	0.41
1:A:169:PHE:HE1	46:1:274:VAL:HG21	1.85	0.41
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.82	0.41
1:A:713:LEU:HA	1:A:713:LEU:HD12	1.85	0.41
1:A:804:GLU:OE2	1:A:805:GLU:N	2.53	0.41
1:A:1339:ASP:O	1:A:1340:LEU:C	2.63	0.41
1:A:1776:ILE:CB	1:A:1858:PRO:HA	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:408:LEU:HD12	3:C:408:LEU:HA	1.78	0.41
5:E:75:HIS:HB2	5:E:80:THR:CG2	2.50	0.41
5:E:214:ASP:OD1	5:E:214:ASP:N	2.42	0.41
6:F:93:G:H2'	6:F:94:C:H6	1.85	0.41
10:I:565:ILE:CB	10:I:576:ALA:HB1	2.50	0.41
11:J:238:ASN:C	11:J:240:THR:N	2.74	0.41
16:O:59:PRO:HD2	16:O:63:MET:HB2	2.03	0.41
16:O:76:LYS:HG2	24:W:111:LEU:CD2	2.51	0.41
17:P:44:ARG:HH11	17:P:49:ASP:HB3	1.85	0.41
26:Y:27:LYS:NZ	26:Y:64:GLN:HE21	2.18	0.41
34:i:18:ARG:HB3	34:i:81:THR:HG23	2.02	0.41
36:k:28:PRO:O	37:m:43:GLN:CB	2.68	0.41
36:k:103:GLY:O	37:m:65:ARG:HD2	2.20	0.41
37:m:20:MET:CE	37:m:30:LYS:HE3	2.49	0.41
39:n:5:HIS:O	39:n:36:PRO:HB3	2.20	0.41
40:o:22:ARG:HG3	40:o:65:ARG:HH22	1.86	0.41
41:p:72:PHE:O	41:p:78:PRO:HA	2.20	0.41
1:A:298:ASP:OD1	1:A:300:ASN:N	2.54	0.41
1:A:312:TYR:N	1:A:312:TYR:CD1	2.87	0.41
1:A:1863:VAL:CG1	1:A:1886:GLY:HA2	2.51	0.41
2:B:97:G:H2'	2:B:98:G:H8	1.82	0.41
3:C:854:ARG:NH1	3:C:879:ASP:OD2	2.53	0.41
9:H:82:G:H2'	9:H:83:A:H8	1.86	0.41
13:L:159:LEU:HD23	13:L:159:LEU:HA	1.91	0.41
18:R:132:LEU:O	18:R:132:LEU:HG	2.21	0.41
20:T:329:HIS:NE2	20:T:355:ARG:HG3	2.36	0.41
23:V:166:ILE:HG23	23:V:197:LEU:HD12	2.02	0.41
23:V:197:LEU:O	23:V:201:VAL:HG23	2.20	0.41
23:V:221:ILE:HD11	23:V:225:LYS:HE2	2.03	0.41
23:V:569:LYS:HG2	23:V:570:LEU:N	2.35	0.41
23:V:577:SER:O	23:V:581:ILE:HG12	2.20	0.41
27:Z:606:GLY:HA2	27:Z:618:CYS:O	2.20	0.41
29:u:46:ARG:NH1	29:u:102:ILE:HD11	2.36	0.41
37:m:36:VAL:CG1	37:m:40:MET:HA	2.50	0.41
38:l:31:ILE:HD13	38:l:89:SER:CB	2.50	0.41
46:1:246:VAL:CG2	46:1:254:LYS:HB3	2.50	0.41
47:2:105:SER:O	47:2:140:PRO:HD2	2.20	0.41
1:A:1282:GLN:N	1:A:1282:GLN:CD	2.78	0.41
1:A:1640:SER:OG	1:A:1641:ARG:N	2.54	0.41
3:C:129:ILE:HA	3:C:199:LEU:O	2.20	0.41
3:C:213:ASP:HB2	3:C:615:PRO:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:487:GLY:HA3	3:C:489:GLN:OE1	2.21	0.41
3:C:731:SER:OG	3:C:746:VAL:HG13	2.20	0.41
4:D:149:ARG:C	4:D:151:LYS:H	2.25	0.41
4:D:1211:ASP:O	4:D:1215:HIS:N	2.52	0.41
5:E:71:CYS:SG	5:E:115:LEU:HG	2.60	0.41
6:F:22:A:O4'	15:N:118:ILE:HG22	2.19	0.41
6:F:45:A:N7	8:6:3:A:C4	2.89	0.41
6:F:64:U:H2'	6:F:65:G:O4'	2.20	0.41
9:H:81:G:H2'	9:H:82:G:C8	2.55	0.41
11:J:294:HIS:CE1	13:L:227:THR:OG1	2.74	0.41
11:J:413:GLU:O	11:J:414:HIS:C	2.64	0.41
11:J:440:LEU:HG	11:J:445:LYS:CE	2.50	0.41
12:K:164:ASN:HB3	12:K:168:LYS:NZ	2.35	0.41
14:M:151:ARG:HD3	14:M:151:ARG:C	2.46	0.41
20:T:253:ILE:HD13	20:T:253:ILE:HA	1.94	0.41
23:V:286:THR:O	23:V:290:VAL:HG13	2.20	0.41
23:V:467:LEU:O	23:V:468:ASP:HB2	2.20	0.41
23:V:640:THR:O	23:V:644:ARG:HG3	2.20	0.41
24:W:185:ASP:N	24:W:185:ASP:OD1	2.53	0.41
26:Y:134:MET:HE3	27:Z:1128:GLU:H	1.85	0.41
28:q:56:LYS:HG2	28:q:57:VAL:N	2.36	0.41
29:u:137:CYS:HA	29:u:159:VAL:O	2.19	0.41
29:u:198:LYS:HE2	29:u:231:LYS:HZ2	1.86	0.41
29:u:335:ASP:OD2	29:u:360:LEU:HD13	2.20	0.41
35:j:17:ILE:HG12	35:j:68:PHE:CE2	2.56	0.41
36:k:109:VAL:O	37:m:62:VAL:HA	2.21	0.41
37:m:3:LEU:O	37:m:4:PRO:C	2.64	0.41
38:l:34:TRP:HD1	38:l:88:GLN:N	2.19	0.41
1:A:91:ALA:HB3	1:A:503:MET:HE2	2.01	0.41
1:A:191:ILE:HG13	1:A:571:ALA:HB1	2.02	0.41
1:A:212:PRO:HD2	1:A:225:TYR:OH	2.20	0.41
1:A:984:MET:SD	1:A:1048:MET:HE1	2.60	0.41
1:A:1176:SER:OG	1:A:1185:LEU:HD12	2.21	0.41
1:A:1197:LEU:HA	1:A:1197:LEU:HD12	1.83	0.41
1:A:1418:ARG:HB2	1:A:1461:ASP:O	2.21	0.41
1:A:1633:ALA:HB2	1:A:1637:TRP:CZ3	2.56	0.41
1:A:1692:MET:O	1:A:1692:MET:HE3	2.20	0.41
1:A:1823:HIS:ND1	1:A:1825:SER:OG	2.43	0.41
2:B:10:U:H2'	2:B:11:U:H6	1.85	0.41
2:B:19:A:C2	2:B:59:G:C4	3.09	0.41
2:B:95:G:H21	2:B:96:A:H5''	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:LYS:NZ	17:P:209:ARG:HH12	2.18	0.41
3:C:416:LEU:HD23	3:C:416:LEU:HA	1.93	0.41
3:C:826:ARG:HH12	3:C:910:ASP:CG	2.29	0.41
5:E:89:LEU:CD2	5:E:106:LYS:HG2	2.51	0.41
5:E:309:VAL:HB	5:E:323:LEU:HB2	2.03	0.41
13:L:767:LEU:HD23	13:L:767:LEU:HA	1.90	0.41
14:M:179:ILE:HG13	14:M:180:ASP:N	2.35	0.41
16:O:35:ARG:HD3	24:W:129:ARG:HE	1.85	0.41
16:O:78:LYS:HE3	16:O:94:ILE:HG21	2.02	0.41
16:O:104:LYS:C	16:O:106:ASP:H	2.29	0.41
18:R:51:ILE:N	18:R:52:PRO:CD	2.83	0.41
18:R:137:GLU:HG2	18:R:138:GLU:N	2.36	0.41
20:T:224:ALA:HA	20:T:248:THR:HG23	2.02	0.41
20:T:366:VAL:HG21	20:T:402:ASP:HA	2.02	0.41
23:V:577:SER:CA	23:V:580:ARG:HH11	2.33	0.41
24:W:549:HIS:C	24:W:551:LYS:N	2.79	0.41
25:X:33:GLU:O	25:X:37:ILE:HG13	2.20	0.41
26:Y:9:LYS:HE2	26:Y:9:LYS:HB2	1.82	0.41
29:u:258:VAL:HB	29:u:263:TRP:HB2	2.01	0.41
30:v:88:GLN:NE2	30:v:106:ILE:HG12	2.35	0.41
1:A:84:ASP:O	1:A:88:TYR:HB2	2.21	0.41
1:A:1053:LEU:HD21	1:A:1088:PHE:CD1	2.56	0.41
1:A:1781:ASP:HB3	1:A:1808:PHE:HB3	2.03	0.41
1:A:1921:ASP:HB3	1:A:1966:HIS:CG	2.56	0.41
1:A:1943:LEU:HA	1:A:1943:LEU:HD23	1.94	0.41
3:C:240:GLU:CD	3:C:240:GLU:C	2.88	0.41
3:C:441:PRO:HA	3:C:444:GLY:HA3	2.02	0.41
6:F:3:G:O2'	6:F:4:C:H5'	2.21	0.41
9:H:101:U:N3	33:h:64:ARG:CZ	2.83	0.41
9:H:174:A:C2	9:H:175:G:C4	3.09	0.41
13:L:102:PHE:CD1	13:L:102:PHE:C	2.98	0.41
15:N:73:GLU:O	15:N:76:GLU:HG3	2.21	0.41
18:R:204:LYS:HB2	18:R:204:LYS:HE3	1.86	0.41
20:T:288:LEU:HD23	20:T:288:LEU:HA	1.83	0.41
20:T:483:ASP:O	20:T:485:THR:HG23	2.20	0.41
24:W:87:THR:OG1	24:W:88:MET:N	2.54	0.41
25:X:13:HIS:CE1	26:Y:98:TYR:HH	2.38	0.41
26:Y:86:GLU:OE2	26:Y:86:GLU:N	2.46	0.41
29:u:140:CYS:HB3	29:u:167:VAL:HG12	2.03	0.41
38:l:77:ILE:HA	38:l:77:ILE:HD13	1.84	0.41
46:1:312:GLU:HB2	46:1:315:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1:319:GLN:N	46:1:319:GLN:OE1	2.53	0.41
46:1:440:THR:O	46:1:453:LEU:HD12	2.21	0.41
47:2:104:ASP:OD2	47:2:104:ASP:N	2.54	0.41
1:A:338:VAL:O	1:A:338:VAL:HG13	2.21	0.41
1:A:750:TRP:CD1	1:A:778:ARG:NH2	2.88	0.41
1:A:1275:ARG:O	1:A:1369:TYR:HE1	2.02	0.41
1:A:1593:LEU:HD23	1:A:1593:LEU:HA	1.69	0.41
1:A:1762:TYR:CB	1:A:1888:GLU:HB2	2.49	0.41
1:A:1838:LYS:HG2	1:A:1868:MET:HE1	2.03	0.41
1:A:1862:ILE:CG2	1:A:1887:SER:HB2	2.51	0.41
2:B:14:U:H2'	2:B:15:C:H6	1.85	0.41
2:B:19:A:C6	2:B:59:G:C6	3.08	0.41
2:B:63:A:C4	2:B:64:G:C8	3.08	0.41
2:B:103:G:N1	2:B:111:A:C6	2.89	0.41
3:C:187:THR:HA	3:C:200:PHE:O	2.21	0.41
3:C:445:ALA:O	3:C:449:ILE:N	2.38	0.41
3:C:445:ALA:O	3:C:449:ILE:HG13	2.20	0.41
3:C:493:PHE:CZ	3:C:549:TRP:HB3	2.56	0.41
3:C:743:ASN:HA	3:C:787:VAL:O	2.20	0.41
5:E:66:GLU:CD	5:E:66:GLU:H	2.28	0.41
6:F:40:U:H2'	6:F:41:A:C8	2.54	0.41
9:H:142:C:N4	9:H:143:A:N6	2.69	0.41
9:H:157:G:H5'	9:H:158:G:OP2	2.21	0.41
11:J:439:ALA:HA	11:J:442:ARG:HB3	2.01	0.41
13:L:226:ASP:OD1	18:R:83:SER:HB3	2.21	0.41
14:M:176:THR:O	14:M:179:ILE:N	2.54	0.41
15:N:63:LEU:HD23	15:N:63:LEU:HA	1.90	0.41
18:R:126:ASN:ND2	18:R:128:ASP:O	2.53	0.41
18:R:196:VAL:HG11	24:W:120:ILE:HD12	2.03	0.41
18:R:238:THR:HB	18:R:241:GLU:OE1	2.21	0.41
20:T:284:TYR:CE2	20:T:320:LYS:HA	2.56	0.41
23:V:261:ALA:HB2	23:V:296:PHE:CD1	2.56	0.41
23:V:399:LYS:N	23:V:399:LYS:HD3	2.35	0.41
23:V:600:ASN:HA	23:V:639:LEU:HD11	2.02	0.41
24:W:145:ASN:CG	24:W:146:HIS:N	2.79	0.41
28:r:56:LYS:HD3	28:r:56:LYS:HA	1.76	0.41
29:u:242:LYS:HD3	30:v:48:ILE:HD13	2.02	0.41
29:u:358:ARG:HH12	32:x:191:HIS:HA	1.85	0.41
34:i:18:ARG:NH2	34:i:83:GLU:OE2	2.35	0.41
34:i:46:ASP:OD1	34:i:66:VAL:HA	2.21	0.41
35:j:1:MET:O	36:k:60:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:45:MET:HE2	35:j:47:LEU:HG	2.02	0.41
36:k:40:THR:HG23	37:m:61:GLU:OE2	2.21	0.41
36:k:108:VAL:HG12	36:k:109:VAL:O	2.20	0.41
38:l:34:TRP:CG	38:l:86:LEU:O	2.74	0.41
39:n:30:ILE:N	39:n:42:ILE:HG23	2.36	0.41
46:1:282:HIS:NE2	46:1:309:ARG:HB2	2.36	0.41
46:1:302:CYS:HB2	46:1:335:PRO:HG2	2.03	0.41
47:2:60:ILE:HG12	47:2:99:ALA:HB2	2.02	0.41
1:A:630:TRP:O	1:A:631:ALA:C	2.62	0.41
1:A:712:HIS:CE1	18:R:250:CYS:HB2	2.55	0.41
1:A:863:GLU:HG3	1:A:913:PRO:HB3	2.03	0.41
1:A:880:ARG:HH11	1:A:880:ARG:HD3	1.77	0.41
1:A:1189:MET:CG	1:A:1190:CYS:N	2.84	0.41
1:A:1364:LEU:C	1:A:1365:ILE:HG12	2.46	0.41
1:A:1757:GLU:HA	1:A:1757:GLU:OE2	2.21	0.41
1:A:1781:ASP:OD1	1:A:1783:THR:OG1	2.30	0.41
1:A:1863:VAL:HG22	1:A:1865:ARG:N	2.36	0.41
1:A:1963:GLU:OE1	1:A:1965:HIS:CD2	2.74	0.41
2:B:17:U:O2	2:B:60:G:N2	2.41	0.41
2:B:37:G:C2	2:B:46:U:C2	3.08	0.41
3:C:485:ASP:OD1	3:C:486:ASP:N	2.54	0.41
5:E:198:ALA:O	5:E:210:SER:HA	2.21	0.41
5:E:305:ALA:HA	5:E:329:SER:OG	2.21	0.41
6:F:72:G:C6	6:F:75:G:C8	3.08	0.41
6:F:93:G:H2'	6:F:94:C:C6	2.55	0.41
11:J:212:GLN:NE2	13:L:182:LEU:HD13	2.36	0.41
13:L:733:LYS:HA	13:L:736:ASN:CG	2.46	0.41
18:R:148:ARG:HH11	18:R:148:ARG:HG3	1.86	0.41
18:R:184:GLN:O	18:R:185:GLY:C	2.63	0.41
20:T:185:MET:CB	20:T:186:PRO:HD3	2.49	0.41
25:X:6:LEU:HD11	25:X:10:LYS:HE2	2.02	0.41
29:u:97:LEU:HB3	29:u:133:MET:CE	2.40	0.41
29:u:382:LYS:HG2	29:u:383:ASN:H	1.85	0.41
30:v:59:MET:HA	30:v:62:LEU:HD12	2.02	0.41
39:n:19:LEU:HD21	39:n:42:ILE:HD11	2.02	0.41
1:A:76:MET:HB2	1:A:76:MET:HE3	1.48	0.40
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.93	0.40
1:A:442:LYS:HD2	1:A:610:HIS:NE2	2.37	0.40
1:A:723:ASN:OD1	1:A:785:LYS:HE3	2.21	0.40
1:A:843:LEU:HD23	1:A:843:LEU:HA	1.81	0.40
1:A:1621:LYS:HD3	46:1:272:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:LEU:N	1:A:1647:ASP:OD2	2.41	0.40
1:A:1811:ASN:O	1:A:1815:GLY:N	2.44	0.40
49:A:3000:IHP:P6	49:A:3000:IHP:O25	2.79	0.40
3:C:323:PHE:HE2	3:C:424:PHE:HE1	1.69	0.40
3:C:516:LEU:HD12	3:C:517:GLU:HG3	2.03	0.40
3:C:652:ASP:OD1	3:C:652:ASP:N	2.53	0.40
5:E:206:ASP:CG	5:E:223:ARG:HH12	2.29	0.40
11:J:296:ARG:HD2	13:L:225:TYR:CE2	2.56	0.40
11:J:308:ARG:HA	11:J:308:ARG:HD2	1.64	0.40
11:J:440:LEU:O	11:J:445:LYS:HD2	2.21	0.40
13:L:150:GLU:OE1	13:L:150:GLU:HA	2.21	0.40
15:N:15:TRP:HE3	15:N:74:LEU:HD11	1.87	0.40
15:N:38:GLU:C	15:N:40:LYS:N	2.76	0.40
16:O:57:TRP:O	16:O:65:PHE:HA	2.21	0.40
18:R:142:GLU:OE1	18:R:142:GLU:N	2.54	0.40
21:Q:288:LEU:O	21:Q:295:GLY:HA3	2.20	0.40
23:V:583:VAL:O	23:V:587:PHE:HD2	2.03	0.40
24:W:180:LYS:HG2	24:W:199:TYR:HA	2.04	0.40
25:X:29:LYS:HE3	25:X:33:GLU:OE1	2.21	0.40
26:Y:132:ASN:N	26:Y:133:PRO:HD2	2.36	0.40
29:u:111:ILE:HG21	29:u:122:ILE:HG21	2.03	0.40
36:k:52:LEU:HD22	36:k:99:MET:HE1	2.03	0.40
36:k:108:VAL:HG13	37:m:64:ILE:HG12	2.02	0.40
37:m:17:LYS:O	37:m:19:VAL:HG13	2.21	0.40
46:1:227:CYS:O	46:1:229:CYS:N	2.54	0.40
1:A:34:ALA:HA	5:E:213:ILE:CD1	2.52	0.40
1:A:213:LEU:O	1:A:214:ARG:C	2.65	0.40
1:A:348:PRO:HB3	1:A:394:TYR:CE1	2.57	0.40
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.73	0.40
1:A:886:LEU:HA	1:A:886:LEU:HD23	1.74	0.40
1:A:1001:VAL:HG23	1:A:1002:ASP:O	2.22	0.40
1:A:1621:LYS:HD3	46:1:272:TYR:CE1	2.55	0.40
1:A:1807:ILE:O	1:A:1819:LEU:HD12	2.21	0.40
2:B:97:G:C2	2:B:98:G:C5	3.09	0.40
3:C:276:TYR:HD1	3:C:276:TYR:HA	1.77	0.40
3:C:333:ASP:OD2	39:f:4:ALA:N	2.54	0.40
3:C:363:SER:O	3:C:364:SER:OG	2.26	0.40
6:F:17:C:C2	6:F:18:A:N7	2.89	0.40
11:J:187:VAL:O	11:J:188:GLN:HG2	2.21	0.40
11:J:375:ASP:HB3	11:J:378:ASN:ND2	2.37	0.40
13:L:100:TYR:O	13:L:104:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:177:GLU:HA	14:M:180:ASP:OD2	2.21	0.40
15:N:70:ILE:HG22	15:N:71:SER:O	2.20	0.40
16:O:28:LEU:HB3	18:R:195:ARG:NH2	2.36	0.40
16:O:160:ASN:OD1	16:O:160:ASN:N	2.53	0.40
18:R:91:ASP:OD2	18:R:95:LYS:HG2	2.21	0.40
20:T:333:VAL:HA	20:T:349:SER:HB2	2.03	0.40
29:u:23:MET:SD	29:u:26:VAL:HG11	2.61	0.40
29:u:215:VAL:HG12	29:u:217:ILE:HG12	2.04	0.40
29:u:275:LEU:HD11	29:u:350:ILE:HD11	2.02	0.40
29:u:399:GLN:NE2	31:w:108:ARG:HH12	2.19	0.40
30:v:29:ARG:HG2	30:v:29:ARG:NH1	2.36	0.40
31:w:100:LYS:HB3	31:w:120:GLU:OE2	2.20	0.40
36:k:60:ASP:CG	36:k:64:ASN:HB2	2.46	0.40
36:k:70:VAL:HB	36:k:96:ILE:HB	2.02	0.40
37:m:62:VAL:CG1	37:m:63:LEU:N	2.78	0.40
38:l:86:LEU:CB	39:n:63:ARG:H	2.31	0.40
1:A:480:LYS:CB	15:N:110:ASP:HA	2.51	0.40
1:A:545:HIS:ND1	1:A:548:ARG:NH2	2.69	0.40
1:A:901:LEU:C	1:A:903:SER:H	2.29	0.40
1:A:1443:LYS:HD3	1:A:1443:LYS:HA	1.66	0.40
1:A:1657:THR:OG1	1:A:1658:GLN:N	2.55	0.40
1:A:1883:VAL:O	1:A:1884:ILE:HD13	2.21	0.40
3:C:489:GLN:CD	3:C:489:GLN:H	2.30	0.40
3:C:898:LEU:HD23	3:C:898:LEU:HA	1.73	0.40
6:F:76:A:H2'	6:F:77:C:O4'	2.21	0.40
9:H:27:U:O2'	9:H:28:C:H5'	2.22	0.40
9:H:157:G:C6	9:H:174:A:C6	3.09	0.40
11:J:282:TYR:CZ	11:J:298:ILE:HD11	2.57	0.40
14:M:150:GLU:HA	14:M:153:ARG:HB3	2.04	0.40
16:O:153:THR:OG1	16:O:154:THR:HG23	2.21	0.40
22:U:82:TYR:C	22:U:84:GLU:H	2.27	0.40
29:u:164:PRO:HG3	29:u:192:MET:HE1	2.02	0.40
35:j:10:LEU:HD21	35:j:79:LEU:HD13	2.04	0.40
40:o:97:ASN:H	40:o:122:ARG:HB2	1.85	0.40
47:2:47:TRP:CD1	47:2:91:PRO:HD2	2.56	0.40
1:A:795:LEU:HA	1:A:795:LEU:HD23	1.68	0.40
1:A:835:ASP:OD1	1:A:835:ASP:N	2.53	0.40
1:A:1328:LEU:HD23	1:A:1470:TYR:CE2	2.57	0.40
1:A:1489:LEU:O	1:A:1490:PHE:C	2.64	0.40
1:A:1808:PHE:CE1	1:A:1817:LEU:HD13	2.56	0.40
2:B:9:G:H2'	2:B:10:U:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:SER:OG	3:C:302:PRO:HD2	2.22	0.40
3:C:444:GLY:O	3:C:447:PRO:HD2	2.20	0.40
3:C:510:LEU:HB3	3:C:514:TYR:HD2	1.86	0.40
3:C:531:TRP:HA	3:C:539:ILE:O	2.22	0.40
3:C:749:THR:O	3:C:753:GLU:HB2	2.22	0.40
3:C:857:VAL:HA	3:C:873:ALA:CB	2.51	0.40
6:F:1:G:C6	6:F:2:U:C4	3.10	0.40
9:H:74:U:H2'	9:H:75:A:C8	2.55	0.40
12:K:39:GLU:HG3	28:r:116:VAL:CG2	2.51	0.40
13:L:216:PHE:HB3	16:O:116:TYR:CE2	2.56	0.40
16:O:72:GLN:HA	16:O:82:GLN:HE21	1.85	0.40
16:O:80:VAL:CG1	16:O:94:ILE:HD11	2.51	0.40
16:O:164:ILE:HD11	16:O:184:GLU:H	1.85	0.40
19:S:136:ILE:HA	19:S:139:VAL:HG12	2.04	0.40
26:Y:154:LEU:HA	26:Y:154:LEU:HD23	1.84	0.40
28:q:58:ALA:HB1	28:r:6:SER:CA	2.50	0.40
29:u:214:VAL:CG2	29:u:233:MET:HG2	2.51	0.40
30:v:64:ARG:HH21	30:v:65:ILE:HG12	1.87	0.40
32:x:189:PHE:CE1	32:x:191:HIS:HB2	2.56	0.40
36:k:44:ILE:HG22	36:k:46:CYS:SG	2.62	0.40
37:m:28:GLU:OE2	37:m:73:ARG:NH1	2.54	0.40
46:l:306:ALA:HA	46:l:334:ILE:HA	2.04	0.40
1:A:701:ILE:HG22	1:A:705:LYS:NZ	2.36	0.40
1:A:1900:GLU:H	1:A:1900:GLU:CD	2.30	0.40
2:B:62:G:N1	2:B:63:A:C5	2.90	0.40
2:B:108:G:H3'	2:B:109:G:C8	2.56	0.40
3:C:313:GLN:HB2	50:C:1500:GTP:C5	2.57	0.40
3:C:474:LEU:HA	3:C:498:SER:O	2.22	0.40
3:C:532:ILE:HD13	3:C:532:ILE:HA	1.87	0.40
3:C:589:LYS:HG3	3:C:628:VAL:CG1	2.51	0.40
3:C:622:GLU:O	3:C:625:GLY:N	2.55	0.40
3:C:668:GLU:H	3:C:824:THR:CG2	2.34	0.40
3:C:863:ILE:CG1	3:C:870:THR:HG23	2.51	0.40
5:E:147:LEU:HD22	5:E:179:TRP:HE3	1.86	0.40
5:E:336:HIS:CD2	5:E:337:PRO:HD2	2.57	0.40
6:F:16:G:C2	6:F:17:C:C2	3.10	0.40
8:6:28:A:H4'	16:O:266:ARG:HD2	2.02	0.40
11:J:276:ILE:HG13	11:J:277:THR:N	2.33	0.40
14:M:139:THR:O	14:M:142:ILE:HG22	2.21	0.40
18:R:162:ALA:O	18:R:164:PRO:HD3	2.20	0.40
20:T:343:PRO:HD3	20:T:401:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:576:THR:O	23:V:579:SER:N	2.54	0.40
29:u:28:PHE:HD1	29:u:226:LEU:HD12	1.87	0.40
32:x:181:TYR:CE2	32:x:183:PRO:HG3	2.57	0.40
33:h:22:THR:HA	33:h:67:LYS:O	2.22	0.40
39:n:60:VAL:HG12	39:n:61:VAL:H	1.85	0.40
46:1:428:ASP:HB2	46:1:476:ARG:HD3	2.02	0.40
46:1:437:LEU:HD21	46:1:455:PHE:HD2	1.86	0.40
47:2:254:ASP:HB2	47:2:257:CYS:HB2	2.04	0.40
35:b:33:ASP:H	35:b:37:ASN:N	2.20	0.40
39:f:40:LEU:O	39:f:62:ILE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2247/2335 (96%)	2098 (93%)	127 (6%)	22 (1%)	12	40
3	C	856/972 (88%)	783 (92%)	61 (7%)	12 (1%)	9	31
4	D	1900/2136 (89%)	1838 (97%)	53 (3%)	9 (0%)	24	54
5	E	297/357 (83%)	281 (95%)	16 (5%)	0	100	100
10	I	662/855 (77%)	585 (88%)	75 (11%)	2 (0%)	36	65
11	J	530/848 (62%)	502 (95%)	20 (4%)	8 (2%)	8	30
12	K	144/225 (64%)	136 (94%)	5 (4%)	3 (2%)	5	24
13	L	401/802 (50%)	381 (95%)	19 (5%)	1 (0%)	43	71
14	M	89/243 (37%)	79 (89%)	9 (10%)	1 (1%)	11	38
15	N	141/144 (98%)	121 (86%)	15 (11%)	5 (4%)	3	16
16	O	279/420 (66%)	250 (90%)	25 (9%)	4 (1%)	9	31
17	P	92/229 (40%)	84 (91%)	6 (6%)	2 (2%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	235/536 (44%)	205 (87%)	25 (11%)	5 (2%)	5	24
19	S	157/166 (95%)	148 (94%)	8 (5%)	1 (1%)	21	50
20	T	311/514 (60%)	279 (90%)	24 (8%)	8 (3%)	4	21
21	Q	1304/1485 (88%)	1280 (98%)	24 (2%)	0	100	100
22	U	68/2752 (2%)	63 (93%)	5 (7%)	0	100	100
23	V	444/908 (49%)	430 (97%)	12 (3%)	2 (0%)	24	54
24	W	436/579 (75%)	397 (91%)	34 (8%)	5 (1%)	11	38
25	X	69/425 (16%)	62 (90%)	6 (9%)	1 (1%)	9	31
26	Y	202/323 (62%)	181 (90%)	19 (9%)	2 (1%)	12	40
27	Z	746/1227 (61%)	730 (98%)	15 (2%)	1 (0%)	48	78
28	q	130/504 (26%)	123 (95%)	7 (5%)	0	100	100
28	r	129/504 (26%)	123 (95%)	6 (5%)	0	100	100
28	s	65/504 (13%)	61 (94%)	2 (3%)	2 (3%)	3	18
28	t	65/504 (13%)	64 (98%)	1 (2%)	0	100	100
29	u	388/411 (94%)	379 (98%)	9 (2%)	0	100	100
30	v	142/146 (97%)	140 (99%)	2 (1%)	0	100	100
31	w	89/174 (51%)	88 (99%)	1 (1%)	0	100	100
32	x	23/703 (3%)	23 (100%)	0	0	100	100
33	g	77/126 (61%)	70 (91%)	7 (9%)	0	100	100
33	h	76/126 (60%)	74 (97%)	2 (3%)	0	100	100
34	a	84/240 (35%)	78 (93%)	6 (7%)	0	100	100
34	i	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
35	b	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
35	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
36	c	95/118 (80%)	84 (88%)	11 (12%)	0	100	100
36	k	81/118 (69%)	74 (91%)	6 (7%)	1 (1%)	10	35
37	d	72/86 (84%)	66 (92%)	6 (8%)	0	100	100
37	m	72/86 (84%)	64 (89%)	6 (8%)	2 (3%)	4	19
38	e	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
38	l	73/92 (79%)	63 (86%)	7 (10%)	3 (4%)	2	15
39	f	71/76 (93%)	66 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	n	64/76 (84%)	53 (83%)	8 (12%)	3 (5%)	2	12
40	o	160/255 (63%)	152 (95%)	8 (5%)	0	100	100
41	p	92/225 (41%)	92 (100%)	0	0	100	100
42	y	77/301 (26%)	76 (99%)	1 (1%)	0	100	100
43	z	76/285 (27%)	70 (92%)	5 (7%)	1 (1%)	9	33
44	3	448/646 (69%)	419 (94%)	29 (6%)	0	100	100
45	4	12/450 (3%)	9 (75%)	3 (25%)	0	100	100
46	1	387/654 (59%)	320 (83%)	64 (16%)	3 (1%)	16	44
47	2	165/258 (64%)	159 (96%)	6 (4%)	0	100	100
48	5	1/37 (3%)	0	1 (100%)	0	100	100
All	All	15145/26756 (57%)	14208 (94%)	828 (6%)	109 (1%)	20	47

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
3	C	388	VAL
3	C	801	LEU
3	C	802	HIS
3	C	824	THR
4	D	956	LEU
4	D	957	VAL
11	J	216	ASP
15	N	3	LYS
15	N	37	HIS
18	R	233	PRO
20	T	186	PRO
20	T	406	ILE
20	T	458	SER
36	k	29	LEU
37	m	46	ASN
38	l	37	GLU
39	n	22	ASN
39	n	65	ASN
1	A	330	THR
1	A	368	GLN
1	A	382	GLU
1	A	1763	LEU

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Mol	Chain	Res	Type
3	C	94	ILE
4	D	1583	ASP
4	D	2097	PRO
4	D	2099	THR
11	J	188	GLN
11	J	205	LEU
11	J	217	GLU
11	J	241	VAL
11	J	358	GLU
12	K	66	MET
13	L	200	LYS
15	N	39	GLY
15	N	41	ARG
17	P	205	LYS
18	R	126	ASN
18	R	186	VAL
20	T	329	HIS
23	V	596	LEU
23	V	597	PRO
24	W	155	SER
24	W	156	VAL
28	s	72	PRO
39	n	12	PHE
43	z	63	ALA
46	1	568	VAL
1	A	109	PRO
1	A	167	PRO
1	A	570	ASP
1	A	1211	ASP
1	A	1362	ASP
3	C	363	SER
3	C	441	PRO
11	J	495	PHE
17	P	48	GLN
18	R	223	PRO
20	T	327	SER
24	W	550	ASP
25	X	64	LYS
26	Y	24	LYS
1	A	346	ASP
1	A	364	SER
1	A	366	LYS

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Mol	Chain	Res	Type
3	C	426	GLU
4	D	532	ASN
4	D	1666	THR
4	D	2098	ALA
12	K	78	PRO
14	M	195	LYS
24	W	319	TYR
26	Y	97	ASP
38	l	84	ILE
1	A	56	ALA
1	A	1092	ILE
3	C	83	GLU
3	C	440	SER
3	C	803	ARG
4	D	150	ASP
11	J	341	PRO
16	O	20	PHE
16	O	173	CYS
18	R	70	ALA
20	T	343	PRO
20	T	400	PHE
28	s	71	ILE
37	m	40	MET
1	A	192	GLN
1	A	378	PHE
16	O	106	ASP
38	l	83	ASN
46	1	571	PRO
46	1	616	SER
10	I	51	PRO
10	I	375	ILE
15	N	4	VAL
16	O	134	VAL
24	W	200	VAL
1	A	942	PRO
1	A	1212	GLY
3	C	93	ILE
19	S	12	PRO
1	A	108	MET
1	A	1419	ILE
12	K	77	GLN
20	T	342	GLU

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Mol	Chain	Res	Type
27	Z	986	ARG
1	A	1567	PRO

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	1778/2108 (84%)	1737 (98%)	41 (2%)	44	63
3	C	760/866 (88%)	727 (96%)	33 (4%)	26	51
5	E	256/300 (85%)	252 (98%)	4 (2%)	55	68
10	I	24/749 (3%)	24 (100%)	0	100	100
11	J	241/751 (32%)	236 (98%)	5 (2%)	47	64
12	K	51/196 (26%)	50 (98%)	1 (2%)	48	65
13	L	193/709 (27%)	184 (95%)	9 (5%)	23	50
14	M	85/209 (41%)	80 (94%)	5 (6%)	18	44
15	N	130/130 (100%)	125 (96%)	5 (4%)	29	54
16	O	253/361 (70%)	249 (98%)	4 (2%)	55	68
17	P	90/203 (44%)	85 (94%)	5 (6%)	19	46
18	R	210/457 (46%)	199 (95%)	11 (5%)	21	48
19	S	129/134 (96%)	125 (97%)	4 (3%)	35	59
20	T	269/441 (61%)	261 (97%)	8 (3%)	36	59
22	U	21/2432 (1%)	19 (90%)	2 (10%)	8	29
23	V	324/838 (39%)	316 (98%)	8 (2%)	42	62
24	W	125/502 (25%)	120 (96%)	5 (4%)	28	53
25	X	33/381 (9%)	32 (97%)	1 (3%)	36	59
26	Y	114/289 (39%)	106 (93%)	8 (7%)	14	40
28	q	76/435 (18%)	72 (95%)	4 (5%)	20	47
28	r	75/435 (17%)	71 (95%)	4 (5%)	20	47
28	t	40/435 (9%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	u	344/361 (95%)	343 (100%)	1 (0%)	86	84
30	v	132/134 (98%)	131 (99%)	1 (1%)	73	77
31	w	76/143 (53%)	75 (99%)	1 (1%)	61	71
32	x	23/581 (4%)	23 (100%)	0	100	100
33	h	68/101 (67%)	68 (100%)	0	100	100
34	i	77/177 (44%)	76 (99%)	1 (1%)	61	71
35	j	77/101 (76%)	75 (97%)	2 (3%)	40	61
36	k	80/110 (73%)	73 (91%)	7 (9%)	9	31
37	m	63/74 (85%)	48 (76%)	15 (24%)	1	2
38	l	70/84 (83%)	55 (79%)	15 (21%)	1	3
39	n	59/66 (89%)	54 (92%)	5 (8%)	10	33
40	o	138/218 (63%)	135 (98%)	3 (2%)	45	63
41	p	82/195 (42%)	82 (100%)	0	100	100
43	z	33/240 (14%)	33 (100%)	0	100	100
44	3	18/572 (3%)	18 (100%)	0	100	100
45	4	11/411 (3%)	11 (100%)	0	100	100
46	1	234/572 (41%)	234 (100%)	0	100	100
47	2	135/223 (60%)	134 (99%)	1 (1%)	76	78
48	5	1/1 (100%)	1 (100%)	0	100	100
All	All	6998/17725 (40%)	6779 (97%)	219 (3%)	36	59

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	76	MET
1	A	99	VAL
1	A	330	THR
1	A	336	ASN
1	A	390	ASP
1	A	413	LEU
1	A	439	GLN
1	A	569	VAL
1	A	579	GLN
1	A	621	VAL

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Mol	Chain	Res	Type
1	A	671	THR
1	A	771	VAL
1	A	851	SER
1	A	855	ARG
1	A	897	GLU
1	A	1012	LYS
1	A	1021	ASP
1	A	1041	VAL
1	A	1089	CYS
1	A	1168	VAL
1	A	1286	ASP
1	A	1315	VAL
1	A	1407	ASP
1	A	1416	ILE
1	A	1449	LYS
1	A	1526	LEU
1	A	1529	ILE
1	A	1536	LEU
1	A	1568	THR
1	A	1570	LYS
1	A	1613	THR
1	A	1615	HIS
1	A	1626	CYS
1	A	1765	SER
1	A	1790	ILE
1	A	1800	THR
1	A	1813	ARG
1	A	1838	LYS
1	A	1870	ASP
1	A	1890	GLN
3	C	62	ASP
3	C	68	THR
3	C	71	GLU
3	C	84	GLU
3	C	86	THR
3	C	94	ILE
3	C	112	THR
3	C	146	VAL
3	C	256	CYS
3	C	298	LEU
3	C	300	LEU
3	C	357	THR

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Mol	Chain	Res	Type
3	C	359	LYS
3	C	387	ASP
3	C	419	VAL
3	C	427	PHE
3	C	442	LYS
3	C	452	THR
3	C	458	ASP
3	C	465	MET
3	C	474	LEU
3	C	475	MET
3	C	480	LYS
3	C	489	GLN
3	C	490	PHE
3	C	495	ARG
3	C	517	GLU
3	C	673	LYS
3	C	680	ASN
3	C	704	VAL
3	C	749	THR
3	C	939	ARG
3	C	943	LEU
5	E	81	LEU
5	E	215	ASN
5	E	272	ARG
5	E	290	ARG
11	J	195	LEU
11	J	214	ILE
11	J	239	ARG
11	J	240	THR
11	J	308	ARG
12	K	90	PRO
13	L	24	MET
13	L	25	LYS
13	L	33	ARG
13	L	41	LYS
13	L	138	ARG
13	L	158	ARG
13	L	222	LEU
13	L	235	LEU
13	L	766	ARG
14	M	125	SER
14	M	160	PHE

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Mol	Chain	Res	Type
14	M	172	HIS
14	M	179	ILE
14	M	197	SER
15	N	17	LEU
15	N	34	THR
15	N	101	CYS
15	N	102	CYS
15	N	142	CYS
16	O	45	CYS
16	O	77	LEU
16	O	134	VAL
16	O	198	ILE
17	P	34	ASP
17	P	62	GLU
17	P	65	GLU
17	P	189	ASP
17	P	215	LEU
18	R	72	TYR
18	R	86	LEU
18	R	131	ASP
18	R	134	ARG
18	R	175	GLN
18	R	188	PHE
18	R	212	PHE
18	R	279	HIS
18	R	280	ILE
18	R	297	LYS
18	R	302	VAL
19	S	9	TRP
19	S	10	GLN
19	S	102	ASN
19	S	146	GLU
20	T	220	VAL
20	T	281	ILE
20	T	282	ARG
20	T	400	PHE
20	T	402	ASP
20	T	412	HIS
20	T	455	GLN
20	T	496	THR
22	U	1	MET
22	U	11	ARG

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Mol	Chain	Res	Type
23	V	458	THR
23	V	465	SER
23	V	468	ASP
23	V	502	THR
23	V	535	THR
23	V	553	HIS
23	V	590	LEU
23	V	597	PRO
24	W	97	ASN
24	W	101	THR
24	W	139	LEU
24	W	156	VAL
24	W	160	GLU
25	X	37	ILE
26	Y	4	ARG
26	Y	7	LEU
26	Y	20	ILE
26	Y	22	LYS
26	Y	51	TYR
26	Y	65	ASN
26	Y	108	PHE
26	Y	163	ARG
28	q	19	PRO
28	q	46	PRO
28	q	52	LEU
28	q	117	ILE
28	r	19	PRO
28	r	46	PRO
28	r	60	PRO
28	r	96	LEU
29	u	337	TRP
30	v	13	VAL
31	w	103	HIS
34	i	83	GLU
35	j	35	SER
35	j	54	GLN
36	k	23	GLU
36	k	31	VAL
36	k	40	THR
36	k	42	VAL
36	k	69	ASN
36	k	104	ASP

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Mol	Chain	Res	Type
36	k	107	ILE
37	m	2	SER
37	m	5	LEU
37	m	11	LEU
37	m	14	LEU
37	m	21	VAL
37	m	23	LEU
37	m	25	TRP
37	m	27	MET
37	m	32	TYR
37	m	37	ASP
37	m	44	LEU
37	m	47	THR
37	m	52	ASP
37	m	56	SER
37	m	72	ILE
38	l	21	ILE
38	l	24	TYR
38	l	29	SER
38	l	33	VAL
38	l	34	TRP
38	l	40	ASN
38	l	54	MET
38	l	66	SER
38	l	68	THR
38	l	70	SER
38	l	83	ASN
38	l	86	LEU
38	l	87	LEU
38	l	88	GLN
38	l	90	VAL
39	n	34	PHE
39	n	42	ILE
39	n	60	VAL
39	n	61	VAL
39	n	67	ILE
40	o	55	ARG
40	o	71	VAL
40	o	120	ILE
47	2	119	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	73	HIS
1	A	97	HIS
1	A	112	GLN
1	A	181	ASN
1	A	192	GLN
1	A	294	ASN
1	A	297	ASN
1	A	321	ASN
1	A	361	HIS
1	A	439	GLN
1	A	563	GLN
1	A	584	HIS
1	A	587	GLN
1	A	601	GLN
1	A	659	GLN
1	A	675	GLN
1	A	792	HIS
1	A	957	GLN
1	A	1003	HIS
1	A	1004	ASN
1	A	1014	ASN
1	A	1035	GLN
1	A	1075	GLN
1	A	1122	ASN
1	A	1359	HIS
1	A	1367	ASN
1	A	1450	GLN
1	A	1460	HIS
1	A	1563	HIS
1	A	1580	HIS
1	A	1615	HIS
1	A	1717	ASN
1	A	1816	GLN
1	A	1875	HIS
1	A	1894	GLN
1	A	1944	HIS
1	A	1965	HIS
3	C	87	GLN
3	C	137	HIS
3	C	139	HIS
3	C	245	HIS
3	C	437	HIS

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Mol	Chain	Res	Type
3	C	892	GLN
5	E	165	GLN
11	J	181	ASN
11	J	188	GLN
11	J	259	GLN
11	J	373	HIS
11	J	389	HIS
13	L	73	HIS
13	L	175	GLN
13	L	211	ASN
14	M	134	GLN
14	M	136	HIS
14	M	156	HIS
14	M	172	HIS
14	M	189	GLN
15	N	54	HIS
15	N	99	ASN
16	O	82	GLN
16	O	163	HIS
16	O	196	GLN
16	O	254	GLN
16	O	294	ASN
17	P	204	GLN
18	R	68	HIS
18	R	106	GLN
18	R	126	ASN
18	R	194	GLN
18	R	279	HIS
18	R	314	GLN
19	S	63	GLN
19	S	150	GLN
20	T	217	GLN
20	T	269	GLN
20	T	285	HIS
20	T	350	HIS
20	T	413	ASN
20	T	446	ASN
20	T	455	GLN
23	V	174	ASN
23	V	262	HIS
23	V	306	GLN
23	V	383	ASN

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Mol	Chain	Res	Type
23	V	394	ASN
23	V	553	HIS
24	W	97	ASN
24	W	102	GLN
24	W	172	GLN
25	X	7	ASN
25	X	41	GLN
26	Y	57	ASN
26	Y	64	GLN
26	Y	102	HIS
29	u	138	HIS
29	u	285	ASN
29	u	345	GLN
29	u	379	ASN
30	v	41	ASN
30	v	114	GLN
31	w	67	GLN
31	w	105	ASN
31	w	128	GLN
31	w	137	GLN
32	x	178	ASN
33	h	23	ASN
33	h	60	GLN
34	i	22	GLN
34	i	76	ASN
35	j	12	HIS
35	j	39	HIS
35	j	64	ASN
36	k	62	HIS
36	k	69	ASN
36	k	112	ASN
37	m	58	HIS
38	l	19	ASN
38	l	73	GLN
38	l	83	ASN
38	l	88	GLN
39	n	28	GLN
39	n	65	ASN
40	o	130	HIS
41	p	7	HIS
43	z	48	GLN
46	1	180	HIS

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Mol	Chain	Res	Type
46	1	231	GLN
46	1	236	GLN
46	1	271	GLN
46	1	278	ASN
46	1	329	GLN
46	1	362	ASN
46	1	370	HIS
46	1	480	HIS
47	2	52	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	31 (32%)	3 (3%)
6	F	96/107 (89%)	38 (39%)	12 (12%)
7	G	17/46 (36%)	4 (23%)	1 (5%)
8	6	68/174 (39%)	44 (64%)	5 (7%)
9	H	132/188 (70%)	23 (17%)	1 (0%)
All	All	409/632 (64%)	140 (34%)	22 (5%)

All (140) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	25	C
2	B	26	A
2	B	28	A
2	B	35	U
2	B	36	C
2	B	38	C
2	B	39	C
2	B	45	C
2	B	52	U
2	B	57	G
2	B	71	C
2	B	85	C

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Mol	Chain	Res	Type
2	B	86	C
2	B	87	A
2	B	88	A
2	B	89	U
2	B	90	U
2	B	92	U
2	B	93	U
2	B	94	U
2	B	95	G
2	B	96	A
2	B	97	G
2	B	98	G
2	B	117	A
6	F	6	C
6	F	7	G
6	F	10	U
6	F	12	G
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	33	G
6	F	34	G
6	F	36	A
6	F	37	C
6	F	38	G
6	F	45	A
6	F	46	G
6	F	48	A
6	F	49	G
6	F	51	U
6	F	54	G
6	F	56	A
6	F	58	G
6	F	59	G
6	F	60	C
6	F	61	C
6	F	67	G
6	F	68	C
6	F	74	U
6	F	78	A

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Mol	Chain	Res	Type
6	F	79	C
6	F	80	G
6	F	81	C
6	F	82	A
6	F	83	A
6	F	84	A
6	F	85	U
6	F	86	U
6	F	87	C
7	G	-11	G
7	G	-9	C
7	G	-6	C
7	G	-1	G
8	6	2	U
8	6	3	A
8	6	5	G
8	6	7	G
8	6	8	C
8	6	10	U
8	6	11	A
8	6	12	G
8	6	13	C
8	6	14	A
8	6	16	G
8	6	17	U
8	6	20	A
8	6	21	A
8	6	22	C
8	6	23	U
8	6	24	G
8	6	25	G
8	6	27	U
8	6	30	C
8	6	31	U
8	6	73	G
8	6	74	G
8	6	75	U
8	6	76	U
8	6	77	U
8	6	78	C
8	6	79	C
8	6	80	U

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Mol	Chain	Res	Type
8	6	81	U
8	6	82	G
8	6	83	A
8	6	91	A
8	6	92	U
8	6	97	A
8	6	99	C
8	6	100	C
8	6	101	U
8	6	102	G
8	6	103	U
8	6	104	C
8	6	105	C
8	6	106	C
8	6	107	U
9	H	15	U
9	H	16	U
9	H	17	U
9	H	19	G
9	H	20	G
9	H	24	A
9	H	25	G
9	H	29	A
9	H	30	A
9	H	31	G
9	H	40	C
9	H	101	U
9	H	102	U
9	H	106	G
9	H	112	G
9	H	147	G
9	H	153	A
9	H	154	C
9	H	156	U
9	H	157	G
9	H	164	C
9	H	178	A
9	H	179	C

All (22) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
2	B	20	G
2	B	27	U
2	B	94	U
6	F	5	U
6	F	25	C
6	F	26	U
6	F	33	G
6	F	47	A
6	F	48	A
6	F	50	A
6	F	58	G
6	F	59	G
6	F	81	C
6	F	84	A
6	F	86	U
7	G	-12	G
8	6	16	G
8	6	20	A
8	6	21	A
8	6	22	C
8	6	105	C
9	H	15	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	SEP	R	224	18	8,9,10	1.44	1 (12%)	7,12,14	0.88	0
18	SEP	R	232	18	8,9,10	1.57	1 (12%)	7,12,14	1.76	1 (14%)

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
18	SEP	R	224	18	-	3/6/8/10	-
18	SEP	R	232	18	-	4/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.40	1.61	1.50
18	R	224	SEP	P-O1P	3.17	1.60	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	232	SEP	OG-CB-CA	4.28	112.31	108.14

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	224	SEP	CB-OG-P-O2P
18	R	224	SEP	CB-OG-P-O3P
18	R	232	SEP	CA-CB-OG-P
18	R	232	SEP	CB-OG-P-O1P
18	R	232	SEP	N-CA-CB-OG
18	R	224	SEP	CB-OG-P-O1P
18	R	232	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	232	SEP	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
50	GTP	C	1500	51	33,34,34	1.06	2 (6%)	50,54,54	1.69	10 (20%)
49	IHP	A	3000	-	36,36,36	1.11	0	60,60,60	1.96	18 (30%)

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
50	GTP	C	1500	51	-	6/22/38/38	0/3/3/3
49	IHP	A	3000	-	-	4/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	1500	GTP	C5-N7	-2.42	1.34	1.39
50	C	1500	GTP	O4'-C4'	-2.07	1.40	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	A	3000	IHP	P5-O15-C5	-5.45	108.87	123.43
50	C	1500	GTP	C5-C4-N3	-5.27	120.00	128.39
49	A	3000	IHP	C6-C5-C4	4.95	121.29	110.43
50	C	1500	GTP	C2-N3-C4	4.33	119.76	112.30
49	A	3000	IHP	C6-C1-C2	4.05	119.31	110.43
49	A	3000	IHP	C3-C2-C1	3.74	118.64	110.43
49	A	3000	IHP	C5-C6-C1	3.54	118.18	110.43
50	C	1500	GTP	C2-N1-C6	-3.51	118.75	125.11
49	A	3000	IHP	C4-C3-C2	3.43	117.94	110.43

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C	1500	GTP	N9-C4-N3	3.38	132.71	125.95
50	C	1500	GTP	N9-C8-N7	-2.85	108.11	113.40
49	A	3000	IHP	O11-C1-C2	2.78	114.67	108.76
50	C	1500	GTP	C2'-C1'-N9	-2.65	105.87	113.25
50	C	1500	GTP	C5-C6-N1	2.64	119.96	113.25
49	A	3000	IHP	P3-O13-C3	-2.61	116.46	123.43
50	C	1500	GTP	C8-N7-C5	2.56	108.82	104.26
49	A	3000	IHP	C5-C4-C3	2.46	115.82	110.43
49	A	3000	IHP	O12-P2-O22	-2.32	101.07	109.33
49	A	3000	IHP	P6-O16-C6	-2.31	117.25	123.43
50	C	1500	GTP	O6-C6-C5	-2.30	120.47	126.53
49	A	3000	IHP	O45-P5-O25	2.28	119.74	110.83
49	A	3000	IHP	O43-P3-O33	2.26	116.27	107.80
50	C	1500	GTP	O2B-PB-O3B	2.24	113.33	107.27
49	A	3000	IHP	O12-C2-C1	2.18	113.40	108.76
49	A	3000	IHP	O11-P1-O21	-2.14	101.72	109.33
49	A	3000	IHP	O14-P4-O24	-2.08	101.93	109.33
49	A	3000	IHP	O16-C6-C5	2.03	113.07	108.76
49	A	3000	IHP	O42-P2-O32	2.01	115.33	107.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

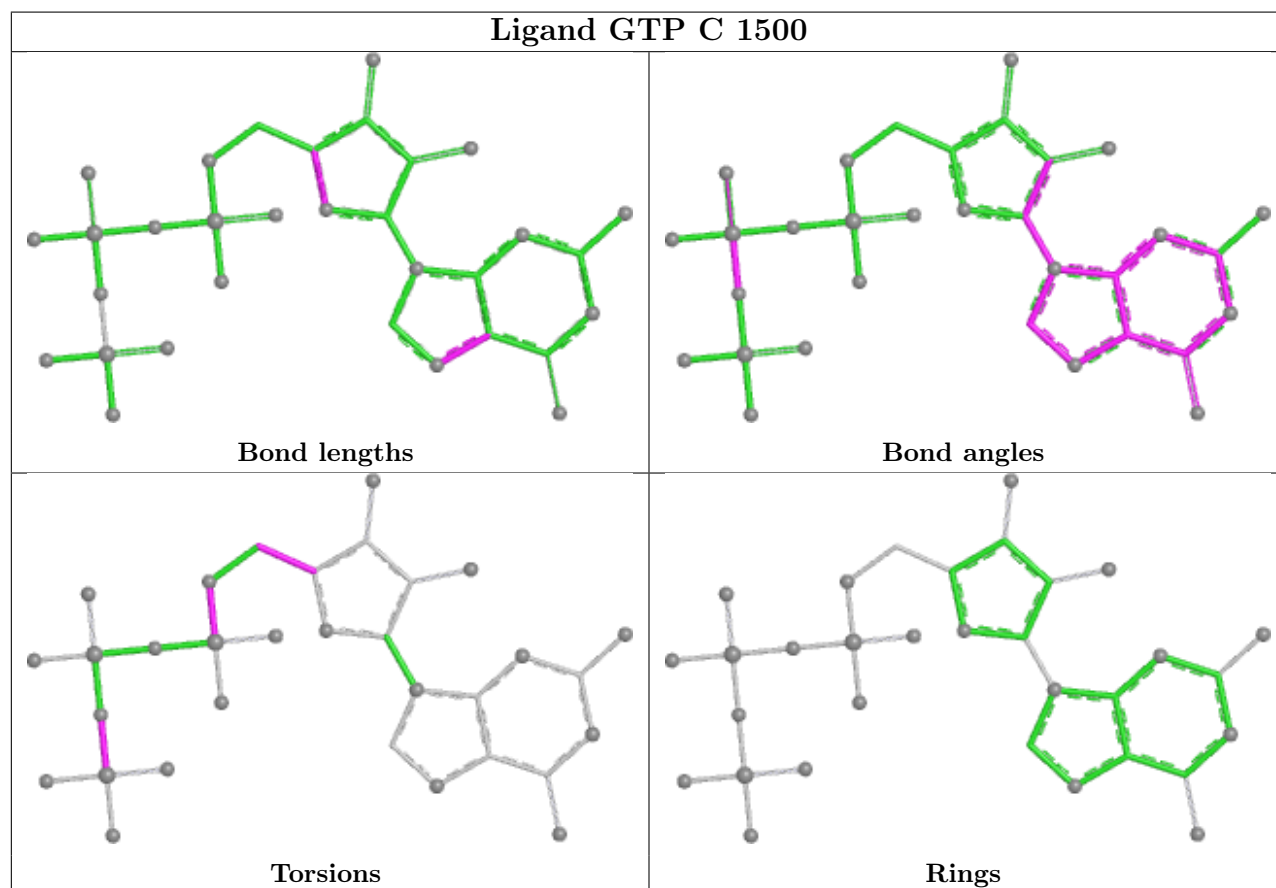
Mol	Chain	Res	Type	Atoms
49	A	3000	IHP	C2-C1-O11-P1
50	C	1500	GTP	PB-O3B-PG-O3G
50	C	1500	GTP	C5'-O5'-PA-O3A
50	C	1500	GTP	C5'-O5'-PA-O1A
50	C	1500	GTP	C5'-O5'-PA-O2A
50	C	1500	GTP	C3'-C4'-C5'-O5'
50	C	1500	GTP	O4'-C4'-C5'-O5'
49	A	3000	IHP	C3-C4-O14-P4
49	A	3000	IHP	C6-O16-P6-O26
49	A	3000	IHP	C2-O12-P2-O22

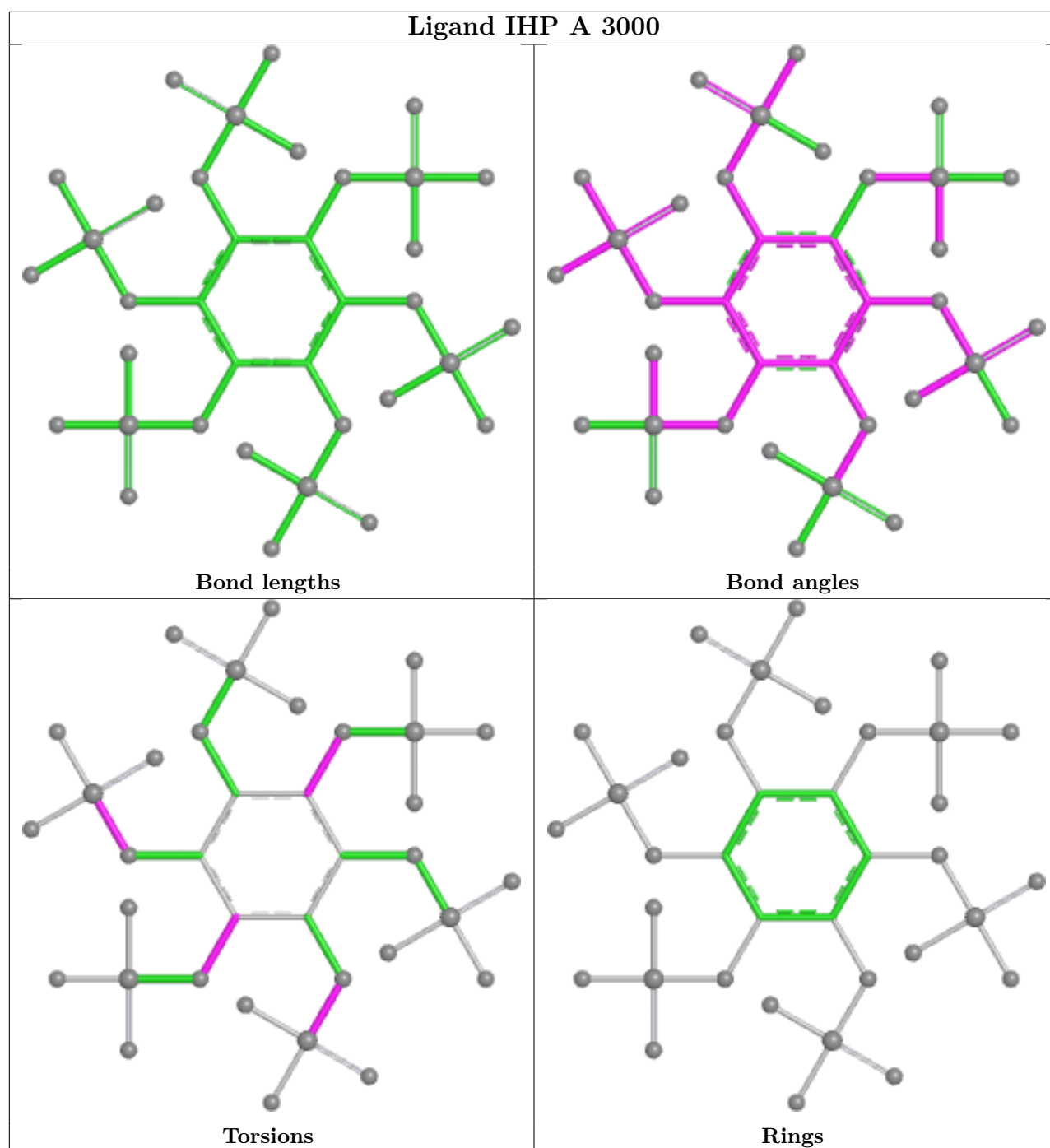
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	C	1500	GTP	6	0
49	A	3000	IHP	8	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

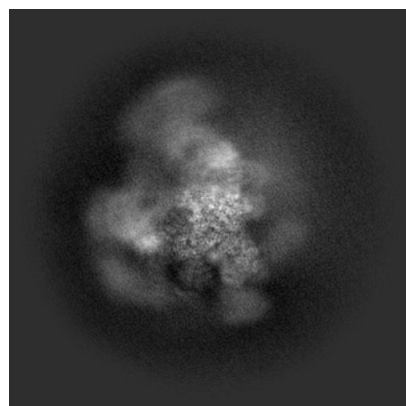
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35113. These allow visual inspection of the internal detail of the map and identification of artifacts.

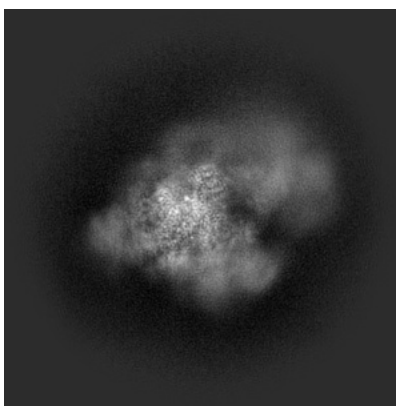
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

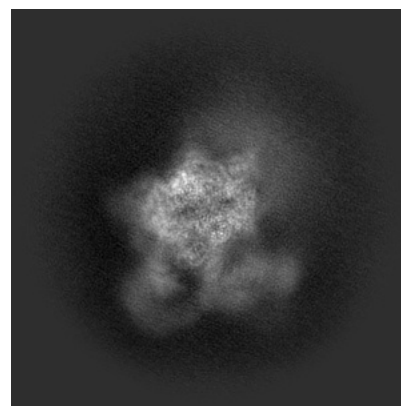
6.1.1 Primary map



X

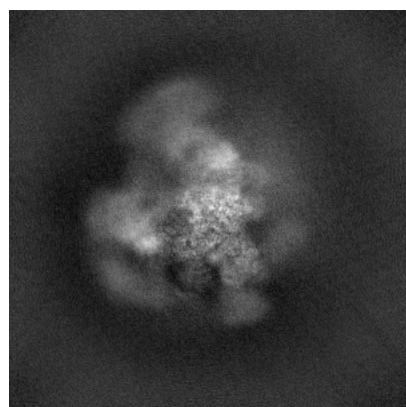


Y

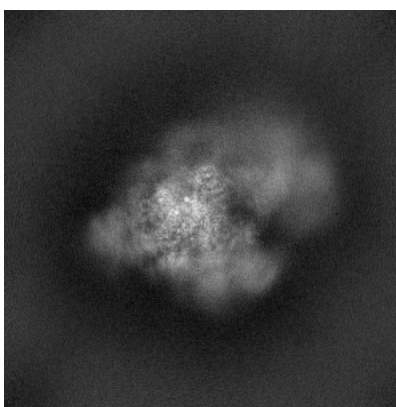


Z

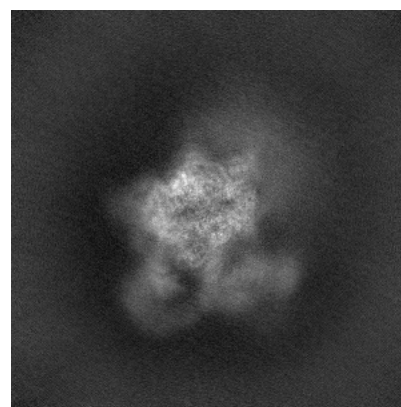
6.1.2 Raw map



X



Y

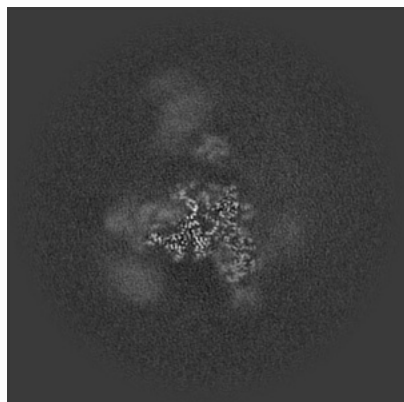


Z

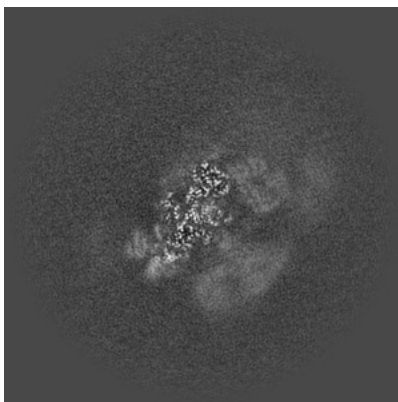
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

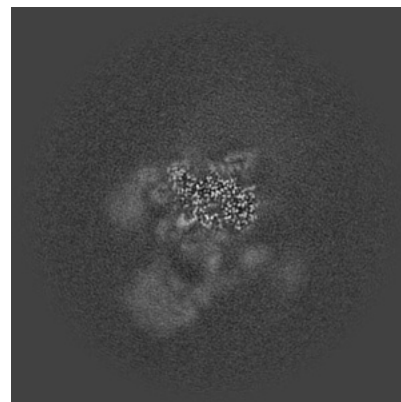
6.2.1 Primary map



X Index: 240

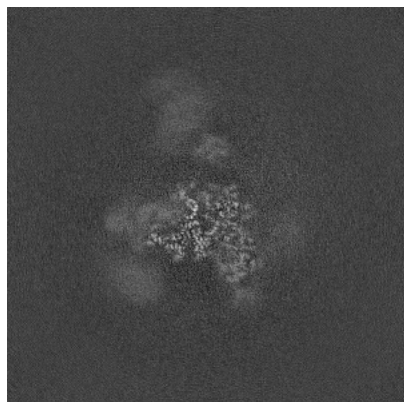


Y Index: 240

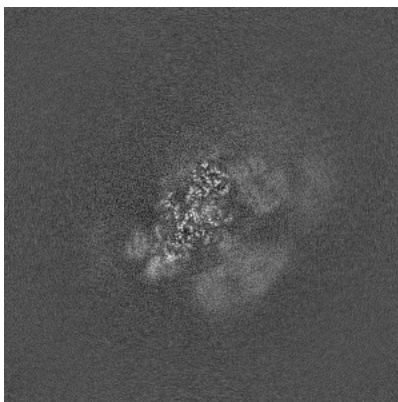


Z Index: 240

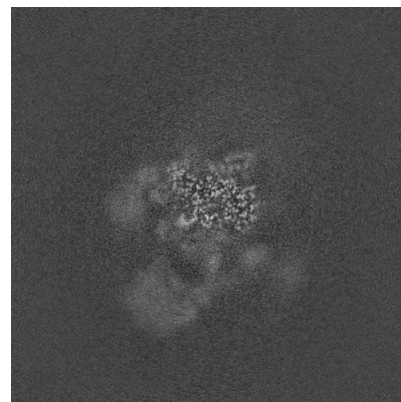
6.2.2 Raw map



X Index: 240



Y Index: 240

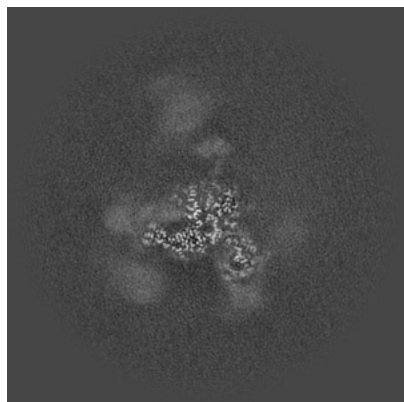


Z Index: 240

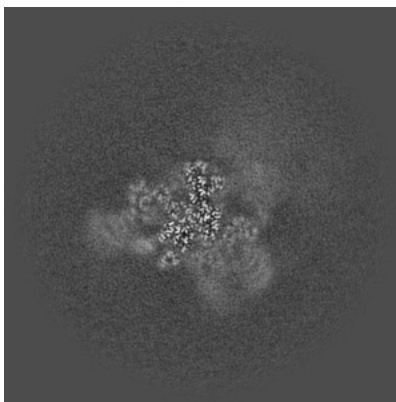
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

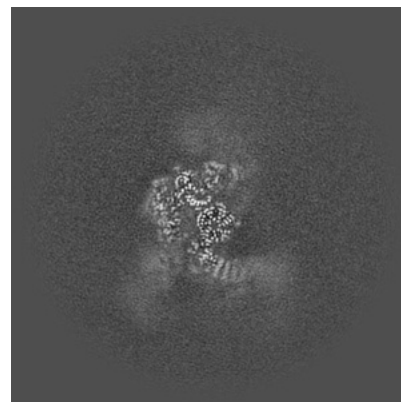
6.3.1 Primary map



X Index: 236

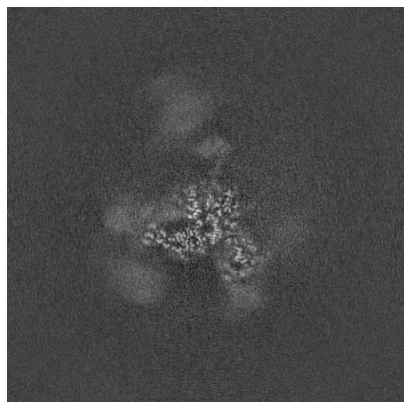


Y Index: 262

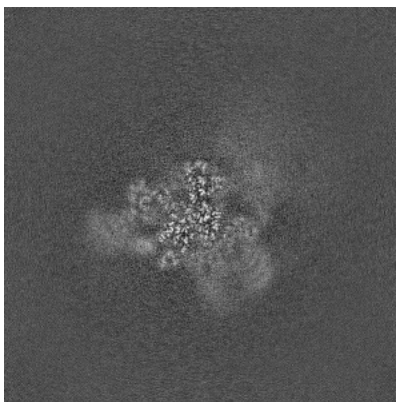


Z Index: 200

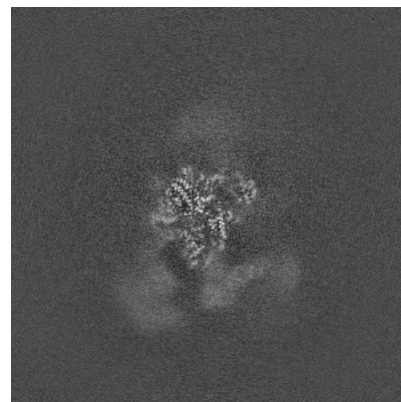
6.3.2 Raw map



X Index: 236



Y Index: 262

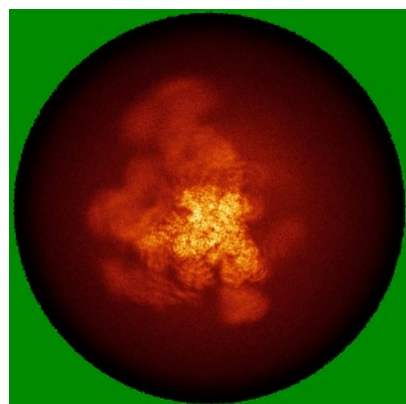


Z Index: 218

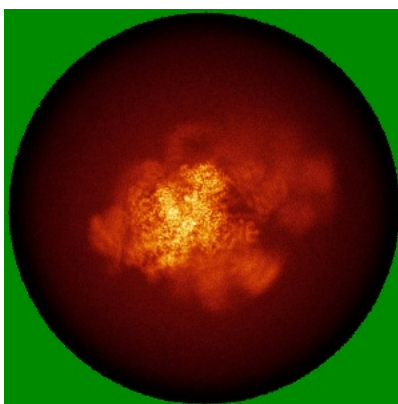
The images above show the largest variance slices of the map in three orthogonal directions.

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

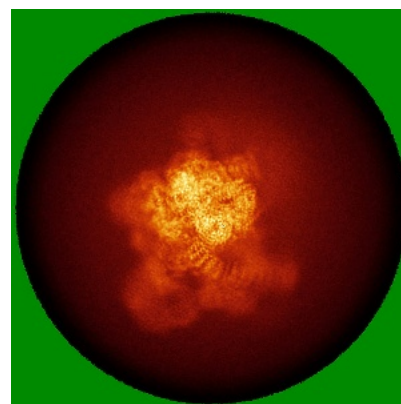
6.4.1 Primary map



X

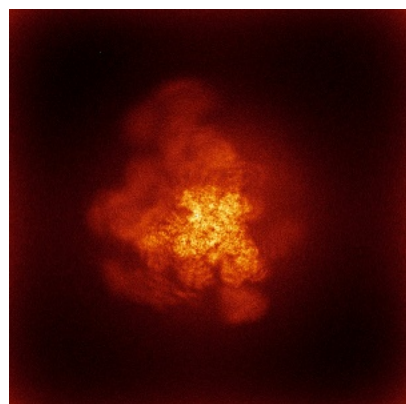


Y

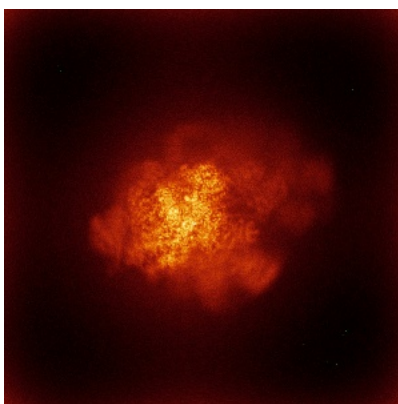


Z

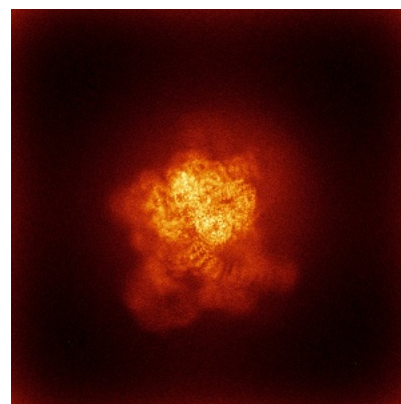
6.4.2 Raw map



X



Y

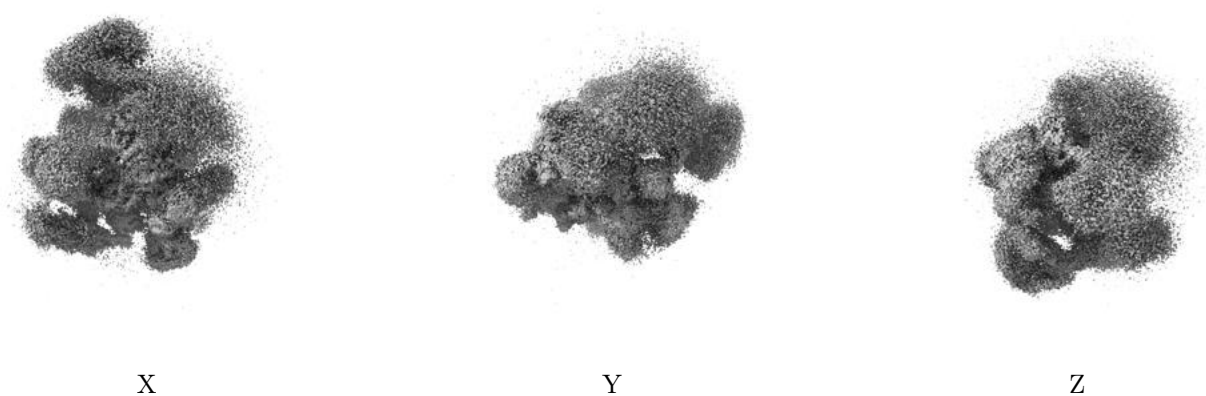


Z

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

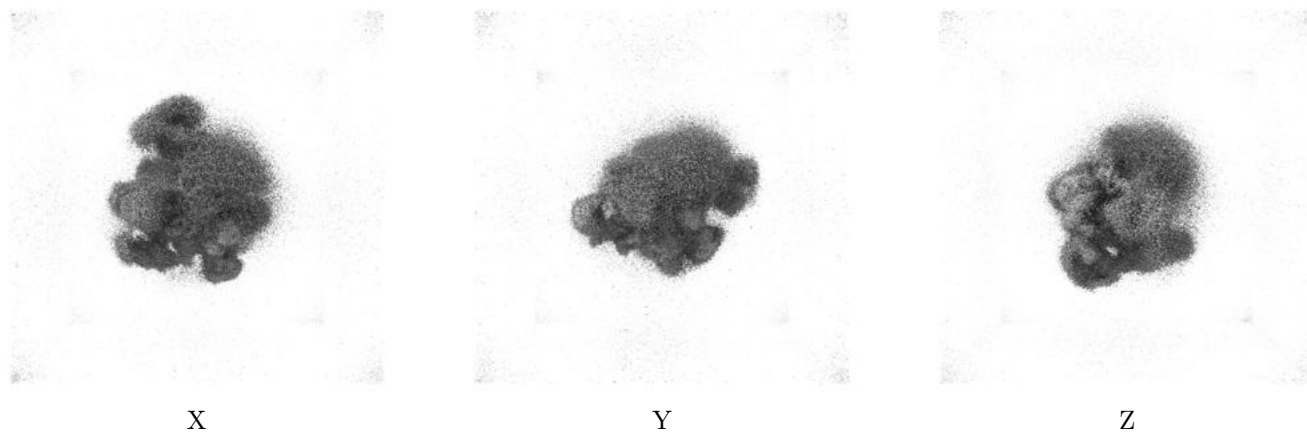
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

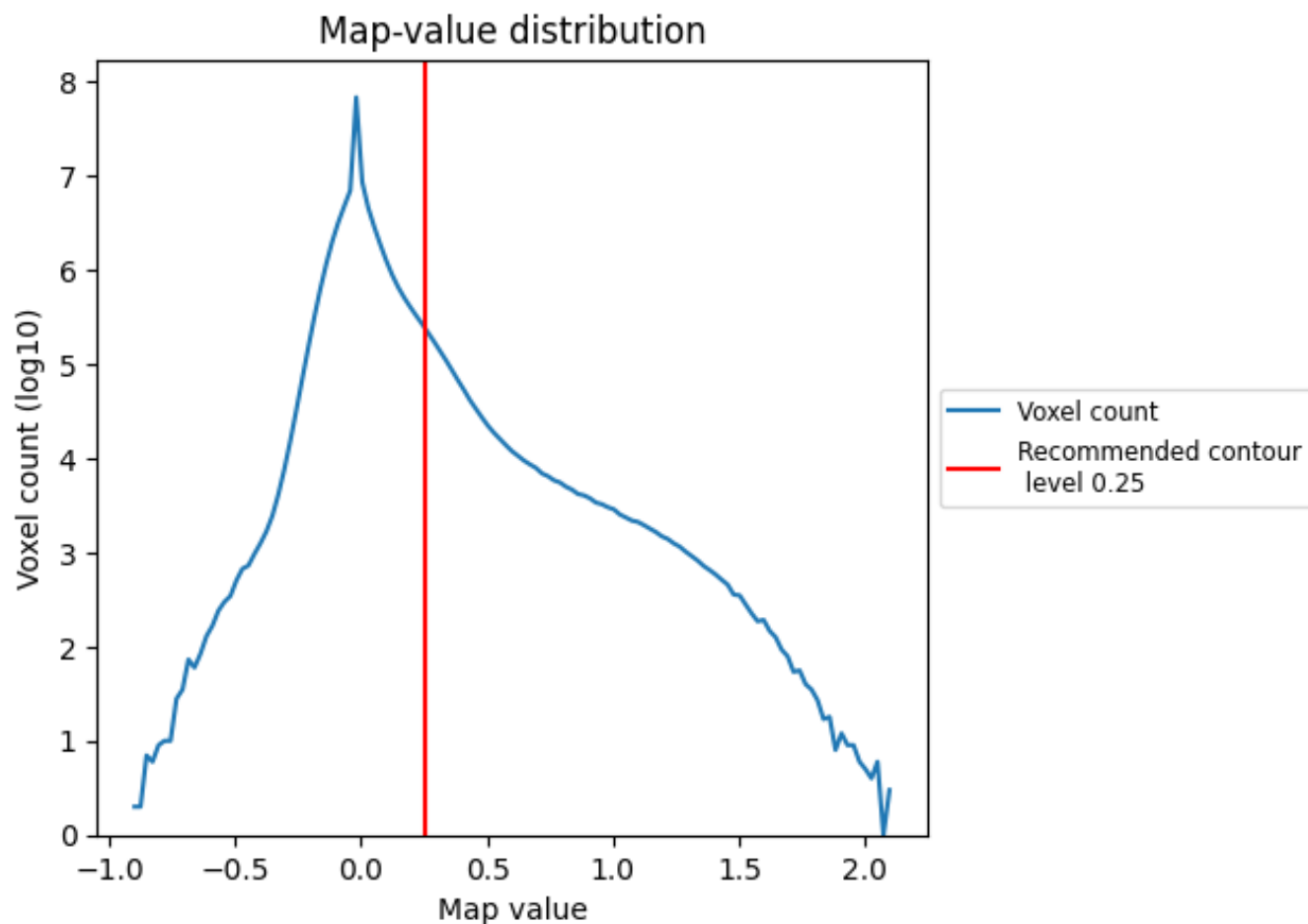
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

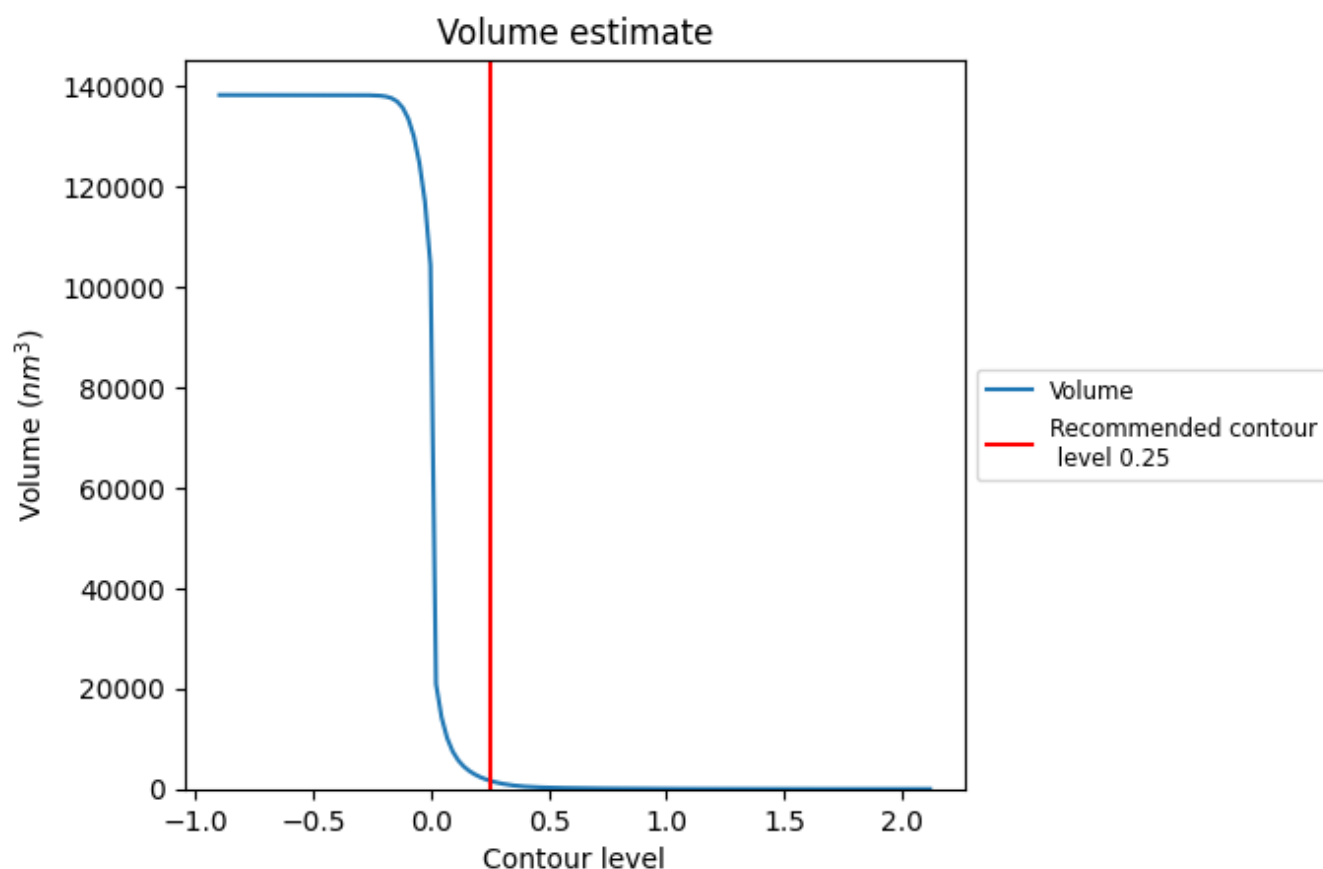
This section contains the results of statistical analysis of the map.

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.

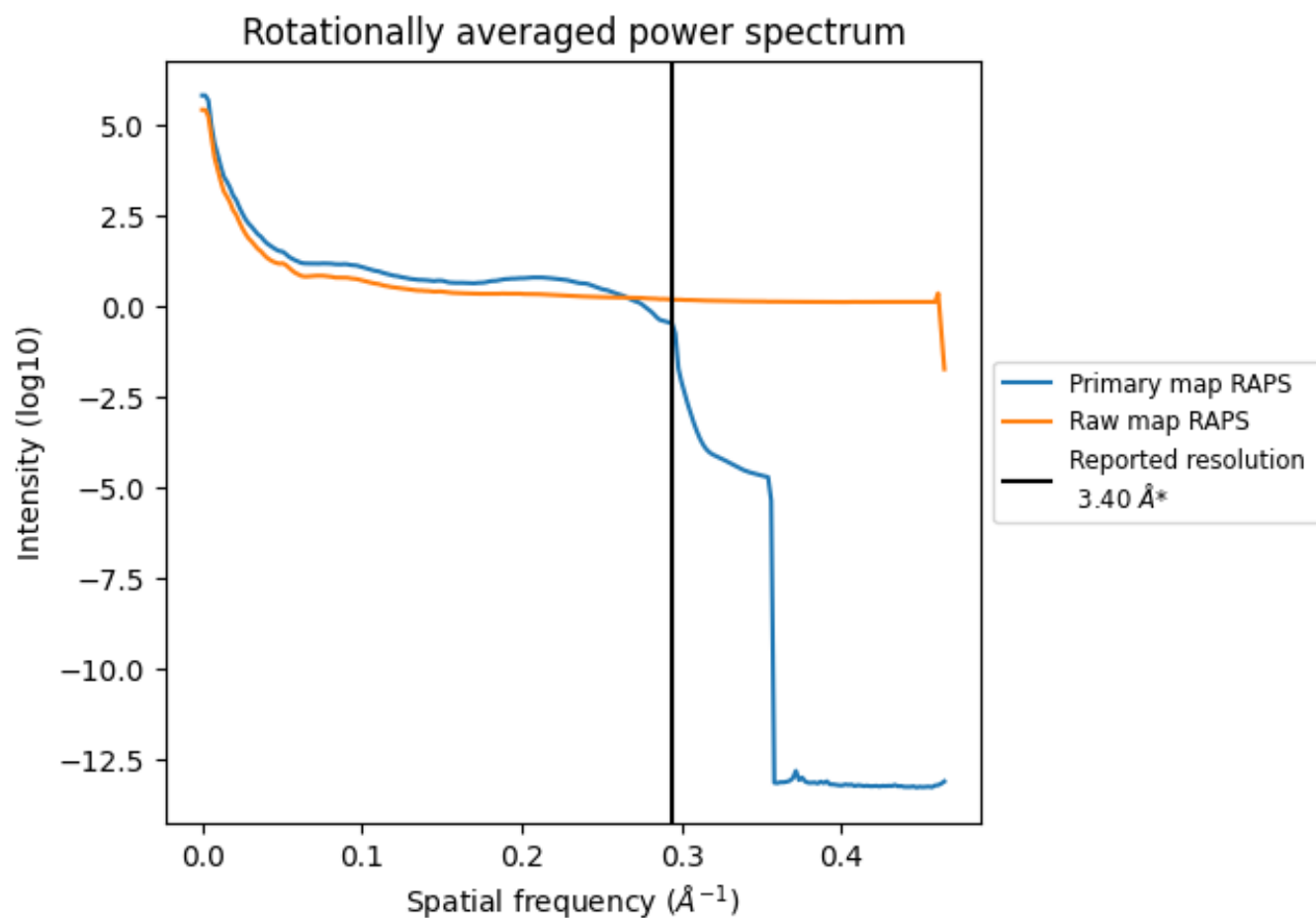
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1654 nm^3 ; this corresponds to an approximate mass of 1495 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

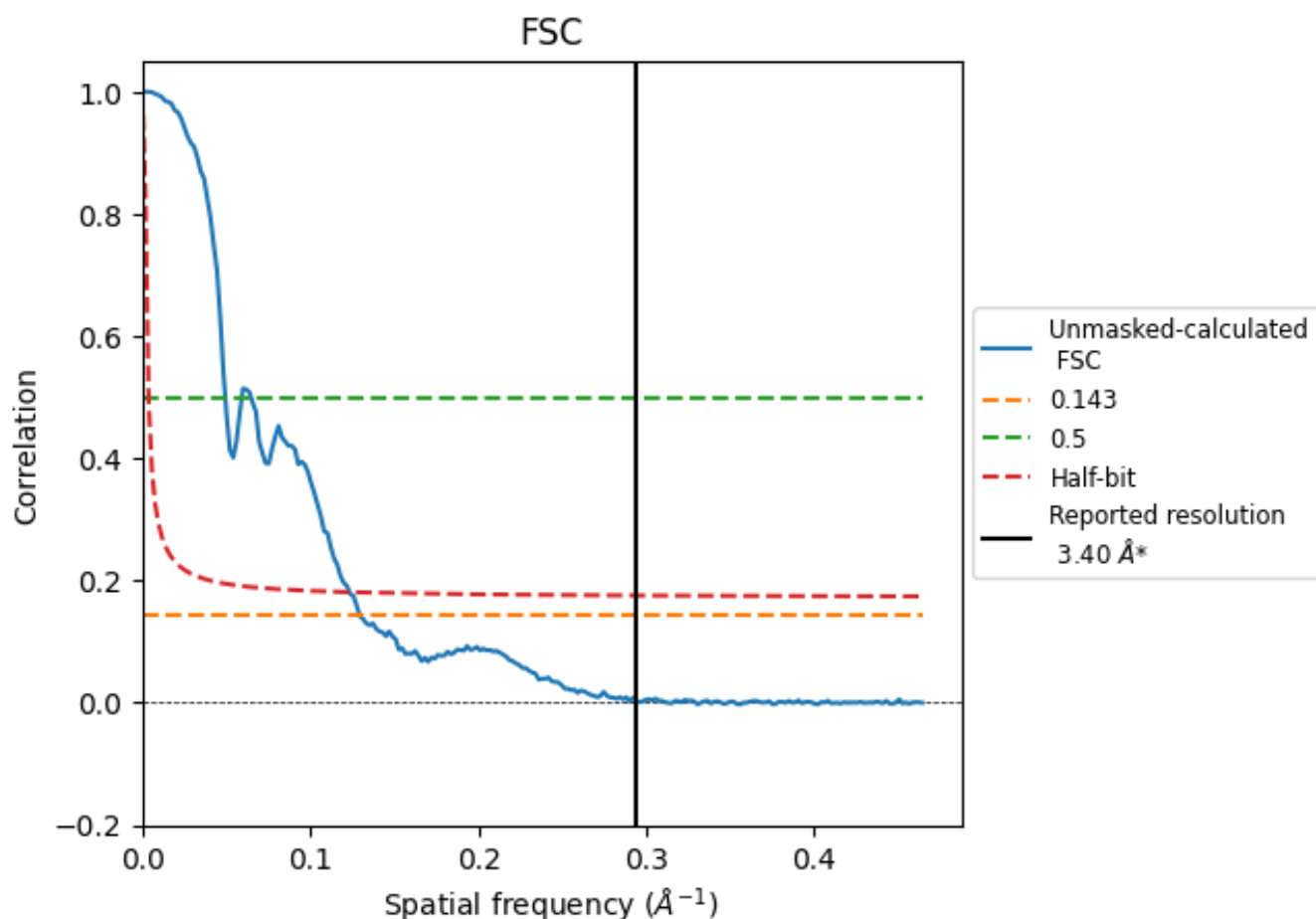


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

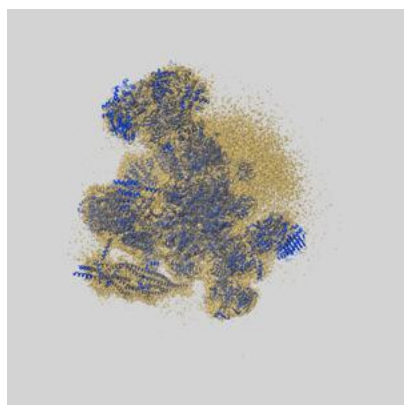
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.73	20.24	8.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.73 differs from the reported value 3.4 by more than 10 %

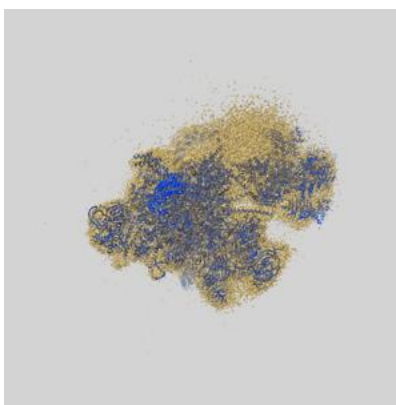
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35113 and PDB model 8I0W. Per-residue inclusion information can be found in section [3](#) on page [15](#).

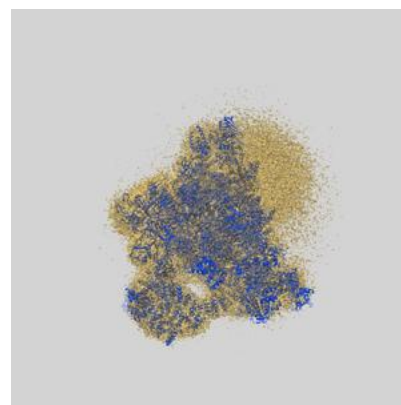
9.1 Map-model overlay [i](#)



X



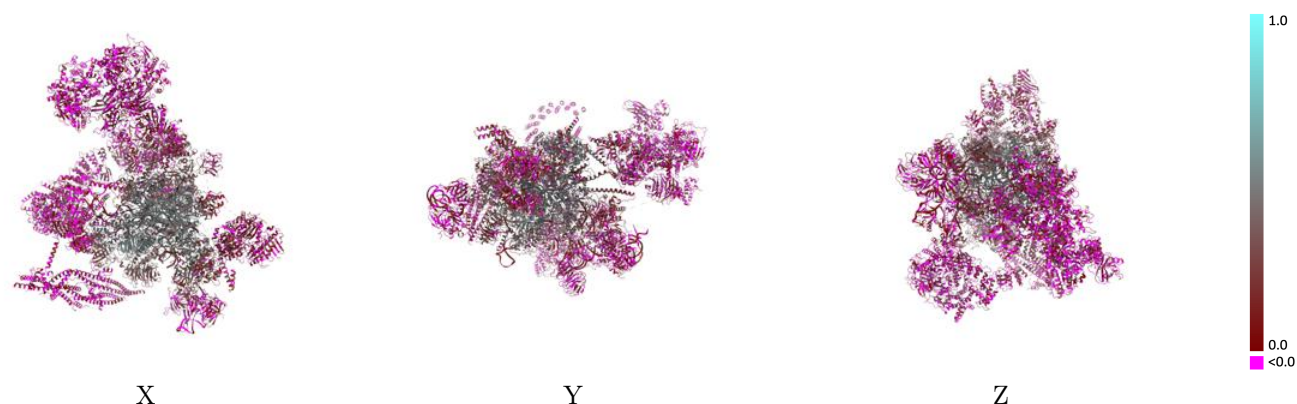
Y



Z

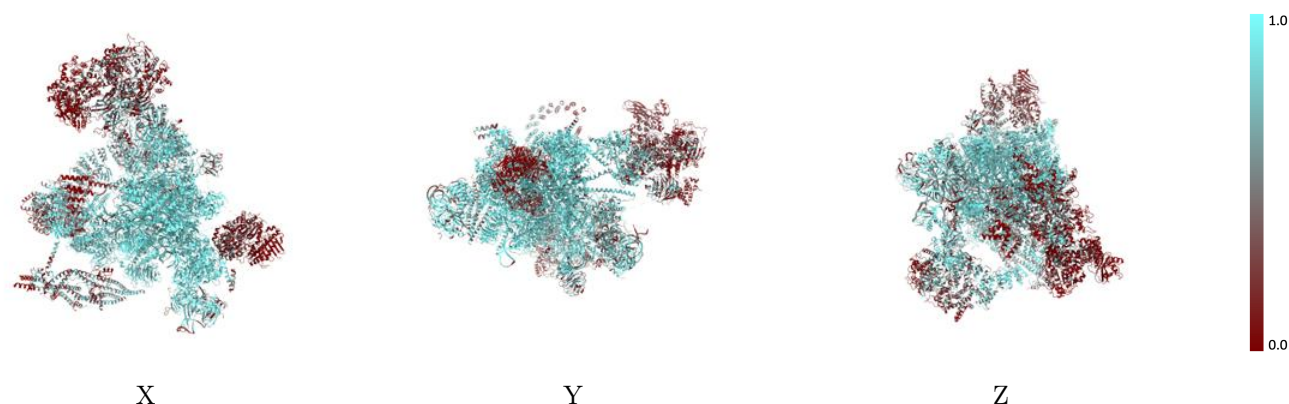
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



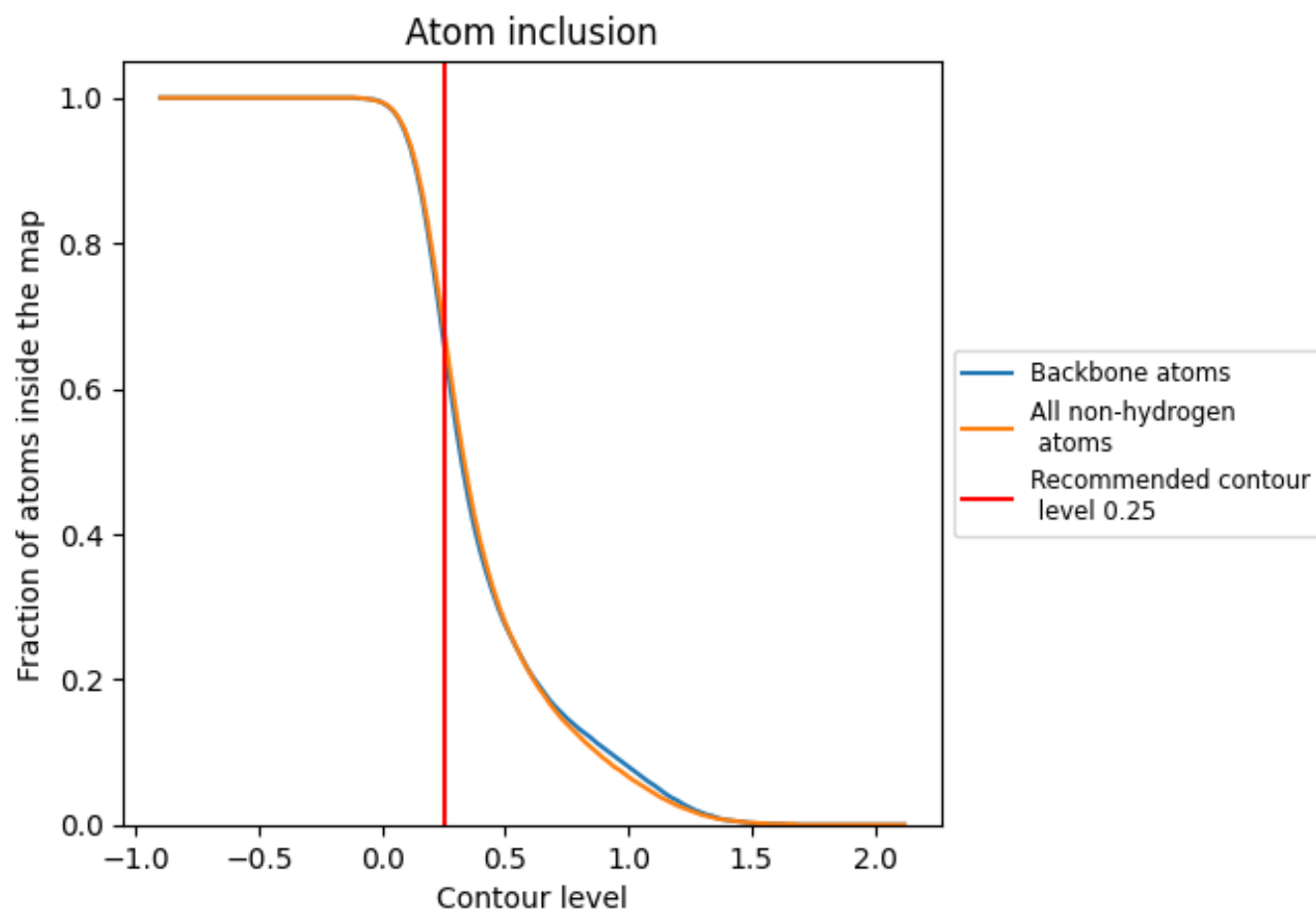
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 68% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.2310
1	 0.7650	 0.2030
2	 0.4860	 0.1790
3	 0.5550	 0.0900
4	 0.4770	 0.1300
5	 0.7070	 0.3070
6	 0.8500	 0.2460
A	 0.8970	 0.4280
B	 0.8620	 0.2550
C	 0.9070	 0.3610
D	 0.1970	 0.0360
E	 0.9250	 0.2880
F	 0.8900	 0.3270
G	 0.6580	 0.3060
H	 0.7390	 0.1200
I	 0.7980	 0.1070
J	 0.7170	 0.2580
K	 0.5170	 0.0640
L	 0.7310	 0.2630
M	 0.7730	 0.2440
N	 0.9240	 0.4300
O	 0.8530	 0.3150
P	 0.8360	 0.3900
Q	 0.3980	 0.0480
R	 0.8710	 0.3850
S	 0.8950	 0.2700
T	 0.9720	 0.5180
U	 0.7280	 0.2950
V	 0.5520	 0.1830
W	 0.6510	 0.1820
X	 0.8570	 0.3260
Y	 0.8390	 0.3640
Z	 0.7080	 0.1440
a	 0.7530	 0.0930
b	 0.8840	 0.1120



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Chain	Atom inclusion	Q-score
c	 0.7630	 0.0580
d	 0.7130	 0.0330
e	 0.7660	 0.1150
f	 0.6710	 0.0530
g	 0.8300	 0.1580
h	 0.5970	 0.0860
i	 0.4440	 0.0620
j	 0.6200	 0.1210
k	 0.6260	 0.0720
l	 0.6980	 0.0900
m	 0.7700	 0.0630
n	 0.6110	 0.0300
o	 0.4800	 0.0920
p	 0.6940	 0.0770
q	 0.2690	 0.0640
r	 0.4390	 0.0700
s	 0.5860	 -0.0050
t	 0.4720	 0.0260
u	 0.1910	 0.1160
v	 0.0310	 0.0980
w	 0.0360	 0.0930
x	 0.0380	 0.0740
y	 0.7280	 0.1030
z	 0.8960	 0.3010