



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 10:51 PM UTC

PDB ID : 8I0R / pdb_00008i0r
EMDB ID : EMD-35107
Title : The cryo-EM structure of human Bact-I complex
Authors : Zhan, X.; Lu, Y.; Shi, Y.
Deposited on : 2023-01-11
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

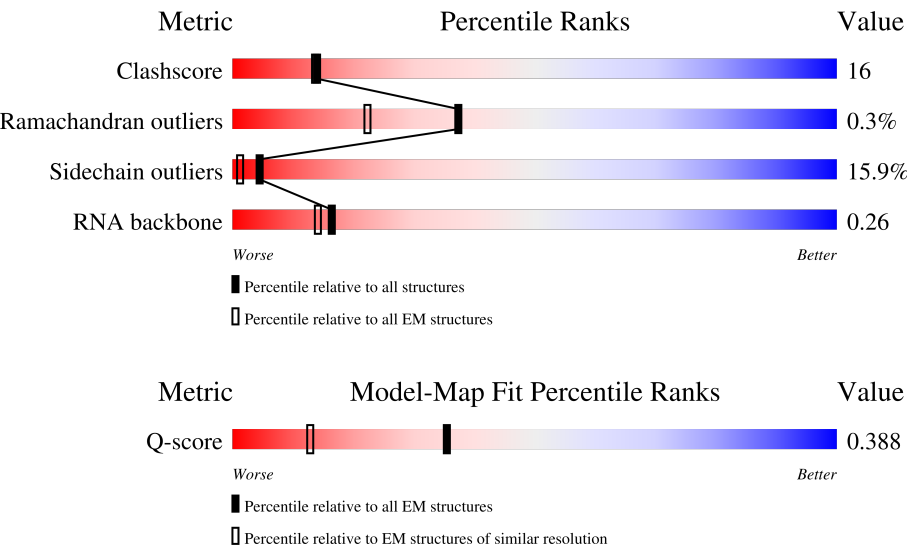
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2335	56%32%7%.
2	B	117	28%44%11%16%
3	C	972	45%36%8%12%

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Mol	Chain	Length	Quality of chain
4	D	2136	
5	E	357	
6	F	107	
7	G	220	
8	H	188	
9	I	855	
10	J	848	
11	K	343	
12	L	802	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	1041	
19	T	514	
20	U	2752	
21	V	908	
22	W	122	
23	X	396	
24	Y	322	
25	Z	619	
26	1	1304	
27	3	1217	
28	p	225	

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Mol	Chain	Length	Quality of chain
29	w	501	
30	u	793	
31	2	895	
32	4	424	
33	6	125	
34	7	110	
35	5	86	
36	9	520	
37	8	904	
38	y	301	
39	v	464	
40	o	255	
41	c	118	
41	h	118	
42	d	86	
42	i	86	
43	a	240	
43	m	240	
44	g	126	
44	l	126	
45	f	76	
45	k	76	
46	e	92	
46	j	92	
47	b	119	

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Mol	Chain	Length	Quality of chain
47	n	119	30% 60% 8% 33%
48	z	472	23% 13% 62%

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 115060 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	2242	Total	C	N	O	S	0	0
			18543	11943	3241	3280	79		

- 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	860	Total	C	N	O	S	0	0
			6724	4298	1122	1272	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1722	Total	C	N	O		0	0
			8528	5084	1722	1722			

- 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	71	Total	C	N	O	P	0	0
			1481	663	243	504	71		

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	P	0	0
			3539	1581	607	1184	167		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	593	Total	C	N	O	0	0
			2991	1805	593	593		

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	249	Total	C	N	O	S	0	0
			2116	1355	380	375	6		

- Molecule 11 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	128	Total	C	N	O	S	0	0
			1059	660	190	204	5		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	99	Total	C	N	O	S	0	0
			829	532	149	144	4		

- Molecule 13 is a protein called Protein BUD31 homolog.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	290	Total	C	N	O	0	0
			1433	853	290	290		

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	42	Total	C	N	O	S	0	0
			362	231	63	66	2		

- Molecule 16 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	1329	Total	C	N	O	0	0
			6730	4072	1329	1329		

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	237	Total	C	N	O	S	0	0
			1889	1171	347	360	11		

- Molecule 18 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	643	Total	C	N	O	0	0
			3180	1894	643	643		

- Molecule 19 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	320	Total	C	N	O	S	0	0
			2507	1582	456	462	7		

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	468	Total	C	N	O	S	0	0
			3008	1873	546	576	13		

- Molecule 22 is a protein called Unknown polymer.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	43	Total	C	N	O	0	0
			229	140	46	43		

- Molecule 23 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	154	Total	C	N	O	S	0	0
			1279	819	231	227	2		

- Molecule 24 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	118	Total	C	N	O	S	0	0
			948	605	163	176	4		

- Molecule 25 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	137	Total	C	N	O	S	0	0
			1142	708	213	216	5		

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	1	993	Total	C	N	O	P	S	0	0
			7866	5018	1363	1438	1	46		

- Molecule 27 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	169	Total	C	N	O	0	0
			851	513	169	169		

- Molecule 29 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	434	Total	C	N	O	S	0	0
			2275	1287	491	493	4		

- Molecule 30 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	u	187	Total	C	N	O	0	0
			834	460	187	187		

- Molecule 31 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	250	Total	C	N	O	S	0	0
			1807	1134	340	326	7		

- Molecule 32 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	4	161	Total	C	N	O	0	0
			792	470	161	161		

- Molecule 33 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	109	Total	C	N	O	S	0	0
			906	582	157	163	4		

- Molecule 34 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	105	Total	C	N	O	S	0	0
			811	502	145	151	13		

- Molecule 35 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5	81	Total	C	N	O	S	0	0
			669	422	117	124	6		

- Molecule 36 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	379	Total	C	N	O	S	0	0
			2636	1633	479	516	8		

- Molecule 37 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	8	115	Total	C	N	O	S	0	0
			931	602	154	170	5		

- Molecule 38 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	y	79	Total	C	N	O	S	0	0
			390	232	79	79			

- Molecule 39 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	v	173	Total	C	N	O	S	0	0
			1041	602	219	217	3		

- 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
			816	492	162	162			

- Molecule 41 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	95	Total	C	N	O	S	0	0
			482	292	95	95			
41	c	97	Total	C	N	O	S	0	0
			388	194	97	97			

- Molecule 42 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	i	72	Total	C	N	O	0	0
			359	215	72	72		
42	d	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 43 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	m	82	Total	C	N	O	0	0
			413	249	82	82		
43	a	86	Total	C	N	O	0	0
			344	172	86	86		

- Molecule 44 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	l	83	Total	C	N	O	0	0
			415	249	83	83		
44	g	81	Total	C	N	O	0	0
			324	162	81	81		

- Molecule 45 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	k	73	Total	C	N	O	0	0
			364	218	73	73		
45	f	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 46 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	j	81	Total	C	N	O	0	0
			403	241	81	81		
46	e	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 47 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	n	80	Total	C	N	O	0	0
			402	242	80	80		

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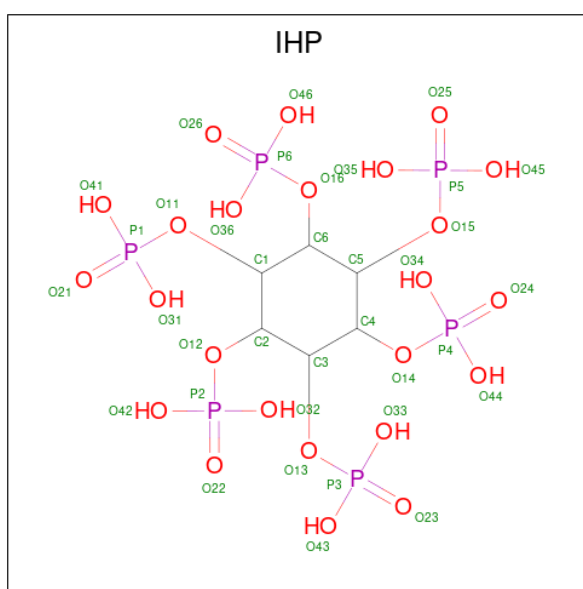
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Mol	Chain	Residues	Atoms				AltConf	Trace
47	b	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 48 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

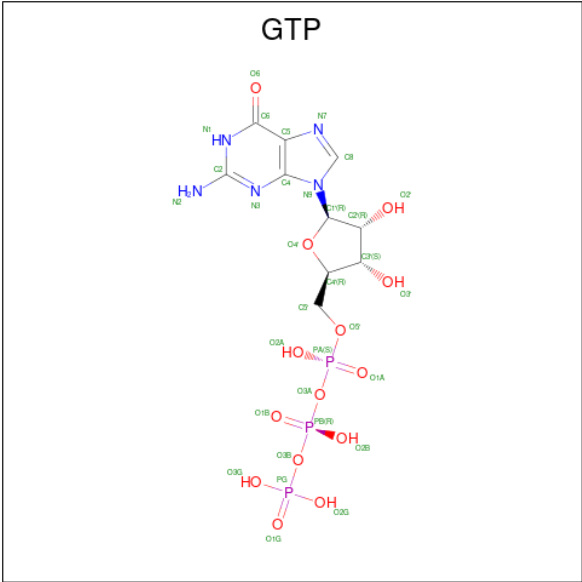
Mol	Chain	Residues	Atoms					AltConf	Trace
48	z	177	Total	C	N	O	S	1	0
			1402	884	243	270	5		

- 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	5	Total	Mg	0
			5	5	

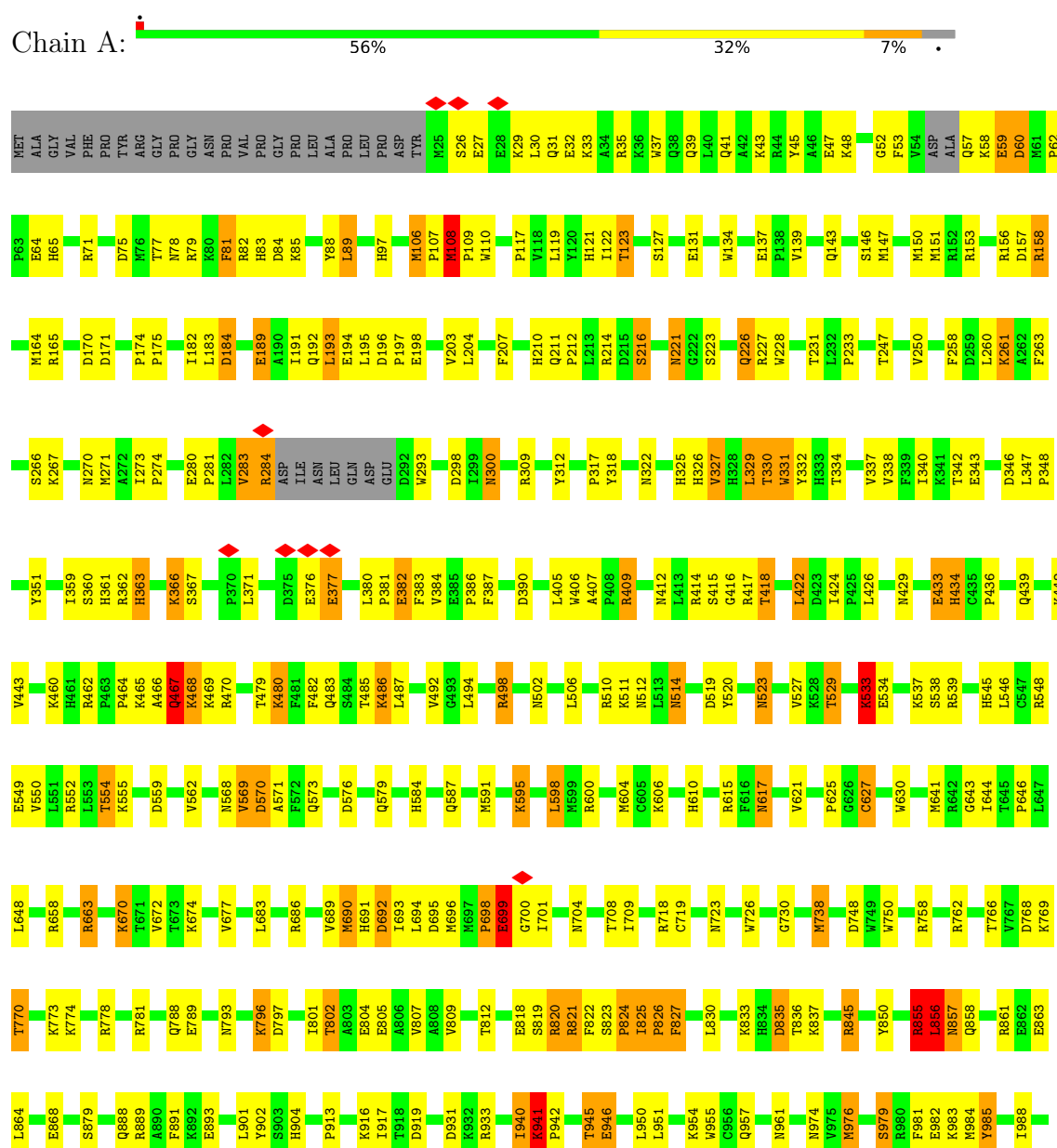
- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	K	1	Total	Zn	0
			1	1	
52	N	3	Total	Zn	0
			3	3	
52	7	3	Total	Zn	0
			3	3	

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.

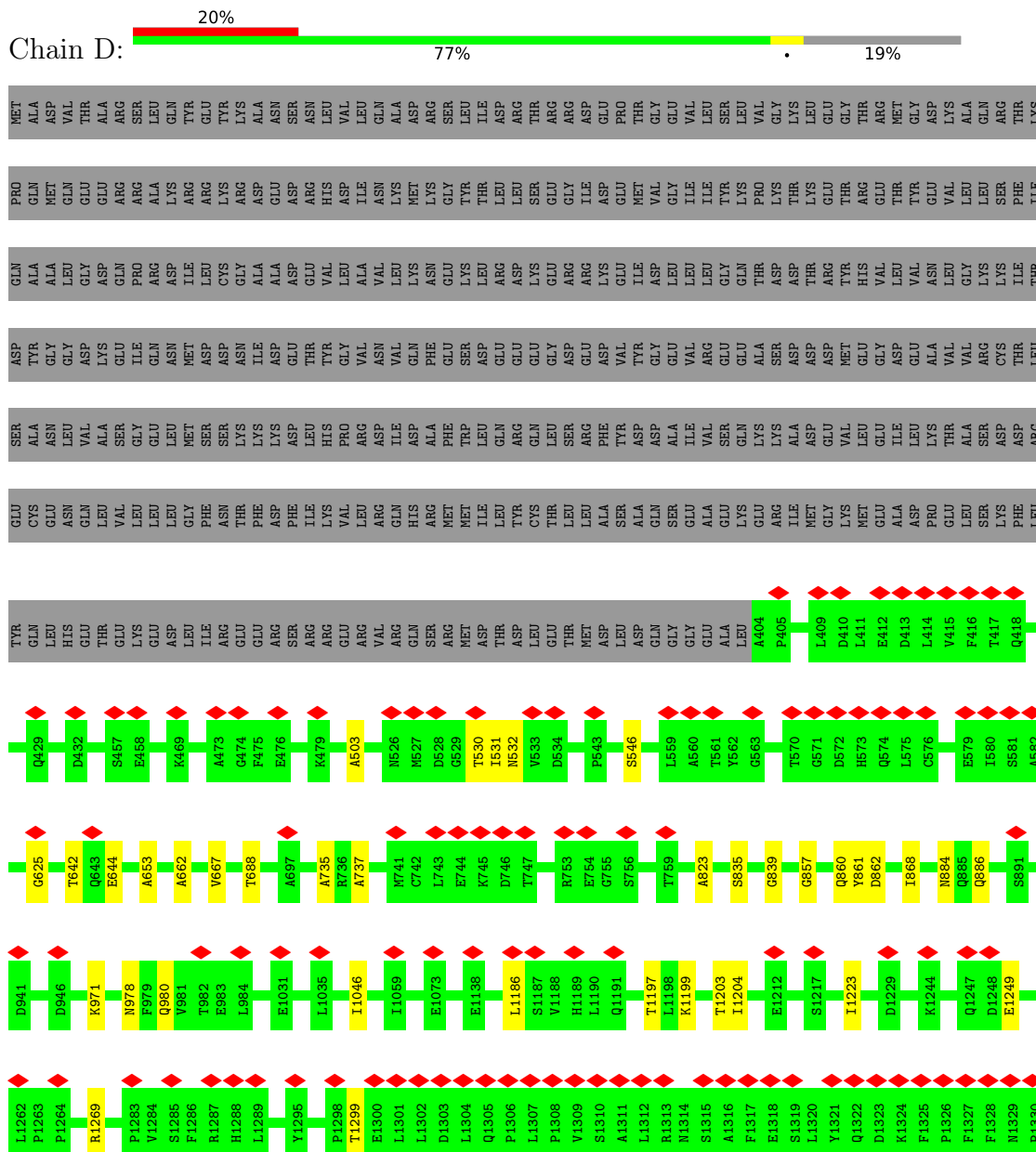
- Molecule 1: Pre-mRNA-processing-splicing factor 8

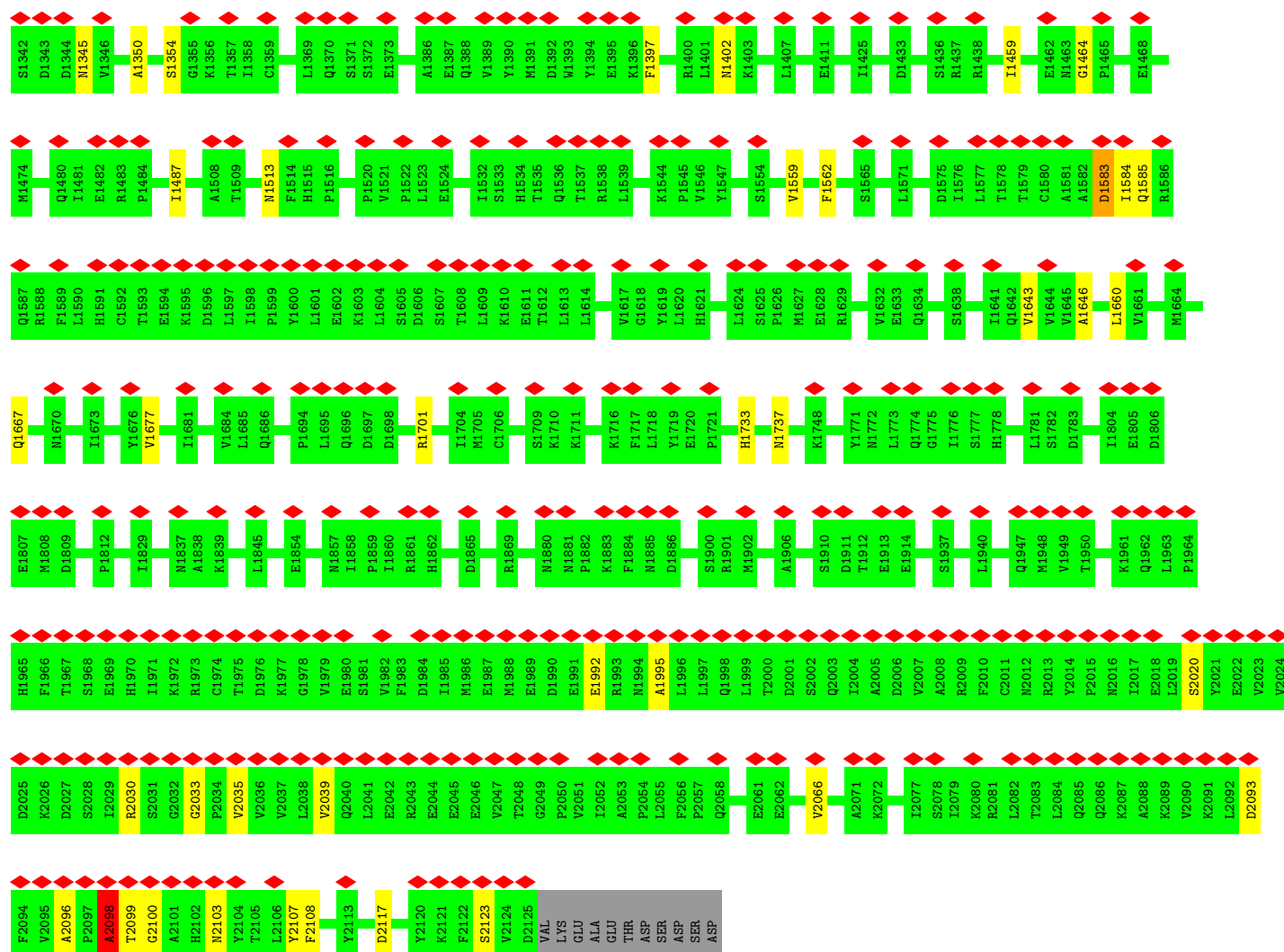




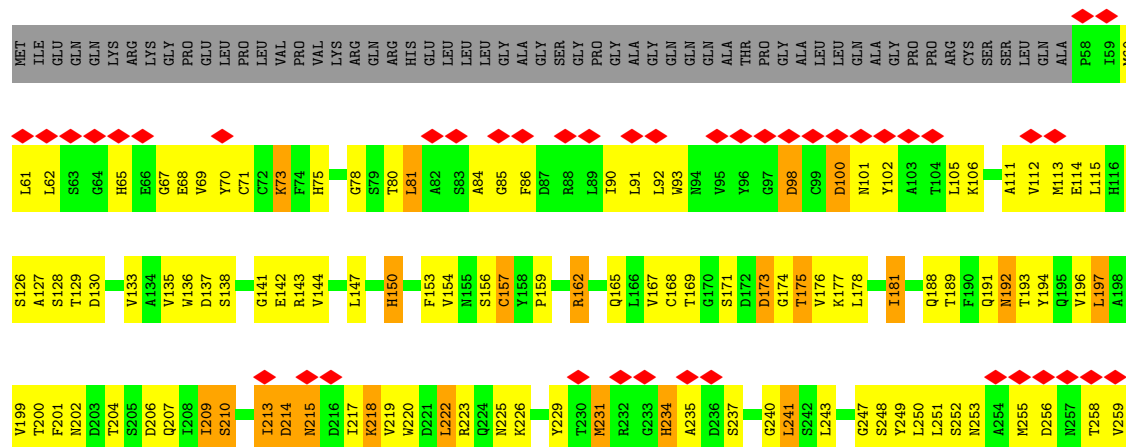


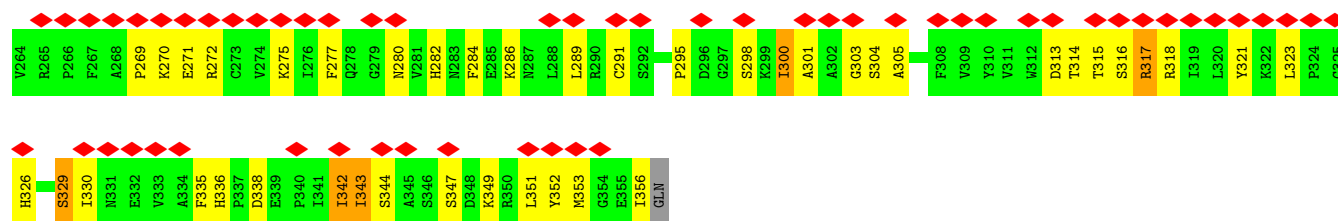
- Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase



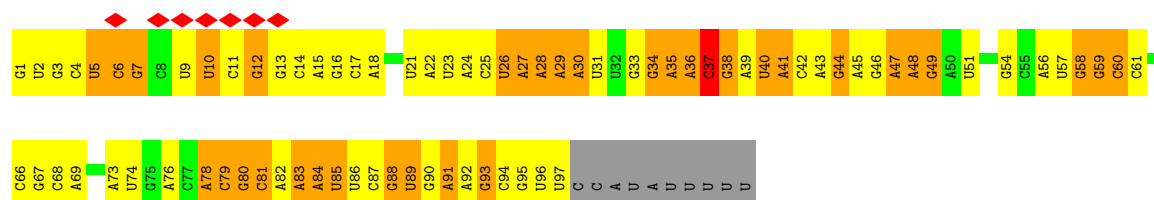
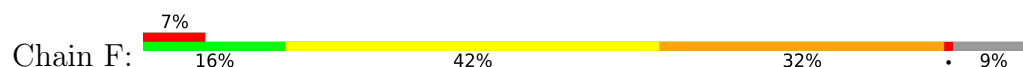


• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

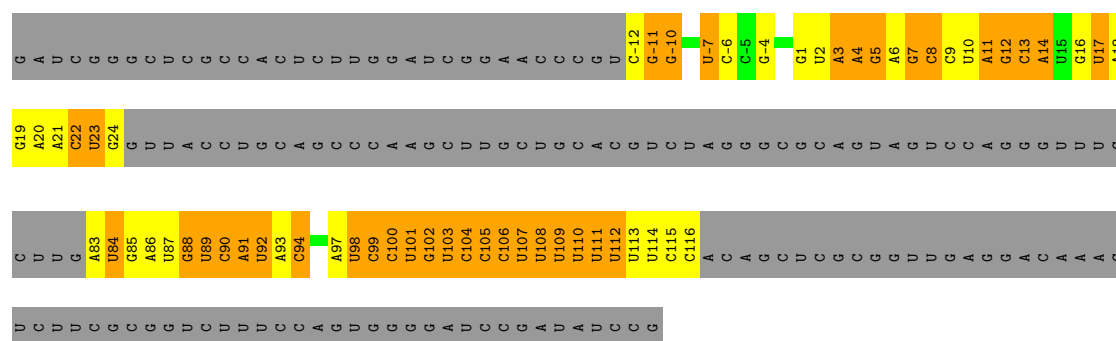




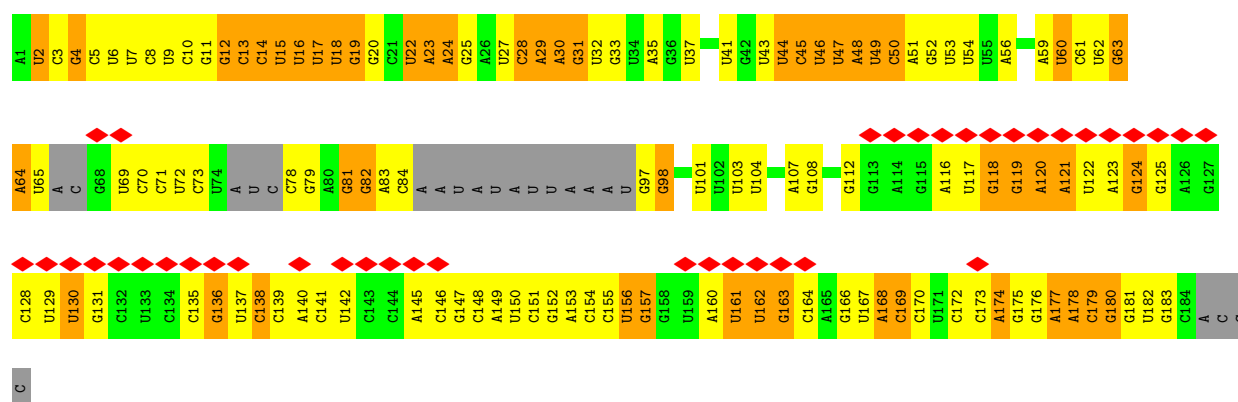
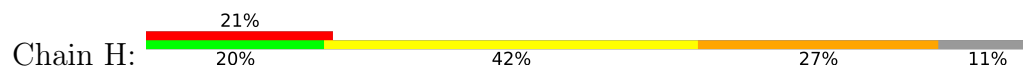
• Molecule 6: U6 snRNA



• Molecule 7: pre-mRNA

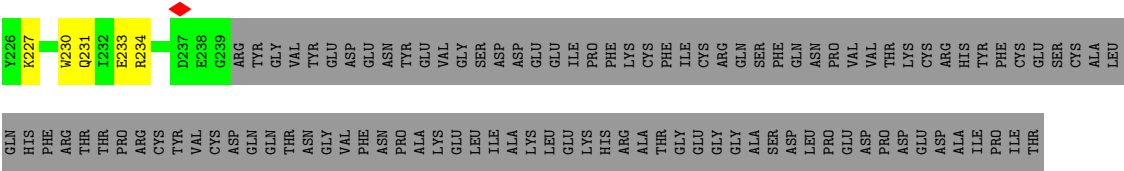


• Molecule 8: U2 snRNA



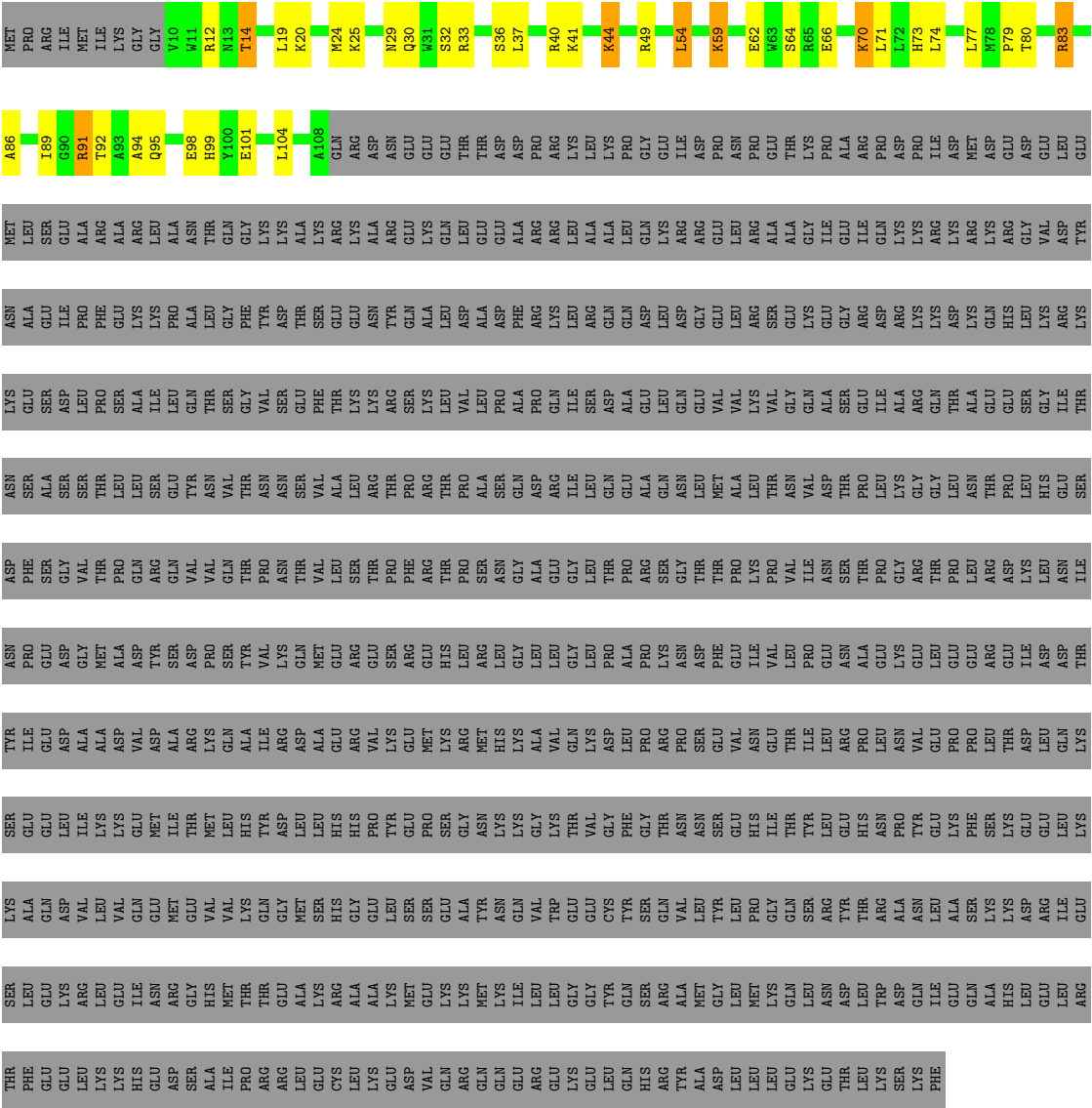
• Molecule 9: Pre-mRNA-splicing factor SYF1





● Molecule 12: Cell division cycle 5-like protein

Chain L: 7% . . 88%



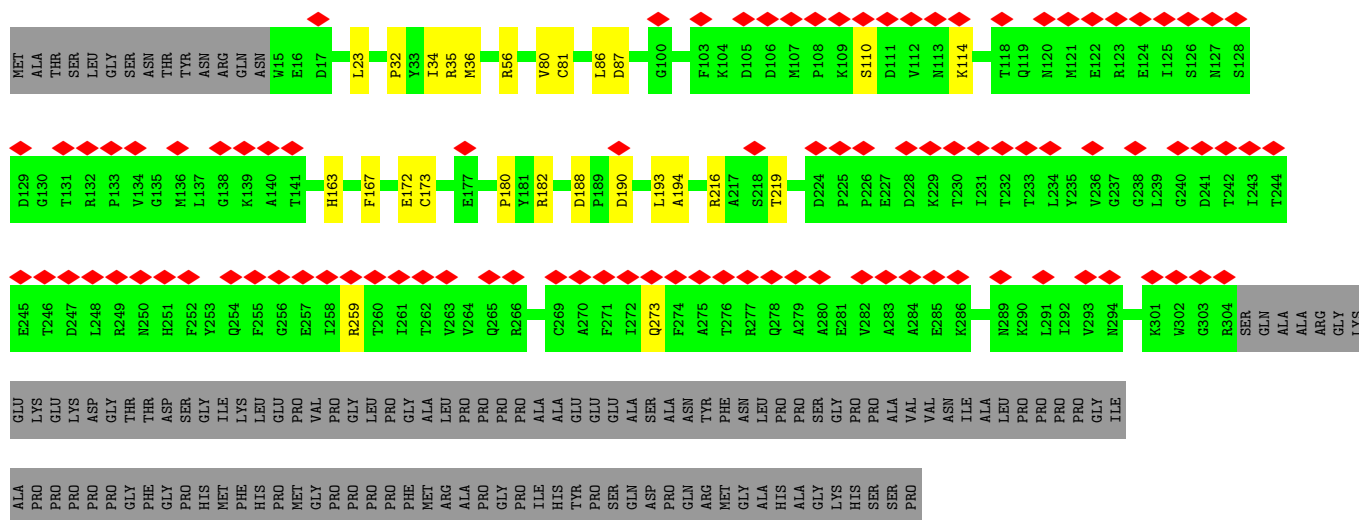
● Molecule 13: Protein BUD31 homolog

Chain N: 50% 42% 8% .

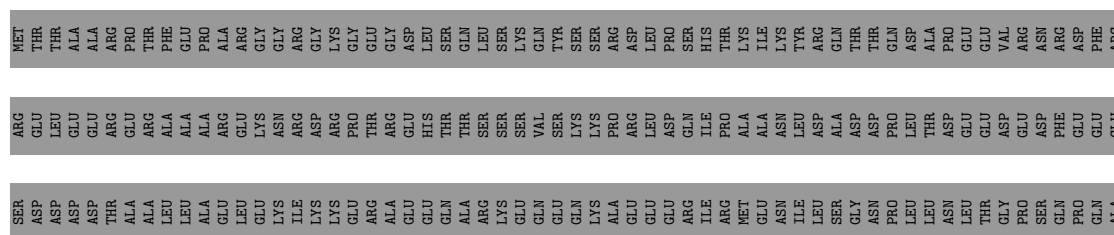




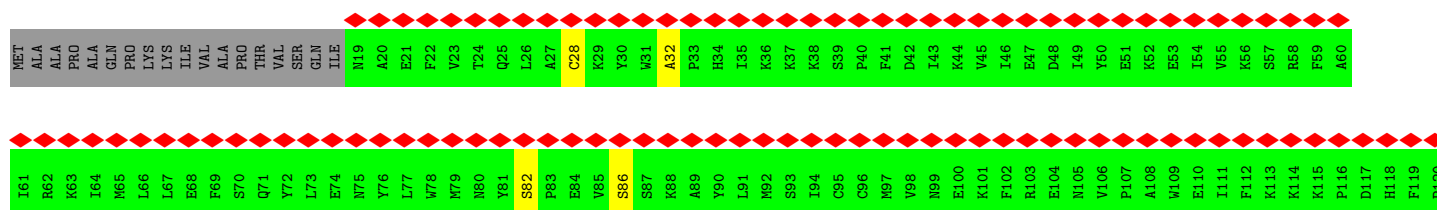
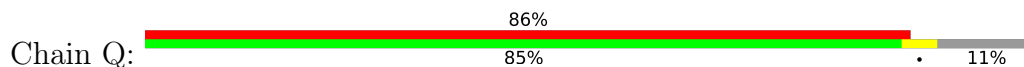
• Molecule 14: Pre-mRNA-splicing factor RBM22



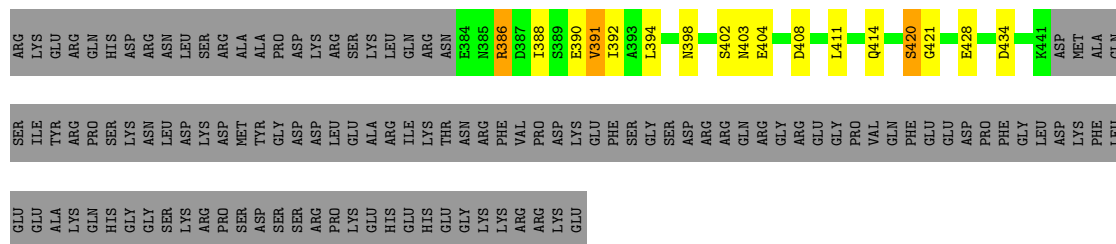
• Molecule 15: Spliceosome-associated protein CWC15 homolog



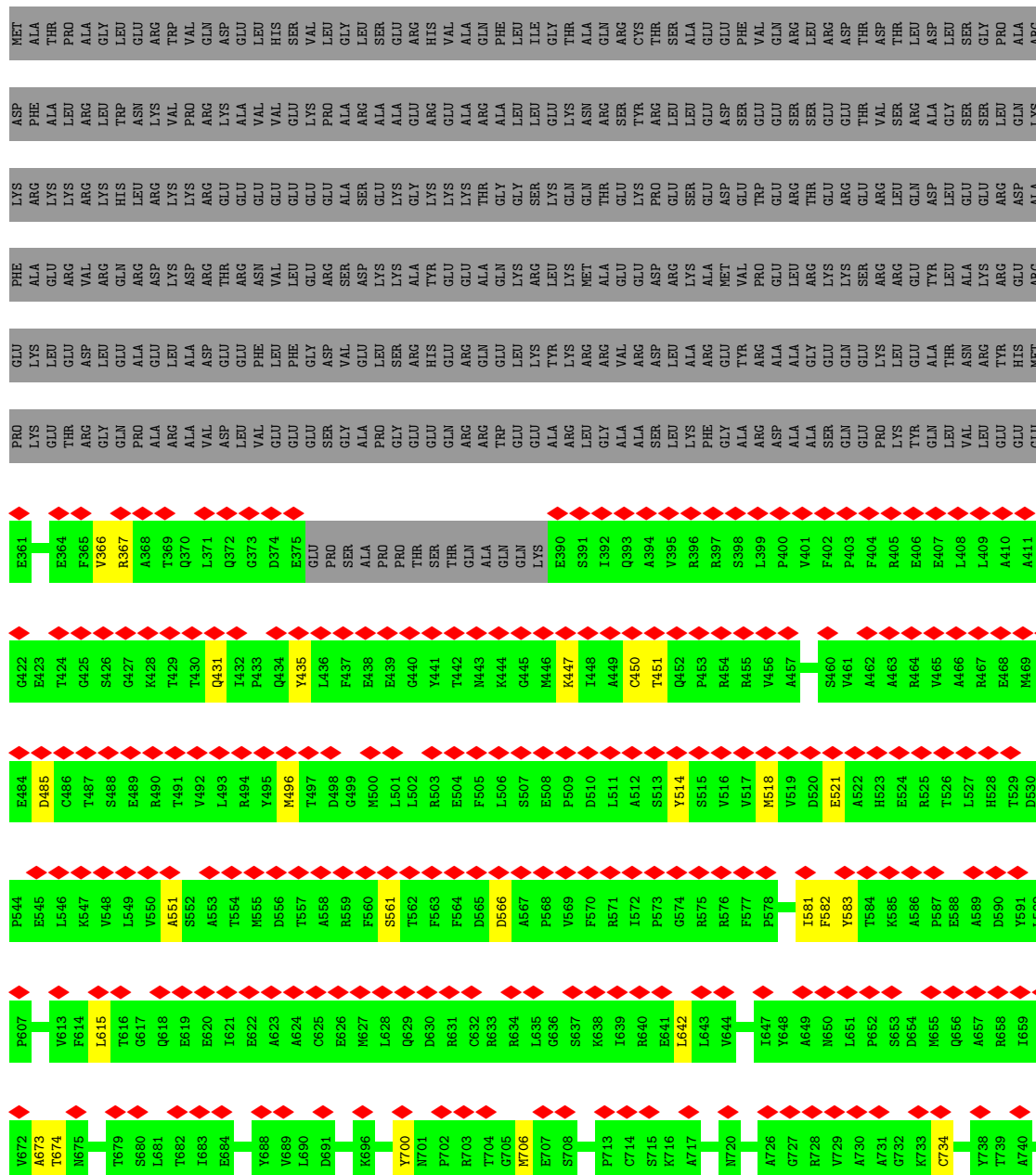
• Molecule 16: RNA helicase aquarius

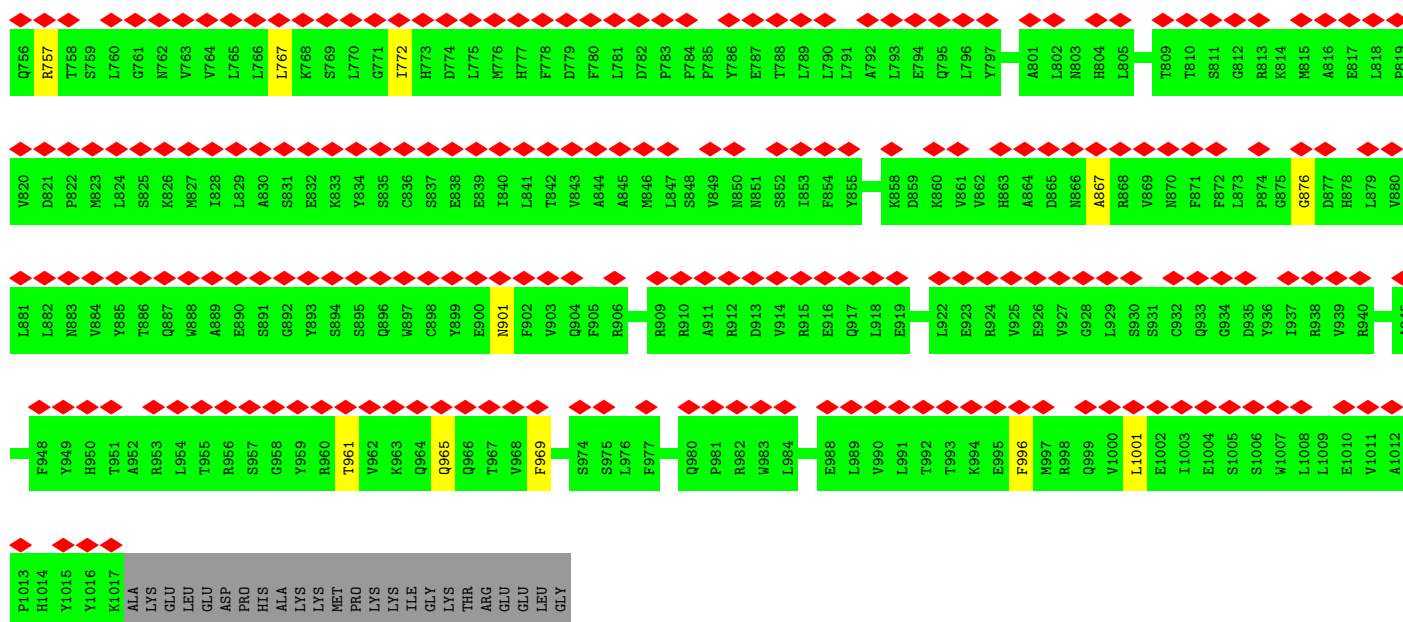


R905	R906	E907	L908	L909	E910	E911	V912	R913	R914	L915	Q916	R917	S918	L919	Q920	V921	P922	G923	D924	A925	S926	Y927	T928	C929	E930	T931	G933	Y934	F935	F936	L937	Y938	Q939	V940	N941	S942	E943	W944	E945	E946	Y947	I948	S949	K950	V951	K952	N953	LYS	GLY	SER	LEU	P959	D960	V961	T962	E963	V964																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
N843	F844	P845	E846	Q847	R848	T849	L850	I851	V852	T853	H854	S855	N856	Q857	A858	L859	N860	Q861	L862	F863	E864	K865	I866	N867	A868	L869	D870	I871	D872	E873	R874	H875	L876	L877																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</



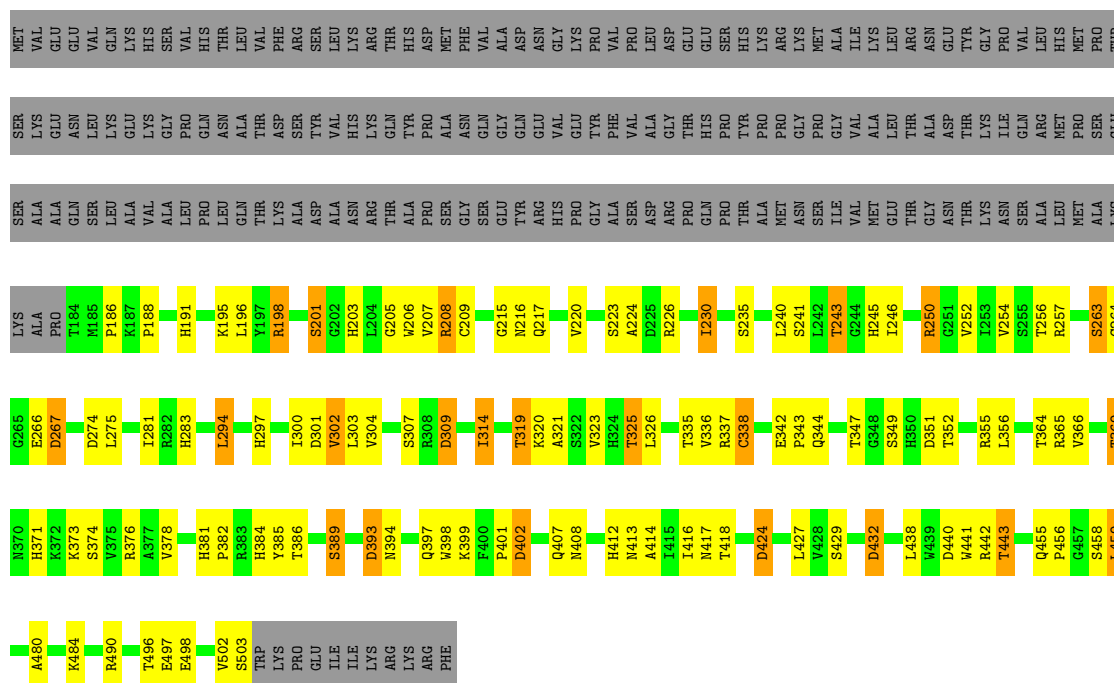
• Molecule 18: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16





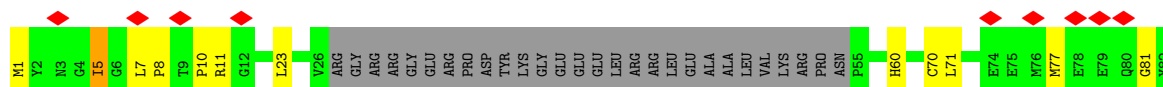
• Molecule 19: Pleiotropic regulator 1

Chain T: 39% 19% 38%



• Molecule 20: Serine/arginine repetitive matrix protein 2

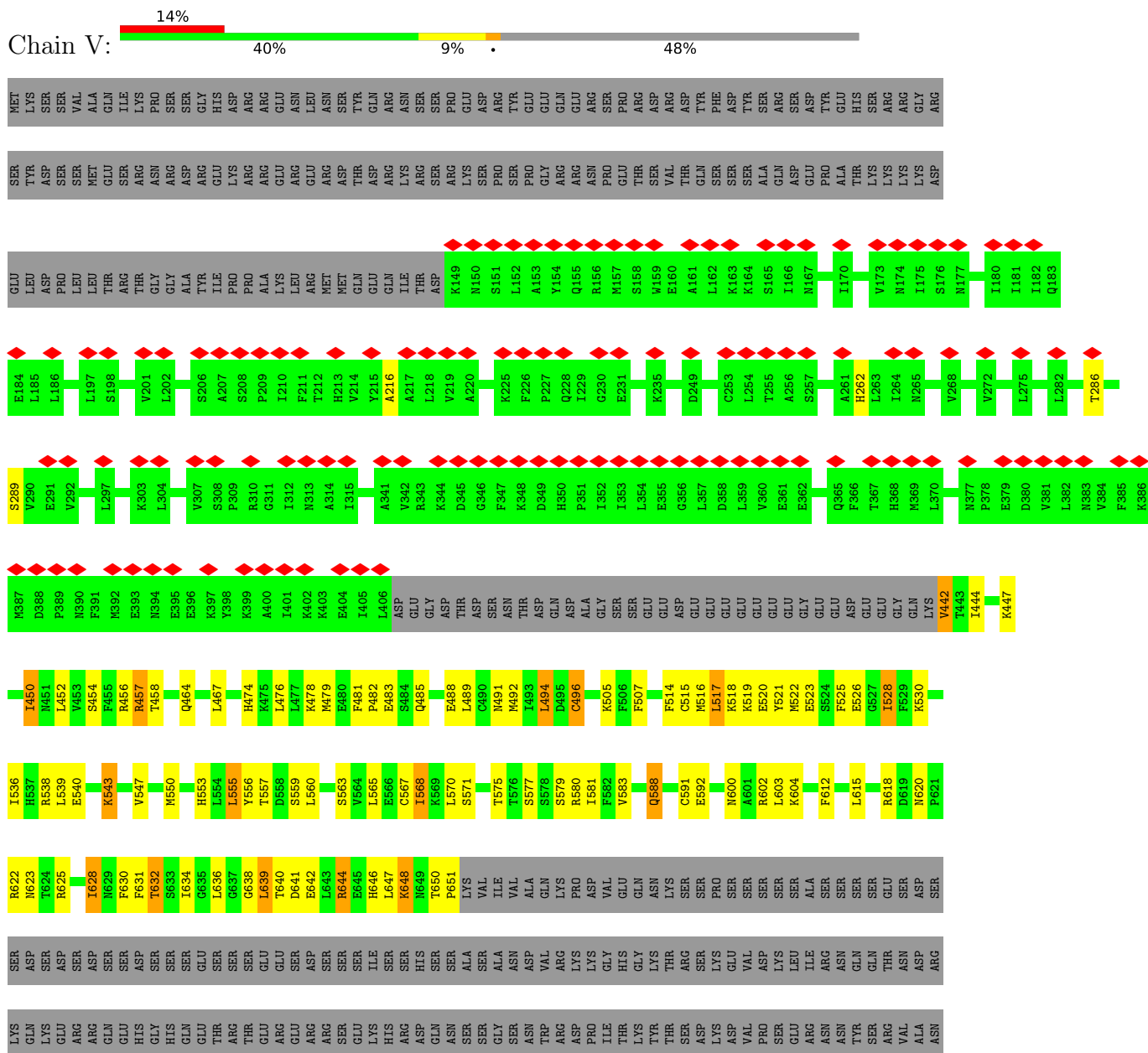
Chain U: 97%







- Molecule 21: Pre-mRNA-splicing factor CWC22 homolog



[illegible]

- Molecule 25: BUD13 homolog



MET	ALA	ALA	ALA	ALA	PRO	PRO	LEU	SER	LYS	ALA	ALA	GLU	TYR	LEU	LYS	ARG	TYR	SER	GLY	ALA	ASP	GLY	VAL	ASP	ARG	GLY	SER	SER	GLY	ARG	LYS	ARG	ARG	ARG	LYS	LYS	PRO	PRO	PRO	GLY	GLY	ALA	GLY	GLY	LYS	GLY	MET	ARG	ILE	VAL	ASP	ASP	ASP	VAL	SER	SER	TRP	THR	ALA
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ILE	SER	THR	THR	LYS	LEU	GLU	LYS	GLU	GLU	GLU	GLU	ASP	ASP	GLY	ASP	LEU	PRO	VAL	VAL	ALA	ALA	PHE	VAL	ASP	GLU	GLU	GLU	GLU	VAL	LYS	GLN	ARG	ARG	PRO	GLU	GLU	GLU	ALA	ALA	PHE	ARG	SER	SER	SER	ALA	ALA	LYS	TRP	LYS	LEU	LEU	LEU	GLY	GLY	HIS	ASN	ASN	ARG	HIS	PHE	ARG
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HIS	ASP	THR	PRO	ASP	SER	SER	PRO	ARG	ARG	VAL	ARG	HIS	GLY	THR	ASP	PRO	SER	SER	PRO	ARG	LYS	ASP	ARG	ASP	HIS	ASP	THR	PRO	PRO	PRO	SER	PRO	PRO	LEU	ALA	GLY	GLA	ALA	ARG	HIS	ASP	SER	SER	ASP	THR	SER	PRO	PRO	ARG	ARG	ALA	THR
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ARG ASP ASP SER SER ASP THR SER PRO PRO ARG ARG ALA ARG ARG ASP SER PRO PRO PRO PRO ARG ARG ARG GLN HIS HIS ASN SER SER GLY VAL VAL ARG ARG ARG HIS HIS ASP SER PRO PRO ARG ARG ALA ARG ARG ARG HIS GLY SER SER ASP ASP SER

PRO	ARG	ARG	VAL	HIS	ASN	ASN	SER	PRO	PRO	ASP	THR	THR	SER	ARG	ARG	THR	THR	GLN	GLN	LEU	LEU	ARG	ARG	ALA	ALA	HIS	HIS	ASP	ASP	SER	SER	PRO	PRO	ASP	LEU	LEU	ALA	PRO	PRO	ASN	ASN	VAL	THR	THR	TYR	SER	SER	LEU	LEU	PRO	ARG	THR	THR	LYS	LYS	SER	SER	GLY	GLY	LYS	PRO	PRO	GLU	GLU	ALA	ALA	SER	SER	LYS	LYS	THR	THR	SER	SER	PRO	PRO
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HIS	TRP	LYS	GLU	GLY	ALA	ALA	SER	HIS	LEU	SER	PHE	PRO	ASN	SER	LYS	TYR	GLU	TYR	ASP	PRO	ASP	ASP	ILE	SER	SER	PRO	PRO	ARG	LYS	LYS	GLN	ALA	ALA	LYS	SER	SER	HIS	PHE	GLY	LYS	ASP	LYS	LYS	GLN	GLN	LEU	ASP	SER	SER	LYS	GLY	GLY	ASP	CYS	GLN	LYS	ALA	ALA	THR	ASP	SER	SER	ASP	LEU	SER	SER	PRO	PRO	ARG
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HIS	LYS	GLN	GLN	SER	PRO	GLY	HIS	GLN	ASP	ASP	SER	SER	ASP	LEU	SER	PRO	ARG	ASN	ARG	ARG	ARG	ARG	HIS	ARG	SER	SER	ASP	ASP	LEU	SER	SER	PRO	PRO	ARG	ARG	ARG	ARG	GLN	ARG	THR	THR	LYS	SER	SER	SER	ASP	SER	ASP	LEU	GLN	SER	PRO	PRO	PRO	GLY	LYS	LYS	ALA	ALA
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HIS MET THR TYR SER GLY ALA LYS THR THR GLY LEU VAL LEU THR ASP LEU GLN ARG GLU GLN GLN GLU LYS GLU GLN ASP GLN GLU THR MET ALA PHE GLU ALA PHE GLU TYR THR THR VAL PHE ASP ASP LYS SER GLY ARG LYS ARG ASN LEU LYS LEU LEU ARG LEU GLU THR

- Molecule 26: Splicing factor 3B subunit 1

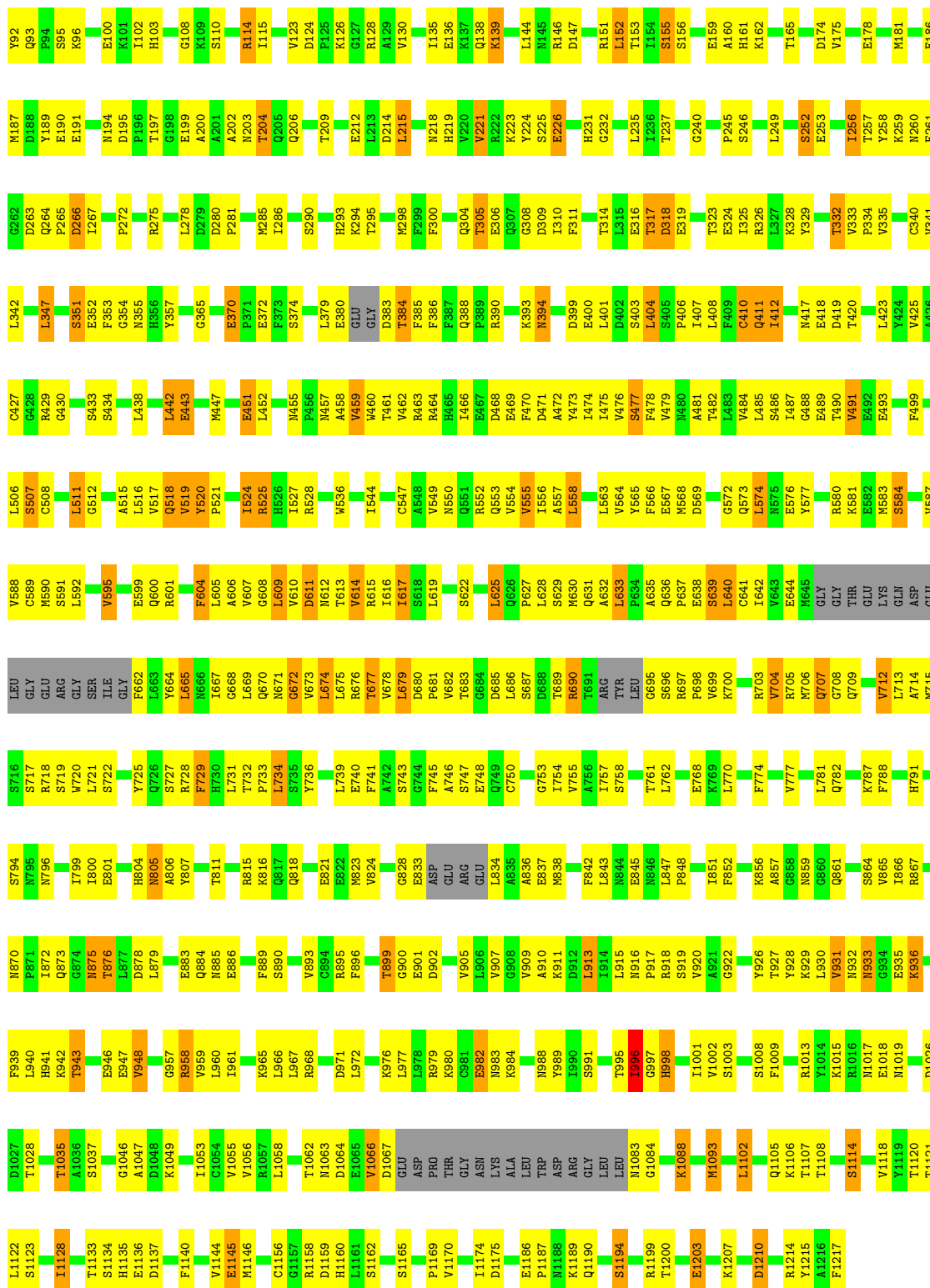


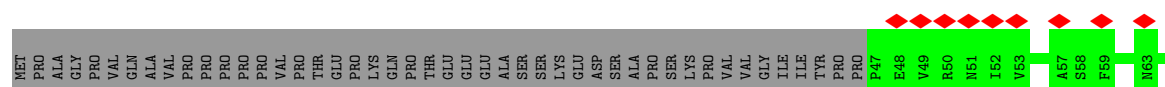
MET	ALA	LYS	ILE	ALA	LYS	THR	HIS	GLU	ASP	LEU	GLU	ALA	GLN	ILE	ARG	GLU	ILE	GLN	LYS	LYS	ALA	ALA	LEU	ASP	GLU	GLN	ALA	GLN	GLY	VAL	GLY	LEU	ASP	SER	THR	GLY	TYR	TYR	ASP	ASP	GLN	GLU	ILE	TYR	GLY	GLY	SER	SER	ARG	PHE	ALA	GLY	GLY	TYR	VAL	THR	SER	ILE	ALA	ALA
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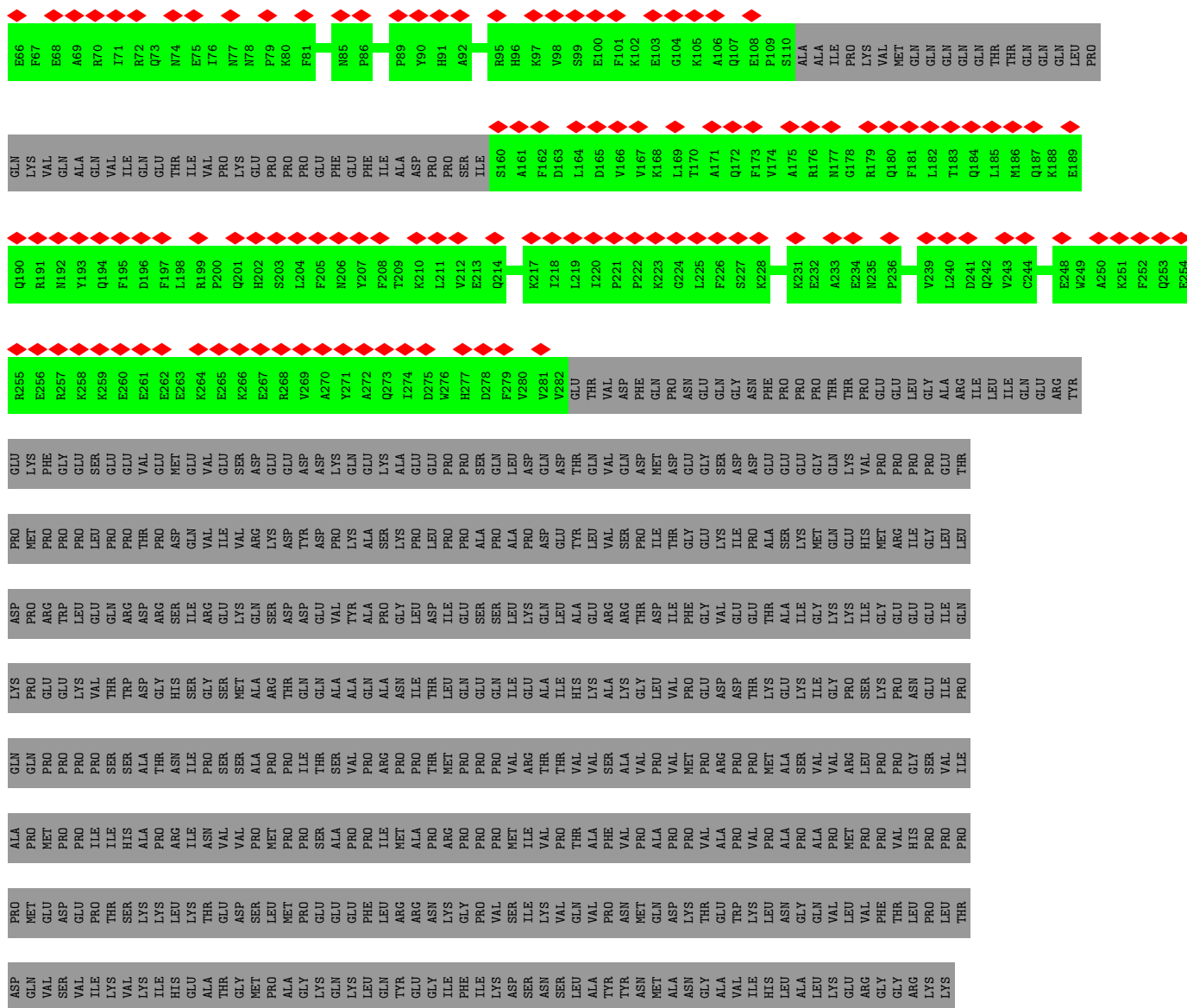
[illegible]

P130	D134	P135	D138	K141	T142	P145	K146	R150	T151	Y152	M153	D154	V155	M156	R157	E158	L161	T162	K163	E164	E165	R166	R169	Q170	Q171	L172	A173	E174	K175	A176	LYS	ALA	ALA	GLY	GLY	GLU	LEU	LYS	LYS	VAL	VAL	ASN	GLY	ALA	ALA	ALA	ALA	SER	SER	GLN	PRO	PRO	PRO	SER	LYS	ARG	LYS	ARG	PRO
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ARG TRP ASP GLN THR ALA ASP GLN THR PRO PRO GLY GLY ALA THR PRO PRO LYS LYS LEU SER SER TRP TRP ASP GLN GLN ALA ALA GLU THR PRO PRO GLY GLY HIS THR PRO PRO SER LEU SER ARG ARG TRP TRP ASP GLU GLU THR THR PRO PRO GLY GLY ARG ARG LYS GLY SER SER GLU THR THR PRO PRO GLY GLY ALA THR THR PRO PRO GLY GLY LYS LYS LLE TRP TRP PRO PRO THR PRO PRO

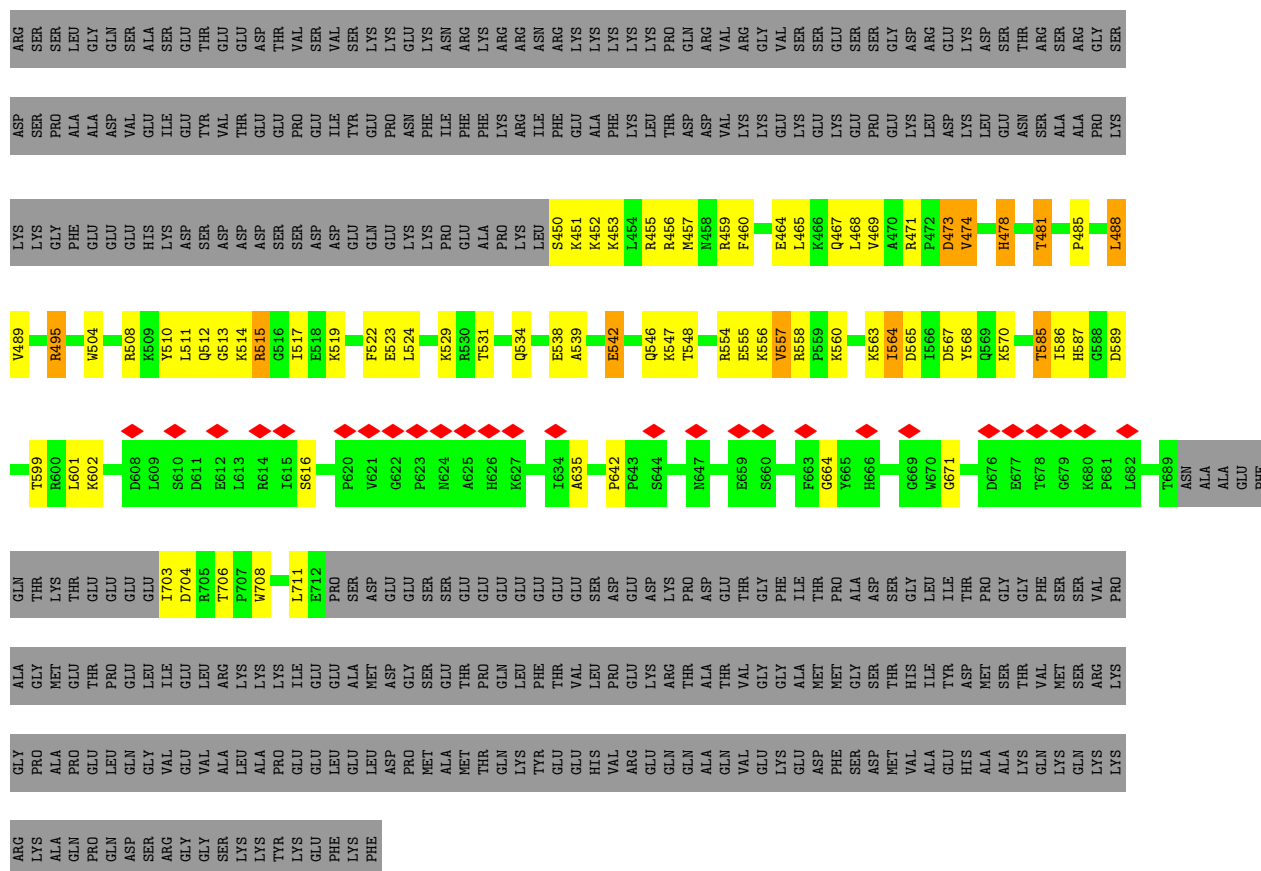




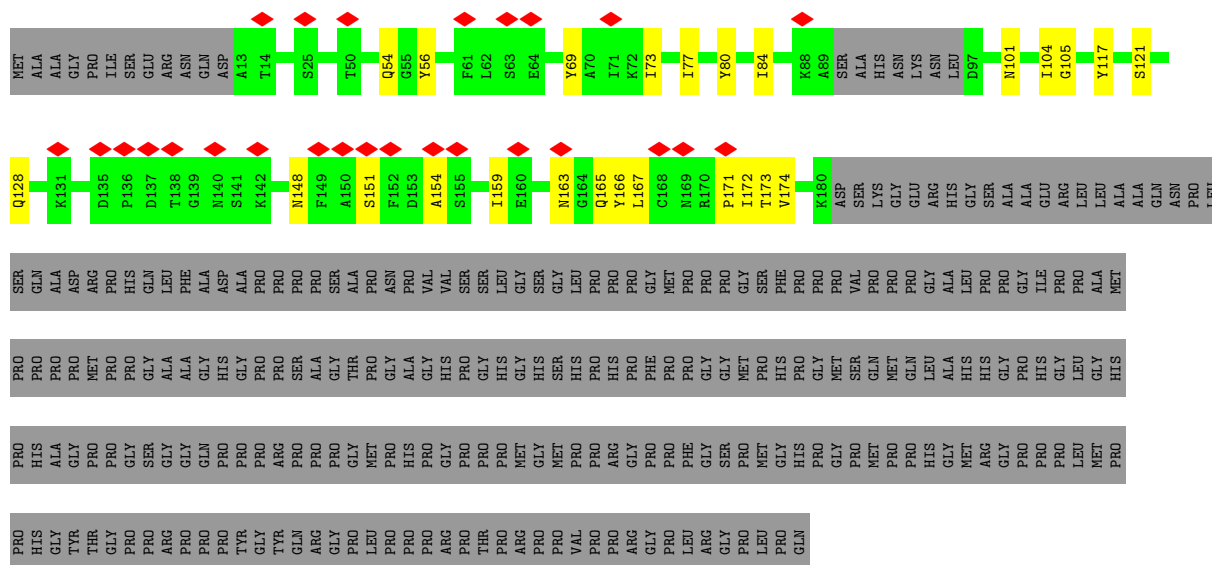


- Molecule 31: Splicing factor 3B subunit 2



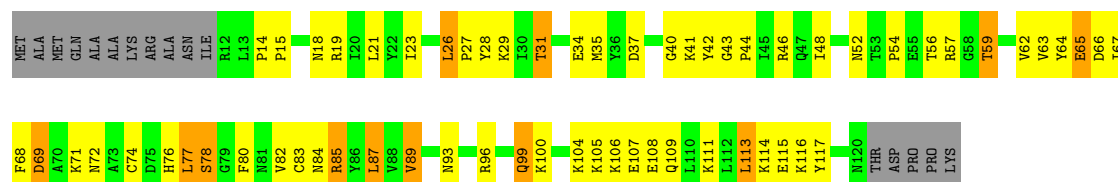


• Molecule 32: Splicing factor 3B subunit 4

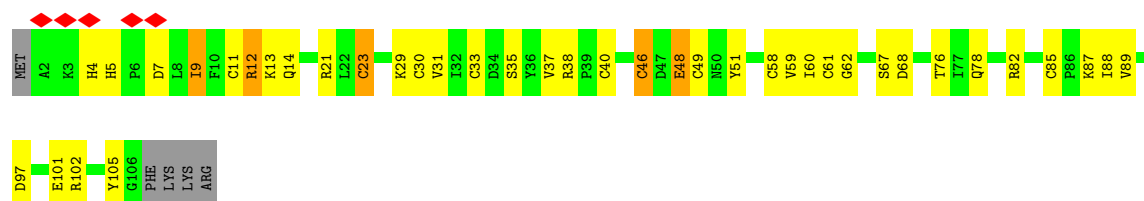


• Molecule 33: Splicing factor 3B subunit 6





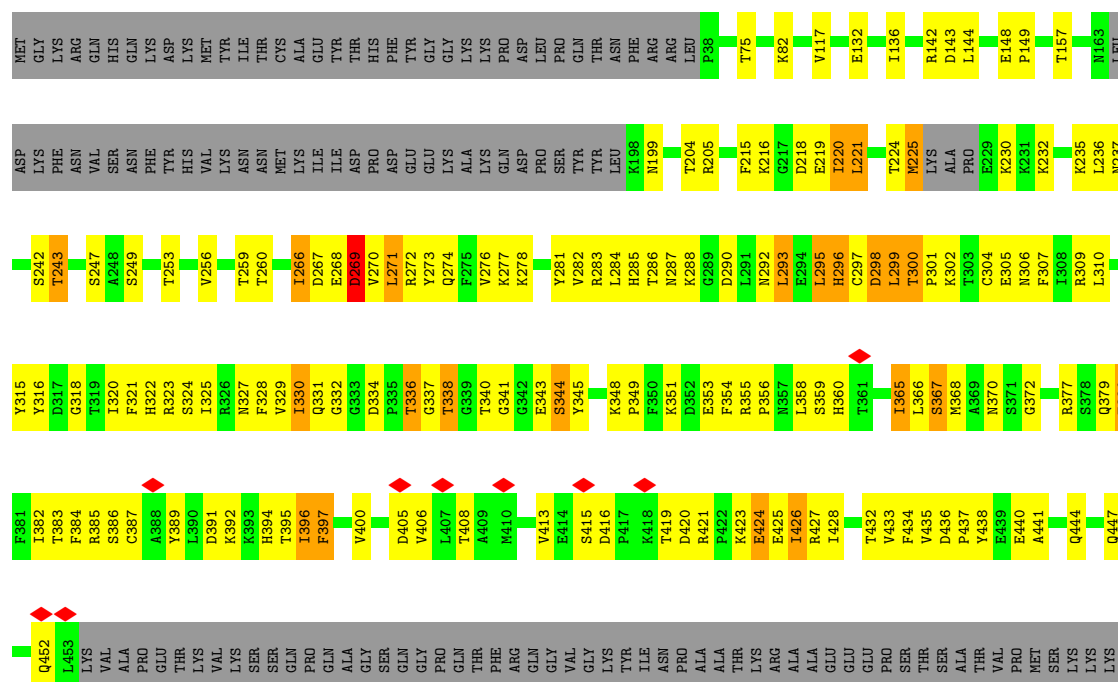
• Molecule 34: PHD finger-like domain-containing protein 5A



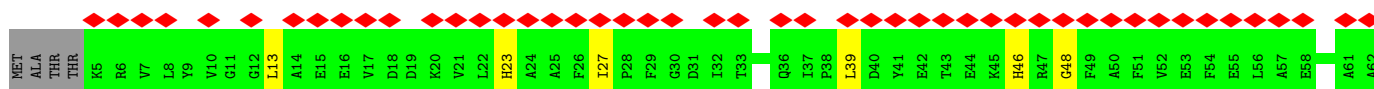
• Molecule 35: Splicing factor 3B subunit 5

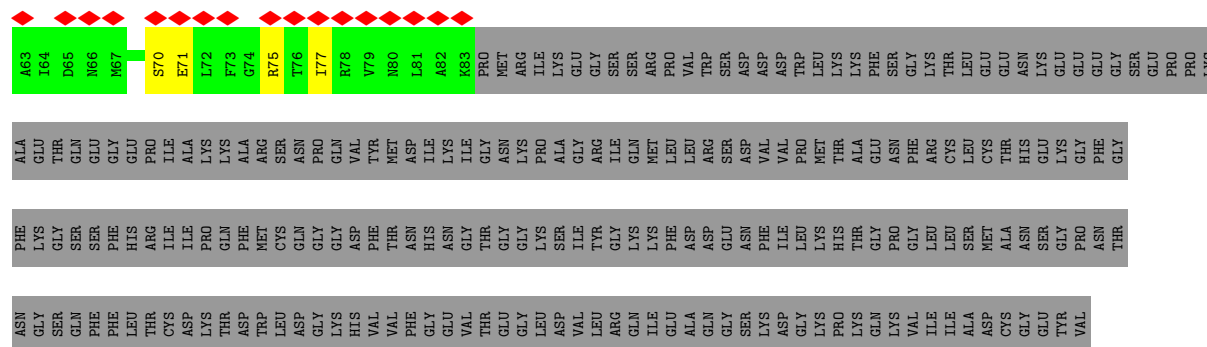


• Molecule 36: RING-type E3 ubiquitin-protein ligase PPIL2

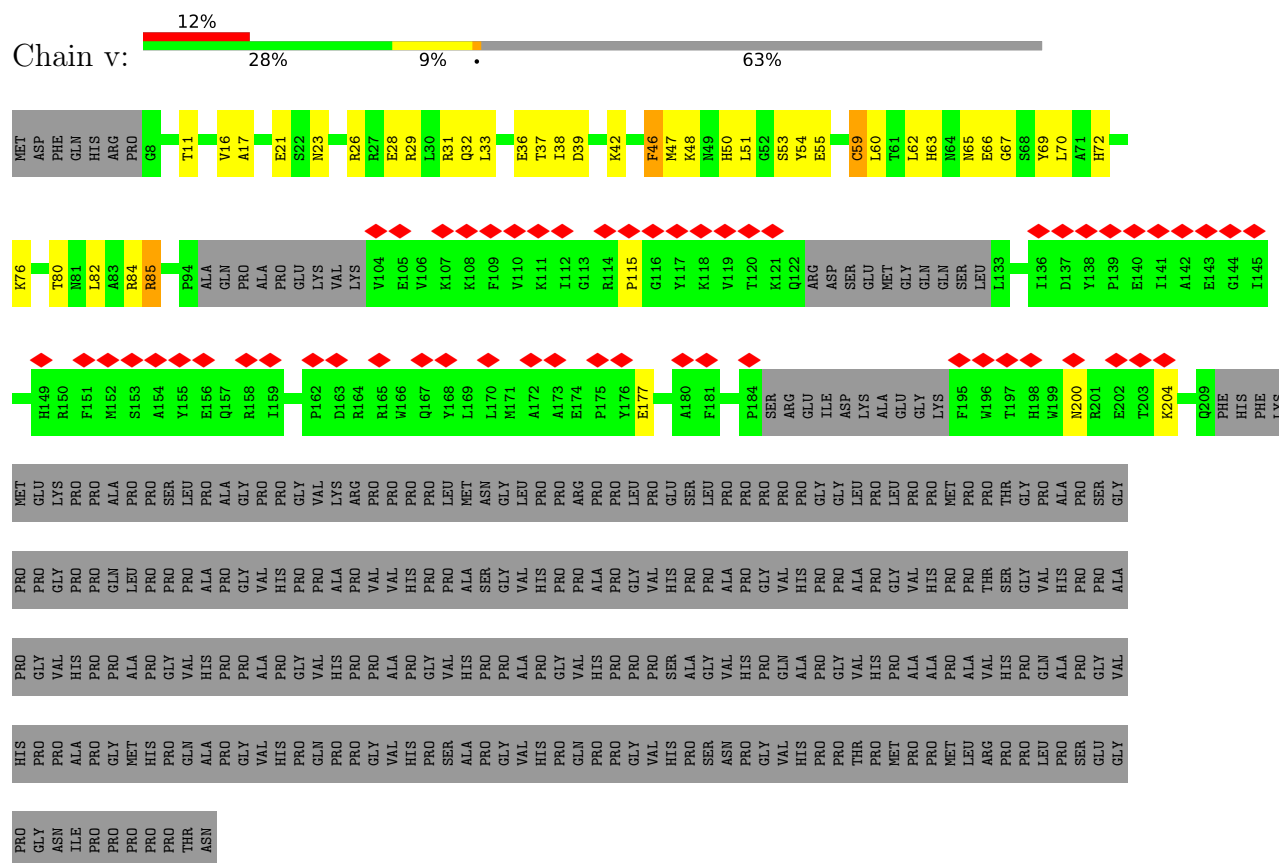


Chain 8: 7% 5% 87%

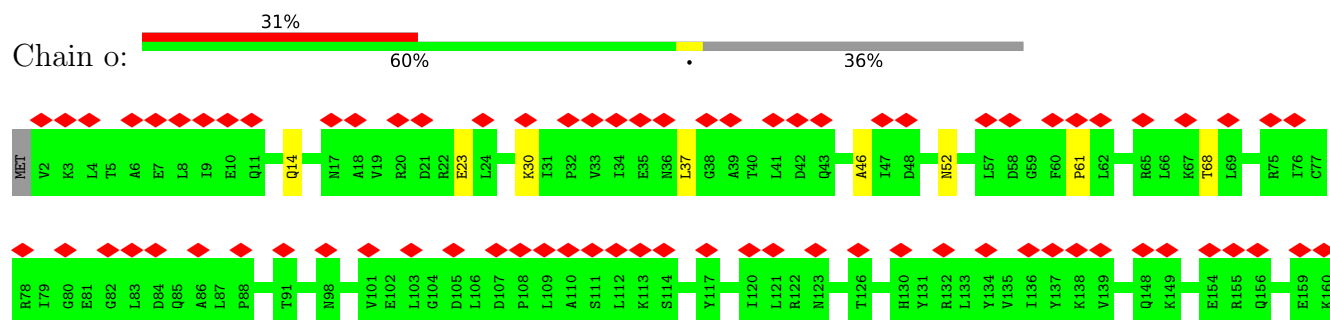


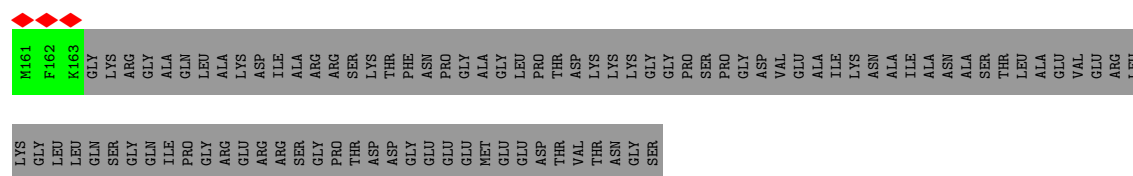


- Molecule 39: Splicing factor 3A subunit 2

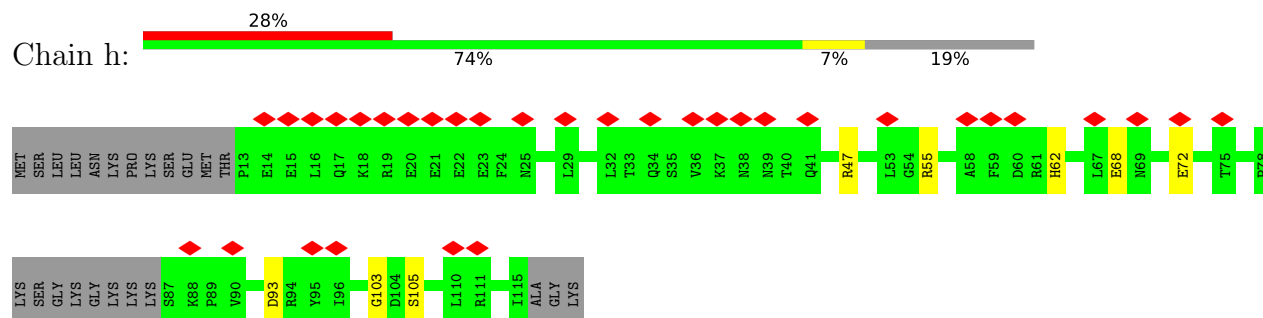


- Molecule 40: U2 small nuclear ribonucleoprotein A'

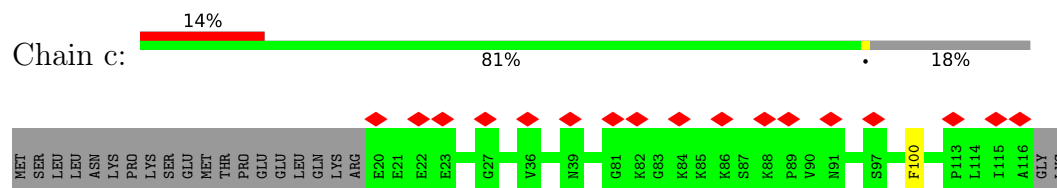




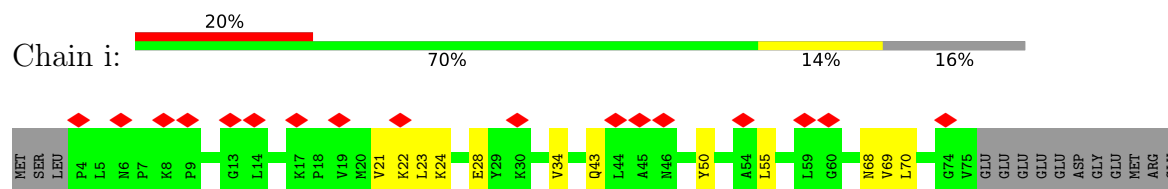
• Molecule 41: Small nuclear ribonucleoprotein Sm D2



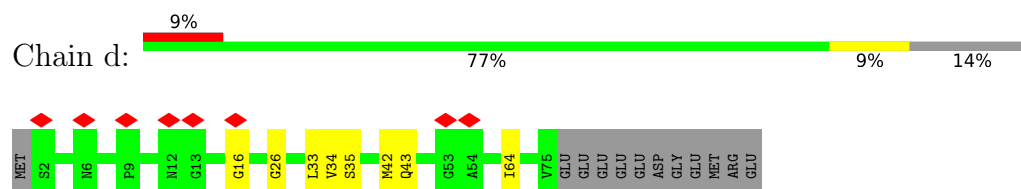
• Molecule 41: Small nuclear ribonucleoprotein Sm D2



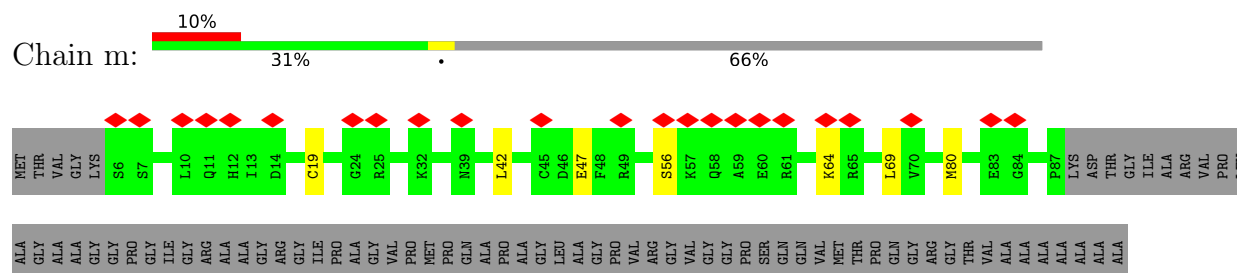
• Molecule 42: Small nuclear ribonucleoprotein F



• Molecule 42: Small nuclear ribonucleoprotein F

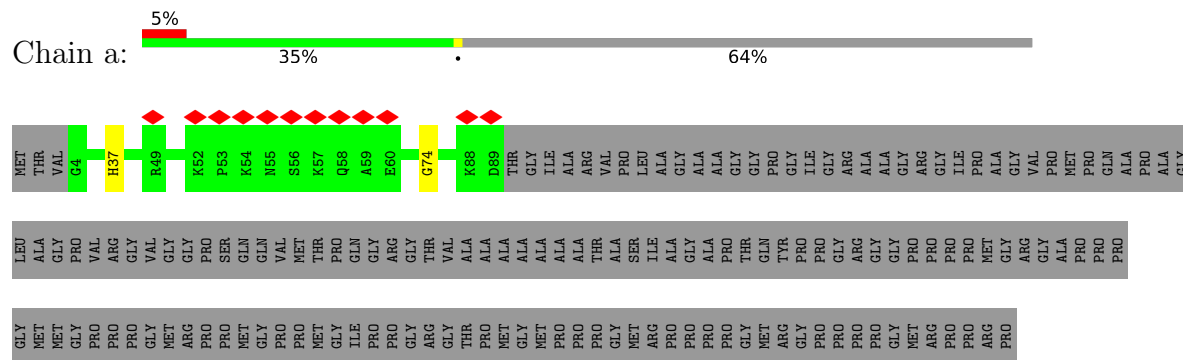


• Molecule 43: Small nuclear ribonucleoprotein-associated proteins B and B'

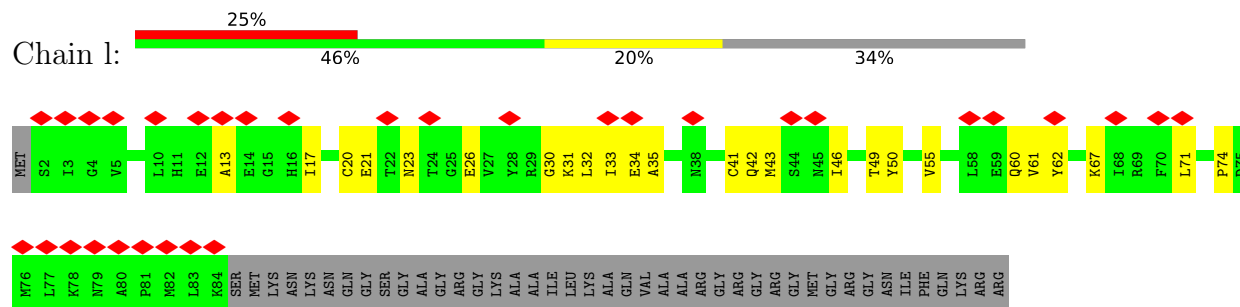




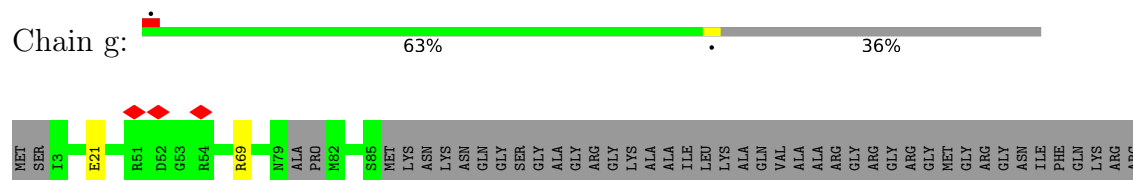
- Molecule 43: Small nuclear ribonucleoprotein-associated proteins B and B'



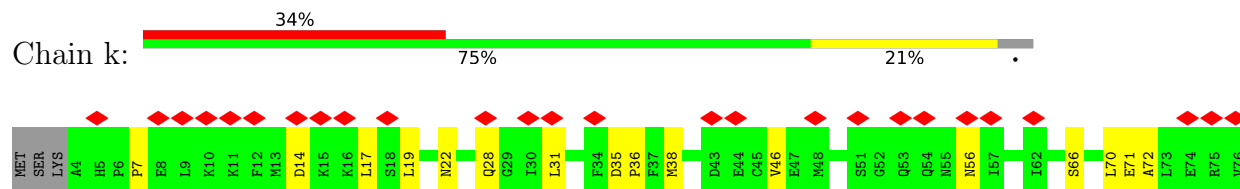
- Molecule 44: Small nuclear ribonucleoprotein Sm D3



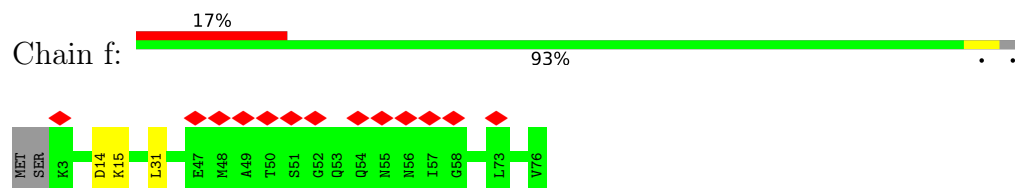
- Molecule 44: Small nuclear ribonucleoprotein Sm D3



- Molecule 45: Small nuclear ribonucleoprotein G



- Molecule 45: Small nuclear ribonucleoprotein G



- | |
|-----|
| VAL | GLU | SER | GLY | LYS | GLY | ASP | ALA | PRO | ASP | LEU | VAL | ASP | GLY | GLU | ASP | GLU | Tyr | ILE | ASP | ASN | MET | ARG | GLU | ARG | ILE | ALA | LYS | LYS | LEU | LYS | LYS | ASP | THR | SER | ALA | ASN | VAL | LYS | LYS | SER | ALA | GLY | GLU | GLY | GLU | VAL | GLU |
|-----|

GLU	LYS
ALA	SER
LEU	VAL
ARG	SER
LYS	ARG
GLN	SER
GLU	GLU
SER	GLU
LYS	LEU
LYS	ARG
GLY	LYS
THR	GLU
SER	ALA
ARG	ARG
GLU	GLN
ASP	LEU
THR	LYS
PHE	GLN
GLU	ARG
ILE	GLU
TYR	LEU
ASP	LEU
PRO	ALA
ARG	ASN
ASN	ALA
PRO	LYS
VAL	GLN
ASN	LYS
LYS	LYS
ARG	VAL
ARG	LEU
ARG	ASN
ARG	THR
GLU	ASN
GLU	ALA
SER	ALA
LYS	LYS
LYS	GLN
LYS	ALA
LEU	GLU
MET	THR
LEU	LYS
ARG	ARG
ARG	SER
ARG	GLU
GLU	ASP
LYS	ILE
LYS	GLU
GLU	PRO
ARG	GLU
ARG	ALA
ARG	THR
ARG	GLU
ARG	GLU
ARG	VAL
ARG	PRO
ARG	GLU
ARG	VAL
ARG	GLY
ARG	TRP
ARG	MET
ARG	TYR
ARG	GLU
ARG	GLU
ARG	LYS
ARG	GLN
ARG	LYS
ARG	TYR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136665	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	3.781	Depositor
Minimum map value	-1.945	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.24	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: MG, GTP, ZN, SEP, IHP

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	0.76	10/19056 (0.1%)	0.75	20/25857 (0.1%)
2	B	0.53	0/2303	0.46	0/3579
3	C	0.40	0/6873	0.67	4/9346 (0.0%)
4	D	0.18	0/8527	0.48	0/11887
5	E	0.24	0/2392	0.63	0/3242
6	F	0.58	0/2323	0.58	1/3619 (0.0%)
7	G	0.48	0/1648	0.60	0/2558
8	H	0.37	0/3947	0.50	0/6138
9	I	0.20	0/3013	0.53	0/4223
10	J	0.26	0/2171	0.60	0/2929
11	K	0.54	0/1081	0.63	1/1447 (0.1%)
12	L	0.61	0/850	0.67	0/1146
13	N	0.27	0/1210	0.62	0/1622
14	O	0.20	0/1432	0.48	0/1993
15	P	0.72	0/369	0.76	0/489
16	Q	0.18	0/6796	0.43	0/9527
17	R	0.50	0/1920	0.68	0/2576
18	S	0.18	0/3178	0.46	0/4425
19	T	0.92	5/2574 (0.2%)	0.79	0/3511
20	U	0.36	0/424	0.82	2/582 (0.3%)
21	V	0.34	0/3043	0.54	0/4156
22	W	0.73	0/33	0.75	0/42
23	X	0.33	0/1312	0.59	0/1769
24	Y	0.55	0/966	0.59	0/1303
25	Z	0.39	0/1166	0.64	0/1559
26	1	0.80	30/8004 (0.4%)	0.82	18/10830 (0.2%)
27	3	0.55	0/9408	0.71	4/12767 (0.0%)
28	p	0.19	0/857	0.46	0/1196
29	w	0.23	0/2311	0.48	0/3008
30	u	0.15	0/842	0.38	0/1110
31	2	0.50	0/1837	0.75	3/2473 (0.1%)
32	4	0.21	0/790	0.49	0/1095

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.29	0/925	0.61	0/1247
34	7	0.43	0/825	0.62	0/1106
35	5	0.68	0/688	0.74	0/930
36	9	0.32	0/2675	0.61	0/3631
37	8	0.33	0/946	0.54	0/1270
38	y	0.20	0/389	0.45	0/540
39	v	0.45	0/1054	0.61	0/1385
40	o	0.18	0/821	0.53	0/1149
41	c	0.17	0/387	0.52	0/482
41	h	0.18	0/485	0.41	0/677
42	d	0.18	0/295	0.49	0/367
42	i	0.19	0/362	0.47	0/502
43	a	0.18	0/343	0.53	0/427
43	m	0.19	0/416	0.51	0/581
44	g	0.17	0/322	0.48	0/399
44	l	0.21	0/417	0.54	0/581
45	f	0.16	0/295	0.45	0/367
45	k	0.19	0/366	0.50	0/509
46	e	0.16	0/315	0.50	0/392
46	j	0.20	0/403	0.46	0/561
47	b	0.18	0/327	0.47	0/407
47	n	0.21	0/404	0.50	0/564
48	z	0.53	0/1436	0.61	0/1945
All	All	0.51	45/117552 (0.0%)	0.63	53/162023 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
3	C	0	7
4	D	0	2
9	I	0	1
13	N	0	1
15	P	0	2
16	Q	0	2
17	R	0	1
23	X	0	1
26	1	0	5
27	3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	2	0	1
48	z	0	1
All	All	0	42

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	827	PHE	C-N	14.66	1.50	1.33
19	T	307	SER	C-O	-13.31	1.09	1.23
1	A	826	PRO	C-O	-13.10	1.07	1.23
1	A	824	PRO	C-O	-9.99	1.12	1.23
19	T	307	SER	CA-CB	-9.89	1.40	1.53
26	1	1115	ALA	C-O	-9.18	1.13	1.24
19	T	349	SER	C-O	-9.04	1.12	1.24
1	A	825	ILE	C-O	-9.02	1.12	1.24
26	1	1108	ASN	C-O	-8.91	1.13	1.24
26	1	949	GLN	C-O	-8.76	1.13	1.24
26	1	938	TRP	C-O	-8.69	1.14	1.24
26	1	1114	VAL	C-O	-8.66	1.13	1.24
1	A	823	SER	C-O	-8.39	1.14	1.24
26	1	1106	ARG	C-O	-8.37	1.14	1.24
26	1	944	SER	C-O	-8.26	1.14	1.24
26	1	952	ALA	C-O	-7.96	1.13	1.24
26	1	950	GLN	C-O	-7.81	1.14	1.24
26	1	1105	GLU	C-O	-7.77	1.14	1.23
26	1	1100	ASN	C-O	-7.53	1.15	1.24
26	1	939	ARG	C-O	-7.49	1.14	1.24
26	1	1109	ARG	C-O	-7.40	1.15	1.24
26	1	951	ALA	C-O	-7.16	1.14	1.24
19	T	349	SER	CA-CB	-7.14	1.41	1.53
26	1	946	LYS	C-O	-7.03	1.16	1.24
26	1	935	THR	C-O	-6.94	1.16	1.24
26	1	940	LEU	C-O	-6.90	1.16	1.24
26	1	1112	THR	C-O	-6.74	1.15	1.24
26	1	1069	HIS	CA-C	-6.44	1.43	1.52
1	A	821	ARG	C-O	-6.37	1.15	1.23
1	A	827	PHE	C-O	-6.31	1.16	1.24
26	1	1111	CYS	C-O	-6.20	1.16	1.24
19	T	266	GLU	CA-C	-6.01	1.44	1.52
26	1	1099	ASN	C-O	-5.93	1.17	1.24
26	1	943	LYS	C-O	-5.93	1.16	1.24
26	1	1025	LYS	CA-C	-5.85	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	1113	THR	C-O	-5.80	1.17	1.24
26	1	1101	LEU	C-O	-5.71	1.16	1.24
1	A	822	PHE	C-O	-5.61	1.16	1.23
26	1	933	CYS	C-O	-5.59	1.17	1.24
1	A	537	LYS	C-O	-5.55	1.17	1.24
26	1	1102	LYS	C-O	-5.47	1.16	1.24
1	A	533	LYS	C-O	-5.37	1.17	1.24
26	1	941	ASN	C-O	-5.30	1.17	1.24
26	1	936	VAL	C-O	-5.09	1.18	1.24
26	1	901	GLN	CA-C	-5.09	1.45	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	PHE	CA-C-N	14.20	135.00	120.38
1	A	827	PHE	C-N-CA	14.20	135.00	120.38
26	1	1108	ASN	CB-CA-C	-11.62	91.49	110.79
26	1	935	THR	CB-CA-C	-9.57	95.85	110.88
26	1	942	ASN	CB-CA-C	-9.23	94.57	109.80
26	1	935	THR	CA-CB-OG1	-8.96	96.17	109.60
26	1	435	PRO	N-CA-C	-8.64	94.67	112.47
6	F	37	C	P-O5'-C5'	8.13	133.10	120.90
1	A	827	PHE	CA-C-O	-7.61	112.59	119.75
3	C	534	VAL	N-CA-C	-7.28	102.11	110.05
31	2	510	TYR	CA-C-N	-7.22	109.77	122.26
31	2	510	TYR	C-N-CA	-7.22	109.77	122.26
1	A	820	ARG	CB-CA-C	-7.02	97.37	110.01
1	A	825	ILE	N-CA-CB	-6.88	103.68	110.08
26	1	1113	THR	CA-CB-OG1	-6.82	99.37	109.60
1	A	824	PRO	N-CA-C	6.79	121.73	111.14
26	1	1114	VAL	CA-C-O	-6.79	113.14	120.47
1	A	826	PRO	CB-CA-C	-6.61	101.48	110.60
26	1	1101	LEU	O-C-N	-6.60	113.65	122.43
26	1	944	SER	CA-C-O	-6.60	113.23	120.36
26	1	1111	CYS	CB-CA-C	6.39	121.71	110.85
26	1	1105	GLU	CB-CA-C	6.11	119.85	109.53
26	1	1112	THR	OG1-CB-CG2	-6.10	97.10	109.30
1	A	1019	TYR	N-CA-C	-5.94	100.29	109.14
1	A	825	ILE	CA-C-O	-5.91	114.21	119.71
20	U	83	GLU	CA-C-N	5.91	132.83	121.54
20	U	83	GLU	C-N-CA	5.91	132.83	121.54
1	A	704	ASN	N-CA-C	-5.87	106.75	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1091	TYR	N-CA-C	-5.87	101.84	110.52
3	C	823	ALA	N-CA-C	5.84	117.30	110.41
3	C	822	MET	CA-C-N	-5.77	112.70	121.53
3	C	822	MET	C-N-CA	-5.77	112.70	121.53
27	3	917	PRO	N-CA-C	-5.75	100.61	112.47
1	A	568	ASN	CA-C-N	-5.67	111.76	121.97
1	A	568	ASN	C-N-CA	-5.67	111.76	121.97
11	K	122	LEU	N-CA-C	-5.66	104.25	113.19
26	1	1108	ASN	CA-C-O	-5.63	114.58	120.55
26	1	1106	ARG	CA-C-O	-5.57	114.52	120.42
1	A	824	PRO	N-CA-CB	-5.54	98.38	103.31
1	A	1252	GLY	N-CA-C	-5.53	100.07	113.18
27	3	805	ASN	N-CA-CB	-5.37	103.26	111.74
1	A	821	ARG	CG-CD-NE	-5.29	100.36	112.00
1	A	692	ASP	CA-C-N	-5.27	112.12	120.55
1	A	692	ASP	C-N-CA	-5.27	112.12	120.55
26	1	952	ALA	CA-C-N	5.26	127.28	120.44
26	1	952	ALA	C-N-CA	5.26	127.28	120.44
31	2	510	TYR	N-CA-CB	-5.24	101.64	110.49
27	3	84	SER	CA-C-N	-5.20	111.21	121.41
27	3	84	SER	C-N-CA	-5.20	111.21	121.41
1	A	672	VAL	CA-C-N	-5.15	111.71	121.54
1	A	672	VAL	C-N-CA	-5.15	111.71	121.54
26	1	1101	LEU	N-CA-C	-5.06	106.80	112.87
26	1	948	ARG	CG-CD-NE	-5.02	100.95	112.00

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	1101	LEU	Mainchain
26	1	1178	MET	Peptide
26	1	1179	ASP	Peptide
26	1	717	THR	Peptide
26	1	944	SER	Mainchain
31	2	515	ARG	Peptide
27	3	916	ASN	Peptide
27	3	996	ILE	Peptide
1	A	1019	TYR	Peptide
1	A	1189	MET	Peptide
1	A	1416	ILE	Peptide
1	A	1547	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	1548	TYR	Peptide
1	A	1765	SER	Peptide
1	A	2320	LEU	Peptide
1	A	2329	ASP	Peptide
1	A	433	GLU	Peptide
1	A	467	GLN	Peptide
1	A	699	GLU	Peptide
1	A	700	GLY	Peptide
1	A	81	PHE	Peptide
1	A	855	ARG	Peptide
1	A	940	ILE	Peptide
1	A	941	LYS	Peptide
3	C	359	LYS	Peptide
3	C	360	ALA	Peptide
3	C	443	VAL	Peptide
3	C	560	VAL	Peptide
3	C	572	GLU	Peptide
3	C	736	GLY	Peptide
3	C	823	ALA	Peptide
4	D	1583	ASP	Peptide
4	D	2098	ALA	Peptide
9	I	337	LEU	Peptide
13	N	36	PRO	Peptide
15	P	202	ASP	Peptide
15	P	203	ASP	Peptide
16	Q	488	SER	Peptide
16	Q	489	VAL	Peptide
17	R	235	ARG	Peptide
23	X	296	HIS	Peptide
48	z	151	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18543	0	18403	647	0
2	B	2066	0	1047	57	0
3	C	6724	0	6696	317	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8528	0	3745	45	0
5	E	2338	0	2275	130	0
6	F	2075	0	1048	103	0
7	G	1481	0	755	81	0
8	H	3539	0	1791	130	0
9	I	2991	0	1473	12	0
10	J	2116	0	1977	105	0
11	K	1059	0	1012	38	0
12	L	829	0	837	29	0
13	N	1184	0	1193	52	0
14	O	1433	0	621	18	0
15	P	362	0	356	16	0
16	Q	6730	0	3268	33	0
17	R	1889	0	1866	75	0
18	S	3180	0	1441	20	0
19	T	2507	0	2451	81	0
20	U	422	0	291	16	0
21	V	3008	0	2288	93	0
22	W	229	0	86	3	0
23	X	1279	0	1284	65	0
24	Y	948	0	954	36	0
25	Z	1142	0	1112	38	0
26	1	7866	0	7964	292	0
27	3	9220	0	9139	426	0
28	p	851	0	423	7	0
29	w	2275	0	1347	53	0
30	u	834	0	325	0	0
31	2	1807	0	1622	60	0
32	4	792	0	367	16	0
33	6	906	0	913	51	0
34	7	811	0	790	29	0
35	5	669	0	631	20	0
36	9	2636	0	2228	130	0
37	8	931	0	960	46	0
38	y	390	0	190	5	0
39	v	1041	0	800	30	0
40	o	816	0	386	4	0
41	c	388	0	102	1	0
41	h	482	0	220	5	0
42	d	296	0	87	5	0
42	i	359	0	179	6	0
43	a	344	0	93	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	m	413	0	194	5	0
44	g	324	0	89	1	0
44	l	415	0	198	15	0
45	f	296	0	84	2	0
45	k	364	0	176	10	0
46	e	316	0	85	3	0
46	j	403	0	173	4	0
47	b	328	0	89	6	0
47	n	402	0	184	5	0
48	z	1402	0	1336	39	0
49	A	36	0	6	2	0
50	C	32	0	12	3	0
51	C	1	0	0	0	0
51	F	5	0	0	0	0
52	7	3	0	0	0	0
52	K	1	0	0	0	0
52	N	3	0	0	0	0
All	All	115060	0	89662	3208	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 16.

All (3208) 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)
26:1:933:CYS:SG	26:1:970:LEU:HD21	1.63	1.38
26:1:933:CYS:SG	26:1:970:LEU:HD11	1.74	1.27
26:1:933:CYS:SG	26:1:970:LEU:CD2	2.35	1.13
26:1:933:CYS:SG	26:1:970:LEU:CD1	2.43	1.06
21:V:580:ARG:HE	25:Z:545:MET:HB2	1.19	1.04
23:X:273:MET:HE1	26:1:433:ALA:HB1	1.10	1.04
1:A:2087:THR:HG21	1:A:2112:LYS:HA	1.39	1.01
23:X:273:MET:HE1	26:1:433:ALA:CB	1.89	1.01
27:3:642:ILE:H	27:3:703:ARG:HH21	1.09	0.99
23:X:273:MET:CE	26:1:433:ALA:HB1	1.93	0.98
5:E:91:LEU:HB3	5:E:101:ASN:HD21	1.28	0.98
1:A:59:GLU:HG3	13:N:103:LEU:HB3	1.45	0.97
26:1:933:CYS:HG	26:1:970:LEU:HD21	0.95	0.95
7:G:98:U:H3	8:H:33:G:H1	1.01	0.94
3:C:670:SER:HA	3:C:823:ALA:HB3	1.48	0.94
23:X:274:TYR:HE1	26:1:436:THR:N	1.64	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:54:U:O2	8:H:59:A:N6	2.02	0.91
6:F:38:G:H2'	6:F:39:A:H8	1.33	0.91
26:1:578:ILE:HG13	26:1:596:ILE:HD11	1.52	0.91
31:2:456:ARG:HA	31:2:459:ARG:HD3	1.51	0.90
2:B:17:U:O2	2:B:60:G:N1	2.05	0.90
6:F:79:C:H4'	6:F:80:G:H5''	1.50	0.90
7:G:85:G:N2	8:H:45:C:N3	2.19	0.89
26:1:933:CYS:SG	26:1:970:LEU:CG	2.61	0.89
23:X:274:TYR:CE1	26:1:436:THR:N	2.37	0.89
27:3:1026:ASP:OD2	31:2:495:ARG:NH2	2.04	0.89
1:A:1851:SER:HG	21:V:442:VAL:N	1.71	0.89
36:9:285:HIS:HE2	36:9:432:THR:HG1	1.03	0.88
19:T:343:PRO:HG3	19:T:356:LEU:HD23	1.56	0.87
23:X:352:LEU:HD21	23:X:358:LEU:HD11	1.57	0.87
36:9:370:ASN:ND2	36:9:372:GLY:O	2.07	0.87
1:A:2166:HIS:HB3	1:A:2169:LEU:H	1.40	0.87
8:H:19:G:N2	8:H:20:G:O6	2.09	0.85
21:V:644:ARG:NH2	22:W:114:UNK:O	2.10	0.85
27:3:552:ARG:HH11	27:3:600:GLN:HB3	1.42	0.84
23:X:277:ARG:HH22	26:1:437:PRO:CB	1.90	0.84
3:C:727:LEU:HD23	20:U:71:LEU:CB	2.08	0.84
1:A:226:GLN:OE1	1:A:417:ARG:NH2	2.11	0.84
45:k:7:PRO:HD3	45:k:36:PRO:HA	1.59	0.83
21:V:580:ARG:NH2	25:Z:545:MET:SD	2.51	0.83
23:X:274:TYR:CE1	26:1:436:THR:HA	2.13	0.83
21:V:580:ARG:NE	25:Z:545:MET:HB2	1.94	0.83
5:E:90:ILE:HB	5:E:105:LEU:HB3	1.57	0.83
6:F:27:A:N6	7:G:17:U:OP1	2.12	0.82
10:J:354:LEU:HD11	10:J:362:ALA:HB2	1.60	0.82
27:3:870:ASN:HD21	27:3:872:ILE:HB	1.44	0.82
31:2:563:LYS:HG2	31:2:564:ILE:HG13	1.58	0.82
3:C:534:VAL:HB	3:C:537:TYR:HB2	1.58	0.82
13:N:120:ARG:NH1	13:N:142:CYS:SG	2.51	0.82
19:T:336:VAL:HG23	19:T:347:THR:HG22	1.62	0.82
27:3:472:ALA:HA	27:3:487:ILE:HG12	1.62	0.82
1:A:371:LEU:HD11	3:C:347:ILE:HD11	1.61	0.82
34:7:13:LYS:NZ	34:7:48:GLU:OE1	2.13	0.82
31:2:473:ASP:OD1	31:2:473:ASP:N	2.12	0.81
26:1:734:GLY:O	26:1:738:HIS:HB2	1.79	0.81
26:1:1260:LYS:NZ	31:2:504:TRP:O	2.14	0.81
34:7:58:CYS:HB3	34:7:62:GLY:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:371:HIS:HE2	19:T:389:SER:HG	1.28	0.81
3:C:750:LEU:HD11	20:U:70:CYS:CB	2.11	0.81
6:F:37:C:OP1	6:F:37:C:H3'	1.81	0.80
27:3:508:CYS:SG	27:3:518:GLN:NE2	2.54	0.80
6:F:59:G:H1	6:F:76:A:H61	1.30	0.80
11:K:127:GLU:O	11:K:136:ARG:NH2	2.15	0.80
27:3:932:ASN:O	27:3:933:ASN:ND2	2.14	0.80
19:T:274:ASP:HB2	19:T:281:ILE:HD13	1.63	0.80
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.00	0.80
44:l:62:TYR:N	45:k:70:LEU:O	2.15	0.80
47:n:19:LEU:HA	47:n:65:ILE:HA	1.64	0.80
13:N:41:ARG:HB2	13:N:44:GLU:HG2	1.64	0.79
36:9:341:GLY:O	36:9:379:GLN:NE2	2.15	0.79
3:C:746:VAL:O	3:C:790:LYS:HA	1.81	0.79
2:B:18:C:N3	2:B:59:G:N1	2.27	0.79
21:V:575:THR:O	21:V:580:ARG:NH2	2.15	0.79
17:R:386:ARG:NH2	23:X:356:ASP:OD2	2.16	0.79
6:F:38:G:H2'	6:F:39:A:C8	2.18	0.79
3:C:457:VAL:HA	3:C:462:GLY:HA3	1.65	0.78
1:A:762:ARG:HH22	15:P:226:LYS:HZ3	1.29	0.78
26:1:717:THR:HA	26:1:756:LEU:HD11	1.65	0.78
27:3:304:GLN:HE21	27:3:308:GLY:HA2	1.47	0.78
1:A:1870:ASP:N	1:A:1870:ASP:OD1	2.13	0.78
3:C:732:ILE:HA	3:C:746:VAL:HG22	1.65	0.78
26:1:802:GLU:OE1	26:1:805:TYR:N	2.15	0.78
1:A:57:GLN:O	13:N:107:GLN:NE2	2.15	0.78
5:E:214:ASP:N	5:E:214:ASP:OD1	2.17	0.78
31:2:523:GLU:OE1	31:2:529:LYS:NZ	2.16	0.78
3:C:593:GLU:HG2	3:C:594:PRO:HD2	1.65	0.78
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.02	0.78
26:1:1257:PRO:HD3	31:2:488:LEU:HD11	1.66	0.78
1:A:821:ARG:HG2	1:A:821:ARG:NH1	1.97	0.78
5:E:81:LEU:O	5:E:92:LEU:HA	1.84	0.78
8:H:43:U:H2'	8:H:44:U:H6	1.49	0.78
36:9:397:PHE:H	36:9:397:PHE:HD1	1.30	0.77
19:T:371:HIS:NE2	19:T:389:SER:OG	2.14	0.77
27:3:1200:THR:N	27:3:1203:GLU:OE1	2.14	0.77
1:A:332:TYR:O	3:C:888:ARG:NH2	2.16	0.77
26:1:1004:ILE:HD11	26:1:1008:LYS:HB2	1.66	0.77
1:A:380:LEU:HD22	1:A:384:VAL:HG21	1.67	0.77
1:A:1146:ASP:OD2	1:A:1182:ASN:ND2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:LEU:HD23	3:C:128:LEU:HD23	1.65	0.77
27:3:352:GLU:OE2	27:3:429:ARG:NH1	2.18	0.77
1:A:835:ASP:N	1:A:835:ASP:OD1	2.11	0.77
27:3:317:THR:OG1	27:3:318:ASP:O	2.03	0.77
48:z:136[A]:ASP:OD1	48:z:136[A]:ASP:N	2.18	0.77
7:G:111:U:H3	24:Y:105:ARG:HG2	1.48	0.77
26:1:804:ASN:O	26:1:808:THR:OG1	2.02	0.77
1:A:1124:ASN:ND2	1:A:1148:ASN:OD1	2.15	0.77
3:C:853:ARG:NH1	3:C:879:ASP:O	2.17	0.77
27:3:114:ARG:NH1	35:5:38:ASP:OD1	2.17	0.77
1:A:1690:ASP:OD1	1:A:1691:ASN:N	2.18	0.76
1:A:519:ASP:OD2	1:A:523:ASN:ND2	2.16	0.76
1:A:1804:ASN:HD22	1:A:1823:HIS:HA	1.50	0.76
1:A:2146:VAL:HA	1:A:2272:MET:HB3	1.65	0.76
27:3:200:ALA:O	27:3:204:THR:OG1	2.04	0.76
36:9:268:GLU:O	36:9:271:LEU:N	2.18	0.76
2:B:18:C:N4	2:B:59:G:O6	2.18	0.76
12:L:77:LEU:HD12	36:9:221:LEU:HD21	1.65	0.76
26:1:138:ASP:HB3	26:1:141:LYS:HB2	1.66	0.76
2:B:20:G:O6	2:B:57:G:N1	2.15	0.76
3:C:666:VAL:HG12	3:C:668:GLU:H	1.49	0.76
8:H:151:C:H2'	8:H:152:G:C8	2.21	0.76
19:T:220:VAL:HG22	19:T:230:ILE:HD13	1.66	0.76
27:3:316:GLU:OE2	27:3:326:ARG:NH2	2.19	0.76
27:3:199:GLU:O	27:3:203:ASN:ND2	2.19	0.76
36:9:321:PHE:HA	36:9:332:GLY:HA3	1.67	0.76
26:1:420:GLY:O	26:1:424:ILE:N	2.17	0.76
7:G:85:G:H1	8:H:45:C:H42	1.32	0.76
8:H:14:C:H1'	8:H:15:U:H5'	1.68	0.76
13:N:58:ARG:NH2	13:N:98:GLU:O	2.18	0.76
26:1:883:ASP:OD2	26:1:883:ASP:N	2.14	0.76
27:3:639:SER:OG	27:3:699:VAL:O	2.03	0.76
4:D:835:SER:O	4:D:839:GLY:N	2.18	0.75
1:A:584:HIS:HE1	49:A:2401:IHP:O26	1.69	0.75
26:1:714:GLU:O	34:7:51:TYR:OH	2.03	0.75
36:9:360:HIS:HB3	36:9:365:ILE:HG21	1.67	0.75
1:A:548:ARG:NH2	1:A:549:GLU:OE2	2.20	0.75
36:9:269:ASP:HA	36:9:272:ARG:HE	1.49	0.75
1:A:766:THR:HG22	1:A:768:ASP:H	1.51	0.75
14:O:259:ARG:N	14:O:273:GLN:O	2.18	0.75
16:Q:514:ILE:H	16:Q:655:ILE:HA	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:613:THR:HG22	27:3:632:ALA:HA	1.69	0.75
29:w:438:LEU:HD11	29:w:452:ILE:HG23	1.68	0.75
23:X:277:ARG:NH2	26:1:434:THR:CB	2.49	0.74
27:3:705:ARG:HH22	27:3:708:GLY:H	1.34	0.74
36:9:219:GLU:HG2	36:9:220:ILE:HD12	1.69	0.74
1:A:2191:GLN:O	1:A:2195:THR:OG1	2.05	0.74
26:1:471:ASP:OD1	26:1:471:ASP:N	2.19	0.74
27:3:128:ARG:NH2	27:3:178:GLU:O	2.20	0.74
1:A:1314:VAL:O	1:A:1318:THR:OG1	2.04	0.74
5:E:90:ILE:HD12	5:E:105:LEU:HD13	1.69	0.74
24:Y:86:ASP:OD1	24:Y:86:ASP:N	2.16	0.74
7:G:-11:G:O2'	7:G:-10:G:O4'	2.06	0.74
1:A:821:ARG:HG2	1:A:821:ARG:HH11	1.51	0.74
8:H:46:U:O2'	8:H:47:U:OP2	2.05	0.74
29:w:408:CYS:SG	29:w:425:HIS:NE2	2.59	0.74
1:A:891:PHE:O	12:L:83:ARG:NH2	2.21	0.74
3:C:846:VAL:HG22	3:C:887:LEU:HD11	1.70	0.74
6:F:40:U:H3	7:G:7:G:H1	1.36	0.74
5:E:261:VAL:HB	5:E:275:LYS:HB2	1.68	0.73
42:i:21:VAL:O	42:i:28:GLU:HA	1.88	0.73
27:3:718:ARG:HB2	27:3:720:TRP:HE1	1.52	0.73
17:R:403:ASN:OD1	23:X:253:ARG:NH2	2.22	0.73
6:F:92:A:H2'	6:F:93:G:C8	2.24	0.73
23:X:298:SER:O	23:X:335:ASN:ND2	2.22	0.73
5:E:251:LEU:HD22	5:E:300:ILE:HG12	1.68	0.73
6:F:30:A:H61	7:G:16:G:H1'	1.53	0.73
6:F:83:A:O2'	6:F:84:A:N7	2.21	0.73
26:1:866:LYS:NZ	26:1:907:ASP:OD2	2.22	0.73
36:9:298:ASP:OD1	36:9:298:ASP:N	2.16	0.73
10:J:438:TYR:O	10:J:442:ARG:HB2	1.88	0.73
24:Y:32:TYR:OH	26:1:822:ARG:NH2	2.19	0.73
8:H:161:U:O2	8:H:163:G:N2	2.20	0.73
26:1:826:ASP:OD2	26:1:829:ASN:ND2	2.22	0.73
27:3:576:GLU:OE1	27:3:580:ARG:NH2	2.20	0.73
17:R:174:ALA:HA	17:R:199:MET:O	1.88	0.73
27:3:473:TYR:HB3	27:3:475:ILE:HD11	1.71	0.73
33:6:74:CYS:O	33:6:78:SER:OG	2.07	0.73
1:A:1199:LYS:NZ	1:A:1206:GLU:OE2	2.22	0.73
6:F:36:A:N1	7:G:10:U:C4	2.57	0.73
6:F:48:A:O2'	12:L:33:ARG:NH1	2.21	0.73
19:T:497:GLU:OE1	19:T:497:GLU:N	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:285:MET:SD	27:3:305:THR:OG1	2.47	0.73
27:3:326:ARG:NH1	27:3:372:GLU:OE2	2.21	0.73
1:A:1104:ASP:OD1	1:A:1104:ASP:N	2.18	0.72
7:G:92:U:OP1	12:L:40:ARG:NH2	2.20	0.72
15:P:205:LYS:HG2	15:P:208:LYS:HD3	1.68	0.72
23:X:274:TYR:CE1	26:1:436:THR:CA	2.71	0.72
27:3:280:ASP:H	27:3:857:ALA:HB3	1.54	0.72
28:p:72:PHE:O	28:p:78:PRO:HA	1.89	0.72
1:A:1991:TYR:OH	1:A:2015:GLU:OE2	2.07	0.72
5:E:300:ILE:HD12	5:E:314:THR:HG22	1.70	0.72
39:v:115:PRO:HG2	39:v:177:GLU:H	1.54	0.72
4:D:1992:GLU:HA	4:D:1995:ALA:HB3	1.71	0.72
1:A:2189:SER:HB3	1:A:2191:GLN:HE21	1.53	0.72
26:1:1301:ASP:N	26:1:1301:ASP:OD1	2.21	0.72
4:D:2098:ALA:O	4:D:2100:GLY:N	2.23	0.72
1:A:1762:TYR:O	1:A:1768:TYR:OH	2.03	0.72
5:E:250:LEU:O	5:E:261:VAL:HA	1.90	0.72
20:U:23:LEU:H	21:V:474:HIS:HD2	1.38	0.72
24:Y:44:PRO:HG2	24:Y:47:LEU:HD13	1.70	0.72
26:1:699:GLN:OE1	26:1:702:ARG:NH2	2.22	0.72
27:3:484:VAL:HG11	27:3:499:PHE:HD2	1.55	0.72
39:v:200:ASN:O	39:v:204:LYS:N	2.22	0.72
1:A:858:GLN:HE22	8:H:30:A:H5''	1.55	0.72
3:C:187:THR:OG1	3:C:201:ASN:OD1	2.07	0.71
8:H:43:U:H2'	8:H:44:U:C6	2.25	0.71
10:J:231:PHE:HE1	10:J:247:LYS:HG3	1.55	0.71
27:3:864:SER:OG	27:3:886:GLU:O	2.08	0.71
6:F:36:A:H2'	6:F:37:C:H5''	1.72	0.71
7:G:16:G:H5''	7:G:17:U:O4'	1.91	0.71
17:R:332:ARG:HH22	23:X:267:ASP:H	1.38	0.71
19:T:216:ASN:O	19:T:216:ASN:ND2	2.23	0.71
48:z:20:THR:OG1	48:z:159:HIS:ND1	2.22	0.71
2:B:97:G:H1	2:B:116:U:H3	1.37	0.71
10:J:230:THR:O	10:J:234:ASN:ND2	2.23	0.71
4:D:862:ASP:HA	27:3:599:GLU:HA	1.73	0.71
6:F:34:G:H2'	6:F:35:A:O4'	1.90	0.71
48:z:136[B]:ASP:OD1	48:z:136[B]:ASP:N	2.24	0.71
1:A:1761:PRO:O	1:A:1763:LEU:N	2.23	0.71
3:C:445:ALA:HB1	3:C:449:ILE:HD11	1.73	0.71
7:G:8:C:H2'	7:G:9:C:C6	2.25	0.71
10:J:242:ILE:HA	10:J:245:TRP:HD1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:536:ILE:HG13	21:V:539:LEU:HD12	1.72	0.71
27:3:696:SER:O	27:3:696:SER:OG	2.08	0.71
27:3:878:ASP:OD1	27:3:879:LEU:N	2.24	0.71
26:1:967:GLU:O	26:1:971:MET:CB	2.38	0.71
1:A:182:ILE:HD11	1:A:562:VAL:HG13	1.73	0.71
1:A:1188:ASN:ND2	1:A:1193:GLU:OE1	2.22	0.71
31:2:616:SER:O	32:4:80:TYR:N	2.22	0.71
36:9:310:LEU:HD21	36:9:345:TYR:HA	1.72	0.71
1:A:211:GLN:OE1	1:A:214:ARG:NH1	2.24	0.71
1:A:1546:ASN:ND2	11:K:183:ILE:O	2.18	0.71
19:T:424:ASP:OD1	19:T:424:ASP:N	2.20	0.71
27:3:412:ILE:HG12	27:3:423:LEU:HG	1.73	0.71
37:8:38:VAL:HG22	37:8:113:GLN:HE22	1.55	0.71
23:X:345:GLU:OE2	23:X:348:ARG:NH1	2.24	0.70
5:E:80:THR:HA	5:E:93:TRP:O	1.91	0.70
3:C:300:LEU:HA	3:C:306:ASN:HD22	1.57	0.70
1:A:298:ASP:OD1	1:A:300:ASN:ND2	2.24	0.70
1:A:2275:ALA:HA	1:A:2297:GLN:HG2	1.73	0.70
5:E:60:MET:HB2	5:E:353:MET:HB3	1.73	0.70
7:G:91:A:OP1	12:L:12:ARG:NH2	2.24	0.70
10:J:287:MET:HE1	10:J:319:MET:HB3	1.73	0.70
27:3:260:ASN:OD1	27:3:261:PHE:N	2.24	0.70
2:B:46:U:O2	20:U:11:ARG:NH2	2.19	0.70
7:G:85:G:H2'	7:G:86:A:C8	2.26	0.70
10:J:414:HIS:HA	10:J:417:VAL:HG22	1.74	0.70
27:3:246:SER:O	27:3:258:TYR:OH	2.09	0.70
36:9:360:HIS:ND1	36:9:391:ASP:OD1	2.25	0.70
1:A:1941:ARG:NH2	1:A:2012:LEU:O	2.18	0.70
3:C:677:GLU:HA	3:C:683:ASN:O	1.91	0.70
35:5:36:HIS:ND1	35:5:76:CYS:SG	2.65	0.70
10:J:220:LEU:HD13	10:J:224:LYS:HD2	1.72	0.70
26:1:460:PRO:HB2	26:1:464:LEU:HD12	1.74	0.70
2:B:100:C:H2'	2:B:101:U:C6	2.27	0.70
23:X:296:HIS:O	23:X:298:SER:N	2.25	0.70
27:3:442:LEU:H	27:3:734:LEU:HA	1.57	0.70
27:3:461:THR:HA	27:3:473:TYR:O	1.92	0.70
5:E:295:PRO:HD3	5:E:335:PHE:HB3	1.72	0.70
6:F:84:A:H1'	6:F:85:U:H5'	1.74	0.70
8:H:78:C:H2'	8:H:79:G:H8	1.57	0.69
1:A:2105:ILE:HD11	1:A:2141:GLU:HG3	1.72	0.69
19:T:496:THR:OG1	19:T:498:GLU:OE2	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:87:GLN:O	24:Y:90:THR:OG1	2.09	0.69
26:1:544:LEU:HD21	26:1:549:ARG:HB2	1.74	0.69
3:C:453:TYR:OH	3:C:575:GLN:HB2	1.92	0.69
1:A:78:ASN:HD22	1:A:79:ARG:N	1.91	0.69
6:F:37:C:H3'	6:F:37:C:P	2.33	0.69
3:C:826:ARG:HA	3:C:911:PRO:HG3	1.73	0.69
26:1:967:GLU:O	26:1:971:MET:HB2	1.93	0.69
27:3:806:ALA:HA	27:3:856:LYS:HB3	1.75	0.69
27:3:388:GLN:NE2	27:3:845:GLU:OE2	2.25	0.69
27:3:499:PHE:O	27:3:525:ARG:NH1	2.18	0.69
27:3:875:ASN:HD22	27:3:875:ASN:H	1.39	0.69
1:A:2330:ARG:H	1:A:2330:ARG:HD3	1.57	0.69
27:3:640:LEU:HD22	27:3:667:ILE:HG23	1.74	0.69
1:A:1764:SER:O	1:A:1766:GLN:N	2.26	0.68
1:A:2259:VAL:HG12	1:A:2260:GLN:H	1.58	0.68
5:E:262:TRP:HB3	5:E:272:ARG:HG3	1.74	0.68
27:3:115:ILE:O	27:3:138:GLN:NE2	2.26	0.68
27:3:266:ASP:OD1	27:3:266:ASP:N	2.22	0.68
27:3:452:LEU:HD21	27:3:476:VAL:HG11	1.76	0.68
36:9:75:THR:HA	36:9:82:LYS:HA	1.73	0.68
47:n:20:LYS:N	47:n:64:ASN:O	2.26	0.68
1:A:41:GLN:O	1:A:45:TYR:HB2	1.93	0.68
9:I:169:TYR:O	9:I:173:LEU:CB	2.41	0.68
25:Z:601:LEU:O	25:Z:604:LYS:HG3	1.93	0.68
26:1:776:GLU:HG3	26:1:784:MET:HE2	1.75	0.68
32:4:101:ASN:HA	32:4:148:ASN:HA	1.74	0.68
34:7:30:CYS:SG	34:7:31:VAL:N	2.66	0.68
36:9:300:THR:O	36:9:300:THR:OG1	2.06	0.68
5:E:259:VAL:HB	5:E:277:PHE:HB2	1.75	0.68
7:G:7:G:H2'	7:G:8:C:C6	2.28	0.68
10:J:242:ILE:HA	10:J:245:TRP:CD1	2.27	0.68
26:1:614:ARG:NH2	26:1:618:ASP:OD2	2.26	0.68
27:3:528:ARG:NH1	27:3:572:GLY:O	2.26	0.68
48:z:23:ASP:N	48:z:23:ASP:OD1	2.27	0.68
1:A:1296:GLN:HG2	1:A:1327:MET:HE1	1.74	0.68
5:E:241:LEU:HD23	5:E:250:LEU:HD21	1.75	0.68
16:Q:1066:GLN:HA	16:Q:1102:PRO:HD3	1.75	0.68
27:3:275:ARG:HG2	27:3:388:GLN:HB2	1.75	0.68
34:7:46:CYS:HB3	34:7:85:CYS:HB2	1.76	0.68
6:F:92:A:H2'	6:F:93:G:H8	1.57	0.68
26:1:624:VAL:O	26:1:628:THR:OG1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:383:LEU:HB2	29:w:391:PRO:HB3	1.75	0.68
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.76	0.68
1:A:270:ASN:HD21	20:U:8:PRO:HB3	1.58	0.68
1:A:1201:ARG:O	1:A:1203:SER:N	2.26	0.68
2:B:98:G:H2'	2:B:99:C:C6	2.28	0.68
27:3:429:ARG:NH2	35:5:59:GLU:O	2.22	0.68
1:A:1855:GLU:OE1	11:K:136:ARG:NH1	2.27	0.68
8:H:107:A:H2'	8:H:108:G:C8	2.29	0.68
36:9:132:GLU:O	36:9:136:ILE:N	2.22	0.68
1:A:1792:LYS:HB3	1:A:1798:LEU:HG	1.74	0.68
1:A:2106:LEU:HB2	1:A:2142:ILE:HD12	1.76	0.68
31:2:450:SER:HB3	31:2:453:LYS:HG2	1.76	0.68
48:z:52:THR:HG22	48:z:68:PRO:HA	1.76	0.68
6:F:41:A:H2'	6:F:42:C:C6	2.29	0.68
1:A:330:THR:O	3:C:177:ARG:NH1	2.27	0.67
8:H:151:C:H2'	8:H:152:G:H8	1.57	0.67
17:R:174:ALA:HB2	17:R:200:VAL:HG23	1.75	0.67
23:X:274:TYR:HE1	26:1:436:THR:CA	2.06	0.67
39:v:39:ASP:O	39:v:42:LYS:HD2	1.94	0.67
42:i:23:LEU:HA	42:i:69:VAL:HA	1.74	0.67
48:z:3:ASN:O	48:z:3:ASN:ND2	2.27	0.67
48:z:32:GLU:N	48:z:32:GLU:OE1	2.27	0.67
1:A:979:SER:HB3	1:A:1173:SER:HB2	1.76	0.67
1:A:1217:GLN:OE1	1:A:1224:ARG:NE	2.27	0.67
3:C:674:CYS:HB3	3:C:818:SER:HB2	1.75	0.67
13:N:70:ILE:HG23	13:N:74:LEU:HD23	1.75	0.67
3:C:509:VAL:HG12	3:C:565:ILE:HG12	1.75	0.67
4:D:1559:VAL:O	4:D:1643:VAL:HA	1.94	0.67
5:E:214:ASP:OD2	5:E:218:LYS:NZ	2.26	0.67
6:F:80:G:H1'	6:F:81:C:H2'	1.77	0.67
27:3:782:GLN:HG3	27:3:867:ARG:HH22	1.60	0.67
1:A:2076:ARG:NH1	1:A:2305:TYR:OH	2.27	0.67
10:J:370:VAL:HG22	10:J:378:ASN:HB3	1.76	0.67
21:V:517:LEU:HD23	21:V:518:LYS:HG3	1.75	0.67
27:3:353:PHE:HD1	27:3:406:PRO:HD3	1.59	0.67
1:A:1000:ILE:HG22	1:A:1001:VAL:HG22	1.76	0.67
1:A:863:GLU:HG3	1:A:913:PRO:HB3	1.77	0.67
1:A:1925:LYS:HE2	21:V:457:ARG:NH2	2.09	0.67
27:3:326:ARG:HE	27:3:372:GLU:HG2	1.59	0.67
1:A:1786:TYR:CE1	1:A:1837:ALA:HB2	2.30	0.67
3:C:731:SER:HB2	3:C:746:VAL:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:70:C:H2'	8:H:71:C:C6	2.30	0.67
27:3:430:GLY:O	27:3:433:SER:OG	2.11	0.67
42:i:22:LYS:O	42:i:70:LEU:N	2.27	0.67
1:A:2067:PHE:HB2	1:A:2072:GLU:HB3	1.77	0.67
1:A:2086:ARG:O	1:A:2089:HIS:N	2.22	0.67
27:3:616:ILE:HB	27:3:629:SER:O	1.95	0.67
27:3:672:GLY:H	27:3:696:SER:HA	1.58	0.67
27:3:806:ALA:HB1	27:3:856:LYS:HD3	1.75	0.67
47:b:28:THR:O	47:b:41:LYS:N	2.24	0.67
3:C:561:LYS:NZ	3:C:614:TYR:O	2.27	0.66
12:L:64:SER:OG	12:L:66:GLU:OE1	2.12	0.66
7:G:13:C:H2'	7:G:14:A:H8	1.60	0.66
10:J:234:ASN:O	10:J:238:ASN:ND2	2.17	0.66
10:J:240:THR:OG1	10:J:241:VAL:N	2.26	0.66
26:1:1210:HIS:ND1	31:2:585:THR:OG1	2.29	0.66
27:3:41:LEU:HD22	27:3:52:THR:HG22	1.77	0.66
27:3:195:ASP:OD2	27:3:200:ALA:N	2.21	0.66
1:A:52:GLY:O	2:B:64:G:O2'	2.12	0.66
1:A:1412:TRP:O	1:A:1420:ASN:ND2	2.21	0.66
16:Q:515:VAL:N	16:Q:540:THR:O	2.28	0.66
16:Q:1227:LEU:O	16:Q:1273:LEU:HA	1.95	0.66
1:A:1106:ALA:O	1:A:1110:ILE:HG13	1.95	0.66
1:A:2312:SER:O	1:A:2316:ASN:ND2	2.27	0.66
3:C:690:GLU:HG3	3:C:788:LYS:HB3	1.77	0.66
7:G:108:U:H4'	7:G:109:U:OP2	1.96	0.66
24:Y:3:PRO:HA	24:Y:6:LYS:HG3	1.75	0.66
27:3:464:ARG:HG3	27:3:516:LEU:HD11	1.76	0.66
36:9:324:SER:OG	36:9:415:SER:OG	2.13	0.66
37:8:115:ASN:OD1	37:8:116:ILE:N	2.28	0.66
2:B:99:C:H2'	2:B:100:C:C6	2.31	0.66
26:1:477:LYS:HB3	26:1:499:LYS:NZ	2.11	0.66
1:A:982:GLU:O	1:A:983:LYS:HG3	1.96	0.66
33:6:48:ILE:HG12	33:6:62:VAL:HG12	1.76	0.66
36:9:267:ASP:OD1	36:9:268:GLU:N	2.29	0.66
5:E:175:THR:HA	5:E:191:GLN:HA	1.77	0.66
16:Q:1182:VAL:N	16:Q:1305:ALA:O	2.28	0.66
21:V:646:HIS:O	21:V:650:THR:OG1	2.14	0.66
29:w:421:ALA:HA	29:w:424:ARG:HE	1.61	0.66
1:A:533:LYS:HZ2	1:A:533:LYS:HB3	1.61	0.66
1:A:1957:ASP:OD2	1:A:1959:THR:OG1	2.14	0.66
8:H:50:C:H2'	8:H:51:A:H8	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1166:ILE:O	26:1:1170:THR:HG22	1.95	0.66
6:F:17:C:H2'	6:F:18:A:H8	1.61	0.65
1:A:325:HIS:HD2	1:A:326:HIS:HD2	1.43	0.65
1:A:1317:TYR:HB3	1:A:1474:MET:HE3	1.76	0.65
27:3:552:ARG:NH2	27:3:568:MET:O	2.27	0.65
1:A:552:ARG:HG2	1:A:552:ARG:HH11	1.62	0.65
3:C:323:PHE:CD2	3:C:373:ILE:HG12	2.32	0.65
3:C:560:VAL:HG12	3:C:561:LYS:H	1.59	0.65
10:J:408:ASP:OD1	10:J:408:ASP:N	2.30	0.65
27:3:507:SER:HB2	27:3:547:CYS:SG	2.35	0.65
36:9:368:MET:O	36:9:394:HIS:ND1	2.30	0.65
1:A:1384:ARG:HH22	1:A:1414:ARG:HH22	1.45	0.65
1:A:1591:MET:SD	1:A:1611:LYS:NZ	2.61	0.65
3:C:727:LEU:O	3:C:731:SER:OG	2.13	0.65
25:Z:547:ASN:OD1	25:Z:547:ASN:N	2.20	0.65
27:3:670:GLN:HA	27:3:698:PRO:HA	1.79	0.65
36:9:337:GLY:O	36:9:421:ARG:NH2	2.28	0.65
17:R:295:ASP:OD2	17:R:296:ARG:N	2.30	0.65
21:V:618:ARG:HB3	21:V:646:HIS:HE1	1.62	0.65
3:C:925:PRO:HG2	3:C:928:HIS:CE1	2.31	0.65
15:P:198:ALA:HB1	15:P:201:VAL:HG21	1.77	0.65
27:3:351:SER:OG	27:3:355:ASN:O	2.13	0.65
27:3:1187:PRO:HA	27:3:1190:GLN:HB2	1.78	0.65
36:9:299:LEU:HD12	36:9:300:THR:HG22	1.79	0.65
1:A:2105:ILE:HG22	1:A:2262:LEU:HB2	1.79	0.65
1:A:331:TRP:HB2	3:C:177:ARG:HH11	1.62	0.65
1:A:1076:ASP:OD1	1:A:1077:ILE:N	2.30	0.65
1:A:2164:PRO:HB3	1:A:2296:LEU:HD11	1.78	0.65
27:3:556:ILE:HG13	27:3:564:VAL:HB	1.78	0.65
1:A:529:THR:HG22	11:K:197:TYR:HB3	1.79	0.64
3:C:441:PRO:O	3:C:444:GLY:HA3	1.97	0.64
19:T:257:ARG:NH2	19:T:300:ILE:O	2.30	0.64
1:A:1760:GLU:HG2	1:A:1760:GLU:O	1.98	0.64
3:C:836:VAL:HG22	3:C:897:SER:HB2	1.78	0.64
8:H:12:G:O2'	8:H:13:C:O4'	2.11	0.64
26:1:607:ALA:O	26:1:611:SER:OG	2.14	0.64
18:S:366:VAL:N	18:S:583:TYR:O	2.26	0.64
3:C:338:GLU:OE2	3:C:342:ARG:NH1	2.29	0.64
3:C:687:MET:HE2	3:C:791:ILE:HG12	1.79	0.64
6:F:43:A:H2	7:G:4:A:H61	1.46	0.64
17:R:134:ARG:NH2	19:T:385:TYR:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:431:GLN:O	18:S:435:TYR:N	2.26	0.64
4:D:2020:SER:O	4:D:2039:VAL:HA	1.97	0.64
19:T:245:HIS:NE2	19:T:263:SER:OG	2.28	0.64
23:X:273:MET:CE	26:1:433:ALA:CB	2.65	0.64
23:X:275:ILE:O	23:X:308:TYR:OH	2.11	0.64
26:1:1262:ARG:NH1	35:5:24:ALA:O	2.30	0.64
27:3:84:SER:OG	27:3:85:GLY:N	2.31	0.64
27:3:604:PHE:HD1	27:3:628:LEU:HD23	1.62	0.64
29:w:334:LEU:O	29:w:338:ARG:N	2.18	0.64
31:2:456:ARG:HH21	31:2:457:MET:HE3	1.61	0.64
3:C:60:HIS:O	3:C:63:LYS:HB2	1.98	0.64
5:E:125:PHE:HE1	5:E:159:PRO:HB3	1.63	0.64
10:J:251:TRP:CE2	10:J:255:LEU:HD11	2.33	0.64
33:6:68:PHE:HA	33:6:71:LYS:HG2	1.80	0.64
39:v:31:ARG:HD3	39:v:48:LYS:NZ	2.13	0.64
21:V:515:CYS:HA	21:V:521:TYR:HB2	1.79	0.64
27:3:583:MET:HG3	27:3:584:SER:H	1.63	0.64
5:E:90:ILE:HD11	5:E:112:VAL:HG11	1.79	0.64
7:G:-12:C:O2'	7:G:-11:G:N7	2.31	0.64
26:1:531:LEU:HD23	26:1:559:ILE:HD12	1.79	0.64
44:g:21:GLU:O	44:g:69:ARG:N	2.31	0.64
8:H:28:C:O2'	8:H:29:A:O5'	2.16	0.63
25:Z:509:GLN:NE2	25:Z:510:ASN:OD1	2.31	0.63
27:3:875:ASN:HD22	27:3:875:ASN:N	1.95	0.63
29:w:495:LEU:HA	29:w:498:GLN:HB2	1.80	0.63
35:5:3:ASP:O	35:5:7:ILE:HG12	1.98	0.63
1:A:146:SER:HB2	1:A:193:LEU:HD22	1.80	0.63
1:A:781:ARG:HH21	8:H:24:A:H5''	1.63	0.63
21:V:640:THR:O	21:V:644:ARG:HG3	1.98	0.63
26:1:1100:ASN:O	26:1:1103:VAL:HG22	1.98	0.63
26:1:1289:ASN:HB3	26:1:1295:TYR:H	1.63	0.63
27:3:215:LEU:H	27:3:215:LEU:HD12	1.63	0.63
1:A:78:ASN:HD22	1:A:79:ARG:H	1.46	0.63
1:A:2229:LYS:O	1:A:2257:GLU:N	2.32	0.63
5:E:304:SER:O	5:E:330:ILE:N	2.31	0.63
1:A:658:ARG:NH1	6:F:67:G:OP2	2.32	0.63
3:C:496:VAL:HG23	3:C:546:ALA:HA	1.79	0.63
26:1:1120:ALA:HB2	26:1:1128:VAL:HG21	1.80	0.63
27:3:511:LEU:HD23	27:3:512:GLY:H	1.63	0.63
44:l:61:VAL:HA	45:k:71:GLU:HA	1.81	0.63
3:C:489:GLN:OE1	3:C:489:GLN:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:8:ARG:HB2	13:N:9:LYS:HE2	1.81	0.63
25:Z:575:ARG:NH1	25:Z:594:GLU:OE1	2.32	0.63
26:1:1030:LYS:O	26:1:1034:ASN:ND2	2.32	0.63
27:3:93:GLN:NE2	27:3:100:GLU:OE1	2.31	0.63
29:w:416:TYR:CE1	29:w:425:HIS:HB2	2.33	0.63
36:9:360:HIS:NE2	36:9:394:HIS:O	2.32	0.63
1:A:617:ASN:HA	1:A:621:VAL:HG23	1.78	0.63
1:A:1021:ASP:N	1:A:1021:ASP:OD1	2.31	0.63
5:E:118:ASN:HD21	5:E:122:SER:H	1.47	0.63
10:J:280:LEU:HD21	10:J:315:LYS:HD2	1.80	0.63
21:V:525:PHE:HB3	21:V:560:LEU:HD21	1.80	0.63
26:1:150:ARG:NH1	26:1:158:GLU:OE1	2.31	0.63
27:3:399:ASP:OD1	27:3:400:GLU:N	2.32	0.63
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.20	0.63
1:A:1655:THR:OG1	1:A:1656:THR:N	2.31	0.63
5:E:73:LYS:HE3	5:E:117:TYR:H	1.63	0.63
13:N:26:ASP:O	13:N:30:ARG:HG2	1.98	0.63
17:R:240:LYS:O	17:R:244:GLU:HG3	1.99	0.63
23:X:366:GLU:N	23:X:366:GLU:OE2	2.32	0.63
27:3:911:LYS:HB3	27:3:922:GLY:O	1.98	0.63
31:2:547:LYS:NZ	31:2:555:GLU:OE2	2.20	0.63
32:4:117:TYR:O	32:4:121:SER:CB	2.47	0.63
1:A:1295:ILE:HD11	1:A:1327:MET:HE2	1.79	0.63
21:V:641:ASP:HA	21:V:644:ARG:HD2	1.81	0.63
23:X:279:SER:O	23:X:307:GLN:NE2	2.31	0.63
1:A:266:SER:OG	1:A:271:MET:O	2.16	0.63
3:C:540:GLU:H	3:C:540:GLU:CD	2.05	0.63
5:E:219:VAL:HG23	5:E:231:MET:HE1	1.81	0.63
8:H:27:U:C2'	8:H:28:C:H5'	2.29	0.63
9:I:374:ILE:O	9:I:377:THR:N	2.31	0.63
10:J:350:ILE:HD11	10:J:362:ALA:HA	1.81	0.63
1:A:382:GLU:HB3	3:C:354:ARG:HD2	1.79	0.62
6:F:93:G:OP1	10:J:318:TYR:OH	2.15	0.62
12:L:79:PRO:O	12:L:80:THR:OG1	2.14	0.62
39:v:23:ASN:OD1	39:v:26:ARG:NH2	2.32	0.62
5:E:209:ILE:HG12	5:E:219:VAL:HG22	1.79	0.62
10:J:431:ARG:O	10:J:435:ILE:HD12	1.99	0.62
27:3:1160:HIS:NE2	27:3:1175:ASP:OD2	2.23	0.62
1:A:1816:GLN:HG2	1:A:1916:LEU:HD11	1.81	0.62
3:C:604:LEU:HD21	3:C:627:HIS:CE1	2.34	0.62
3:C:937:THR:HG22	3:C:941:LYS:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:488:GLU:O	21:V:492:MET:HB2	2.00	0.62
27:3:511:LEU:HD21	27:3:574:LEU:HD11	1.81	0.62
27:3:918:ARG:HG2	27:3:918:ARG:HH11	1.64	0.62
1:A:837:LYS:NZ	26:1:101:TYR:HB3	2.14	0.62
1:A:1365:ILE:HG23	1:A:1474:MET:HE1	1.82	0.62
3:C:534:VAL:HG23	3:C:539:ILE:HD11	1.80	0.62
21:V:648:LYS:O	21:V:648:LYS:NZ	2.21	0.62
23:X:335:ASN:O	23:X:343:ARG:NE	2.32	0.62
27:3:895:ARG:NE	27:3:901:GLU:OE1	2.32	0.62
36:9:271:LEU:HA	36:9:274:GLN:NE2	2.15	0.62
36:9:366:LEU:HD13	36:9:382:ILE:HG13	1.79	0.62
1:A:2181:GLN:O	1:A:2217:SER:HA	1.99	0.62
16:Q:875:HIS:O	16:Q:1033:LYS:N	2.32	0.62
27:3:1009:PHE:HZ	27:3:1046:GLY:HA3	1.62	0.62
3:C:770:PHE:HE1	3:C:789:PHE:CD1	2.18	0.62
8:H:182:U:H2'	8:H:183:G:C8	2.34	0.62
21:V:647:LEU:O	21:V:651:PRO:HD2	2.00	0.62
23:X:338:PHE:HB3	23:X:341:ASN:HA	1.80	0.62
27:3:341:VAL:HG22	27:3:347:LEU:HD12	1.81	0.62
27:3:1140:PHE:O	27:3:1144:VAL:HG23	2.00	0.62
1:A:698:PRO:HG2	19:T:373:LYS:HZ1	1.64	0.62
4:D:860:GLN:O	27:3:601:ARG:NH1	2.33	0.62
7:G:98:U:H4'	34:7:4:HIS:HD2	1.64	0.62
8:H:53:U:OP1	31:2:450:SER:OG	2.15	0.62
10:J:347:HIS:O	10:J:351:ASN:ND2	2.33	0.62
19:T:215:GLY:O	19:T:217:GLN:NE2	2.28	0.62
19:T:394:ASN:ND2	19:T:408:ASN:OD1	2.32	0.62
27:3:715:MET:HE3	27:3:739:LEU:H	1.64	0.62
36:9:449:ARG:HA	36:9:452:GLN:HE21	1.65	0.62
46:j:44:GLU:O	46:j:61:ALA:HA	2.00	0.62
4:D:1583:ASP:O	4:D:1585:GLN:N	2.33	0.62
33:6:111:LYS:HZ2	33:6:115:GLU:HG3	1.65	0.62
1:A:699:GLU:HA	1:A:701:ILE:HG13	1.82	0.62
9:I:139:ALA:C	9:I:141:PRO:HD3	2.25	0.62
26:1:583:ILE:HD11	26:1:623:TYR:HE1	1.64	0.62
27:3:718:ARG:HB2	27:3:720:TRP:NE1	2.15	0.62
36:9:277:LYS:HA	36:9:298:ASP:HB3	1.80	0.62
47:b:13:GLU:O	47:b:29:ILE:N	2.32	0.62
3:C:685:ILE:HD11	3:C:808:ILE:HD11	1.81	0.61
5:E:90:ILE:HG13	5:E:105:LEU:HD22	1.80	0.61
10:J:220:LEU:O	10:J:224:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:23:LEU:H	21:V:474:HIS:CD2	2.16	0.61
2:B:99:C:H2'	2:B:100:C:H6	1.64	0.61
5:E:217:ILE:HB	5:E:231:MET:HG2	1.82	0.61
23:X:314:THR:HG22	23:X:318:GLY:HA2	1.82	0.61
1:A:693:ILE:HG22	1:A:694:LEU:HD23	1.83	0.61
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.36	0.61
5:E:91:LEU:HB3	5:E:101:ASN:ND2	2.09	0.61
8:H:50:C:H2'	8:H:51:A:C8	2.36	0.61
21:V:481:PHE:HD2	21:V:485:GLN:HB2	1.65	0.61
1:A:2178:ILE:HB	1:A:2214:ILE:HD13	1.80	0.61
6:F:42:C:H2'	6:F:43:A:O4'	2.00	0.61
27:3:223:LYS:NZ	27:3:224:TYR:OH	2.22	0.61
1:A:1384:ARG:HH22	1:A:1414:ARG:NH2	1.97	0.61
3:C:495:ARG:HB2	3:C:495:ARG:HH11	1.64	0.61
6:F:81:C:H42	8:H:18:U:H3	1.49	0.61
14:O:163:HIS:O	14:O:182:ARG:N	2.34	0.61
27:3:412:ILE:HB	27:3:1105:GLN:HE21	1.65	0.61
27:3:511:LEU:HD23	27:3:512:GLY:N	2.15	0.61
27:3:675:LEU:HB3	27:3:686:LEU:HD12	1.81	0.61
3:C:679:PRO:HD2	3:C:807:GLN:HB3	1.82	0.61
5:E:133:VAL:HG22	5:E:154:VAL:HG11	1.82	0.61
14:O:23:LEU:HA	14:O:81:CYS:HA	1.82	0.61
27:3:933:ASN:ND2	27:3:935:GLU:OE2	2.33	0.61
1:A:546:LEU:HD11	1:A:595:LYS:HG3	1.81	0.61
1:A:1018:ASN:ND2	1:A:1023:ASN:OD1	2.34	0.61
17:R:390:GLU:H	17:R:390:GLU:CD	2.09	0.61
5:E:222:LEU:HB3	5:E:223:ARG:HH11	1.64	0.61
3:C:269:LEU:O	3:C:378:TYR:OH	2.09	0.61
3:C:559:ILE:HD12	3:C:560:VAL:O	2.00	0.61
3:C:737:PRO:HG3	3:C:774:THR:HB	1.82	0.61
7:G:111:U:O2	24:Y:105:ARG:NE	2.32	0.61
27:3:587:VAL:HG11	27:3:590:MET:HE2	1.82	0.61
38:y:23:HIS:O	38:y:27:ILE:CB	2.48	0.61
1:A:1502:PHE:HE2	1:A:1505:LYS:HB2	1.66	0.61
3:C:809:ILE:HB	3:C:810:PRO:HD3	1.81	0.61
3:C:931:ARG:HE	3:C:935:ILE:HD11	1.64	0.61
7:G:88:G:N2	8:H:41:U:H3	1.98	0.61
27:3:946:GLU:OE1	27:3:946:GLU:N	2.33	0.61
31:2:471:ARG:HH21	31:2:474:VAL:HG23	1.66	0.61
37:8:39:ASP:OD2	37:8:41:SER:OG	2.19	0.61
24:Y:86:ASP:O	24:Y:89:SER:OG	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:260:ASN:HB3	27:3:264:GLN:HG2	1.83	0.60
1:A:1769:GLY:HA2	1:A:1772:PHE:CZ	2.36	0.60
13:N:102:CYS:SG	13:N:137:CYS:HB2	2.41	0.60
1:A:1994:LYS:O	1:A:1995:ASN:ND2	2.27	0.60
3:C:843:VAL:HG22	3:C:871:ILE:HD11	1.82	0.60
10:J:246:ILE:HG23	10:J:281:LYS:HE3	1.84	0.60
10:J:262:ARG:NH2	10:J:286:GLU:OE1	2.34	0.60
13:N:30:ARG:O	13:N:34:THR:OG1	2.19	0.60
26:1:151:THR:N	26:1:154:ASP:OD2	2.32	0.60
26:1:477:LYS:HB3	26:1:499:LYS:HZ1	1.65	0.60
27:3:138:GLN:HG2	27:3:161:HIS:ND1	2.15	0.60
27:3:893:VAL:HG22	27:3:905:VAL:HG22	1.84	0.60
1:A:858:GLN:OE1	1:A:861:ARG:NH2	2.34	0.60
3:C:118:PHE:O	3:C:122:LEU:HD12	2.01	0.60
5:E:171:SER:OG	5:E:173:ASP:OD2	2.19	0.60
24:Y:62:ILE:HD13	24:Y:82:LEU:HD21	1.83	0.60
26:1:128:ILE:HB	33:6:96:ARG:HB3	1.83	0.60
26:1:400:SER:N	26:1:403:GLU:OE1	2.32	0.60
26:1:690:ILE:HD11	26:1:708:ALA:HB3	1.83	0.60
26:1:866:LYS:HG3	26:1:909:VAL:HG11	1.81	0.60
27:3:70:LEU:HD11	27:3:152:LEU:HD13	1.84	0.60
27:3:697:ARG:NH2	27:3:717:SER:HB3	2.16	0.60
36:9:425:GLU:OE1	36:9:427:ARG:NH1	2.34	0.60
1:A:216:SER:O	1:A:216:SER:OG	2.16	0.60
1:A:274:PRO:HG3	20:U:1:MET:HG3	1.83	0.60
1:A:2128:LEU:HD23	1:A:2142:ILE:HG21	1.83	0.60
18:S:451:THR:HA	18:S:496:MET:O	2.02	0.60
24:Y:7:VAL:HG22	24:Y:108:ARG:HB2	1.84	0.60
37:8:110:LEU:HA	37:8:113:GLN:HE21	1.66	0.60
1:A:43:LYS:HZ3	6:F:21:U:H3	1.50	0.60
1:A:1878:ASP:OD1	1:A:1878:ASP:N	2.34	0.60
1:A:2121:ARG:HA	1:A:2182:PRO:HB3	1.84	0.60
3:C:488:VAL:HG13	3:C:609:LYS:HE2	1.84	0.60
6:F:29:A:N6	7:G:16:G:O2'	2.34	0.60
21:V:491:ASN:HA	21:V:528:ILE:HD11	1.83	0.60
27:3:206:GLN:HE21	27:3:231:HIS:HA	1.66	0.60
27:3:249:LEU:HD22	27:3:256:ILE:HD11	1.83	0.60
39:v:66:GLU:H	39:v:66:GLU:CD	2.10	0.60
47:n:18:GLU:O	47:n:66:ARG:N	2.34	0.60
3:C:286:ASN:OD1	3:C:300:LEU:N	2.26	0.60
6:F:36:A:N6	7:G:10:U:O4	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:72:U:H2'	8:H:73:C:C6	2.36	0.60
17:R:434:ASP:N	17:R:434:ASP:OD1	2.35	0.60
21:V:489:LEU:HD23	21:V:521:TYR:HE1	1.67	0.60
26:1:524:ARG:HG3	35:5:1:MET:HE3	1.83	0.60
27:3:407:ILE:HG23	27:3:425:VAL:HG13	1.83	0.60
27:3:637:PRO:HB3	27:3:640:LEU:HD21	1.84	0.60
27:3:899:THR:OG1	27:3:900:GLY:N	2.33	0.60
48:z:49:TYR:O	48:z:52:THR:OG1	2.16	0.60
27:3:525:ARG:NE	27:3:527:ILE:HD11	2.16	0.60
27:3:1136:GLU:OE1	27:3:1136:GLU:N	2.23	0.60
1:A:1850:ARG:NH1	1:A:1878:ASP:OD2	2.34	0.60
3:C:352:LYS:H	3:C:352:LYS:HD3	1.67	0.60
5:E:69:VAL:HG23	5:E:349:LYS:HA	1.82	0.60
5:E:175:THR:HG22	5:E:191:GLN:HB3	1.83	0.60
7:G:98:U:H4'	34:7:4:HIS:CD2	2.37	0.60
8:H:37:U:OP2	26:1:517:ARG:NH1	2.35	0.60
36:9:296:HIS:H	36:9:296:HIS:CD2	2.18	0.60
37:8:115:ASN:ND2	37:8:119:ILE:O	2.29	0.60
1:A:1535:THR:HG22	1:A:1569:LEU:HD13	1.84	0.60
1:A:2177:TRP:HZ3	1:A:2179:HIS:HB3	1.66	0.60
7:G:83:A:N1	29:w:400:HIS:NE2	2.49	0.60
8:H:98:G:C6	41:h:62:HIS:HA	2.37	0.60
9:I:231:ASN:O	9:I:233:ASP:N	2.27	0.60
27:3:725:TYR:O	27:3:728:ARG:HB2	2.02	0.60
32:4:105:GLY:N	32:4:173:THR:O	2.29	0.60
42:d:34:VAL:N	42:d:43:GLN:O	2.32	0.60
1:A:1548:TYR:CE2	1:A:1550:GLY:HA2	2.36	0.59
5:E:305:ALA:HA	5:E:329:SER:HB3	1.84	0.59
23:X:231:ALA:HA	24:Y:103:LYS:HE3	1.84	0.59
27:3:475:ILE:HG21	27:3:508:CYS:SG	2.42	0.59
1:A:2275:ALA:HB3	1:A:2295:GLU:HB2	1.83	0.59
3:C:86:THR:OG1	3:C:87:GLN:N	2.35	0.59
3:C:642:HIS:HE1	3:C:646:LYS:HD3	1.65	0.59
5:E:215:ASN:ND2	5:E:235:ALA:O	2.35	0.59
11:K:159:TYR:CE2	21:V:450:ILE:HG21	2.36	0.59
29:w:461:LYS:HA	29:w:464:LEU:HD12	1.84	0.59
1:A:529:THR:HG23	11:K:230:TRP:NE1	2.16	0.59
1:A:692:ASP:HA	19:T:376:ARG:HH22	1.67	0.59
1:A:1581:LEU:O	1:A:1585:ILE:HG13	2.02	0.59
5:E:344:SER:O	5:E:351:LEU:HA	2.01	0.59
26:1:1291:ASP:OD1	26:1:1292:LYS:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:HIS:O	3:C:142:LYS:NZ	2.26	0.59
4:D:530:THR:C	4:D:532:ASN:H	2.10	0.59
19:T:267:ASP:OD1	19:T:267:ASP:N	2.17	0.59
21:V:579:SER:O	21:V:583:VAL:HG23	2.03	0.59
24:Y:110:ASP:OD1	24:Y:111:HIS:N	2.35	0.59
26:1:907:ASP:OD1	26:1:907:ASP:N	2.35	0.59
36:9:436:ASP:O	36:9:440:GLU:HG3	2.01	0.59
1:A:1808:PHE:CE2	1:A:1893:PHE:HB3	2.37	0.59
6:F:39:A:H2'	6:F:40:U:O4'	2.03	0.59
7:G:98:U:O2'	34:7:5:HIS:NE2	2.33	0.59
21:V:622:ARG:HA	21:V:625:ARG:HE	1.67	0.59
38:y:70:SER:N	38:y:77:ILE:O	2.33	0.59
1:A:436:PRO:HB2	1:A:439:GLN:CD	2.27	0.59
3:C:774:THR:HG22	3:C:784:ILE:HD11	1.84	0.59
14:O:110:SER:O	14:O:114:LYS:CB	2.51	0.59
27:3:485:LEU:HB3	27:3:491:VAL:HG12	1.83	0.59
31:2:567:ASP:OD2	31:2:570:LYS:NZ	2.26	0.59
1:A:1502:PHE:CE2	1:A:1505:LYS:HB2	2.38	0.59
4:D:884:ASN:O	4:D:886:GLN:N	2.31	0.59
6:F:87:C:H4'	36:9:356:PRO:HG3	1.85	0.59
26:1:701:VAL:HA	26:1:704:ILE:HG22	1.83	0.59
27:3:947:GLU:HG3	27:3:948:VAL:H	1.68	0.59
3:C:514:TYR:CE2	3:C:522:SER:HB2	2.38	0.59
8:H:2:U:H2'	8:H:3:C:C6	2.38	0.59
11:K:136:ARG:O	11:K:140:ILE:HG12	2.02	0.59
27:3:547:CYS:HA	27:3:555:VAL:HG12	1.85	0.59
48:z:122:GLU:OE1	48:z:122:GLU:N	2.36	0.59
48:z:123:LEU:HD22	48:z:127:HIS:CD2	2.38	0.59
1:A:2106:LEU:O	1:A:2264:SER:N	2.36	0.59
3:C:922:GLU:O	3:C:924:GLN:NE2	2.35	0.59
5:E:318:ARG:HB3	5:E:318:ARG:HH11	1.67	0.59
27:3:520:TYR:HB2	27:3:521:PRO:HD2	1.85	0.59
42:d:35:SER:O	42:d:43:GLN:N	2.25	0.59
1:A:37:TRP:O	1:A:41:GLN:HG2	2.03	0.58
2:B:97:G:H2'	2:B:98:G:C8	2.38	0.58
7:G:19:G:N2	14:O:193:LEU:O	2.30	0.58
26:1:652:CYS:SG	26:1:692:HIS:HE1	2.26	0.58
26:1:1078:VAL:HG12	26:1:1118:ILE:HD12	1.83	0.58
27:3:108:GLY:O	34:7:82:ARG:NH1	2.35	0.58
31:2:451:LYS:O	31:2:455:ARG:NH1	2.35	0.58
44:l:49:THR:HA	44:l:55:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:SER:O	1:A:1251:SER:OG	2.15	0.58
1:A:1838:LYS:O	1:A:1841:THR:OG1	2.19	0.58
3:C:731:SER:HB3	3:C:747:ASP:O	2.03	0.58
6:F:85:U:H1'	6:F:86:U:C5	2.38	0.58
10:J:251:TRP:CZ2	10:J:255:LEU:HD11	2.39	0.58
13:N:18:ILE:HG21	13:N:70:ILE:HD11	1.84	0.58
27:3:547:CYS:HB2	27:3:556:ILE:HG22	1.85	0.58
37:8:64:ASP:O	37:8:68:ILE:HG12	2.03	0.58
48:z:20:THR:HG1	48:z:159:HIS:HD1	1.48	0.58
6:F:38:G:P	6:F:38:G:H8	2.26	0.58
10:J:326:VAL:HG13	10:J:352:PHE:HZ	1.68	0.58
31:2:511:LEU:O	31:2:514:LYS:N	2.36	0.58
44:l:17:ILE:HA	44:l:31:LYS:HA	1.85	0.58
1:A:280:GLU:OE2	2:B:47:A:H1'	2.04	0.58
1:A:2076:ARG:HD3	1:A:2121:ARG:HE	1.68	0.58
1:A:2190:PRO:O	1:A:2194:THR:HG22	2.03	0.58
5:E:202:ASN:HD21	5:E:206:ASP:H	1.51	0.58
18:S:447:LYS:H	18:S:514:TYR:HA	1.69	0.58
26:1:1208:LEU:HB2	26:1:1241:ILE:HD11	1.85	0.58
27:3:442:LEU:HB2	27:3:734:LEU:HB3	1.84	0.58
27:3:739:LEU:HD23	27:3:758:SER:HB3	1.86	0.58
6:F:88:G:H2'	6:F:89:U:H5''	1.86	0.58
26:1:962:MET:O	26:1:967:GLU:HB2	2.03	0.58
27:3:939:PHE:HZ	27:3:942:LYS:HG2	1.68	0.58
1:A:663:ARG:CB	1:A:663:ARG:HH11	2.16	0.58
6:F:59:G:H1	6:F:76:A:N6	1.98	0.58
8:H:27:U:H2'	8:H:28:C:H5'	1.86	0.58
10:J:267:ARG:O	10:J:271:VAL:HG23	2.04	0.58
10:J:376:VAL:HA	10:J:379:TRP:HD1	1.68	0.58
16:Q:1224:ILE:O	16:Q:1255:ASN:N	2.34	0.58
17:R:176:TYR:CE2	17:R:198:ARG:HB3	2.38	0.58
18:S:367:ARG:HA	18:S:582:PHE:HA	1.86	0.58
26:1:493:LYS:O	26:1:497:ILE:HG23	2.04	0.58
27:3:1019:ASN:O	27:3:1019:ASN:ND2	2.36	0.58
36:9:143:ASP:N	36:9:148:GLU:O	2.35	0.58
1:A:2174:PRO:HB2	1:A:2206:TRP:CD1	2.39	0.58
3:C:785:ARG:HB2	3:C:785:ARG:HH11	1.69	0.58
3:C:928:HIS:ND1	3:C:928:HIS:N	2.52	0.58
27:3:458:ALA:HB1	27:3:460:TRP:HZ3	1.68	0.58
1:A:134:TRP:HB3	1:A:418:THR:HG21	1.85	0.58
1:A:267:LYS:NZ	2:B:49:A:OP1	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:TRP:O	1:A:1440:THR:HG23	2.03	0.58
1:A:2093:SER:HB2	1:A:2226:THR:HG23	1.85	0.58
3:C:670:SER:HB3	3:C:688:ILE:HB	1.85	0.58
3:C:925:PRO:HG2	3:C:928:HIS:HE1	1.69	0.58
10:J:232:GLU:O	10:J:236:ARG:HB2	2.03	0.58
24:Y:106:THR:O	24:Y:106:THR:OG1	2.22	0.58
25:Z:532:ASP:O	25:Z:536:ARG:HG3	2.03	0.58
29:w:497:ARG:HA	29:w:497:ARG:NH1	2.18	0.58
36:9:310:LEU:HB2	36:9:316:TYR:CE2	2.39	0.58
37:8:14:ASP:OD1	37:8:15:ASN:N	2.37	0.58
1:A:331:TRP:HB2	3:C:177:ARG:HD3	1.85	0.58
1:A:693:ILE:HG13	1:A:738:MET:HB2	1.84	0.58
1:A:837:LYS:HZ3	26:1:101:TYR:HB3	1.69	0.58
1:A:1617:ARG:HD3	11:K:233:GLU:HG2	1.86	0.58
8:H:156:U:H2'	8:H:157:G:C8	2.38	0.58
27:3:544:ILE:HD11	27:3:556:ILE:HB	1.85	0.58
27:3:615:ARG:CZ	27:3:630:MET:HB3	2.34	0.58
27:3:848:PRO:HG2	27:3:851:ILE:HG22	1.86	0.58
34:7:23:CYS:HB3	34:7:58:CYS:HB2	1.84	0.58
36:9:366:LEU:HD11	36:9:380:PHE:CD2	2.39	0.58
42:i:50:TYR:HA	42:i:55:LEU:HA	1.85	0.58
44:l:26:GLU:HA	44:l:50:TYR:HA	1.85	0.58
1:A:1949:ARG:O	1:A:1953:ILE:HG13	2.04	0.58
3:C:117:ASP:OD1	3:C:117:ASP:N	2.37	0.58
3:C:618:THR:HB	3:C:630:LEU:HB2	1.85	0.58
5:E:253:ASN:ND2	5:E:291:CYS:HB3	2.18	0.58
18:S:969:PHE:O	18:S:996:PHE:HA	2.04	0.58
24:Y:58:GLN:NE2	25:Z:588:ASP:OD1	2.37	0.58
26:1:1092:ASP:O	26:1:1096:THR:HG23	2.03	0.58
27:3:685:ASP:OD1	27:3:686:LEU:N	2.37	0.58
31:2:460:PHE:HB3	31:2:464:GLU:HB3	1.86	0.58
3:C:434:CYS:O	3:C:438:ILE:HB	2.03	0.57
3:C:692:LEU:HD22	3:C:696:LEU:HD11	1.85	0.57
7:G:88:G:H22	8:H:41:U:H3	1.51	0.57
19:T:412:HIS:ND1	19:T:429:SER:OG	2.31	0.57
27:3:614:VAL:HB	27:3:633:LEU:HD11	1.86	0.57
36:9:351:LYS:H	36:9:351:LYS:HD2	1.68	0.57
1:A:595:LYS:NZ	2:B:30:A:OP1	2.34	0.57
1:A:2124:ILE:HG13	1:A:2147:MET:HE1	1.86	0.57
3:C:812:ALA:O	3:C:816:VAL:HG23	2.04	0.57
8:H:13:C:H1'	8:H:14:C:H5'	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:122:HIS:ND1	26:1:125:THR:OG1	2.37	0.57
26:1:826:ASP:OD1	26:1:827:ARG:N	2.37	0.57
26:1:1010:THR:OG1	26:1:1011:PRO:HD3	2.04	0.57
33:6:42:TYR:OH	33:6:76:HIS:HB3	2.04	0.57
34:7:21:ARG:NH2	34:7:68:ASP:OD1	2.36	0.57
2:B:66:A:H2'	2:B:67:A:C8	2.40	0.57
3:C:514:TYR:HE2	3:C:522:SER:HB2	1.69	0.57
3:C:719:GLN:HG3	3:C:724:TRP:O	2.04	0.57
5:E:125:PHE:CE1	5:E:159:PRO:HB3	2.39	0.57
7:G:22:C:O2'	7:G:23:U:OP1	2.20	0.57
11:K:230:TRP:CD1	11:K:230:TRP:H	2.22	0.57
16:Q:852:VAL:O	16:Q:1061:MET:HA	2.04	0.57
23:X:230:GLY:O	23:X:234:GLU:HB2	2.04	0.57
31:2:478:HIS:O	31:2:481:THR:OG1	2.20	0.57
44:l:30:GLY:HA3	44:l:46:ILE:HA	1.86	0.57
44:l:35:ALA:HA	44:l:41:CYS:HA	1.86	0.57
1:A:1352:HIS:CD2	20:U:5:ILE:HG21	2.39	0.57
19:T:195:LYS:HE3	19:T:490:ARG:NH2	2.19	0.57
23:X:328:ILE:HB	23:X:352:LEU:HD11	1.86	0.57
27:3:960:LEU:HD22	27:3:967:LEU:HD11	1.87	0.57
1:A:748:ASP:OD2	19:T:484:LYS:NZ	2.37	0.57
3:C:335:ASN:ND2	3:C:338:GLU:H	2.03	0.57
23:X:222:GLU:OE1	23:X:222:GLU:N	2.38	0.57
26:1:529:GLY:O	26:1:533:ASN:ND2	2.37	0.57
27:3:1159:ASP:HB3	27:3:1162:SER:HB3	1.86	0.57
36:9:440:GLU:O	36:9:444:GLN:HG3	2.03	0.57
3:C:491:HIS:HB3	3:C:551:LEU:HD22	1.86	0.57
3:C:673:LYS:HB3	3:C:686:THR:HG23	1.87	0.57
3:C:774:THR:HA	3:C:784:ILE:HD11	1.86	0.57
9:I:406:GLU:HA	9:I:410:GLN:HA	1.87	0.57
27:3:636:GLN:HB3	27:3:670:GLN:HE22	1.69	0.57
36:9:306:ASN:OD1	36:9:345:TYR:N	2.32	0.57
39:v:85:ARG:HH11	39:v:85:ARG:HB2	1.69	0.57
1:A:2150:GLN:HG2	1:A:2279:TRP:O	2.05	0.57
5:E:156:SER:HB2	5:E:199:VAL:HG12	1.87	0.57
8:H:181:G:H2'	8:H:182:U:C6	2.39	0.57
10:J:263:SER:O	10:J:267:ARG:NE	2.37	0.57
16:Q:851:ILE:O	16:Q:1036:ALA:HA	2.05	0.57
26:1:696:ASP:OD1	26:1:697:GLU:N	2.36	0.57
27:3:720:TRP:HE3	27:3:731:LEU:HG	1.69	0.57
37:8:45:LEU:O	37:8:48:ILE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2173:GLU:HG2	1:A:2174:PRO:HD2	1.87	0.57
3:C:123:MET:HE2	3:C:548:ASN:ND2	2.20	0.57
3:C:343:LEU:HD13	3:C:373:ILE:HD11	1.87	0.57
13:N:53:HIS:NE2	13:N:85:ASP:OD2	2.35	0.57
27:3:206:GLN:NE2	27:3:232:GLY:H	2.02	0.57
27:3:475:ILE:HG23	27:3:484:VAL:HG22	1.85	0.57
36:9:281:TYR:HA	36:9:293:LEU:O	2.05	0.57
1:A:1089:CYS:SG	1:A:1096:HIS:HD2	2.28	0.57
1:A:2142:ILE:HG12	1:A:2175:LEU:HD23	1.85	0.57
1:A:2271:PHE:O	1:A:2298:LEU:HD23	2.05	0.57
10:J:238:ASN:C	10:J:240:THR:H	2.12	0.57
10:J:360:ASP:OD1	10:J:360:ASP:N	2.33	0.57
27:3:1017:ASN:OD1	27:3:1018:GLU:HG3	2.04	0.57
44:I:34:GLU:O	44:I:42:GLN:N	2.38	0.57
3:C:465:MET:HA	3:C:498:SER:OG	2.05	0.57
7:G:101:U:C2	7:G:102:G:H8	2.22	0.57
8:H:69:U:H2'	8:H:70:C:C6	2.40	0.57
14:O:81:CYS:N	14:O:86:LEU:O	2.30	0.57
17:R:256:ASN:OD1	17:R:256:ASN:N	2.38	0.57
19:T:319:THR:O	19:T:321:ALA:N	2.38	0.57
26:1:1276:SER:O	26:1:1276:SER:OG	2.17	0.57
27:3:1199:ARG:NH2	27:3:1207:LYS:HE3	2.20	0.57
42:d:42:MET:O	42:d:64:ILE:N	2.21	0.57
1:A:1318:THR:HB	1:A:1324:GLY:HA3	1.87	0.56
3:C:669:THR:HG22	3:C:690:GLU:HB3	1.86	0.56
6:F:49:G:N7	12:L:33:ARG:NH1	2.53	0.56
10:J:245:TRP:O	10:J:248:TYR:N	2.38	0.56
21:V:476:LEU:O	21:V:479:MET:HG3	2.06	0.56
27:3:136:GLU:OE2	27:3:189:TYR:OH	2.18	0.56
27:3:554:VAL:HB	27:3:566:PHE:HB2	1.87	0.56
1:A:247:THR:OG1	1:A:429:ASN:OD1	2.21	0.56
1:A:309:ARG:NH2	20:U:1:MET:HE2	2.20	0.56
1:A:762:ARG:NH2	15:P:226:LYS:HZ3	2.00	0.56
25:Z:493:LEU:O	25:Z:496:GLN:HG2	2.06	0.56
27:3:719:SER:OG	27:3:734:LEU:HG	2.05	0.56
28:p:223:ALA:HB1	29:w:498:GLN:HG2	1.87	0.56
31:2:635:ALA:HB3	32:4:73:ILE:HA	1.86	0.56
1:A:1960:THR:O	25:Z:524:ARG:NH1	2.38	0.56
1:A:2121:ARG:O	1:A:2182:PRO:HG3	2.05	0.56
3:C:749:THR:HB	3:C:792:LEU:O	2.06	0.56
5:E:73:LYS:HE3	5:E:117:TYR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:60:C:H4'	17:R:217:LYS:HD2	1.87	0.56
8:H:9:U:H2'	8:H:10:C:H6	1.70	0.56
20:U:7:LEU:HD13	20:U:10:PRO:HA	1.87	0.56
23:X:359:LYS:NZ	23:X:366:GLU:HB3	2.21	0.56
26:1:869:MET:HE1	26:1:896:ILE:HD13	1.85	0.56
26:1:1076:ALA:O	26:1:1080:THR:HG22	2.05	0.56
27:3:1083:ASN:OD1	27:3:1084:GLY:N	2.39	0.56
37:8:34:LEU:HG	37:8:82:SER:HB2	1.87	0.56
1:A:1843:GLU:HB3	1:A:1875:HIS:ND1	2.20	0.56
1:A:1957:ASP:OD1	1:A:1958:LYS:N	2.38	0.56
2:B:21:A:O3'	2:B:22:U:H4'	2.06	0.56
10:J:224:LYS:HE2	10:J:255:LEU:HD13	1.87	0.56
26:1:609:MET:O	26:1:613:MET:HG2	2.04	0.56
27:3:671:ASN:O	27:3:673:VAL:HG23	2.05	0.56
36:9:237:ASN:O	36:9:266:ILE:HG22	2.06	0.56
36:9:416:ASP:O	36:9:420:ASP:N	2.27	0.56
1:A:312:TYR:OH	3:C:886:ASP:OD2	2.13	0.56
1:A:826:PRO:HG2	1:A:826:PRO:O	2.05	0.56
8:H:118:G:O2'	8:H:119:G:H5'	2.05	0.56
10:J:231:PHE:CE1	10:J:247:LYS:HG3	2.40	0.56
25:Z:507:GLN:O	25:Z:511:VAL:HG23	2.06	0.56
26:1:781:ASP:OD1	26:1:783:GLU:N	2.38	0.56
34:7:46:CYS:SG	34:7:49:CYS:N	2.66	0.56
39:v:59:CYS:SG	39:v:72:HIS:NE2	2.78	0.56
3:C:464:ALA:HB1	3:C:473:PRO:HG3	1.88	0.56
6:F:94:C:OP1	10:J:355:ARG:NH2	2.39	0.56
27:3:931:VAL:HG23	27:3:936:LYS:HD2	1.87	0.56
1:A:796:LYS:HG3	17:R:279:HIS:HB2	1.87	0.56
3:C:471:ASP:H	3:C:499:GLY:HA2	1.70	0.56
19:T:207:VAL:HG12	19:T:480:ALA:HB1	1.88	0.56
20:U:23:LEU:HD12	21:V:478:LYS:HB2	1.88	0.56
21:V:577:SER:O	21:V:581:ILE:HG13	2.05	0.56
1:A:191:ILE:HG13	1:A:571:ALA:HB1	1.86	0.56
1:A:1257:THR:HG22	1:A:1320:LYS:HE3	1.87	0.56
1:A:1853:PRO:HB2	1:A:1856:GLU:OE2	2.06	0.56
3:C:187:THR:HA	3:C:200:PHE:O	2.06	0.56
10:J:326:VAL:HG13	10:J:352:PHE:CZ	2.41	0.56
19:T:402:ASP:OD1	19:T:402:ASP:N	2.37	0.56
21:V:618:ARG:HB3	21:V:646:HIS:CE1	2.41	0.56
26:1:492:GLN:NE2	26:1:495:ARG:HE	2.04	0.56
27:3:226:GLU:OE1	27:3:259:LYS:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:77:ILE:O	32:4:84:ILE:N	2.21	0.56
1:A:698:PRO:HG2	19:T:373:LYS:NZ	2.20	0.56
1:A:770:THR:O	1:A:774:LYS:HG3	2.05	0.56
2:B:98:G:H2'	2:B:99:C:H6	1.71	0.56
21:V:543:LYS:O	21:V:547:VAL:HG23	2.05	0.56
26:1:1273:TYR:O	26:1:1277:GLN:HB3	2.06	0.56
27:3:404:LEU:HD21	27:3:438:LEU:HD11	1.87	0.56
27:3:794:SER:O	27:3:796:ASN:ND2	2.39	0.56
33:6:28:TYR:CE1	33:6:57:ARG:HG3	2.41	0.56
1:A:283:VAL:HG13	1:A:284:ARG:H	1.71	0.56
1:A:1539:SER:HB2	1:A:1569:LEU:HD11	1.88	0.56
26:1:117:ASP:OD1	26:1:120:LYS:N	2.23	0.56
1:A:1301:ILE:HD11	1:A:1306:LYS:HD3	1.87	0.55
1:A:2193:VAL:HG11	1:A:2251:TYR:HE1	1.70	0.55
5:E:65:HIS:CD2	5:E:91:LEU:HD23	2.41	0.55
26:1:153:MET:O	26:1:157:ARG:HG3	2.05	0.55
36:9:334:ASP:HB3	36:9:337:GLY:H	1.70	0.55
1:A:533:LYS:HD3	6:F:37:C:H6	1.71	0.55
8:H:63:G:N1	8:H:64:A:N6	2.52	0.55
12:L:14:THR:HG22	39:v:67:GLY:C	2.31	0.55
17:R:148:ARG:HH22	17:R:152:GLU:HB2	1.71	0.55
27:3:605:LEU:HB3	27:3:617:ILE:O	2.06	0.55
1:A:701:ILE:H	1:A:701:ILE:HD12	1.71	0.55
1:A:974:ASN:OD1	1:A:1100:ARG:NH1	2.36	0.55
3:C:351:PRO:O	3:C:354:ARG:HG2	2.06	0.55
7:G:13:C:H2'	7:G:14:A:C8	2.39	0.55
8:H:63:G:H1	8:H:64:A:N6	2.04	0.55
23:X:282:LEU:N	23:X:291:ASP:OD2	2.38	0.55
27:3:240:GLY:HA2	27:3:245:PRO:O	2.05	0.55
36:9:370:ASN:H	36:9:394:HIS:HE1	1.53	0.55
1:A:117:PRO:HD2	1:A:131:GLU:OE1	2.06	0.55
2:B:69:A:H3'	2:B:70:A:H8	1.71	0.55
6:F:41:A:C2	7:G:7:G:C2	2.94	0.55
19:T:257:ARG:NH1	19:T:301:ASP:OD1	2.28	0.55
20:U:77:MET:O	20:U:81:GLY:N	2.40	0.55
27:3:452:LEU:HD22	27:3:762:LEU:HD22	1.87	0.55
27:3:473:TYR:CE1	27:3:486:SER:HB2	2.42	0.55
27:3:617:ILE:HG12	27:3:627:PRO:HA	1.86	0.55
36:9:282:VAL:HB	36:9:293:LEU:HD12	1.89	0.55
36:9:366:LEU:HD11	36:9:380:PHE:HD2	1.69	0.55
38:y:13:LEU:H	38:y:48:GLY:HA2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD23	1:A:422:LEU:H	1.72	0.55
2:B:64:G:H2'	2:B:65:G:C8	2.41	0.55
3:C:227:LEU:HD22	3:C:243:ILE:HD13	1.89	0.55
3:C:811:THR:O	3:C:815:VAL:HG23	2.05	0.55
33:6:66:ASP:OD2	33:6:69:ASP:N	2.32	0.55
1:A:81:PHE:O	1:A:83:HIS:N	2.40	0.55
1:A:1258:LYS:O	1:A:1262:LYS:HG3	2.06	0.55
5:E:133:VAL:HB	5:E:147:LEU:HB2	1.89	0.55
10:J:300:ASP:HA	10:J:303:ILE:HG12	1.89	0.55
13:N:118:ILE:HD11	13:N:132:ILE:HG21	1.88	0.55
19:T:394:ASN:N	19:T:394:ASN:OD1	2.35	0.55
26:1:905:THR:HG22	26:1:906:GLU:H	1.71	0.55
27:3:380:GLU:O	27:3:383:ASP:N	2.39	0.55
27:3:511:LEU:HD22	27:3:517:VAL:HG23	1.89	0.55
27:3:565:TYR:OH	27:3:567:GLU:OE1	2.20	0.55
27:3:996:ILE:O	27:3:998:HIS:N	2.39	0.55
27:3:1013:ARG:HD3	27:3:1064:ASP:OD1	2.07	0.55
1:A:957:GLN:O	1:A:961:ASN:ND2	2.37	0.55
1:A:1419:ILE:HG13	1:A:1419:ILE:O	2.05	0.55
1:A:2083:LEU:HD22	1:A:2116:CYS:HA	1.89	0.55
1:A:2113:LYS:HA	1:A:2116:CYS:SG	2.46	0.55
1:A:2127:TYR:HD2	1:A:2164:PRO:HG2	1.71	0.55
1:A:2330:ARG:NH2	1:A:2331:GLU:HG2	2.22	0.55
5:E:127:ALA:HB2	5:E:157:CYS:SG	2.47	0.55
6:F:45:A:OP2	31:2:554:ARG:NH1	2.40	0.55
8:H:46:U:O4	29:w:383:LEU:HG	2.06	0.55
11:K:207:GLU:OE2	31:2:558:ARG:NH1	2.35	0.55
17:R:198:ARG:HD2	17:R:198:ARG:O	2.07	0.55
19:T:343:PRO:HB3	19:T:365:ARG:NH1	2.21	0.55
27:3:123:VAL:HG23	27:3:130:VAL:HG12	1.88	0.55
27:3:459:VAL:HA	27:3:475:ILE:O	2.07	0.55
32:4:165:GLN:O	32:4:172:ILE:N	2.39	0.55
35:5:15:GLN:O	35:5:18:TYR:C	2.50	0.55
37:8:107:PRO:HA	37:8:110:LEU:HD12	1.88	0.55
1:A:1505:LYS:HG3	25:Z:615:SER:HB3	1.89	0.55
1:A:2075:VAL:O	1:A:2078:ILE:HD13	2.06	0.55
3:C:390:THR:OG1	3:C:391:SER:N	2.38	0.55
14:O:167:PHE:O	14:O:172:GLU:N	2.29	0.55
27:3:720:TRP:CZ2	27:3:733:PRO:HG3	2.42	0.55
36:9:322:HIS:HB3	36:9:337:GLY:O	2.06	0.55
37:8:52:ILE:O	37:8:56:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:THR:OG1	1:A:486:LYS:N	2.35	0.55
3:C:129:ILE:HD11	3:C:441:PRO:HG3	1.88	0.55
3:C:515:THR:H	3:C:518:ASP:HB3	1.70	0.55
27:3:425:VAL:HG12	27:3:427:CYS:HB2	1.89	0.55
27:3:451:GLU:HG2	27:3:761:THR:HG22	1.88	0.55
37:8:90:THR:HG23	37:8:95:GLY:HA2	1.89	0.55
46:j:63:GLU:O	46:j:71:ARG:HA	2.07	0.55
21:V:525:PHE:HA	21:V:528:ILE:HB	1.89	0.55
29:w:383:LEU:HD13	29:w:392:ILE:O	2.06	0.55
1:A:409:ARG:HD2	1:A:409:ARG:C	2.30	0.54
1:A:1868:MET:HE2	1:A:1872:LEU:HG	1.88	0.54
3:C:119:LEU:HD23	3:C:123:MET:HG3	1.89	0.54
5:E:121:GLY:O	5:E:138:SER:OG	2.19	0.54
7:G:102:G:N2	7:G:103:U:H2'	2.21	0.54
8:H:135:C:H2'	8:H:136:G:C8	2.42	0.54
10:J:241:VAL:HG22	10:J:243:SER:H	1.72	0.54
10:J:391:TYR:HB3	10:J:394:HIS:ND1	2.22	0.54
26:1:972:GLY:HA2	26:1:1010:THR:HG21	1.88	0.54
27:3:77:TYR:HD1	27:3:91:GLU:HB2	1.71	0.54
1:A:1339:ASP:OD1	1:A:1339:ASP:N	2.40	0.54
1:A:2108:LYS:N	1:A:2264:SER:O	2.37	0.54
1:A:2236:GLU:O	1:A:2239:ARG:HD3	2.08	0.54
3:C:453:TYR:CE1	3:C:465:MET:HE1	2.42	0.54
10:J:332:VAL:HA	10:J:335:ARG:HD2	1.89	0.54
11:K:163:MET:SD	21:V:479:MET:HB3	2.48	0.54
14:O:35:ARG:HA	17:R:198:ARG:NH1	2.23	0.54
16:Q:408:VAL:O	16:Q:412:GLU:CB	2.56	0.54
19:T:335:THR:HG21	19:T:378:VAL:HG13	1.88	0.54
26:1:565:ASP:O	26:1:568:ARG:HG3	2.07	0.54
29:w:408:CYS:SG	29:w:431:HIS:ND1	2.81	0.54
1:A:1379:PHE:O	1:A:1383:GLN:HG2	2.07	0.54
1:A:1570:LYS:HZ3	1:A:1574:ILE:HD12	1.70	0.54
2:B:63:A:H2'	2:B:64:G:H8	1.71	0.54
3:C:85:ASP:OD1	3:C:85:ASP:N	2.33	0.54
6:F:84:A:C1'	6:F:85:U:H5'	2.37	0.54
8:H:8:C:H2'	8:H:9:U:H6	1.73	0.54
8:H:22:U:HO2'	8:H:23:A:H8	1.56	0.54
16:Q:1270:TYR:HA	16:Q:1300:GLY:O	2.07	0.54
19:T:342:GLU:HG2	19:T:343:PRO:HA	1.89	0.54
26:1:1140:GLU:HB2	26:1:1143:VAL:HG13	1.89	0.54
26:1:1303:ILE:HD11	27:3:989:TYR:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:727:SER:O	27:3:728:ARG:HD2	2.07	0.54
29:w:424:ARG:O	29:w:428:GLU:HG3	2.07	0.54
31:2:664:GLY:H	31:2:671:GLY:N	2.05	0.54
13:N:38:GLU:C	13:N:40:LYS:H	2.13	0.54
15:P:196:ASN:OD1	15:P:198:ALA:N	2.34	0.54
17:R:253:ASN:HB3	17:R:254:TRP:CE3	2.43	0.54
27:3:418:GLU:HG3	27:3:420:THR:H	1.73	0.54
27:3:587:VAL:HA	27:3:608:GLY:O	2.08	0.54
1:A:985:TYR:CD1	1:A:985:TYR:N	2.75	0.54
3:C:126:SER:O	3:C:126:SER:OG	2.24	0.54
3:C:595:VAL:HG23	3:C:596:ASN:ND2	2.22	0.54
8:H:15:U:O2'	8:H:16:U:H5'	2.07	0.54
8:H:69:U:H2'	8:H:70:C:H6	1.72	0.54
11:K:154:ARG:O	11:K:158:ASN:ND2	2.35	0.54
19:T:198:ARG:HH12	19:T:235:SER:HA	1.73	0.54
27:3:488:GLY:H	27:3:491:VAL:HG22	1.72	0.54
27:3:1210:ASP:O	27:3:1214:ARG:HG2	2.07	0.54
29:w:496:LYS:HA	29:w:501:LEU:C	2.33	0.54
33:6:111:LYS:NZ	33:6:115:GLU:HG3	2.22	0.54
41:h:62:HIS:O	41:h:103:GLY:HA3	2.07	0.54
1:A:726:TRP:O	36:9:247:SER:OG	2.24	0.54
1:A:1948:ASP:HB3	25:Z:518:MET:HE2	1.90	0.54
4:D:2066:VAL:HA	4:D:2107:TYR:O	2.07	0.54
8:H:162:U:H4'	8:H:163:G:H5'	1.89	0.54
23:X:239:PHE:CE2	23:X:240:ARG:HG3	2.42	0.54
27:3:895:ARG:HH21	27:3:895:ARG:HG3	1.73	0.54
37:8:30:PHE:CE1	37:8:83:LYS:HD2	2.43	0.54
1:A:134:TRP:HB3	1:A:418:THR:CG2	2.37	0.54
1:A:893:GLU:OE1	1:A:893:GLU:N	2.40	0.54
1:A:1206:GLU:HG2	1:A:1207:PHE:N	2.23	0.54
27:3:458:ALA:HB1	27:3:460:TRP:CZ3	2.43	0.54
44:l:21:GLU:HA	44:l:26:GLU:O	2.08	0.54
1:A:1318:THR:HG23	1:A:1484:ILE:HD13	1.89	0.54
1:A:1554:GLN:HG3	1:A:1561:PHE:CE1	2.42	0.54
1:A:2229:LYS:N	1:A:2257:GLU:O	2.31	0.54
6:F:30:A:N6	7:G:16:G:H1'	2.21	0.54
6:F:81:C:N4	8:H:18:U:H3	2.04	0.54
26:1:977:VAL:O	26:1:981:TYR:HD2	1.91	0.54
1:A:545:HIS:O	1:A:549:GLU:HG2	2.08	0.54
8:H:7:U:H2'	8:H:8:C:H6	1.73	0.54
26:1:1185:ARG:HH11	31:2:511:LEU:HD12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:68:PHE:HB2	27:3:123:VAL:HG21	1.90	0.54
37:8:28:LEU:HB3	37:8:30:PHE:CE2	2.43	0.54
45:k:14:ASP:N	45:k:31:LEU:O	2.30	0.54
1:A:1640:SER:OG	1:A:1641:ARG:N	2.41	0.54
1:A:1953:ILE:HD13	1:A:1982:GLN:HB3	1.88	0.54
1:A:2006:GLU:O	1:A:2010:ILE:HG13	2.08	0.54
1:A:2188:LEU:O	1:A:2251:TYR:OH	2.26	0.54
2:B:117:A:C2	42:d:26:GLY:HA3	2.43	0.54
3:C:213:ASP:OD1	3:C:213:ASP:N	2.39	0.54
3:C:350:ASN:O	3:C:353:THR:OG1	2.25	0.54
7:G:99:C:H42	8:H:32:U:H3	1.55	0.54
8:H:70:C:H2'	8:H:71:C:C5	2.43	0.54
8:H:182:U:H2'	8:H:183:G:H8	1.72	0.54
21:V:494:LEU:HD12	21:V:528:ILE:HD13	1.89	0.54
26:1:967:GLU:O	26:1:971:MET:HB3	2.08	0.54
27:3:943:THR:HG21	27:3:977:LEU:HB2	1.89	0.54
31:2:451:LYS:O	31:2:455:ARG:HD2	2.07	0.54
1:A:467:GLN:HG2	2:B:20:G:H21	1.73	0.53
1:A:919:ASP:OD2	1:A:1012:LYS:NZ	2.40	0.53
3:C:93:ILE:HD12	19:T:275:LEU:HD22	1.89	0.53
17:R:322:GLU:OE2	17:R:325:ARG:NH1	2.41	0.53
26:1:1118:ILE:O	26:1:1122:THR:HG23	2.08	0.53
27:3:1058:LEU:HD22	27:3:1062:THR:HG21	1.90	0.53
43:a:37:HIS:O	43:a:74:GLY:HA3	2.08	0.53
42:d:16:GLY:N	42:d:33:LEU:O	2.38	0.53
1:A:84:ASP:O	1:A:85:LYS:C	2.51	0.53
1:A:109:PRO:HD3	1:A:630:TRP:CZ2	2.43	0.53
1:A:533:LYS:HZ2	1:A:533:LYS:CB	2.21	0.53
3:C:508:LYS:HG3	3:C:524:ILE:HG22	1.89	0.53
3:C:696:LEU:O	3:C:699:ASP:N	2.41	0.53
7:G:12:G:H3'	7:G:13:C:C5	2.43	0.53
17:R:139:ALA:O	17:R:143:ILE:HG13	2.07	0.53
36:9:338:THR:HA	36:9:421:ARG:NH2	2.22	0.53
1:A:533:LYS:CB	1:A:533:LYS:NZ	2.72	0.53
3:C:496:VAL:HG11	3:C:501:ILE:HD12	1.90	0.53
4:D:620:LEU:HA	4:D:625:GLY:HA3	1.89	0.53
6:F:1:G:H2'	6:F:2:U:C6	2.43	0.53
8:H:47:U:H4'	8:H:48:A:OP1	2.08	0.53
10:J:294:HIS:HA	10:J:297:ASN:HD22	1.73	0.53
17:R:279:HIS:HB3	36:9:225:MET:HG2	1.89	0.53
25:Z:590:SER:OG	25:Z:591:ASN:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:487:VAL:HB	29:w:491:THR:OG1	2.08	0.53
36:9:296:HIS:HB2	36:9:299:LEU:HG	1.91	0.53
36:9:322:HIS:CE1	36:9:332:GLY:HA2	2.43	0.53
39:v:76:LYS:O	39:v:80:THR:HG23	2.07	0.53
43:m:19:CYS:HA	43:m:80:MET:HA	1.89	0.53
1:A:60:ASP:OD1	1:A:60:ASP:N	2.42	0.53
1:A:807:VAL:HG12	36:9:204:THR:HG23	1.90	0.53
1:A:1309:SER:OG	1:A:1547:VAL:HG11	2.07	0.53
1:A:2072:GLU:HA	1:A:2075:VAL:HG22	1.91	0.53
1:A:2130:GLY:H	1:A:2172:MET:HB3	1.73	0.53
19:T:393:ASP:OD1	19:T:393:ASP:N	2.41	0.53
21:V:481:PHE:CD2	21:V:485:GLN:HB2	2.44	0.53
21:V:628:ILE:O	21:V:632:THR:OG1	2.27	0.53
26:1:1113:THR:HG21	26:1:1149:LYS:HG2	1.90	0.53
29:w:390:LYS:NZ	39:v:84:ARG:HG2	2.23	0.53
33:6:46:ARG:HB3	33:6:63:VAL:HG12	1.89	0.53
1:A:191:ILE:O	1:A:191:ILE:HG22	2.09	0.53
1:A:1217:GLN:HE21	1:A:1222:LYS:HD2	1.72	0.53
3:C:593:GLU:HA	3:C:603:MET:HE1	1.90	0.53
3:C:605:ASP:O	3:C:609:LYS:HG3	2.09	0.53
5:E:234:HIS:ND1	5:E:256:ASP:OD2	2.41	0.53
10:J:250:GLN:O	10:J:254:SER:HB2	2.09	0.53
11:K:125:GLU:OE2	11:K:127:GLU:HB2	2.09	0.53
24:Y:87:GLN:HE22	24:Y:91:ILE:HD11	1.73	0.53
26:1:949:GLN:O	26:1:949:GLN:HG2	2.06	0.53
27:3:443:GLU:CD	27:3:443:GLU:H	2.15	0.53
27:3:902:ASP:OD2	27:3:929:LYS:NZ	2.41	0.53
1:A:1258:LYS:HG2	17:R:428:GLU:HB2	1.90	0.53
3:C:724:TRP:HE1	3:C:732:ILE:HD11	1.74	0.53
6:F:3:G:H2'	6:F:4:C:C6	2.43	0.53
11:K:129:ASP:OD1	11:K:130:ALA:N	2.41	0.53
11:K:162:TYR:OH	21:V:485:GLN:NE2	2.42	0.53
14:O:36:MET:HA	14:O:56:ARG:O	2.09	0.53
21:V:581:ILE:HG12	25:Z:543:ASP:HB2	1.90	0.53
26:1:1091:HIS:HE2	31:2:568:TYR:HH	1.57	0.53
27:3:232:GLY:HA2	27:3:252:SER:HA	1.91	0.53
27:3:565:TYR:HB3	27:3:577:TYR:HB3	1.90	0.53
27:3:607:VAL:HB	27:3:615:ARG:HB3	1.89	0.53
27:3:804:HIS:NE2	27:3:859:ASN:O	2.42	0.53
1:A:985:TYR:HD2	1:A:1032:ARG:HE	1.55	0.53
1:A:2177:TRP:CZ3	1:A:2179:HIS:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:C:H4'	2:B:40:U:OP1	2.07	0.53
4:D:1459:ILE:HA	4:D:1464:GLY:HA3	1.89	0.53
7:G:12:G:H3'	7:G:13:C:C6	2.43	0.53
8:H:9:U:H2'	8:H:10:C:C6	2.44	0.53
9:I:550:TRP:O	9:I:552:ASN:N	2.42	0.53
26:1:1134:ASN:ND2	31:2:534:GLN:HA	2.24	0.53
27:3:278:LEU:HD23	27:3:815:ARG:HD3	1.91	0.53
27:3:568:MET:HE2	27:3:569:ASP:O	2.09	0.53
36:9:285:HIS:NE2	36:9:432:THR:OG1	2.15	0.53
36:9:360:HIS:NE2	36:9:396:ILE:HG12	2.24	0.53
1:A:1783:THR:HG22	1:A:1865:ARG:HG3	1.91	0.53
4:D:735:ALA:C	4:D:737:ALA:H	2.16	0.53
8:H:8:C:H2'	8:H:9:U:C6	2.44	0.53
23:X:372:GLU:HG2	23:X:373:SER:N	2.23	0.53
27:3:68:PHE:CZ	27:3:144:LEU:HD13	2.43	0.53
36:9:330:ILE:HB	36:9:384:PHE:HZ	1.74	0.53
48:z:121:ASP:N	48:z:121:ASP:OD1	2.41	0.53
1:A:58:LYS:HA	13:N:107:GLN:NE2	2.24	0.53
1:A:1641:ARG:NH1	1:A:1651:VAL:O	2.42	0.53
11:K:137:SER:O	11:K:141:GLN:HG2	2.09	0.53
13:N:118:ILE:HA	13:N:121:VAL:HG23	1.90	0.53
26:1:130:PRO:HG2	26:1:150:ARG:HD2	1.90	0.53
1:A:1119:ASP:OD1	1:A:1123:GLU:HG3	2.08	0.53
1:A:2163:LEU:HD22	1:A:2164:PRO:HD2	1.91	0.53
1:A:2274:PRO:HA	1:A:2296:LEU:HA	1.90	0.53
1:A:2289:ASP:HB3	1:A:2292:MET:HG2	1.89	0.53
5:E:335:PHE:CE2	5:E:342:ILE:HD11	2.44	0.53
10:J:265:TYR:HB3	10:J:282:TYR:CZ	2.43	0.53
11:K:131:GLN:NE2	11:K:184:ARG:H	2.07	0.53
1:A:325:HIS:HD2	1:A:326:HIS:CD2	2.26	0.52
1:A:1552:GLN:HE21	11:K:193:VAL:HG22	1.73	0.52
3:C:302:PRO:HA	3:C:307:VAL:HB	1.90	0.52
6:F:43:A:N6	6:F:44:G:O6	2.41	0.52
6:F:59:G:N2	6:F:76:A:N1	2.51	0.52
24:Y:2:ASN:HD22	24:Y:2:ASN:H	1.56	0.52
27:3:214:ASP:O	27:3:218:ASN:N	2.35	0.52
27:3:1102:LEU:HD12	27:3:1122:LEU:HD12	1.90	0.52
36:9:320:ILE:HG22	36:9:427:ARG:HB2	1.91	0.52
5:E:316:SER:O	5:E:317:ARG:HG3	2.08	0.52
19:T:243:THR:O	19:T:243:THR:OG1	2.24	0.52
21:V:641:ASP:HA	21:V:644:ARG:CD	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:383:ASP:OD1	27:3:384:THR:N	2.42	0.52
27:3:947:GLU:HG3	27:3:948:VAL:N	2.24	0.52
1:A:363:HIS:CD2	3:C:284:GLU:HA	2.44	0.52
3:C:296:GLU:H	3:C:296:GLU:CD	2.17	0.52
3:C:369:PHE:CD1	3:C:373:ILE:HD12	2.43	0.52
6:F:36:A:C6	7:G:10:U:O4	2.63	0.52
27:3:91:GLU:HB3	27:3:102:ILE:HD11	1.91	0.52
27:3:569:ASP:N	27:3:573:GLN:O	2.39	0.52
27:3:983:ASN:OD1	27:3:984:LYS:N	2.43	0.52
44:l:33:ILE:H	44:l:43:MET:HA	1.75	0.52
1:A:2146:VAL:HG13	1:A:2272:MET:HG2	1.90	0.52
1:A:2330:ARG:HD3	1:A:2330:ARG:N	2.24	0.52
3:C:177:ARG:NH2	3:C:638:ASP:OD2	2.42	0.52
3:C:841:ASP:OD2	3:C:841:ASP:N	2.39	0.52
10:J:244:ASN:HA	10:J:247:LYS:NZ	2.24	0.52
26:1:1103:VAL:HG23	26:1:1109:ARG:HG3	1.91	0.52
34:7:46:CYS:HB3	34:7:85:CYS:CB	2.38	0.52
39:v:200:ASN:O	39:v:204:LYS:CA	2.58	0.52
1:A:1376:GLU:O	1:A:1380:ILE:HG13	2.09	0.52
1:A:1527:ASN:HD22	11:K:215:ASP:HB3	1.73	0.52
1:A:2196:HIS:CG	1:A:2213:ILE:HD11	2.43	0.52
1:A:2280:ASN:OD1	1:A:2282:ASN:ND2	2.32	0.52
3:C:264:ILE:HG12	3:C:378:TYR:CE1	2.44	0.52
16:Q:1059:ILE:O	16:Q:1091:TRP:HA	2.10	0.52
23:X:270:LEU:HB3	23:X:271:PRO:HD2	1.91	0.52
26:1:1260:LYS:O	26:1:1264:VAL:HG23	2.09	0.52
27:3:463:ARG:HG3	27:3:471:ASP:HA	1.90	0.52
27:3:727:SER:O	27:3:727:SER:OG	2.22	0.52
36:9:287:ASN:HD21	36:9:426:ILE:HG12	1.74	0.52
38:y:39:LEU:HA	38:y:46:HIS:HA	1.90	0.52
48:z:174:ILE:O	48:z:175:ILE:HD13	2.09	0.52
1:A:1541:THR:O	1:A:1544:ARG:HG2	2.10	0.52
1:A:1548:TYR:HE2	1:A:1550:GLY:HA2	1.73	0.52
1:A:2106:LEU:HD21	1:A:2111:LEU:HB2	1.91	0.52
1:A:2304:PHE:HB3	1:A:2305:TYR:CD2	2.45	0.52
3:C:614:TYR:OH	3:C:643:ASP:OD2	2.10	0.52
5:E:86:PHE:HA	5:E:111:ALA:HB1	1.91	0.52
8:H:162:U:H4'	8:H:163:G:C5'	2.38	0.52
10:J:293:ASN:HA	10:J:296:ARG:HD2	1.91	0.52
12:L:98:GLU:O	12:L:101:GLU:HG3	2.09	0.52
13:N:29:MET:HB2	13:N:52:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:411:CYS:HB3	29:w:430:ARG:HD2	1.92	0.52
44:l:13:ALA:HB1	44:l:74:PRO:HD2	1.91	0.52
1:A:359:ILE:HA	3:C:864:PRO:HB2	1.92	0.52
1:A:1802:PRO:HB3	1:A:1827:TRP:CZ3	2.45	0.52
1:A:2228:TYR:CD1	1:A:2228:TYR:N	2.78	0.52
3:C:370:VAL:HA	3:C:374:LEU:HB2	1.90	0.52
6:F:10:U:C2	6:F:11:C:H1'	2.44	0.52
8:H:7:U:H2'	8:H:8:C:C6	2.45	0.52
8:H:12:G:H2'	8:H:13:C:C2	2.45	0.52
19:T:381:HIS:HD2	19:T:441:TRP:NE1	2.08	0.52
27:3:162:LYS:HG2	27:3:165:THR:HG21	1.92	0.52
27:3:705:ARG:NH2	27:3:708:GLY:H	2.05	0.52
27:3:707:GLN:HB2	27:3:770:LEU:HD12	1.91	0.52
35:5:3:ASP:HA	35:5:6:THR:HG22	1.92	0.52
36:9:292:ASN:O	36:9:400:VAL:HA	2.09	0.52
36:9:295:LEU:HD22	36:9:397:PHE:O	2.09	0.52
44:l:20:CYS:HA	44:l:71:LEU:HA	1.91	0.52
48:z:103:ASN:HB2	48:z:108:ASP:HB3	1.92	0.52
46:e:36:TYR:N	46:e:83:ASN:O	2.42	0.52
45:f:15:LYS:O	45:f:31:LEU:N	2.38	0.52
1:A:158:ARG:HH12	1:A:573:GLN:HE21	1.58	0.52
1:A:1393:ARG:NH1	26:1:90:LEU:HD22	2.25	0.52
3:C:215:VAL:HG11	3:C:242:LEU:CD2	2.40	0.52
6:F:87:C:H2'	6:F:88:G:O4'	2.10	0.52
6:F:93:G:H2'	6:F:94:C:C6	2.44	0.52
10:J:375:ASP:HB3	10:J:377:LYS:HG2	1.91	0.52
19:T:191:HIS:NE2	19:T:440:ASP:OD1	2.43	0.52
26:1:1114:VAL:O	26:1:1114:VAL:HG12	2.09	0.52
27:3:263:ASP:OD1	27:3:263:ASP:N	2.43	0.52
1:A:1147:VAL:O	1:A:1151:ARG:HG3	2.10	0.52
1:A:1602:ASP:O	1:A:1605:GLU:N	2.39	0.52
1:A:1972:THR:N	1:A:1975:GLU:OE1	2.18	0.52
3:C:112:THR:O	3:C:112:THR:OG1	2.20	0.52
3:C:758:LEU:O	3:C:762:VAL:HG22	2.10	0.52
6:F:84:A:H4'	6:F:85:U:OP1	2.09	0.52
21:V:620:ASN:ND2	21:V:623:ASN:OD1	2.33	0.52
21:V:630:PHE:HE2	25:Z:544:PRO:HD2	1.75	0.52
26:1:770:MET:HE2	26:1:796:CYS:SG	2.50	0.52
35:5:9:SER:OG	37:8:15:ASN:O	2.22	0.52
39:v:31:ARG:HD3	39:v:48:LYS:HZ1	1.73	0.52
1:A:1136:ARG:HA	1:A:1139:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1833:LEU:HD23	1:A:1833:LEU:H	1.74	0.52
1:A:1876:LEU:HD12	1:A:1884:ILE:HD11	1.92	0.52
1:A:2109:ASN:O	1:A:2112:LYS:HB2	2.09	0.52
2:B:97:G:N2	2:B:117:A:H62	2.07	0.52
3:C:218:GLY:O	3:C:222:SER:HB3	2.10	0.52
8:H:155:C:N3	8:H:176:G:N2	2.57	0.52
10:J:434:VAL:O	10:J:438:TYR:HB3	2.10	0.52
18:S:767:LEU:O	18:S:772:ILE:N	2.38	0.52
26:1:1179:ASP:H	31:2:511:LEU:HD13	1.74	0.52
27:3:485:LEU:HG	27:3:493:GLU:HA	1.92	0.52
43:m:80:MET:O	47:n:58:LEU:HA	2.09	0.52
1:A:1209:HIS:CG	1:A:1210:LYS:N	2.78	0.51
1:A:1792:LYS:HA	1:A:1798:LEU:HA	1.91	0.51
1:A:2305:TYR:HD1	1:A:2310:ARG:NH1	2.08	0.51
3:C:801:LEU:HB2	3:C:803:ARG:HD3	1.91	0.51
3:C:919:ARG:HD2	3:C:922:GLU:OE1	2.10	0.51
5:E:150:HIS:CE1	5:E:177:LYS:HG3	2.45	0.51
8:H:50:C:C2	8:H:64:A:N6	2.75	0.51
27:3:463:ARG:NE	27:3:468:ASP:O	2.42	0.51
27:3:488:GLY:C	27:3:490:THR:H	2.17	0.51
27:3:697:ARG:HH21	27:3:717:SER:HB3	1.75	0.51
27:3:712:VAL:HG22	27:3:722:SER:HB3	1.91	0.51
27:3:828:GLY:O	27:3:834:LEU:N	2.43	0.51
33:6:43:GLY:HA3	33:6:69:ASP:OD2	2.09	0.51
36:9:285:HIS:ND1	36:9:290:ASP:OD1	2.43	0.51
36:9:318:GLY:HA2	36:9:427:ARG:HD2	1.93	0.51
37:8:57:THR:HG22	37:8:63:GLU:HA	1.91	0.51
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.75	0.51
1:A:348:PRO:HG2	1:A:351:TYR:HB2	1.92	0.51
2:B:107:U:H2'	2:B:108:G:O4'	2.10	0.51
3:C:223:ASP:OD1	3:C:495:ARG:NH2	2.42	0.51
4:D:1199:LYS:HA	4:D:1255:PHE:HA	1.92	0.51
7:G:22:C:HO2'	7:G:23:U:P	2.32	0.51
8:H:179:C:N4	8:H:180:G:O6	2.43	0.51
10:J:272:ASP:OD1	10:J:274:ARG:N	2.39	0.51
24:Y:96:ASN:HD21	25:Z:594:GLU:HG2	1.76	0.51
26:1:584:ASP:OD1	26:1:585:GLU:N	2.42	0.51
33:6:104:LYS:O	33:6:107:GLU:HG2	2.09	0.51
38:y:71:GLU:HA	38:y:75:ARG:O	2.10	0.51
1:A:1129:ASN:N	1:A:1129:ASN:OD1	2.44	0.51
3:C:674:CYS:HB2	3:C:822:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:133:VAL:HG21	5:E:169:THR:HG21	1.93	0.51
14:O:32:PRO:HA	17:R:195:ARG:HH12	1.76	0.51
27:3:19:HIS:HD2	27:3:340:CYS:SG	2.34	0.51
31:2:539:ALA:O	31:2:542:GLU:HG3	2.10	0.51
31:2:635:ALA:CB	32:4:73:ILE:HA	2.40	0.51
36:9:358:LEU:HD13	36:9:396:ILE:HG13	1.91	0.51
1:A:143:GLN:NE2	1:A:207:PHE:O	2.43	0.51
3:C:931:ARG:NE	3:C:935:ILE:HD11	2.25	0.51
27:3:675:LEU:HA	27:3:687:SER:O	2.11	0.51
36:9:329:VAL:HG12	36:9:383:THR:HG22	1.92	0.51
1:A:156:ARG:NE	1:A:157:ASP:OD1	2.42	0.51
1:A:750:TRP:CZ2	1:A:778:ARG:HG2	2.45	0.51
5:E:165:GLN:HB3	5:E:181:ILE:HD11	1.93	0.51
10:J:329:ALA:O	10:J:332:VAL:HG22	2.11	0.51
11:K:159:TYR:CZ	21:V:450:ILE:HG21	2.46	0.51
13:N:6:ARG:HG2	13:N:6:ARG:HH11	1.76	0.51
26:1:475:PHE:HB3	26:1:478:LEU:HD12	1.93	0.51
27:3:574:LEU:H	27:3:574:LEU:HD22	1.75	0.51
27:3:609:LEU:HB2	27:3:611:ASP:HB3	1.92	0.51
27:3:943:THR:HB	27:3:976:LYS:HB2	1.91	0.51
36:9:269:ASP:CG	36:9:272:ARG:HH21	2.18	0.51
1:A:467:GLN:HG2	2:B:20:G:N2	2.25	0.51
3:C:277:LYS:HD2	3:C:865:GLY:HA3	1.92	0.51
3:C:481:MET:SD	3:C:559:ILE:HD11	2.51	0.51
5:E:234:HIS:CE1	5:E:260:ARG:HG2	2.45	0.51
6:F:35:A:C6	6:F:36:A:N6	2.79	0.51
17:R:195:ARG:HH11	17:R:195:ARG:HG2	1.76	0.51
17:R:332:ARG:NH2	23:X:366:GLU:OE1	2.44	0.51
27:3:680:ASP:CG	27:3:681:PRO:HD2	2.36	0.51
27:3:695:GLY:HA3	27:3:717:SER:OG	2.11	0.51
27:3:876:THR:O	27:3:876:THR:OG1	2.27	0.51
32:4:167:LEU:H	32:4:171:PRO:HA	1.75	0.51
1:A:170:ASP:OD1	1:A:171:ASP:N	2.42	0.51
1:A:227:ARG:NH2	1:A:415:SER:OG	2.44	0.51
1:A:381:PRO:HG2	3:C:334:ILE:HG22	1.92	0.51
1:A:1458:GLN:OE1	17:R:421:GLY:HA3	2.10	0.51
1:A:1520:ASN:ND2	6:F:51:U:O2	2.44	0.51
1:A:1835:GLN:O	1:A:1839:TRP:HD1	1.93	0.51
1:A:2222:SER:OG	1:A:2223:CYS:N	2.43	0.51
3:C:350:ASN:HD22	3:C:353:THR:HG23	1.75	0.51
3:C:677:GLU:N	3:C:677:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:192:ASN:HB3	5:E:220:TRP:CH2	2.46	0.51
26:1:592:GLU:O	26:1:596:ILE:HG23	2.11	0.51
26:1:718:PRO:O	26:1:719:TYR:CG	2.64	0.51
27:3:75:LYS:NZ	27:3:92:TYR:O	2.44	0.51
27:3:745:PHE:HE2	27:3:750:CYS:HB3	1.75	0.51
27:3:910:ALA:HB2	27:3:948:VAL:HB	1.92	0.51
29:w:489:LYS:HA	29:w:492:TYR:HB3	1.92	0.51
1:A:1591:MET:O	1:A:1595:GLN:HG3	2.11	0.51
2:B:115:C:H2'	2:B:116:U:O4'	2.11	0.51
5:E:259:VAL:O	5:E:260:ARG:HD3	2.11	0.51
7:G:-7:U:H2'	7:G:-6:C:O4'	2.10	0.51
8:H:167:U:N3	28:p:42:ALA:O	2.43	0.51
10:J:411:MET:HG3	10:J:415:LEU:HD23	1.93	0.51
21:V:622:ARG:HA	21:V:625:ARG:HH21	1.76	0.51
27:3:155:SER:OG	27:3:156:SER:N	2.40	0.51
27:3:873:GLN:O	27:3:875:ASN:ND2	2.43	0.51
1:A:1209:HIS:ND1	1:A:1210:LYS:N	2.58	0.51
1:A:1766:GLN:HG3	1:A:1767:ASN:H	1.76	0.51
1:A:1926:THR:O	1:A:1926:THR:OG1	2.26	0.51
1:A:2237:TRP:CH2	1:A:2251:TYR:HB2	2.46	0.51
6:F:38:G:H8	6:F:38:G:OP2	1.94	0.51
17:R:295:ASP:OD2	17:R:295:ASP:C	2.53	0.51
36:9:307:PHE:CD1	36:9:397:PHE:HE2	2.29	0.51
37:8:68:ILE:HG22	37:8:72:PHE:CE2	2.46	0.51
1:A:47:GLU:H	1:A:47:GLU:CD	2.19	0.51
10:J:232:GLU:O	10:J:236:ARG:CB	2.58	0.51
27:3:664:TYR:HA	27:3:677:THR:O	2.11	0.51
27:3:946:GLU:OE2	27:3:968:ARG:NH1	2.44	0.51
39:v:46:PHE:HB2	39:v:69:TYR:CZ	2.46	0.51
1:A:1609:VAL:HG22	1:A:1631:LEU:HD22	1.93	0.50
1:A:2228:TYR:HA	1:A:2258:ARG:HA	1.94	0.50
2:B:20:G:H4'	2:B:20:G:OP1	2.11	0.50
3:C:209:VAL:HG21	3:C:237:LEU:HD23	1.92	0.50
3:C:829:GLU:HB3	3:C:907:VAL:HG22	1.93	0.50
18:S:961:THR:O	18:S:965:GLN:N	2.43	0.50
21:V:636:LEU:O	21:V:640:THR:OG1	2.24	0.50
26:1:967:GLU:HB3	26:1:970:LEU:HB3	1.92	0.50
27:3:1158:ARG:HG3	27:3:1159:ASP:H	1.75	0.50
31:2:485:PRO:O	31:2:489:VAL:HG23	2.10	0.50
31:2:568:TYR:C	31:2:570:LYS:H	2.19	0.50
36:9:283:ARG:HG2	36:9:434:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:k:22:ASN:N	45:k:66:SER:O	2.39	0.50
1:A:550:VAL:O	1:A:554:THR:HG22	2.12	0.50
1:A:789:GLU:HB2	36:9:253:THR:HB	1.92	0.50
1:A:1819:LEU:HD11	1:A:1906:ILE:HD11	1.94	0.50
21:V:588:GLN:O	21:V:592:GLU:HG2	2.10	0.50
27:3:328:LYS:NZ	27:3:365:GLY:O	2.43	0.50
27:3:715:MET:HE3	27:3:739:LEU:O	2.12	0.50
1:A:123:THR:O	1:A:123:THR:OG1	2.23	0.50
1:A:464:PRO:O	1:A:466:ALA:N	2.43	0.50
4:D:1223:ILE:HA	4:D:1269:ARG:O	2.11	0.50
5:E:342:ILE:HG13	5:E:356:ILE:HD11	1.94	0.50
8:H:5:C:H2'	8:H:6:U:C6	2.46	0.50
17:R:402:SER:OG	17:R:403:ASN:N	2.44	0.50
26:1:473:GLN:NE2	33:6:93:ASN:HB2	2.27	0.50
27:3:705:ARG:HH12	27:3:709:GLN:H	1.59	0.50
33:6:28:TYR:CD1	33:6:57:ARG:HG3	2.47	0.50
36:9:323:ARG:HB3	36:9:331:GLN:HB3	1.93	0.50
44:l:23:ASN:N	44:l:67:LYS:O	2.44	0.50
1:A:1575:GLN:HB2	11:K:220:LEU:HD11	1.93	0.50
1:A:1843:GLU:HB3	1:A:1875:HIS:CE1	2.47	0.50
1:A:2176:GLY:HA2	1:A:2206:TRP:CZ2	2.46	0.50
2:B:67:A:H2'	2:B:68:C:C6	2.46	0.50
3:C:352:LYS:HD3	3:C:352:LYS:N	2.27	0.50
10:J:220:LEU:CD1	10:J:224:LYS:HD2	2.41	0.50
10:J:406:PHE:HB3	10:J:411:MET:HB2	1.93	0.50
13:N:72:ARG:HH11	13:N:72:ARG:HG3	1.77	0.50
19:T:297:HIS:HB2	19:T:302:VAL:HG22	1.92	0.50
26:1:911:LEU:HD23	26:1:957:ARG:HE	1.76	0.50
26:1:969:LYS:O	26:1:973:HIS:HB2	2.11	0.50
27:3:1035:THR:HG22	27:3:1047:ALA:HB3	1.92	0.50
1:A:43:LYS:NZ	6:F:21:U:H3	2.09	0.50
1:A:64:GLU:CD	1:A:64:GLU:H	2.20	0.50
1:A:147:MET:O	1:A:151:MET:HG3	2.10	0.50
1:A:945:THR:OG1	1:A:946:GLU:HG3	2.11	0.50
1:A:2191:GLN:NE2	1:A:2246:ASN:OD1	2.39	0.50
1:A:2206:TRP:CG	1:A:2211:THR:HG21	2.46	0.50
1:A:2249:LYS:H	1:A:2249:LYS:HD2	1.75	0.50
3:C:240:GLU:O	3:C:243:ILE:HG22	2.12	0.50
5:E:318:ARG:HB3	5:E:318:ARG:NH1	2.26	0.50
8:H:22:U:O2'	8:H:23:A:H8	1.95	0.50
10:J:303:ILE:HD12	10:J:313:TRP:CZ3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:494:LEU:HG	21:V:550:MET:HE1	1.94	0.50
23:X:277:ARG:NH2	26:1:437:PRO:CB	2.67	0.50
26:1:699:GLN:HE22	26:1:738:HIS:CE1	2.29	0.50
26:1:1179:ASP:HB2	26:1:1185:ARG:NH1	2.26	0.50
27:3:478:PHE:HB2	27:3:481:ALA:H	1.76	0.50
27:3:515:ALA:HB2	27:3:528:ARG:NH2	2.27	0.50
27:3:704:VAL:HG21	27:3:754:ILE:HD11	1.93	0.50
1:A:1570:LYS:NZ	1:A:1574:ILE:HD12	2.26	0.50
3:C:753:GLU:O	3:C:756:LYS:HG3	2.11	0.50
8:H:11:G:C2	8:H:12:G:N7	2.80	0.50
10:J:326:VAL:HA	10:J:329:ALA:HB3	1.94	0.50
11:K:208:THR:HB	31:2:557:VAL:HG22	1.94	0.50
26:1:1195:MET:O	26:1:1199:VAL:HG23	2.10	0.50
36:9:282:VAL:HG22	36:9:433:VAL:HA	1.94	0.50
36:9:367:SER:HB2	36:9:394:HIS:HB3	1.94	0.50
47:b:68:PHE:N	41:c:100:PHE:O	2.35	0.50
1:A:1424:GLN:O	1:A:1427:ARG:NH2	2.44	0.50
1:A:1962:THR:HG21	25:Z:523:ALA:HB1	1.93	0.50
3:C:916:ILE:HB	3:C:931:ARG:HG2	1.93	0.50
4:D:1197:THR:HA	4:D:1257:PRO:HA	1.93	0.50
5:E:84:ALA:HB2	5:E:90:ILE:HG12	1.94	0.50
8:H:140:A:H2'	8:H:141:C:C6	2.46	0.50
27:3:50:VAL:HG21	27:3:401:LEU:HD11	1.94	0.50
27:3:80:VAL:HG11	27:3:1156:CYS:SG	2.51	0.50
29:w:388:ASP:OD2	29:w:390:LYS:HD2	2.10	0.50
36:9:323:ARG:HE	36:9:325:ILE:HD11	1.75	0.50
1:A:2209:GLU:O	1:A:2209:GLU:HG2	2.10	0.50
5:E:192:ASN:HB3	5:E:220:TRP:HH2	1.77	0.50
7:G:19:G:H2'	7:G:20:A:C8	2.47	0.50
16:Q:1273:LEU:O	16:Q:1303:ILE:HA	2.11	0.50
18:S:615:LEU:N	18:S:673:ALA:O	2.41	0.50
21:V:518:LYS:HE2	21:V:520:GLU:OE1	2.11	0.50
27:3:940:LEU:HB3	27:3:941:HIS:ND1	2.27	0.50
33:6:44:PRO:HB2	33:6:65:GLU:HG3	1.93	0.50
36:9:415:SER:HB3	36:9:420:ASP:HA	1.94	0.50
48:z:143:ARG:HH11	48:z:143:ARG:HG3	1.77	0.50
3:C:129:ILE:HA	3:C:199:LEU:O	2.11	0.50
3:C:495:ARG:HB3	3:C:549:TRP:CD1	2.47	0.50
4:D:688:THR:O	4:D:868:ILE:HA	2.12	0.50
6:F:21:U:C4	13:N:125:LYS:HE3	2.47	0.50
19:T:188:PRO:HG2	19:T:502:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:732:TRP:HE1	26:1:768:GLU:HG2	1.77	0.50
27:3:147:ASP:OD1	27:3:151:ARG:N	2.41	0.50
27:3:635:ALA:HB3	27:3:669:LEU:HD13	1.93	0.50
1:A:643:GLY:O	1:A:646:PRO:HD2	2.11	0.49
1:A:1361:GLU:HG2	1:A:1362:ASP:H	1.77	0.49
1:A:1814:THR:OG1	1:A:1816:GLN:HB2	2.12	0.49
1:A:2111:LEU:HG	1:A:2115:ILE:HD12	1.94	0.49
7:G:-11:G:HO2'	7:G:-10:G:C1'	2.25	0.49
7:G:8:C:C4	7:G:9:C:N4	2.80	0.49
10:J:291:GLN:HB3	10:J:294:HIS:ND1	2.26	0.49
45:k:35:ASP:O	45:k:38:MET:N	2.45	0.49
48:z:57:VAL:O	48:z:153:GLU:HB3	2.12	0.49
1:A:793:ASN:HD22	3:C:60:HIS:CE1	2.30	0.49
1:A:1333:VAL:HG11	21:V:467:LEU:HD22	1.93	0.49
16:Q:28:CYS:HA	16:Q:32:ALA:HB3	1.94	0.49
19:T:369:THR:O	19:T:369:THR:OG1	2.29	0.49
26:1:626:ASN:OD1	26:1:630:ARG:NH1	2.45	0.49
27:3:673:VAL:HA	27:3:690:ARG:HA	1.94	0.49
31:2:601:LEU:HD12	31:2:602:LYS:H	1.77	0.49
1:A:325:HIS:CD2	1:A:326:HIS:HD2	2.28	0.49
1:A:406:TRP:HH2	3:C:265:LEU:O	1.95	0.49
1:A:1607:GLU:HG2	1:A:1608:THR:OG1	2.13	0.49
1:A:1745:GLU:OE2	26:1:980:GLU:HB3	2.12	0.49
2:B:64:G:H2'	2:B:65:G:H8	1.77	0.49
3:C:125:ASN:ND2	3:C:128:LEU:HD13	2.27	0.49
3:C:131:ASN:HB2	3:C:223:ASP:OD2	2.12	0.49
16:Q:851:ILE:HA	16:Q:1060:LEU:O	2.12	0.49
26:1:741:LYS:HG3	26:1:742:GLY:N	2.27	0.49
26:1:854:VAL:HG23	26:1:855:ASP:OD1	2.12	0.49
29:w:459:TRP:CZ2	29:w:463:LYS:HE2	2.47	0.49
36:9:419:THR:HG23	36:9:421:ARG:HG3	1.94	0.49
1:A:1519:THR:HG22	1:A:1522:GLN:HG3	1.93	0.49
3:C:587:VAL:HG11	3:C:830:PRO:HG3	1.93	0.49
7:G:106:C:H4'	7:G:107:U:OP2	2.11	0.49
8:H:46:U:H3	29:w:381:LYS:HA	1.77	0.49
8:H:148:C:H2'	8:H:149:A:C8	2.48	0.49
13:N:16:GLU:CD	13:N:16:GLU:H	2.20	0.49
13:N:25:LEU:HD23	13:N:28:LYS:HE2	1.94	0.49
17:R:185:GLY:O	17:R:187:ALA:N	2.45	0.49
24:Y:26:VAL:HG11	26:1:860:GLU:HB2	1.93	0.49
26:1:405:ASP:C	33:6:99:GLN:HE22	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:819:TRP:HH2	26:1:871:THR:HG21	1.77	0.49
27:3:316:GLU:HB2	27:3:324:GLU:HG2	1.94	0.49
27:3:791:HIS:ND1	27:3:930:LEU:HD21	2.28	0.49
29:w:420:LYS:O	29:w:424:ARG:HG3	2.13	0.49
48:z:14:LYS:HE2	48:z:27:GLU:HG2	1.95	0.49
3:C:118:PHE:CZ	3:C:122:LEU:HD11	2.47	0.49
6:F:12:G:H2'	6:F:13:G:C8	2.46	0.49
21:V:575:THR:OG1	21:V:580:ARG:NH1	2.41	0.49
31:2:556:LYS:HB2	31:2:556:LYS:HZ3	1.77	0.49
33:6:31:THR:OG1	33:6:34:GLU:HB2	2.12	0.49
33:6:78:SER:HB3	33:6:89:VAL:HG22	1.94	0.49
1:A:1055:LEU:HB3	22:W:18:LEU:HD11	1.95	0.49
5:E:229:TYR:OH	5:E:270:LYS:HA	2.12	0.49
17:R:124:VAL:HG13	19:T:407:GLN:NE2	2.27	0.49
18:S:581:ILE:HA	18:S:734:CYS:O	2.12	0.49
19:T:264:CYS:HB3	19:T:294:LEU:HD13	1.94	0.49
26:1:577:VAL:HG12	26:1:578:ILE:HD13	1.93	0.49
27:3:745:PHE:HB2	27:3:755:VAL:HG23	1.93	0.49
1:A:502:ASN:O	1:A:506:LEU:HG	2.11	0.49
1:A:1416:ILE:O	1:A:1416:ILE:HG23	2.12	0.49
3:C:465:MET:O	3:C:468:CYS:N	2.45	0.49
5:E:255:MET:HB3	5:E:282:HIS:ND1	2.27	0.49
10:J:395:ALA:HA	10:J:398:VAL:HG12	1.95	0.49
21:V:519:LYS:O	21:V:522:MET:N	2.46	0.49
26:1:738:HIS:CE1	26:1:742:GLY:HA3	2.48	0.49
26:1:1138:VAL:HG22	26:1:1143:VAL:HG21	1.94	0.49
27:3:190:GLU:O	27:3:194:ASN:ND2	2.46	0.49
37:8:28:LEU:HB3	37:8:30:PHE:HE2	1.78	0.49
1:A:533:LYS:HE3	6:F:37:C:C5	2.48	0.49
1:A:984:MET:O	1:A:988:ILE:HG13	2.13	0.49
1:A:994:ASN:O	1:A:998:ARG:HG3	2.13	0.49
5:E:255:MET:SD	5:E:286:LYS:HG2	2.53	0.49
6:F:58:G:O2'	6:F:59:G:OP1	2.27	0.49
18:S:700:TYR:HA	18:S:706:MET:O	2.13	0.49
27:3:258:TYR:HB2	27:3:325:ILE:HD11	1.94	0.49
27:3:787:LYS:HB3	27:3:800:ILE:HD11	1.95	0.49
27:3:1217:PHE:CD1	27:3:1217:PHE:N	2.80	0.49
42:i:24:LYS:N	42:i:68:ASN:O	2.45	0.49
11:K:131:GLN:O	11:K:135:GLU:HG3	2.13	0.49
15:P:206:LYS:HA	15:P:209:ARG:HG3	1.94	0.49
21:V:568:ILE:HG22	21:V:570:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:27:SER:OG	24:Y:29:HIS:HD2	1.95	0.49
27:3:590:MET:HG2	27:3:606:ALA:O	2.12	0.49
27:3:741:PHE:HB3	27:3:757:ILE:HD11	1.93	0.49
48:z:55:HIS:CD2	48:z:72:GLY:HA2	2.48	0.49
1:A:1091:TYR:O	1:A:1092:ILE:C	2.56	0.49
1:A:1770:GLU:O	1:A:1773:SER:HB3	2.12	0.49
3:C:275:TYR:HD1	3:C:369:PHE:HD2	1.61	0.49
3:C:776:GLU:O	3:C:781:ASP:HA	2.12	0.49
13:N:99:ASN:O	13:N:142:CYS:HB2	2.13	0.49
19:T:201:SER:HB3	19:T:455:GLN:HE22	1.78	0.49
23:X:278:GLN:HB2	23:X:281:TYR:CZ	2.48	0.49
26:1:834:VAL:HG22	26:1:871:THR:HG22	1.94	0.49
27:3:616:ILE:O	27:3:628:LEU:N	2.37	0.49
27:3:718:ARG:O	27:3:720:TRP:HD1	1.96	0.49
36:9:441:ALA:HA	36:9:444:GLN:OE1	2.12	0.49
1:A:27:GLU:HA	1:A:30:LEU:HG	1.95	0.48
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.37	0.48
3:C:767:VAL:O	3:C:771:GLN:HG3	2.13	0.48
3:C:831:TYR:HB2	3:C:903:HIS:O	2.13	0.48
5:E:67:GLY:C	5:E:349:LYS:HG2	2.38	0.48
5:E:98:ASP:OD1	5:E:98:ASP:N	2.46	0.48
5:E:249:TYR:CE2	5:E:263:ASP:HB3	2.48	0.48
10:J:286:GLU:OE1	10:J:291:GLN:HB2	2.13	0.48
10:J:294:HIS:HA	10:J:297:ASN:ND2	2.28	0.48
16:Q:82:SER:O	16:Q:86:SER:N	2.45	0.48
17:R:310:ARG:HH11	17:R:310:ARG:HG3	1.78	0.48
23:X:285:ARG:HB2	23:X:299:CYS:HB2	1.95	0.48
26:1:652:CYS:O	26:1:661:ARG:HG2	2.13	0.48
26:1:1036:ILE:HD11	26:1:1062:LEU:HD22	1.95	0.48
27:3:155:SER:OG	27:3:156:SER:O	2.31	0.48
31:2:586:ILE:H	31:2:586:ILE:HD12	1.78	0.48
37:8:48:ILE:O	37:8:51:TRP:N	2.46	0.48
39:v:42:LYS:HA	39:v:42:LYS:HE3	1.95	0.48
48:z:55:HIS:CE1	48:z:67:ASP:HB3	2.48	0.48
1:A:360:SER:O	1:A:360:SER:OG	2.27	0.48
2:B:101:U:H2'	2:B:102:U:H6	1.78	0.48
4:D:2108:PHE:O	4:D:2117:ASP:HA	2.13	0.48
5:E:329:SER:N	5:E:347:SER:OG	2.39	0.48
7:G:89:U:H3	26:1:503:LYS:CD	2.27	0.48
13:N:104:ARG:HD3	13:N:136:HIS:HB3	1.95	0.48
15:P:213:ASP:OD2	15:P:216:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:245:LYS:NZ	23:X:302:GLN:O	2.46	0.48
26:1:697:GLU:OE2	26:1:698:GLN:N	2.46	0.48
26:1:944:SER:O	26:1:944:SER:OG	2.20	0.48
27:3:457:ASN:ND2	27:3:479:VAL:HA	2.27	0.48
33:6:19:ARG:HG2	33:6:67:ILE:HA	1.95	0.48
36:9:242:SER:OG	36:9:243:THR:N	2.44	0.48
36:9:327:ASN:O	36:9:385:ARG:HD3	2.13	0.48
1:A:827:PHE:C	1:A:827:PHE:CD2	2.90	0.48
1:A:2156:THR:OG1	1:A:2157:VAL:N	2.45	0.48
3:C:212:SER:O	3:C:216:THR:HG23	2.13	0.48
5:E:253:ASN:HD21	5:E:291:CYS:HB3	1.77	0.48
6:F:7:G:C6	6:F:15:A:C6	3.02	0.48
6:F:89:U:H3'	6:F:90:G:H8	1.78	0.48
10:J:369:PHE:HA	10:J:372:VAL:HG22	1.96	0.48
16:Q:542:ASN:HA	16:Q:622:SER:HA	1.94	0.48
25:Z:619:MET:HG3	25:Z:619:MET:O	2.12	0.48
31:2:519:LYS:HD3	39:v:50:HIS:CD2	2.48	0.48
36:9:282:VAL:HG22	36:9:433:VAL:HG22	1.94	0.48
36:9:295:LEU:HD22	36:9:397:PHE:C	2.37	0.48
40:o:14:GLN:HA	40:o:23:GLU:O	2.13	0.48
1:A:137:GLU:HG3	1:A:424:ILE:HD13	1.94	0.48
1:A:1841:THR:OG1	1:A:1868:MET:HE3	2.13	0.48
3:C:670:SER:HB2	3:C:689:ALA:H	1.78	0.48
3:C:676:ALA:HB3	3:C:811:THR:HG23	1.94	0.48
3:C:710:ASN:OD1	3:C:712:LYS:HB3	2.13	0.48
8:H:148:C:N4	8:H:149:A:N6	2.62	0.48
27:3:757:ILE:HG22	27:3:762:LEU:HB3	1.95	0.48
27:3:918:ARG:HG2	27:3:918:ARG:NH1	2.28	0.48
47:n:24:GLN:O	47:n:45:MET:HA	2.12	0.48
1:A:221:ASN:HB3	1:A:226:GLN:O	2.13	0.48
1:A:683:LEU:HD11	6:F:57:U:H4'	1.94	0.48
1:A:1764:SER:C	1:A:1766:GLN:N	2.72	0.48
1:A:1840:LYS:HE3	1:A:1840:LYS:HB3	1.58	0.48
3:C:305:GLY:O	3:C:433:MET:HG3	2.14	0.48
3:C:497:LEU:HD13	3:C:577:PHE:CZ	2.48	0.48
3:C:916:ILE:HG21	3:C:928:HIS:HB3	1.96	0.48
4:D:1397:PHE:O	4:D:1402:ASN:N	2.47	0.48
4:D:1660:LEU:HA	4:D:1701:ARG:O	2.13	0.48
6:F:89:U:H3'	6:F:90:G:C8	2.48	0.48
8:H:48:A:C2	8:H:65:U:H2'	2.49	0.48
25:Z:566:TYR:HD1	25:Z:579:TRP:HZ3	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:586:ASP:OD1	26:1:589:ALA:N	2.43	0.48
27:3:353:PHE:CD1	27:3:406:PRO:HD3	2.43	0.48
28:p:213:THR:O	28:p:215:SER:N	2.47	0.48
29:w:410:ILE:HG12	29:w:452:ILE:HG12	1.96	0.48
29:w:479:TYR:N	29:w:487:VAL:O	2.28	0.48
1:A:293:TRP:HE1	1:A:1136:ARG:CZ	2.26	0.48
1:A:2107:PRO:HG2	1:A:2110:VAL:HG22	1.95	0.48
2:B:63:A:H2'	2:B:64:G:C8	2.47	0.48
3:C:680:ASN:O	3:C:682:LYS:N	2.46	0.48
7:G:102:G:H21	7:G:103:U:H5'	1.79	0.48
12:L:41:LYS:HA	12:L:41:LYS:HD3	1.58	0.48
12:L:92:THR:OG1	12:L:95:GLN:HG3	2.13	0.48
23:X:253:ARG:HB3	23:X:324:VAL:HG11	1.95	0.48
26:1:472:ILE:O	26:1:476:ASP:HB3	2.13	0.48
26:1:867:MET:O	26:1:871:THR:HG23	2.14	0.48
27:3:175:VAL:HB	27:3:178:GLU:OE1	2.14	0.48
27:3:485:LEU:HB3	27:3:491:VAL:CG1	2.42	0.48
27:3:565:TYR:HE1	27:3:619:LEU:HD22	1.79	0.48
36:9:370:ASN:H	36:9:394:HIS:CE1	2.31	0.48
1:A:569:VAL:O	1:A:570:ASP:HB2	2.13	0.48
1:A:1561:PHE:HE1	11:K:193:VAL:HG11	1.78	0.48
1:A:1808:PHE:CZ	1:A:1893:PHE:HB3	2.48	0.48
1:A:2228:TYR:N	1:A:2228:TYR:HD1	2.12	0.48
1:A:2252:LEU:H	1:A:2255:HIS:HD1	1.62	0.48
3:C:441:PRO:HA	3:C:444:GLY:HA3	1.96	0.48
4:D:2035:VAL:O	4:D:2093:ASP:HA	2.14	0.48
6:F:40:U:H2'	6:F:41:A:C8	2.48	0.48
10:J:368:ARG:HA	10:J:368:ARG:NE	2.29	0.48
26:1:855:ASP:OD1	26:1:855:ASP:N	2.45	0.48
27:3:328:LYS:NZ	27:3:370:GLU:OE1	2.47	0.48
33:6:116:LYS:HG2	33:6:117:TYR:CD1	2.49	0.48
1:A:1361:GLU:OE1	1:A:1363:GLN:HB2	2.12	0.48
1:A:1782:ASP:O	1:A:1785:VAL:HG23	2.14	0.48
5:E:243:LEU:HD21	5:E:247:GLY:HA2	1.96	0.48
7:G:11:A:H2'	7:G:12:G:O4'	2.13	0.48
8:H:19:G:O2'	8:H:20:G:OP2	2.26	0.48
13:N:79:ILE:HA	13:N:84:ALA:HB3	1.96	0.48
26:1:413:LYS:HB2	33:6:52:ASN:HD21	1.78	0.48
26:1:489:PRO:HB2	26:1:492:GLN:HB2	1.96	0.48
27:3:665:LEU:HD23	27:3:677:THR:HB	1.94	0.48
27:3:791:HIS:CD2	27:3:794:SER:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1900:GLU:H	1:A:1900:GLU:CD	2.22	0.48
1:A:2274:PRO:HG2	1:A:2278:SER:O	2.14	0.48
3:C:131:ASN:HB3	3:C:549:TRP:CZ2	2.48	0.48
3:C:663:CYS:HB2	3:C:828:MET:HB2	1.96	0.48
10:J:366:TYR:HB3	10:J:382:TYR:CD2	2.48	0.48
21:V:522:MET:O	21:V:526:GLU:HG3	2.14	0.48
27:3:866:ILE:HD13	27:3:907:VAL:HG21	1.96	0.48
37:8:115:ASN:HD21	37:8:124:LEU:HD21	1.79	0.48
1:A:569:VAL:HG12	1:A:573:GLN:HB2	1.96	0.48
3:C:650:GLU:H	3:C:650:GLU:CD	2.21	0.48
3:C:711:ARG:NE	3:C:730:ARG:O	2.46	0.48
5:E:174:GLY:HA2	5:E:194:TYR:O	2.13	0.48
8:H:119:G:N2	8:H:139:C:O2	2.47	0.48
10:J:292:VAL:HG11	10:J:323:LEU:HD13	1.96	0.48
13:N:58:ARG:NH2	13:N:99:ASN:HA	2.29	0.48
24:Y:1:MET:HE3	24:Y:6:LYS:HG2	1.96	0.48
26:1:406:ALA:HA	33:6:99:GLN:HE22	1.79	0.48
27:3:958:ARG:NH1	27:3:980:LYS:HG2	2.29	0.48
33:6:18:ASN:OD1	33:6:19:ARG:N	2.47	0.48
36:9:142:ARG:HA	36:9:149:PRO:HA	1.96	0.48
1:A:197:PRO:HG3	1:A:204:LEU:HD21	1.95	0.47
1:A:1233:ASP:OD1	1:A:1234:ASP:N	2.46	0.47
1:A:2150:GLN:HA	1:A:2288:HIS:CE1	2.49	0.47
2:B:101:U:H2'	2:B:102:U:C6	2.48	0.47
3:C:366:GLN:HG3	3:C:371:GLU:HG3	1.96	0.47
3:C:515:THR:O	3:C:518:ASP:N	2.47	0.47
6:F:84:A:N6	8:H:14:C:N4	2.62	0.47
6:F:90:G:H2'	6:F:91:A:H8	1.79	0.47
21:V:603:LEU:HA	21:V:612:PHE:CE2	2.49	0.47
23:X:296:HIS:ND1	23:X:298:SER:OG	2.46	0.47
24:Y:17:GLU:HG3	24:Y:22:VAL:HB	1.96	0.47
26:1:984:GLU:HG3	26:1:986:TYR:H	1.78	0.47
27:3:65:LEU:HD12	27:3:80:VAL:HG22	1.95	0.47
27:3:181:MET:HE1	27:3:224:TYR:CE2	2.49	0.47
27:3:676:ARG:HD2	27:3:729:PHE:CE2	2.49	0.47
1:A:766:THR:CG2	1:A:768:ASP:H	2.26	0.47
3:C:693:GLU:OE1	3:C:695:GLY:N	2.40	0.47
6:F:35:A:N7	7:G:11:A:N1	2.62	0.47
8:H:11:G:O2'	8:H:12:G:H5'	2.15	0.47
10:J:286:GLU:HB3	10:J:295:ALA:HB2	1.96	0.47
10:J:299:TRP:HA	10:J:299:TRP:CE3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:80:VAL:HA	14:O:87:ASP:HA	1.96	0.47
26:1:145:PRO:HB2	26:1:146:LYS:NZ	2.29	0.47
26:1:1143:VAL:O	26:1:1147:VAL:HG13	2.14	0.47
27:3:394:ASN:OD1	27:3:394:ASN:N	2.45	0.47
31:2:457:MET:HE2	31:2:457:MET:HA	1.96	0.47
45:k:19:LEU:HA	45:k:70:LEU:HA	1.95	0.47
1:A:309:ARG:HH21	20:U:1:MET:HE2	1.78	0.47
1:A:1264:ASN:O	1:A:1268:ILE:HG13	2.14	0.47
1:A:1575:GLN:HB2	11:K:220:LEU:CD1	2.44	0.47
1:A:1762:TYR:HB3	1:A:2008:ARG:HD2	1.96	0.47
1:A:2171:GLU:O	1:A:2171:GLU:HG2	2.14	0.47
3:C:439:PRO:O	3:C:443:VAL:HB	2.14	0.47
4:D:823:ALA:O	4:D:857:GLY:N	2.30	0.47
10:J:275:ASN:HB3	10:J:278:LEU:HB2	1.95	0.47
13:N:108:THR:O	13:N:111:THR:HG22	2.15	0.47
13:N:139:CYS:SG	13:N:140:ARG:N	2.87	0.47
19:T:440:ASP:OD2	19:T:443:THR:HG23	2.14	0.47
21:V:648:LYS:HA	21:V:648:LYS:HD2	1.63	0.47
23:X:274:TYR:CD1	26:1:436:THR:N	2.72	0.47
26:1:1037:ASP:O	26:1:1041:ARG:HG2	2.14	0.47
1:A:1405:LEU:HD13	17:R:411:LEU:HD23	1.96	0.47
1:A:1490:PHE:O	1:A:1493:THR:OG1	2.30	0.47
1:A:2190:PRO:HG3	1:A:2251:TYR:CE2	2.49	0.47
8:H:60:U:H2'	8:H:61:C:C6	2.49	0.47
8:H:154:C:H1'	8:H:178:A:H61	1.80	0.47
10:J:429:PHE:CE1	10:J:465:ARG:HA	2.49	0.47
19:T:319:THR:O	19:T:319:THR:OG1	2.27	0.47
19:T:381:HIS:ND1	19:T:382:PRO:HD2	2.30	0.47
27:3:484:VAL:HG11	27:3:499:PHE:CD2	2.43	0.47
27:3:700:LYS:O	27:3:714:ALA:HA	2.14	0.47
29:w:497:ARG:HA	29:w:497:ARG:CZ	2.45	0.47
48:z:44:CYS:SG	48:z:164:CYS:HB3	2.53	0.47
1:A:318:TYR:HB2	3:C:638:ASP:OD1	2.14	0.47
1:A:552:ARG:HG2	1:A:552:ARG:NH1	2.29	0.47
1:A:856:LEU:O	1:A:857:ASN:HB3	2.15	0.47
3:C:244:LYS:HE3	3:C:248:GLN:HE22	1.79	0.47
3:C:514:TYR:HB2	3:C:521:ASP:HB3	1.95	0.47
3:C:600:LEU:HD12	3:C:600:LEU:HA	1.68	0.47
3:C:718:PHE:HB3	3:C:724:TRP:CD1	2.50	0.47
4:D:662:ALA:O	4:D:667:VAL:N	2.47	0.47
5:E:298:SER:O	5:E:314:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:23:U:H2'	6:F:24:A:O4'	2.15	0.47
8:H:130:U:H2'	8:H:131:G:H8	1.79	0.47
10:J:354:LEU:HA	10:J:356:TYR:O	2.14	0.47
10:J:359:VAL:O	10:J:363:ARG:HG2	2.15	0.47
16:Q:877:LEU:O	16:Q:1035:ILE:HA	2.15	0.47
21:V:482:PRO:HD2	21:V:485:GLN:OE1	2.14	0.47
26:1:885:ASP:OD1	26:1:886:HIS:N	2.47	0.47
26:1:1137:ARG:HD2	31:2:522:PHE:O	2.15	0.47
1:A:150:MET:CG	1:A:193:LEU:HB2	2.45	0.47
1:A:1673:SER:O	1:A:1673:SER:OG	2.30	0.47
1:A:2294:TYR:HE2	1:A:2296:LEU:HD21	1.80	0.47
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.96	0.47
3:C:369:PHE:HD1	3:C:373:ILE:HD12	1.80	0.47
3:C:384:VAL:HG11	3:C:416:LEU:HD23	1.96	0.47
3:C:711:ARG:HG2	3:C:730:ARG:HD2	1.97	0.47
5:E:75:HIS:O	5:E:78:GLY:N	2.48	0.47
5:E:128:SER:OG	5:E:130:ASP:OD1	2.24	0.47
9:I:366:LEU:HA	9:I:381:ALA:HB1	1.97	0.47
19:T:337:ARG:HG3	19:T:378:VAL:HG23	1.95	0.47
21:V:602:ARG:HD3	21:V:602:ARG:HA	1.67	0.47
26:1:397:ARG:HD2	26:1:398:PRO:HD2	1.97	0.47
27:3:319:GLU:H	27:3:319:GLU:CD	2.21	0.47
31:2:513:GLY:C	31:2:515:ARG:H	2.23	0.47
34:7:49:CYS:HB3	34:7:87:LYS:HD3	1.95	0.47
37:8:26:LYS:HA	37:8:26:LYS:HD3	1.66	0.47
1:A:480:LYS:HB2	13:N:110:ASP:HA	1.97	0.47
1:A:985:TYR:HD2	1:A:1032:ARG:NE	2.11	0.47
1:A:1527:ASN:ND2	11:K:215:ASP:HB3	2.30	0.47
1:A:1690:ASP:OD1	1:A:1692:MET:N	2.39	0.47
1:A:2174:PRO:HB2	1:A:2206:TRP:NE1	2.30	0.47
1:A:2304:PHE:HB3	1:A:2305:TYR:HD2	1.79	0.47
2:B:62:G:H2'	2:B:63:A:H8	1.79	0.47
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.50	0.47
3:C:319:THR:O	3:C:322:SER:N	2.47	0.47
3:C:446:LYS:HB3	3:C:447:PRO:HD3	1.96	0.47
3:C:938:ARG:HG2	3:C:938:ARG:HH11	1.80	0.47
4:D:1299:THR:N	4:D:1513:ASN:O	2.48	0.47
4:D:1667:GLN:HA	4:D:1677:VAL:O	2.14	0.47
16:Q:370:GLY:H	16:Q:371:PRO:HD2	1.79	0.47
19:T:417:ASN:HD21	19:T:432:ASP:HB2	1.80	0.47
25:Z:548:PHE:O	25:Z:551:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:152:TYR:CE2	26:1:156:MET:HG3	2.49	0.47
26:1:781:ASP:HB3	26:1:784:MET:HB2	1.95	0.47
26:1:1122:THR:OG1	26:1:1123:CYS:N	2.47	0.47
27:3:518:GLN:HG2	27:3:520:TYR:CE2	2.50	0.47
27:3:1026:ASP:OD1	27:3:1088:LYS:HE2	2.15	0.47
29:w:425:HIS:HE2	29:w:431:HIS:HD1	1.63	0.47
31:2:703:ILE:HG22	31:2:704:ASP:H	1.80	0.47
32:4:128:GLN:CB	32:4:148:ASN:H	2.28	0.47
33:6:113:LEU:HA	33:6:116:LYS:HZ1	1.80	0.47
46:e:34:TRP:O	46:e:85:THR:CA	2.63	0.47
3:C:65:TYR:CD2	3:C:65:TYR:N	2.81	0.47
3:C:349:PHE:HB2	3:C:356:PHE:CE1	2.49	0.47
3:C:448:LYS:O	3:C:452:THR:OG1	2.33	0.47
3:C:530:LEU:HD23	3:C:530:LEU:HA	1.68	0.47
3:C:799:GLU:HG3	3:C:801:LEU:HG	1.96	0.47
3:C:913:ASP:H	3:C:931:ARG:NH1	2.13	0.47
5:E:73:LYS:NZ	5:E:115:LEU:HB3	2.29	0.47
5:E:78:GLY:HA3	5:E:336:HIS:CE1	2.50	0.47
17:R:398:ASN:HB2	23:X:237:ASN:HD21	1.79	0.47
18:S:450:CYS:HA	18:S:518:MET:O	2.15	0.47
19:T:343:PRO:HB3	19:T:365:ARG:HH12	1.80	0.47
26:1:478:LEU:HG	26:1:499:LYS:HE3	1.97	0.47
26:1:675:MET:HE3	26:1:675:MET:HB3	1.65	0.47
26:1:1067:LYS:HB2	26:1:1067:LYS:NZ	2.29	0.47
27:3:519:VAL:HB	27:3:524:ILE:HG23	1.97	0.47
27:3:720:TRP:CE2	27:3:733:PRO:HG3	2.49	0.47
27:3:833:GLU:HA	27:3:834:LEU:HB2	1.96	0.47
32:4:54:GLN:C	32:4:56:TYR:H	2.23	0.47
33:6:37:ASP:O	33:6:41:LYS:HG2	2.15	0.47
36:9:328:PHE:CD2	36:9:329:VAL:HG13	2.49	0.47
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.96	0.47
1:A:663:ARG:HH11	1:A:663:ARG:CG	2.28	0.47
1:A:1840:LYS:O	1:A:1844:GLU:HG2	2.15	0.47
1:A:2107:PRO:HA	1:A:2264:SER:O	2.15	0.47
3:C:193:THR:HG23	3:C:428:THR:HB	1.97	0.47
5:E:193:THR:HG23	5:E:194:TYR:CG	2.50	0.47
6:F:78:A:H3'	6:F:79:C:C6	2.49	0.47
21:V:565:LEU:HD12	21:V:612:PHE:HE1	1.80	0.47
24:Y:71:LYS:HB2	24:Y:71:LYS:NZ	2.29	0.47
26:1:648:LEU:O	26:1:649:LYS:C	2.58	0.47
26:1:1185:ARG:NH1	31:2:511:LEU:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1251:LEU:HD11	26:1:1285:PRO:HG3	1.97	0.47
27:3:544:ILE:HD12	27:3:558:LEU:HG	1.97	0.47
31:2:601:LEU:O	31:2:602:LYS:HB2	2.15	0.47
35:5:11:LEU:HD22	35:5:23:HIS:HB3	1.95	0.47
37:8:72:PHE:O	37:8:76:GLU:HG2	2.15	0.47
46:j:61:ALA:H	46:j:75:GLY:HA2	1.79	0.47
48:z:16:LEU:HD13	48:z:25:ASP:OD1	2.14	0.47
1:A:468:LYS:HD3	1:A:469:LYS:H	1.80	0.47
1:A:1923:TRP:HB3	1:A:1927:ILE:HD11	1.97	0.47
1:A:2189:SER:HB2	1:A:2192:ASP:CG	2.40	0.47
6:F:16:G:H2'	6:F:17:C:C6	2.50	0.47
6:F:84:A:H2	8:H:15:U:O2	1.98	0.47
8:H:6:U:H2'	8:H:7:U:C6	2.49	0.47
16:Q:525:PRO:HA	16:Q:532:PRO:HA	1.96	0.47
17:R:125:MET:HG3	19:T:186:PRO:HD2	1.97	0.47
17:R:233:PRO:O	17:R:235:ARG:NH1	2.47	0.47
19:T:226:ARG:HD3	19:T:246:ILE:O	2.15	0.47
21:V:600:ASN:O	21:V:604:LYS:HB2	2.15	0.47
21:V:650:THR:HB	21:V:651:PRO:CD	2.45	0.47
27:3:272:PRO:HG2	27:3:311:PHE:HE1	1.80	0.47
27:3:411:GLN:HE21	27:3:411:GLN:HB2	1.42	0.47
36:9:266:ILE:HG23	36:9:267:ASP:H	1.79	0.47
36:9:321:PHE:HA	36:9:332:GLY:CA	2.39	0.47
1:A:988:ILE:HD12	1:A:1030:ILE:HD12	1.97	0.46
1:A:1833:LEU:O	1:A:1836:LEU:HB3	2.15	0.46
1:A:2107:PRO:HG2	1:A:2110:VAL:CG2	2.45	0.46
1:A:2176:GLY:HA2	1:A:2206:TRP:CE2	2.51	0.46
1:A:2309:HIS:CD2	1:A:2309:HIS:N	2.83	0.46
3:C:264:ILE:HG21	3:C:381:LEU:HD12	1.98	0.46
3:C:278:LEU:HD13	3:C:309:PHE:CE1	2.50	0.46
3:C:709:TRP:HZ3	3:C:717:PHE:HB2	1.80	0.46
6:F:13:G:H2'	6:F:14:C:C6	2.51	0.46
8:H:81:G:H2'	8:H:82:G:O4'	2.14	0.46
13:N:9:LYS:HA	13:N:9:LYS:HD3	1.77	0.46
23:X:261:LEU:HG	23:X:367:TYR:HB3	1.96	0.46
26:1:170:GLN:O	26:1:174:GLU:HG2	2.15	0.46
26:1:843:LYS:HA	26:1:843:LYS:HD2	1.62	0.46
27:3:705:ARG:HH12	27:3:709:GLN:N	2.12	0.46
29:w:426:PHE:O	29:w:442:ASN:ND2	2.29	0.46
33:6:26:LEU:HD12	33:6:87:LEU:HD11	1.96	0.46
1:A:382:GLU:HA	3:C:354:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ARG:HA	1:A:758:ARG:HD2	1.62	0.46
1:A:1881:ASN:OD1	1:A:1881:ASN:N	2.47	0.46
3:C:120:ALA:O	3:C:123:MET:HB2	2.15	0.46
5:E:129:THR:O	5:E:153:PHE:HA	2.14	0.46
11:K:140:ILE:HG12	11:K:140:ILE:H	1.49	0.46
13:N:91:LYS:HD2	13:N:91:LYS:HA	1.64	0.46
19:T:250:ARG:HH11	19:T:250:ARG:CG	2.29	0.46
23:X:310:LEU:HB2	23:X:324:VAL:HG12	1.96	0.46
26:1:967:GLU:HG2	26:1:970:LEU:HD23	1.96	0.46
31:2:557:VAL:HG13	31:2:558:ARG:HG3	1.96	0.46
31:2:642:PRO:HA	32:4:69:TYR:CB	2.45	0.46
32:4:166:TYR:HA	32:4:171:PRO:HA	1.96	0.46
41:h:55:ARG:O	41:h:68:GLU:N	2.46	0.46
44:l:60:GLN:O	45:k:72:ALA:N	2.44	0.46
48:z:39:ASN:HA	48:z:78:ILE:HD11	1.96	0.46
1:A:514:ASN:ND2	1:A:514:ASN:H	2.13	0.46
1:A:820:ARG:HA	1:A:820:ARG:HD2	1.58	0.46
3:C:313:GLN:HB2	50:C:1500:GTP:C5	2.50	0.46
3:C:342:ARG:O	3:C:347:ILE:HD12	2.15	0.46
25:Z:546:ALA:O	25:Z:550:LYS:HG2	2.15	0.46
26:1:760:GLU:C	26:1:760:GLU:CD	2.83	0.46
26:1:1256:HIS:CD2	26:1:1257:PRO:HD2	2.50	0.46
27:3:71:THR:O	27:3:146:ARG:NH2	2.49	0.46
27:3:896:PHE:CD1	27:3:972:LEU:HB2	2.50	0.46
1:A:1975:GLU:O	1:A:1979:VAL:HG13	2.16	0.46
3:C:420:CYS:O	3:C:424:PHE:HB2	2.16	0.46
3:C:711:ARG:NH2	3:C:730:ARG:O	2.48	0.46
8:H:28:C:H4'	8:H:29:A:OP1	2.16	0.46
8:H:138:C:H2'	8:H:139:C:C6	2.50	0.46
8:H:175:G:H2'	8:H:176:G:C4	2.49	0.46
26:1:733:LYS:HE2	26:1:733:LYS:HB3	1.70	0.46
29:w:493:GLU:HA	29:w:496:LYS:HB3	1.96	0.46
37:8:30:PHE:HE1	37:8:83:LYS:HA	1.80	0.46
1:A:325:HIS:CD2	1:A:326:HIS:CD2	3.03	0.46
1:A:363:HIS:NE2	3:C:284:GLU:HA	2.31	0.46
1:A:1860:GLN:OE1	1:A:1885:LYS:NZ	2.47	0.46
1:A:2259:VAL:HG12	1:A:2260:GLN:N	2.30	0.46
2:B:110:C:H2'	2:B:111:A:C8	2.49	0.46
3:C:201:ASN:HB3	3:C:549:TRP:CE3	2.50	0.46
3:C:286:ASN:ND2	3:C:300:LEU:O	2.37	0.46
3:C:453:TYR:HD2	3:C:456:GLY:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:84:A:O2'	6:F:85:U:H2'	2.16	0.46
7:G:104:C:O2	7:G:104:C:H2'	2.15	0.46
8:H:168:A:H5''	8:H:169:C:H5	1.80	0.46
8:H:172:C:H2'	8:H:173:C:C6	2.50	0.46
10:J:236:ARG:HE	10:J:236:ARG:HB3	1.57	0.46
10:J:338:GLU:O	10:J:340:GLN:NE2	2.49	0.46
21:V:641:ASP:O	21:V:642:GLU:C	2.58	0.46
23:X:291:ASP:HB2	23:X:292:ILE:HG13	1.98	0.46
26:1:484:GLU:O	26:1:487:LEU:N	2.49	0.46
26:1:694:LEU:HA	26:1:694:LEU:HD23	1.64	0.46
27:3:552:ARG:HH12	27:3:601:ARG:NH2	2.12	0.46
29:w:386:GLY:N	29:w:390:LYS:O	2.31	0.46
1:A:1807:ILE:HG12	1:A:1841:THR:HG22	1.96	0.46
1:A:2129:TYR:CZ	1:A:2169:LEU:HD13	2.51	0.46
3:C:384:VAL:HG13	3:C:415:LEU:HD23	1.97	0.46
4:D:1562:PHE:HA	4:D:1646:ALA:O	2.16	0.46
8:H:2:U:H2'	8:H:3:C:H6	1.77	0.46
8:H:3:C:H2'	8:H:4:G:H8	1.81	0.46
8:H:16:U:H1'	8:H:17:U:H5'	1.98	0.46
25:Z:533:ARG:O	25:Z:537:GLU:HG2	2.16	0.46
26:1:400:SER:O	26:1:404:LEU:HG	2.15	0.46
26:1:495:ARG:HB3	26:1:495:ARG:CZ	2.44	0.46
26:1:773:LEU:HD11	26:1:791:VAL:HG12	1.98	0.46
26:1:1013:ILE:HG22	26:1:1049:TYR:HB2	1.97	0.46
27:3:608:GLY:HA2	27:3:614:VAL:HG22	1.98	0.46
36:9:268:GLU:O	36:9:269:ASP:C	2.58	0.46
36:9:276:VAL:HG21	36:9:438:TYR:CD1	2.50	0.46
1:A:361:HIS:O	1:A:362:ARG:NE	2.48	0.46
1:A:570:ASP:HB3	1:A:573:GLN:HG3	1.97	0.46
1:A:845:ARG:HH22	1:A:1440:THR:HG22	1.80	0.46
1:A:1271:MET:HE3	1:A:1271:MET:HB3	1.78	0.46
2:B:100:C:H2'	2:B:101:U:C5	2.50	0.46
3:C:441:PRO:C	3:C:444:GLY:HA3	2.40	0.46
3:C:696:LEU:O	3:C:700:ILE:HD12	2.16	0.46
3:C:750:LEU:O	3:C:754:VAL:HG23	2.15	0.46
7:G:9:C:H2'	7:G:10:U:N1	2.31	0.46
17:R:283:ASN:N	17:R:283:ASN:OD1	2.46	0.46
23:X:296:HIS:HB3	23:X:363:SER:OG	2.16	0.46
25:Z:560:LYS:HD3	25:Z:561:LYS:H	1.80	0.46
26:1:531:LEU:O	26:1:535:ILE:HG13	2.16	0.46
26:1:770:MET:HE1	26:1:801:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:565:TYR:CE2	27:3:567:GLU:HB2	2.51	0.46
34:7:11:CYS:SG	34:7:13:LYS:NZ	2.76	0.46
39:v:17:ALA:HB1	39:v:21:GLU:HB2	1.98	0.46
39:v:31:ARG:HD3	39:v:48:LYS:HZ2	1.81	0.46
1:A:82:ARG:HG2	1:A:82:ARG:O	2.15	0.46
1:A:1393:ARG:HH11	26:1:90:LEU:HD22	1.81	0.46
2:B:108:G:H3'	2:B:109:G:H8	1.81	0.46
3:C:137:HIS:HB2	3:C:239:THR:HG23	1.98	0.46
4:D:642:THR:C	4:D:644:GLU:H	2.23	0.46
5:E:248:SER:O	5:E:263:ASP:HA	2.16	0.46
8:H:168:A:N3	8:H:168:A:H2'	2.29	0.46
10:J:236:ARG:HA	10:J:239:ARG:CZ	2.45	0.46
12:L:49:ARG:HG3	12:L:54:LEU:HD22	1.97	0.46
15:P:199:LYS:HA	15:P:199:LYS:HD2	1.61	0.46
15:P:212:ASN:OD1	19:T:458:SER:HB3	2.16	0.46
27:3:102:ILE:HG22	27:3:103:HIS:CD2	2.50	0.46
27:3:429:ARG:HG2	27:3:430:GLY:N	2.31	0.46
27:3:550:ASN:HD21	27:3:595:VAL:N	2.14	0.46
27:3:788:PHE:HB2	27:3:799:ILE:HG12	1.97	0.46
27:3:818:GLN:O	27:3:821:GLU:HB2	2.16	0.46
33:6:104:LYS:HA	33:6:107:GLU:OE2	2.16	0.46
43:m:42:LEU:O	43:m:69:LEU:HA	2.16	0.46
48:z:15:VAL:HG11	48:z:40:PHE:HE2	1.81	0.46
1:A:260:LEU:O	1:A:263:PHE:N	2.49	0.46
1:A:696:MET:C	1:A:698:PRO:HD3	2.40	0.46
1:A:1684:PHE:O	1:A:1688:THR:HG23	2.16	0.46
3:C:712:LYS:O	3:C:716:GLU:HG3	2.16	0.46
5:E:226:LYS:HD2	5:E:226:LYS:HA	1.73	0.46
7:G:88:G:H4'	7:G:89:U:OP1	2.15	0.46
10:J:423:GLU:HA	10:J:426:GLN:HG2	1.98	0.46
12:L:101:GLU:C	12:L:101:GLU:CD	2.84	0.46
26:1:933:CYS:CB	26:1:970:LEU:HD11	2.45	0.46
32:4:159:ILE:O	32:4:163:ASN:CB	2.63	0.46
33:6:106:LYS:O	33:6:109:GLN:HG2	2.16	0.46
36:9:293:LEU:HD11	36:9:295:LEU:HG	1.98	0.46
36:9:315:TYR:OH	36:9:343:GLU:HB2	2.16	0.46
48:z:27:GLU:HG3	48:z:134:THR:HG22	1.97	0.46
1:A:693:ILE:HB	1:A:738:MET:SD	2.56	0.46
1:A:1291:CYS:O	1:A:1295:ILE:HG23	2.15	0.46
1:A:2150:GLN:O	1:A:2281:TYR:N	2.49	0.46
2:B:12:U:H2'	2:B:13:C:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:357:THR:OG1	3:C:358:LYS:O	2.33	0.46
5:E:191:GLN:H	5:E:191:GLN:CD	2.23	0.46
8:H:2:U:C2	8:H:3:C:C5	3.04	0.46
8:H:154:C:N3	8:H:155:C:N4	2.64	0.46
10:J:313:TRP:O	10:J:317:THR:HG23	2.15	0.46
17:R:141:LYS:O	17:R:145:GLU:HG2	2.15	0.46
26:1:152:TYR:OH	37:8:64:ASP:OD1	2.25	0.46
26:1:492:GLN:CD	26:1:495:ARG:HH11	2.24	0.46
27:3:636:GLN:HB3	27:3:670:GLN:NE2	2.30	0.46
27:3:1106:LYS:HD2	31:2:708:TRP:NE1	2.31	0.46
27:3:1199:ARG:HH22	27:3:1207:LYS:HE3	1.80	0.46
39:v:55:GLU:HG2	39:v:62:LEU:HD23	1.97	0.46
44:l:32:LEU:HA	44:l:43:MET:CB	2.47	0.46
1:A:83:HIS:NE2	7:G:16:G:O6	2.49	0.45
1:A:1784:ASN:ND2	1:A:1894:GLN:HB2	2.31	0.45
5:E:174:GLY:HA2	5:E:194:TYR:C	2.42	0.45
7:G:110:U:OP2	24:Y:2:ASN:ND2	2.49	0.45
11:K:129:ASP:O	11:K:133:ILE:HD12	2.16	0.45
16:Q:1217:LEU:O	16:Q:1338:PHE:N	2.49	0.45
26:1:547:GLN:NE2	34:7:101:GLU:OE2	2.49	0.45
26:1:805:TYR:CE1	26:1:809:GLU:HG3	2.51	0.45
26:1:826:ASP:HB3	26:1:829:ASN:HB2	1.96	0.45
27:3:333:VAL:HB	27:3:334:PRO:HD2	1.98	0.45
27:3:354:GLY:O	27:3:403:SER:OG	2.33	0.45
27:3:370:GLU:H	27:3:370:GLU:HG2	1.41	0.45
27:3:1063:ASN:ND2	27:3:1066:VAL:HG12	2.31	0.45
27:3:1123:SER:OG	35:5:48:ASP:OD1	2.34	0.45
33:6:77:LEU:O	33:6:80:PHE:HB2	2.15	0.45
34:7:12:ARG:HD3	34:7:12:ARG:HA	1.46	0.45
36:9:219:GLU:CG	36:9:220:ILE:HD12	2.43	0.45
39:v:60:LEU:HD23	39:v:60:LEU:HA	1.80	0.45
1:A:976:MET:HE2	1:A:1098:PHE:HD1	1.80	0.45
1:A:1386:TRP:CH2	26:1:91:LEU:HD21	2.51	0.45
4:D:1186:LEU:HA	4:D:1203:THR:O	2.17	0.45
5:E:114:GLU:OE2	5:E:156:SER:HA	2.16	0.45
7:G:87:U:H2'	7:G:88:G:O4'	2.16	0.45
7:G:109:U:OP1	24:Y:2:ASN:ND2	2.49	0.45
25:Z:489:GLU:O	25:Z:492:GLU:HG2	2.16	0.45
26:1:568:ARG:HH11	26:1:608:THR:HG21	1.81	0.45
27:3:1114:SER:HB2	27:3:1215:TYR:CE1	2.51	0.45
27:3:1158:ARG:HG3	27:3:1159:ASP:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:464:LEU:O	29:w:468:SER:OG	2.34	0.45
33:6:29:LYS:HE3	33:6:29:LYS:HB3	1.54	0.45
36:9:199:ASN:HD21	36:9:205:ARG:HD3	1.81	0.45
48:z:32:GLU:HG3	48:z:88:HIS:CD2	2.51	0.45
46:e:34:TRP:O	46:e:85:THR:N	2.48	0.45
1:A:818:GLU:OE2	17:R:305:ARG:NH1	2.47	0.45
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.97	0.45
1:A:1570:LYS:O	1:A:1574:ILE:HB	2.17	0.45
1:A:1994:LYS:C	1:A:1995:ASN:HD22	2.17	0.45
1:A:2189:SER:HB3	1:A:2191:GLN:HG2	1.99	0.45
4:D:912:ASN:HA	4:D:978:ASN:HA	1.99	0.45
5:E:301:ALA:HB2	5:E:335:PHE:HE2	1.81	0.45
6:F:49:G:H8	6:F:49:G:OP1	1.98	0.45
7:G:19:G:N2	14:O:194:ALA:HA	2.31	0.45
9:I:619:ALA:O	9:I:623:VAL:CA	2.65	0.45
26:1:413:LYS:HB3	26:1:413:LYS:HE2	1.59	0.45
33:6:34:GLU:O	33:6:35:MET:C	2.59	0.45
33:6:66:ASP:HB3	33:6:69:ASP:HB2	1.97	0.45
36:9:301:PRO:O	36:9:305:GLU:HB2	2.17	0.45
41:h:72:GLU:O	41:h:93:ASP:HA	2.16	0.45
1:A:689:VAL:HG13	1:A:738:MET:SD	2.57	0.45
1:A:2103:THR:HB	1:A:2260:GLN:CD	2.41	0.45
3:C:227:LEU:HD12	3:C:227:LEU:HA	1.74	0.45
3:C:933:PHE:O	3:C:937:THR:OG1	2.27	0.45
5:E:178:LEU:HD11	5:E:222:LEU:HD22	1.98	0.45
8:H:79:G:H2'	8:H:79:G:N3	2.30	0.45
10:J:299:TRP:HB3	10:J:316:TYR:CD2	2.51	0.45
10:J:332:VAL:HA	10:J:335:ARG:CD	2.46	0.45
17:R:144:THR:O	17:R:148:ARG:HB2	2.16	0.45
17:R:332:ARG:HH22	23:X:267:ASP:N	2.10	0.45
21:V:555:LEU:HD23	21:V:555:LEU:HA	1.66	0.45
27:3:971:ASP:OD1	27:3:972:LEU:N	2.43	0.45
29:w:390:LYS:HZ3	39:v:84:ARG:HG2	1.80	0.45
47:b:42:ALA:N	47:b:56:GLU:O	2.49	0.45
1:A:210:HIS:CD2	1:A:210:HIS:C	2.95	0.45
1:A:646:PRO:HG3	2:B:55:C:H4'	1.98	0.45
1:A:976:MET:HE2	1:A:976:MET:HB2	1.80	0.45
1:A:1457:HIS:ND1	1:A:1460:HIS:HD2	2.14	0.45
1:A:1642:PRO:HA	1:A:1716:GLY:O	2.17	0.45
2:B:88:A:H4'	2:B:94:U:O4	2.15	0.45
5:E:84:ALA:HB1	5:E:112:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:G:C6	26:1:1069:HIS:NE2	2.85	0.45
8:H:154:C:H1'	8:H:178:A:N6	2.30	0.45
10:J:313:TRP:HB3	10:J:336:TRP:CE3	2.52	0.45
12:L:30:GLN:HG2	12:L:33:ARG:HE	1.82	0.45
13:N:77:TYR:CE2	13:N:81:GLU:HG3	2.52	0.45
17:R:189:ASN:HB3	17:R:191:GLY:H	1.81	0.45
18:S:480:SER:HA	18:S:485:ASP:HA	1.98	0.45
18:S:521:GLU:N	18:S:551:ALA:O	2.50	0.45
21:V:514:PHE:HB3	21:V:521:TYR:CD1	2.51	0.45
24:Y:48:THR:OG1	24:Y:49:GLU:N	2.47	0.45
26:1:742:GLY:O	26:1:746:PHE:HD2	2.00	0.45
27:3:365:GLY:HA3	27:3:394:ASN:HD21	1.80	0.45
35:5:59:GLU:OE1	35:5:63:ARG:HG2	2.17	0.45
1:A:109:PRO:HD3	1:A:630:TRP:HZ2	1.80	0.45
1:A:338:VAL:HG21	3:C:867:PRO:HD2	1.98	0.45
1:A:1386:TRP:HB3	26:1:87:PRO:HG2	1.97	0.45
1:A:2234:GLY:HA2	1:A:2255:HIS:CD2	2.52	0.45
3:C:641:MET:HE2	3:C:641:MET:HB3	1.80	0.45
6:F:15:A:H2'	6:F:16:G:C8	2.52	0.45
7:G:109:U:H1'	26:1:626:ASN:ND2	2.32	0.45
13:N:44:GLU:HB2	13:N:47:TRP:CZ3	2.52	0.45
26:1:619:ASN:OD1	26:1:620:MET:N	2.50	0.45
26:1:637:SER:HA	26:1:675:MET:SD	2.56	0.45
26:1:699:GLN:HE22	26:1:738:HIS:HE1	1.65	0.45
26:1:1046:GLY:O	26:1:1048:GLU:N	2.48	0.45
27:3:544:ILE:HG13	27:3:557:ALA:O	2.17	0.45
27:3:833:GLU:C	27:3:836:ALA:H	2.21	0.45
31:2:469:VAL:HG11	31:2:489:VAL:CG1	2.46	0.45
36:9:348:LYS:HE3	36:9:348:LYS:HB3	1.66	0.45
41:h:47:ARG:N	41:h:105:SER:O	2.46	0.45
1:A:48:LYS:HA	1:A:53:PHE:CE1	2.52	0.45
1:A:196:ASP:OD2	1:A:198:GLU:HB2	2.16	0.45
1:A:519:ASP:C	1:A:519:ASP:OD1	2.60	0.45
1:A:1699:THR:HA	1:A:1717:ASN:HD22	1.81	0.45
1:A:2188:LEU:HD12	1:A:2188:LEU:HA	1.79	0.45
2:B:66:A:H2'	2:B:67:A:H8	1.80	0.45
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.29	0.45
6:F:47:A:H2'	6:F:48:A:C5	2.50	0.45
7:G:-11:G:H2'	7:G:-10:G:C8	2.52	0.45
21:V:555:LEU:HD23	21:V:560:LEU:HB2	1.99	0.45
24:Y:64:ASN:HB3	24:Y:83:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:66:ASN:HD21	24:Y:118:PRO:HG3	1.82	0.45
26:1:932:ILE:N	26:1:932:ILE:CD1	2.79	0.45
26:1:946:LYS:HA	26:1:946:LYS:HD3	1.51	0.45
27:3:410:CYS:SG	27:3:411:GLN:N	2.89	0.45
27:3:1145:GLU:HG3	27:3:1146:MET:N	2.31	0.45
36:9:268:GLU:OE1	36:9:268:GLU:HA	2.16	0.45
48:z:45:LEU:HD23	48:z:45:LEU:HA	1.78	0.45
1:A:156:ARG:HH21	1:A:157:ASP:CG	2.25	0.45
1:A:226:GLN:HA	1:A:418:THR:HB	1.98	0.45
1:A:1070:ASP:O	1:A:1071:PHE:C	2.58	0.45
1:A:1935:ARG:O	1:A:1939:ILE:HG13	2.17	0.45
1:A:2129:TYR:CE2	1:A:2169:LEU:HB3	2.52	0.45
1:A:2279:TRP:NE1	1:A:2301:PRO:HB3	2.30	0.45
3:C:153:THR:OG1	3:C:154:HIS:N	2.50	0.45
3:C:594:PRO:HD3	3:C:603:MET:SD	2.57	0.45
3:C:673:LYS:HE2	20:U:60:HIS:CB	2.47	0.45
3:C:750:LEU:HD23	3:C:750:LEU:H	1.82	0.45
5:E:73:LYS:HZ1	5:E:115:LEU:HD12	1.82	0.45
7:G:89:U:H4'	7:G:90:C:OP2	2.16	0.45
10:J:231:PHE:HA	10:J:234:ASN:HD22	1.82	0.45
17:R:233:PRO:HG2	17:R:235:ARG:NH1	2.32	0.45
21:V:620:ASN:HB3	21:V:623:ASN:OD1	2.17	0.45
24:Y:88:ARG:NH1	25:Z:503:GLN:OE1	2.49	0.45
27:3:525:ARG:O	27:3:525:ARG:HG2	2.16	0.45
27:3:720:TRP:CE3	27:3:731:LEU:HG	2.49	0.45
27:3:884:GLN:HG3	27:3:885:ASN:OD1	2.17	0.45
29:w:453:GLU:H	29:w:453:GLU:CD	2.22	0.45
39:v:66:GLU:O	39:v:70:LEU:HG	2.17	0.45
1:A:913:PRO:HA	1:A:916:LYS:HB2	1.99	0.45
1:A:1678:ARG:HD3	1:A:1678:ARG:HA	1.70	0.45
1:A:2280:ASN:HD22	1:A:2304:PHE:HA	1.81	0.45
3:C:275:TYR:CD1	3:C:369:PHE:HD2	2.35	0.45
3:C:709:TRP:HB2	3:C:714:LEU:HD12	1.98	0.45
3:C:735:PHE:CE1	3:C:744:ILE:HG12	2.52	0.45
8:H:139:C:H2'	8:H:140:A:C8	2.52	0.45
13:N:72:ARG:HG3	13:N:72:ARG:NH1	2.31	0.45
13:N:118:ILE:CD1	13:N:132:ILE:HG21	2.46	0.45
19:T:195:LYS:HE3	19:T:490:ARG:CZ	2.47	0.45
21:V:530:LYS:HD3	21:V:567:CYS:SG	2.57	0.45
26:1:866:LYS:HB2	26:1:866:LYS:HE2	1.50	0.45
27:3:298:MET:N	27:3:298:MET:SD	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:2:555:GLU:OE1	31:2:560:LYS:HB2	2.16	0.45
34:7:21:ARG:HA	34:7:67:SER:O	2.17	0.45
37:8:46:GLU:H	37:8:46:GLU:CD	2.24	0.45
1:A:460:LYS:NZ	2:B:49:A:OP2	2.48	0.45
1:A:955:TRP:CG	1:A:1189:MET:HE1	2.52	0.45
1:A:2163:LEU:HG	1:A:2203:ASN:ND2	2.31	0.45
2:B:88:A:H2'	2:B:88:A:N3	2.32	0.45
3:C:416:LEU:HD23	3:C:416:LEU:HA	1.65	0.45
3:C:495:ARG:HD2	3:C:497:LEU:HG	1.98	0.45
3:C:564:THR:HG21	3:C:576:ILE:HA	1.99	0.45
3:C:854:ARG:NH1	3:C:879:ASP:OD2	2.50	0.45
6:F:26:U:H2'	14:O:180:PRO:CB	2.47	0.45
7:G:90:C:H2'	7:G:91:A:C8	2.52	0.45
8:H:157:G:C6	8:H:174:A:N1	2.85	0.45
11:K:230:TRP:HA	11:K:233:GLU:HG3	1.98	0.45
12:L:19:LEU:HD23	12:L:54:LEU:HD23	1.99	0.45
19:T:355:ARG:HD3	19:T:364:THR:HG21	1.99	0.45
19:T:503:SER:O	19:T:503:SER:OG	2.16	0.45
27:3:206:GLN:NE2	27:3:232:GLY:N	2.65	0.45
27:3:484:VAL:C	27:3:485:LEU:HD12	2.41	0.45
27:3:614:VAL:HG12	27:3:631:GLN:OE1	2.17	0.45
27:3:870:ASN:ND2	27:3:872:ILE:H	2.14	0.45
27:3:1194:SER:HB2	27:3:1199:ARG:O	2.16	0.45
29:w:452:ILE:O	29:w:456:VAL:HG23	2.17	0.45
36:9:268:GLU:O	36:9:270:VAL:N	2.50	0.45
36:9:354:PHE:HB3	36:9:392:LYS:NZ	2.32	0.45
37:8:51:TRP:HZ3	37:8:105:LEU:HD12	1.82	0.45
1:A:1971:LEU:HB3	1:A:1975:GLU:HB2	1.99	0.44
1:A:2070:LYS:O	1:A:2074:ARG:HG2	2.17	0.44
1:A:2113:LYS:HB3	1:A:2271:PHE:CE2	2.52	0.44
1:A:2147:MET:HB3	1:A:2279:TRP:HB3	1.99	0.44
2:B:14:U:H2'	2:B:15:C:H6	1.82	0.44
3:C:311:SER:O	3:C:311:SER:OG	2.31	0.44
3:C:687:MET:HB3	3:C:815:VAL:HG11	1.99	0.44
3:C:807:GLN:NE2	36:9:144:LEU:O	2.49	0.44
5:E:243:LEU:HD11	5:E:247:GLY:O	2.17	0.44
8:H:123:A:N3	8:H:123:A:H2'	2.31	0.44
8:H:156:U:C2	8:H:175:G:N2	2.85	0.44
16:Q:1322:GLN:HA	16:Q:1325:ALA:HB2	2.00	0.44
24:Y:64:ASN:OD1	24:Y:65:ILE:N	2.50	0.44
26:1:123:ARG:NH2	26:1:124:ARG:HG3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:614:VAL:O	27:3:630:MET:HB2	2.17	0.44
29:w:403:ASN:N	29:w:403:ASN:OD1	2.50	0.44
37:8:30:PHE:CD1	37:8:83:LYS:HD2	2.52	0.44
37:8:82:SER:HB2	37:8:102:MET:HE1	1.98	0.44
1:A:110:TRP:O	1:A:192:GLN:NE2	2.48	0.44
1:A:183:LEU:HD23	13:N:30:ARG:NH2	2.32	0.44
1:A:231:THR:OG1	1:A:233:PRO:HD2	2.18	0.44
1:A:670:LYS:HE2	1:A:670:LYS:HB3	1.35	0.44
1:A:1870:ASP:O	1:A:1874:VAL:HG23	2.17	0.44
1:A:2107:PRO:HD3	1:A:2267:PHE:CZ	2.53	0.44
3:C:63:LYS:C	3:C:63:LYS:HD3	2.42	0.44
3:C:495:ARG:HB3	3:C:549:TRP:HD1	1.82	0.44
5:E:326:HIS:CE1	5:E:352:TYR:HD2	2.36	0.44
8:H:177:A:O2'	8:H:178:A:H5'	2.16	0.44
19:T:455:GLN:HG3	19:T:456:PRO:HD2	2.00	0.44
23:X:359:LYS:HZ1	23:X:366:GLU:HB3	1.82	0.44
26:1:406:ALA:HA	33:6:99:GLN:NE2	2.32	0.44
26:1:869:MET:SD	26:1:913:GLY:HA3	2.57	0.44
29:w:438:LEU:HD23	29:w:438:LEU:HA	1.82	0.44
33:6:21:LEU:HD21	33:6:64:TYR:HE2	1.82	0.44
39:v:69:TYR:O	39:v:72:HIS:HB3	2.17	0.44
1:A:888:GLN:O	1:A:889:ARG:HD3	2.16	0.44
1:A:1681:ARG:HE	1:A:1681:ARG:HB2	1.52	0.44
1:A:2237:TRP:O	1:A:2240:GLN:HB3	2.17	0.44
3:C:273:ASP:N	3:C:273:ASP:OD1	2.46	0.44
13:N:12:PRO:HB2	13:N:74:LEU:HB2	2.00	0.44
16:Q:1110:GLN:HA	16:Q:1115:MET:H	1.82	0.44
19:T:223:SER:OG	19:T:224:ALA:N	2.48	0.44
21:V:520:GLU:HA	21:V:523:GLU:CD	2.42	0.44
21:V:520:GLU:HA	21:V:523:GLU:OE2	2.17	0.44
24:Y:44:PRO:HA	24:Y:105:ARG:HD2	1.99	0.44
26:1:682:HIS:O	26:1:685:SER:OG	2.26	0.44
26:1:1036:ILE:HD12	26:1:1065:LEU:HD22	1.98	0.44
26:1:1055:TRP:HA	26:1:1055:TRP:CE3	2.52	0.44
27:3:69:ARG:HB2	27:3:76:ASP:OD1	2.16	0.44
27:3:581:LYS:HB2	27:3:625:LEU:HD22	1.98	0.44
27:3:847:LEU:HB3	27:3:852:PHE:CD2	2.53	0.44
27:3:946:GLU:CD	27:3:968:ARG:HH12	2.24	0.44
27:3:966:LEU:HD22	27:3:982:GLU:OE2	2.18	0.44
33:6:40:GLY:C	33:6:42:TYR:H	2.26	0.44
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD12	3:C:177:ARG:HG3	1.98	0.44
1:A:1556:ASP:OD1	1:A:1556:ASP:N	2.51	0.44
1:A:1974:GLU:O	1:A:1978:LYS:HG3	2.18	0.44
1:A:2162:GLN:HB3	1:A:2294:TYR:CE1	2.52	0.44
6:F:43:A:H1'	7:G:5:G:N2	2.33	0.44
8:H:46:U:N3	29:w:381:LYS:HA	2.32	0.44
8:H:118:G:O6	8:H:140:A:N6	2.50	0.44
13:N:64:PHE:HE1	13:N:72:ARG:HA	1.81	0.44
14:O:216:ARG:O	14:O:219:THR:N	2.51	0.44
17:R:134:ARG:HH22	19:T:385:TYR:H	1.63	0.44
26:1:162:THR:HA	26:1:165:GLU:HB2	2.00	0.44
26:1:1103:VAL:HB	26:1:1104:GLN:H	1.75	0.44
26:1:1108:ASN:N	26:1:1108:ASN:OD1	2.50	0.44
27:3:212:GLU:OE1	27:3:223:LYS:HD2	2.16	0.44
27:3:550:ASN:HD21	27:3:595:VAL:H	1.63	0.44
27:3:615:ARG:NE	27:3:627:PRO:HB3	2.33	0.44
27:3:842:PHE:HD2	27:3:843:LEU:HD12	1.81	0.44
27:3:870:ASN:ND2	27:3:872:ILE:HB	2.21	0.44
27:3:965:LYS:HG2	27:3:988:ASN:O	2.17	0.44
1:A:617:ASN:HA	1:A:621:VAL:CG2	2.46	0.44
1:A:2118:SER:HB3	1:A:2124:ILE:HD13	1.98	0.44
1:A:2295:GLU:O	1:A:2296:LEU:HD23	2.18	0.44
2:B:36:C:O2	20:U:11:ARG:NH2	2.50	0.44
3:C:493:PHE:HB2	3:C:551:LEU:HD23	1.98	0.44
3:C:902:HIS:ND1	3:C:903:HIS:HD2	2.16	0.44
5:E:343:ILE:HG23	5:E:351:LEU:HD13	2.00	0.44
6:F:28:A:N1	14:O:173:CYS:HA	2.32	0.44
8:H:46:U:HO2'	8:H:47:U:P	2.36	0.44
10:J:227:LYS:HB3	10:J:251:TRP:CZ2	2.53	0.44
13:N:15:TRP:O	13:N:18:ILE:HG12	2.17	0.44
13:N:16:GLU:CD	13:N:16:GLU:N	2.76	0.44
13:N:38:GLU:C	13:N:40:LYS:N	2.75	0.44
17:R:138:GLU:HG3	17:R:139:ALA:H	1.83	0.44
25:Z:534:MET:HE3	25:Z:534:MET:HB3	1.75	0.44
26:1:630:ARG:O	26:1:634:VAL:HG23	2.17	0.44
26:1:1182:LEU:HG	26:1:1226:VAL:HG21	2.00	0.44
27:3:91:GLU:OE1	27:3:102:ILE:HD11	2.18	0.44
27:3:608:GLY:HA2	27:3:614:VAL:CG2	2.48	0.44
28:p:8:THR:HA	28:p:55:ILE:HA	2.00	0.44
29:w:481:ASP:OD1	29:w:485:ASN:N	2.48	0.44
1:A:281:PRO:HG2	1:A:284:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:HIS:ND1	1:A:434:HIS:C	2.75	0.44
1:A:902:TYR:OH	1:A:1249:MET:SD	2.68	0.44
1:A:1303:LEU:HD13	1:A:1311:PHE:CE1	2.53	0.44
2:B:106:U:H2'	2:B:107:U:C6	2.53	0.44
7:G:104:C:H1'	7:G:105:C:OP1	2.18	0.44
10:J:350:ILE:HD12	10:J:350:ILE:HA	1.66	0.44
19:T:314:ILE:HD11	19:T:326:LEU:HD11	1.99	0.44
21:V:641:ASP:OD2	21:V:642:GLU:N	2.51	0.44
26:1:166:ARG:O	26:1:170:GLN:HG2	2.16	0.44
26:1:667:ILE:O	26:1:671:ILE:HG13	2.18	0.44
26:1:1091:HIS:NE2	31:2:568:TYR:OH	2.49	0.44
27:3:365:GLY:HA3	27:3:394:ASN:ND2	2.32	0.44
27:3:607:VAL:O	27:3:614:VAL:HG22	2.17	0.44
29:w:483:SER:O	29:w:483:SER:OG	2.29	0.44
37:8:35:GLU:OE1	37:8:35:GLU:N	2.51	0.44
48:z:99:VAL:HG22	48:z:115:PHE:CD1	2.53	0.44
1:A:39:GLN:O	1:A:43:LYS:HD2	2.17	0.44
1:A:436:PRO:HB2	1:A:439:GLN:NE2	2.32	0.44
1:A:468:LYS:HE2	1:A:468:LYS:HA	2.00	0.44
1:A:1879:PHE:HB3	1:A:1882:ILE:HG13	2.00	0.44
1:A:2246:ASN:C	1:A:2248:PRO:HD3	2.43	0.44
3:C:89:LEU:HG	19:T:240:LEU:HD11	1.98	0.44
3:C:531:TRP:O	3:C:532:ILE:HD13	2.17	0.44
6:F:10:U:H2'	6:F:11:C:O4'	2.17	0.44
7:G:7:G:C2	7:G:8:C:N3	2.86	0.44
10:J:318:TYR:O	10:J:322:MET:HG2	2.18	0.44
10:J:424:GLU:OE1	10:J:464:ASP:HA	2.18	0.44
16:Q:488:SER:O	16:Q:489:VAL:C	2.61	0.44
17:R:185:GLY:O	17:R:188:PHE:N	2.26	0.44
19:T:417:ASN:ND2	19:T:432:ASP:HB2	2.32	0.44
23:X:277:ARG:HH21	26:1:434:THR:CB	2.27	0.44
24:Y:2:ASN:HB2	24:Y:3:PRO:HD2	1.99	0.44
26:1:540:MET:HE3	26:1:540:MET:HB3	1.68	0.44
26:1:897:LEU:O	26:1:901:GLN:HG3	2.18	0.44
27:3:324:GLU:OE1	27:3:374:SER:HB2	2.18	0.44
27:3:384:THR:OG1	27:3:385:PHE:O	2.35	0.44
31:2:464:GLU:O	31:2:468:LEU:HG	2.18	0.44
31:2:586:ILE:HG22	31:2:587:HIS:N	2.33	0.44
36:9:288:LYS:HB2	36:9:406:VAL:HG13	1.99	0.44
1:A:769:LYS:HE2	1:A:1249:MET:O	2.18	0.44
1:A:1876:LEU:CD1	1:A:1884:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2074:ARG:HG2	1:A:2074:ARG:H	1.45	0.44
3:C:780:CYS:O	3:C:941:LYS:NZ	2.46	0.44
5:E:85:GLY:O	5:E:112:VAL:N	2.51	0.44
5:E:202:ASN:ND2	5:E:204:THR:OG1	2.51	0.44
8:H:160:A:H2'	8:H:161:U:C6	2.52	0.44
11:K:105:SER:OG	11:K:106:ALA:N	2.51	0.44
12:L:74:LEU:O	12:L:77:LEU:N	2.50	0.44
19:T:338:CYS:HA	19:T:344:GLN:O	2.17	0.44
23:X:251:GLU:H	23:X:251:GLU:HG3	1.52	0.44
23:X:323:ARG:HE	23:X:325:LYS:HG3	1.82	0.44
26:1:1055:TRP:HB2	26:1:1088:ILE:HD11	2.00	0.44
27:3:165:THR:O	27:3:165:THR:OG1	2.31	0.44
27:3:293:HIS:HD1	27:3:300:PHE:HZ	1.66	0.44
27:3:982:GLU:HG3	27:3:983:ASN:N	2.32	0.44
33:6:56:THR:O	33:6:59:THR:HG23	2.18	0.44
36:9:353:GLU:HG3	36:9:355:ARG:HH21	1.82	0.44
36:9:368:MET:HE1	36:9:377:ARG:O	2.17	0.44
1:A:75:ASP:O	1:A:77:THR:N	2.51	0.44
1:A:381:PRO:O	1:A:383:PHE:N	2.49	0.44
1:A:730:GLY:O	17:R:248:PRO:HG3	2.18	0.44
1:A:1361:GLU:HG2	1:A:1362:ASP:N	2.33	0.44
1:A:1434:LYS:O	1:A:1439:ARG:NH2	2.50	0.44
1:A:2153:THR:HG22	1:A:2154:HIS:H	1.82	0.44
3:C:189:VAL:C	3:C:190:LEU:HD23	2.43	0.44
4:D:971:LYS:N	4:D:980:GLN:O	2.33	0.44
6:F:94:C:H5''	10:J:351:ASN:HD22	1.83	0.44
6:F:96:U:H2'	6:F:97:U:C6	2.53	0.44
8:H:155:C:H2'	8:H:156:U:C6	2.53	0.44
15:P:205:LYS:HE3	15:P:205:LYS:HB3	1.66	0.44
21:V:632:THR:HG22	22:W:115:UNK:HA	2.00	0.44
26:1:1100:ASN:C	26:1:1102:LYS:N	2.75	0.44
26:1:1289:ASN:HD22	26:1:1294:THR:HG23	1.82	0.44
27:3:21:ASN:OD1	27:3:69:ARG:NH2	2.50	0.44
27:3:77:TYR:CD1	27:3:91:GLU:HB2	2.52	0.44
27:3:782:GLN:HG3	27:3:867:ARG:NH2	2.29	0.44
36:9:215:PHE:C	36:9:216:LYS:HD2	2.42	0.44
36:9:320:ILE:HA	36:9:427:ARG:HA	2.00	0.44
1:A:486:LYS:O	1:A:487:LEU:HD23	2.18	0.43
1:A:690:MET:O	1:A:691:HIS:C	2.60	0.43
1:A:913:PRO:O	1:A:917:ILE:HG13	2.18	0.43
1:A:1019:TYR:O	1:A:1020:LYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:LEU:HD22	1:A:2263:LEU:HD11	1.99	0.43
1:A:2192:ASP:HB3	1:A:2213:ILE:HG21	2.00	0.43
3:C:444:GLY:O	3:C:447:PRO:HD2	2.18	0.43
3:C:569:ARG:O	3:C:569:ARG:HG2	2.17	0.43
5:E:68:GLU:HB3	5:E:70:TYR:CE1	2.53	0.43
5:E:200:THR:O	5:E:209:ILE:HB	2.19	0.43
10:J:342:GLU:O	10:J:346:TRP:HD1	2.01	0.43
12:L:36:SER:OG	39:v:29:ARG:NH2	2.51	0.43
15:P:224:MET:HE3	15:P:228:ILE:HD13	1.99	0.43
26:1:112:ILE:HD11	26:1:546:ASP:HA	1.99	0.43
27:3:457:ASN:OD1	27:3:477:SER:OG	2.28	0.43
1:A:805:GLU:O	1:A:809:VAL:HG23	2.18	0.43
1:A:1359:HIS:HB2	1:A:1361:GLU:O	2.17	0.43
1:A:1941:ARG:HH12	1:A:2013:GLY:N	2.16	0.43
1:A:2120:LEU:O	1:A:2182:PRO:HB3	2.18	0.43
1:A:2149:PRO:HB3	1:A:2281:TYR:CE1	2.53	0.43
5:E:217:ILE:HB	5:E:231:MET:CG	2.48	0.43
5:E:304:SER:H	5:E:330:ILE:HB	1.84	0.43
5:E:343:ILE:HD13	5:E:343:ILE:HA	1.71	0.43
8:H:13:C:C1'	8:H:14:C:H5'	2.48	0.43
8:H:59:A:C2'	8:H:60:U:H5'	2.48	0.43
10:J:437:LYS:O	10:J:440:LEU:N	2.51	0.43
18:S:615:LEU:O	18:S:674:THR:HA	2.18	0.43
24:Y:17:GLU:HB2	26:1:825:LEU:HD21	1.99	0.43
26:1:1197:LEU:HD11	34:7:78:GLN:NE2	2.33	0.43
27:3:418:GLU:CD	27:3:419:ASP:H	2.26	0.43
27:3:637:PRO:HB3	27:3:640:LEU:CD2	2.48	0.43
27:3:644:GLU:HG3	27:3:662:PHE:HB3	1.99	0.43
37:8:37:LYS:HG2	37:8:38:VAL:N	2.33	0.43
1:A:950:LEU:O	1:A:954:LYS:HG3	2.17	0.43
1:A:1848:LEU:HD13	1:A:1914:MET:HE3	2.00	0.43
5:E:168:CYS:HB2	5:E:201:PHE:CE1	2.53	0.43
5:E:321:TYR:HD1	5:E:323:LEU:HD21	1.83	0.43
7:G:17:U:H3'	7:G:18:A:H8	1.83	0.43
15:P:206:LYS:HA	15:P:209:ARG:HD2	2.00	0.43
16:Q:567:VAL:HA	16:Q:589:LEU:HA	2.00	0.43
17:R:148:ARG:O	17:R:148:ARG:NH2	2.51	0.43
19:T:283:HIS:O	19:T:320:LYS:HD3	2.19	0.43
23:X:315:ARG:CZ	23:X:321:GLY:HA3	2.48	0.43
26:1:1080:THR:O	26:1:1084:ILE:HG23	2.18	0.43
27:3:226:GLU:HG2	27:3:261:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:286:ILE:HG12	27:3:306:GLU:OE2	2.18	0.43
27:3:310:ILE:C	27:3:311:PHE:HD2	2.26	0.43
27:3:558:LEU:HD12	27:3:558:LEU:N	2.33	0.43
27:3:704:VAL:HG22	27:3:706:MET:HG2	2.00	0.43
27:3:1015:LYS:HZ3	27:3:1067:ASP:HB2	1.82	0.43
31:2:495:ARG:HE	31:2:495:ARG:HB3	1.36	0.43
35:5:14:LEU:HA	35:5:14:LEU:HD23	1.60	0.43
36:9:273:TYR:CG	36:9:301:PRO:HB2	2.53	0.43
42:i:34:VAL:N	42:i:43:GLN:O	2.29	0.43
48:z:45:LEU:HD12	48:z:174:ILE:HG21	1.99	0.43
1:A:1089:CYS:SG	1:A:1096:HIS:CD2	3.11	0.43
1:A:2067:PHE:CE2	1:A:2069:SER:HA	2.53	0.43
3:C:173:THR:O	3:C:177:ARG:HB2	2.18	0.43
3:C:572:GLU:H	3:C:572:GLU:HG3	1.60	0.43
4:D:530:THR:C	4:D:532:ASN:N	2.76	0.43
5:E:277:PHE:HE2	5:E:300:ILE:HD13	1.82	0.43
9:I:512:ASP:C	9:I:514:ARG:H	2.27	0.43
17:R:195:ARG:HG2	17:R:195:ARG:NH1	2.33	0.43
18:S:867:ALA:HB1	18:S:901:ASN:HA	2.00	0.43
21:V:581:ILE:HD11	25:Z:540:ARG:HG3	2.01	0.43
23:X:253:ARG:HD3	23:X:253:ARG:HA	1.73	0.43
27:3:257:THR:HG23	27:3:267:ILE:O	2.18	0.43
27:3:458:ALA:O	27:3:459:VAL:HG23	2.18	0.43
27:3:536:TRP:CE2	27:3:576:GLU:HG3	2.54	0.43
27:3:636:GLN:H	27:3:670:GLN:HE22	1.66	0.43
27:3:700:LYS:HE2	27:3:715:MET:O	2.18	0.43
27:3:939:PHE:CZ	27:3:942:LYS:HG2	2.50	0.43
29:w:495:LEU:HB2	29:w:501:LEU:HD12	2.00	0.43
32:4:151:SER:H	32:4:154:ALA:HB3	1.82	0.43
33:6:27:PRO:HG3	33:6:83:CYS:CB	2.48	0.43
36:9:360:HIS:HB2	36:9:387:CYS:O	2.18	0.43
37:8:55:ARG:HA	37:8:55:ARG:HD2	1.39	0.43
1:A:533:LYS:HE3	6:F:37:C:H5	1.83	0.43
1:A:718:ARG:NH2	17:R:255:LYS:HE2	2.34	0.43
1:A:1310:ARG:NH2	1:A:1563:HIS:O	2.51	0.43
1:A:1821:ILE:HG12	1:A:1906:ILE:HG12	2.01	0.43
1:A:1980:GLU:O	1:A:1984:LYS:HG3	2.19	0.43
1:A:2074:ARG:NH2	4:D:1046:ILE:O	2.51	0.43
2:B:18:C:O2	2:B:59:G:N2	2.26	0.43
3:C:733:TRP:NE1	3:C:747:ASP:OD2	2.52	0.43
8:H:97:G:H2'	8:H:97:G:N3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:124:G:H2'	8:H:125:G:C8	2.54	0.43
26:1:564:ASP:OD1	26:1:564:ASP:N	2.44	0.43
26:1:649:LYS:HG2	26:1:689:ILE:HG12	2.00	0.43
26:1:1134:ASN:HD21	31:2:534:GLN:HA	1.84	0.43
29:w:493:GLU:OE1	29:w:496:LYS:HD3	2.17	0.43
36:9:423:LYS:HD2	36:9:423:LYS:HA	1.77	0.43
1:A:174:PRO:HA	1:A:520:TYR:CD1	2.54	0.43
1:A:598:LEU:C	1:A:600:ARG:N	2.75	0.43
1:A:1407:ASP:O	1:A:1408:LEU:HD23	2.19	0.43
3:C:243:ILE:HD12	3:C:243:ILE:HA	1.65	0.43
3:C:244:LYS:HD2	3:C:292:TYR:CZ	2.54	0.43
3:C:477:HIS:HE1	3:C:562:THR:HG23	1.84	0.43
3:C:696:LEU:HD23	3:C:696:LEU:H	1.84	0.43
4:D:861:TYR:O	27:3:599:GLU:HG3	2.19	0.43
4:D:2103:ASN:HA	4:D:2123:SER:HA	2.00	0.43
5:E:62:LEU:HB3	5:E:93:TRP:CH2	2.54	0.43
6:F:23:U:C4	13:N:118:ILE:HD13	2.52	0.43
6:F:88:G:C2	8:H:11:G:C2	3.06	0.43
10:J:353:GLU:C	10:J:354:LEU:HD12	2.44	0.43
11:K:218:LYS:H	11:K:218:LYS:HG3	1.66	0.43
18:S:700:TYR:N	18:S:757:ARG:O	2.34	0.43
25:Z:497:TRP:CD1	25:Z:501:LEU:HD21	2.53	0.43
26:1:413:LYS:HB2	33:6:52:ASN:ND2	2.34	0.43
26:1:914:PHE:CG	26:1:954:LEU:HD11	2.54	0.43
26:1:929:LEU:N	26:1:930:PRO:HD2	2.34	0.43
27:3:325:ILE:O	27:3:374:SER:HA	2.19	0.43
27:3:615:ARG:NE	27:3:630:MET:HB3	2.33	0.43
33:6:21:LEU:HG	33:6:23:ILE:HD11	2.01	0.43
36:9:236:LEU:HB3	36:9:452:GLN:OE1	2.18	0.43
36:9:405:ASP:OD1	36:9:405:ASP:N	2.52	0.43
37:8:70:PHE:HZ	37:8:88:ASN:HD22	1.65	0.43
39:v:115:PRO:HG2	39:v:177:GLU:N	2.27	0.43
1:A:1593:LEU:HD23	1:A:1593:LEU:HA	1.66	0.43
1:A:1892:PRO:HG2	1:A:1940:LEU:HB3	2.00	0.43
2:B:12:U:H2'	2:B:13:C:C6	2.53	0.43
3:C:137:HIS:CD2	3:C:138:LEU:H	2.37	0.43
3:C:255:VAL:O	3:C:307:VAL:HA	2.18	0.43
3:C:713:LYS:HA	3:C:716:GLU:OE1	2.19	0.43
3:C:801:LEU:C	3:C:803:ARG:N	2.77	0.43
4:D:1733:HIS:O	4:D:1737:ASN:CB	2.66	0.43
6:F:89:U:H2'	6:F:90:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:G:O2'	8:H:120:A:H5'	2.18	0.43
16:Q:849:THR:O	16:Q:1034:ILE:HA	2.17	0.43
19:T:208:ARG:HE	19:T:208:ARG:HB3	1.32	0.43
21:V:570:LEU:HD12	21:V:570:LEU:HA	1.77	0.43
23:X:337:THR:HB	23:X:344:ILE:HD11	2.00	0.43
26:1:818:PHE:O	26:1:823:MET:HG3	2.19	0.43
26:1:1091:HIS:CE1	31:2:568:TYR:HE1	2.36	0.43
27:3:412:ILE:H	27:3:1105:GLN:NE2	2.16	0.43
27:3:470:PHE:HA	27:3:746:ALA:HB3	2.01	0.43
27:3:807:TYR:O	27:3:856:LYS:HE2	2.18	0.43
29:w:445:HIS:H	29:w:445:HIS:CD2	2.37	0.43
32:4:104:ILE:HA	32:4:174:VAL:HA	1.99	0.43
33:6:116:LYS:HG2	33:6:117:TYR:CE1	2.54	0.43
36:9:117:VAL:HA	36:9:157:THR:HA	2.00	0.43
36:9:273:TYR:OH	36:9:302:LYS:HA	2.19	0.43
39:v:53:SER:HB2	39:v:63:HIS:O	2.19	0.43
48:z:86:GLU:O	48:z:128:THR:HG23	2.19	0.43
3:C:404:THR:OG1	3:C:405:LYS:N	2.51	0.43
3:C:705:VAL:HG22	3:C:705:VAL:O	2.17	0.43
3:C:724:TRP:HH2	3:C:788:LYS:HE3	1.84	0.43
14:O:34:ILE:O	17:R:198:ARG:NH1	2.51	0.43
17:R:184:GLN:NE2	17:R:193:LYS:HA	2.34	0.43
17:R:240:LYS:HA	17:R:240:LYS:HD2	1.78	0.43
25:Z:497:TRP:HD1	25:Z:501:LEU:HD21	1.84	0.43
25:Z:579:TRP:CE3	25:Z:580:PRO:HD2	2.53	0.43
27:3:278:LEU:HD21	27:3:816:LYS:HB2	2.00	0.43
27:3:280:ASP:HA	27:3:281:PRO:HD3	1.93	0.43
27:3:469:GLU:H	27:3:469:GLU:CD	2.25	0.43
27:3:838:MET:N	27:3:838:MET:SD	2.92	0.43
36:9:302:LYS:HB2	36:9:353:GLU:CD	2.42	0.43
37:8:39:ASP:OD2	37:8:40:MET:N	2.52	0.43
40:o:30:LYS:HA	40:o:52:ASN:HA	2.00	0.43
48:z:9:PRO:HD2	48:z:91:LEU:HD21	2.01	0.43
1:A:1763:LEU:O	1:A:1764:SER:O	2.37	0.43
1:A:1872:LEU:HD13	1:A:1884:ILE:HD13	2.00	0.43
1:A:1911:GLU:HG2	1:A:1912:PRO:HD2	2.01	0.43
5:E:280:ASN:ND2	5:E:303:GLY:O	2.49	0.43
6:F:85:U:H1'	6:F:86:U:C4	2.54	0.43
7:G:12:G:P	7:G:13:C:H41	2.42	0.43
10:J:236:ARG:O	10:J:239:ARG:NE	2.51	0.43
16:Q:600:MET:O	16:Q:608:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:459:LEU:HA	36:9:259:THR:HB	2.01	0.43
21:V:577:SER:HB2	25:Z:543:ASP:OD2	2.19	0.43
21:V:638:GLY:HA2	21:V:641:ASP:OD1	2.19	0.43
26:1:396:ASN:HB2	33:6:67:ILE:HG23	2.00	0.43
26:1:539:LEU:HD12	26:1:539:LEU:HA	1.66	0.43
26:1:998:LYS:NZ	26:1:1041:ARG:HD3	2.33	0.43
27:3:264:GLN:OE1	27:3:265:PRO:HD2	2.18	0.43
27:3:976:LYS:NZ	29:w:486:VAL:HG11	2.34	0.43
27:3:1186:GLU:O	27:3:1189:LYS:N	2.51	0.43
31:2:524:LEU:HD23	31:2:524:LEU:HA	1.79	0.43
34:7:9:ILE:O	34:7:88:ILE:HA	2.19	0.43
45:k:46:VAL:HA	45:k:56:ASN:HA	2.01	0.43
1:A:139:VAL:HG11	1:A:212:PRO:HG2	2.01	0.43
1:A:386:PRO:HB3	3:C:371:GLU:O	2.19	0.43
1:A:1543:ASN:HB2	1:A:1569:LEU:HD21	2.01	0.43
1:A:2294:TYR:CE2	1:A:2296:LEU:HD21	2.54	0.43
3:C:438:ILE:HD12	3:C:438:ILE:HA	1.70	0.43
9:I:140:LEU:N	9:I:141:PRO:HD3	2.34	0.43
10:J:394:HIS:HA	10:J:397:LYS:HD2	2.01	0.43
13:N:104:ARG:O	13:N:107:GLN:N	2.41	0.43
15:P:195:LYS:O	15:P:196:ASN:C	2.62	0.43
26:1:714:GLU:HB2	26:1:752:TYR:CE1	2.54	0.43
27:3:614:VAL:HG23	27:3:637:PRO:HG2	2.01	0.43
27:3:712:VAL:O	27:3:721:LEU:HD12	2.19	0.43
36:9:310:LEU:HD11	36:9:344:SER:C	2.44	0.43
36:9:380:PHE:HZ	36:9:428:ILE:HD11	1.84	0.43
1:A:65:HIS:CD2	1:A:65:HIS:C	2.97	0.42
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.84	0.42
1:A:1544:ARG:HB2	1:A:1672:ASP:OD2	2.19	0.42
1:A:2179:HIS:CD2	1:A:2215:THR:HA	2.54	0.42
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.35	0.42
3:C:727:LEU:HD12	3:C:727:LEU:HA	1.79	0.42
3:C:934:MET:HE2	3:C:934:MET:HB3	1.76	0.42
5:E:100:ASP:OD1	5:E:100:ASP:N	2.52	0.42
5:E:263:ASP:OD1	5:E:263:ASP:N	2.52	0.42
10:J:226:ARG:O	10:J:230:THR:HG23	2.19	0.42
12:L:59:LYS:HZ2	12:L:59:LYS:HG3	1.77	0.42
13:N:18:ILE:HG22	13:N:63:LEU:HD12	2.00	0.42
17:R:153:LYS:C	17:R:153:LYS:HD3	2.44	0.42
26:1:714:GLU:HB2	26:1:752:TYR:CD1	2.53	0.42
26:1:1017:LEU:HD23	26:1:1050:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:976:LYS:HZ1	29:w:486:VAL:HG11	1.84	0.42
35:5:69:MET:HE2	35:5:69:MET:HB2	1.70	0.42
1:A:106:MET:HA	1:A:107:PRO:HD3	1.76	0.42
1:A:985:TYR:N	1:A:985:TYR:HD1	2.15	0.42
1:A:1458:GLN:HB2	17:R:421:GLY:H	1.83	0.42
3:C:718:PHE:HB3	3:C:724:TRP:HD1	1.84	0.42
3:C:770:PHE:CE1	3:C:789:PHE:CD1	3.03	0.42
3:C:818:SER:O	3:C:822:MET:HB2	2.19	0.42
5:E:113:MET:HA	5:E:113:MET:HE2	2.01	0.42
7:G:2:U:H5''	7:G:3:A:H4'	2.01	0.42
8:H:3:C:H2'	8:H:4:G:C8	2.54	0.42
8:H:149:A:H2'	8:H:150:U:C6	2.54	0.42
10:J:273:TYR:CD1	17:R:226:PRO:HB2	2.54	0.42
23:X:321:GLY:C	23:X:322:ARG:HG3	2.43	0.42
26:1:415:LEU:HD23	26:1:415:LEU:HA	1.86	0.42
26:1:789:LEU:HD12	26:1:789:LEU:HA	1.88	0.42
26:1:1029:GLU:OE2	26:1:1070:LYS:HB2	2.19	0.42
26:1:1065:LEU:C	26:1:1067:LYS:H	2.26	0.42
26:1:1084:ILE:HG21	26:1:1084:ILE:HD13	1.69	0.42
26:1:1289:ASN:HB3	26:1:1294:THR:HA	2.01	0.42
27:3:50:VAL:CG2	27:3:401:LEU:HD11	2.49	0.42
27:3:1118:VAL:HG22	27:3:1128:ILE:HG22	2.00	0.42
33:6:114:LYS:HE3	33:6:114:LYS:HB3	1.73	0.42
35:5:11:LEU:HD12	35:5:12:GLU:N	2.34	0.42
36:9:365:ILE:HG23	36:9:396:ILE:CG2	2.49	0.42
48:z:97:GLY:O	48:z:133:VAL:HG23	2.19	0.42
1:A:762:ARG:NH2	15:P:226:LYS:NZ	2.67	0.42
1:A:1072:LEU:HD22	1:A:1087:LEU:HB3	2.01	0.42
1:A:1855:GLU:HG2	11:K:133:ILE:HG12	2.00	0.42
3:C:736:GLY:O	3:C:738:ASP:N	2.52	0.42
5:E:70:TYR:HB2	5:E:85:GLY:HA2	2.01	0.42
7:G:7:G:C2	7:G:8:C:C2	3.06	0.42
7:G:99:C:C2'	7:G:100:C:H5'	2.50	0.42
10:J:352:PHE:CD1	10:J:352:PHE:C	2.97	0.42
19:T:414:ALA:O	19:T:416:ILE:HG13	2.19	0.42
21:V:580:ARG:HG2	21:V:630:PHE:CE2	2.55	0.42
26:1:1059:CYS:SG	26:1:1084:ILE:HD11	2.58	0.42
26:1:1182:LEU:HA	26:1:1182:LEU:HD12	1.64	0.42
27:3:275:ARG:HA	27:3:386:PHE:CD2	2.55	0.42
27:3:294:LYS:HB3	27:3:294:LYS:HE3	1.73	0.42
27:3:488:GLY:N	27:3:491:VAL:HG22	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:740:GLU:HB2	27:3:757:ILE:HD12	2.01	0.42
27:3:781:LEU:HB3	27:3:801:GLU:OE1	2.18	0.42
27:3:1015:LYS:NZ	27:3:1066:VAL:O	2.49	0.42
36:9:235:LYS:HD3	36:9:452:GLN:HB2	2.01	0.42
36:9:278:LYS:HE3	36:9:278:LYS:HB3	1.81	0.42
36:9:405:ASP:HA	36:9:408:THR:OG1	2.19	0.42
1:A:1571:ILE:HD13	11:K:218:LYS:O	2.19	0.42
1:A:2275:ALA:HB2	1:A:2296:LEU:O	2.19	0.42
3:C:745:LEU:HB2	3:C:770:PHE:CE2	2.55	0.42
3:C:801:LEU:O	3:C:802:HIS:C	2.63	0.42
6:F:35:A:H1'	7:G:12:G:O6	2.19	0.42
6:F:57:U:C2'	6:F:58:G:H5'	2.49	0.42
7:G:85:G:H1	8:H:44:U:H3	1.66	0.42
8:H:46:U:H1'	8:H:47:U:H5''	2.00	0.42
10:J:334:GLU:O	10:J:338:GLU:HG3	2.20	0.42
10:J:419:PHE:HD1	10:J:419:PHE:HA	1.74	0.42
16:Q:708:GLN:HA	16:Q:816:PRO:HD2	2.02	0.42
19:T:297:HIS:HA	19:T:338:CYS:SG	2.60	0.42
21:V:491:ASN:O	21:V:494:LEU:HB3	2.19	0.42
21:V:639:LEU:HA	21:V:642:GLU:OE2	2.20	0.42
23:X:261:LEU:HA	23:X:261:LEU:HD12	1.76	0.42
24:Y:49:GLU:O	24:Y:50:GLY:C	2.61	0.42
26:1:402:GLU:OE1	26:1:402:GLU:HA	2.16	0.42
26:1:687:VAL:HA	26:1:690:ILE:HG22	2.00	0.42
27:3:139:LYS:HB2	27:3:160:ALA:HB3	2.01	0.42
27:3:326:ARG:HH11	27:3:372:GLU:CD	2.25	0.42
27:3:488:GLY:H	27:3:491:VAL:HG13	1.84	0.42
27:3:788:PHE:CD1	27:3:788:PHE:C	2.97	0.42
29:w:410:ILE:HG13	29:w:450:THR:O	2.20	0.42
29:w:433:HIS:O	29:w:434:GLY:C	2.61	0.42
31:2:534:GLN:O	31:2:538:GLU:HG3	2.20	0.42
33:6:35:MET:HE3	33:6:35:MET:HB3	1.88	0.42
35:5:17:LYS:HA	35:5:17:LYS:HD2	1.58	0.42
37:8:75:LEU:HA	37:8:75:LEU:HD23	1.83	0.42
39:v:54:TYR:CE2	39:v:66:GLU:HG3	2.54	0.42
43:m:47:GLU:O	43:m:64:LYS:HA	2.20	0.42
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.79	0.42
1:A:1295:ILE:HG13	1:A:1296:GLN:N	2.35	0.42
1:A:1457:HIS:CD2	17:R:420:SER:HB3	2.54	0.42
1:A:2166:HIS:CG	1:A:2168:TYR:HB2	2.54	0.42
1:A:2188:LEU:HD13	1:A:2228:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:796:VAL:HG12	3:C:800:PRO:HB3	2.01	0.42
5:E:102:TYR:HD1	5:E:102:TYR:H	1.67	0.42
7:G:99:C:H2'	7:G:100:C:C6	2.54	0.42
8:H:11:G:C2	8:H:12:G:C8	3.07	0.42
8:H:13:C:H1'	8:H:14:C:OP2	2.20	0.42
8:H:18:U:H1'	8:H:19:G:OP1	2.20	0.42
10:J:291:GLN:HB3	10:J:294:HIS:HD1	1.85	0.42
13:N:106:ILE:HG22	13:N:116:ASN:HD22	1.85	0.42
16:Q:440:PRO:HG2	16:Q:1108:ALA:HB1	2.01	0.42
17:R:236:LYS:HD3	17:R:236:LYS:HA	1.53	0.42
17:R:251:ILE:HD12	17:R:251:ILE:HA	1.79	0.42
18:S:876:GLY:HA3	18:S:1001:LEU:HA	2.02	0.42
19:T:191:HIS:CD2	19:T:440:ASP:OD1	2.73	0.42
21:V:456:ARG:HG2	21:V:492:MET:HG3	2.02	0.42
21:V:505:LYS:HE3	21:V:553:HIS:NE2	2.34	0.42
25:Z:543:ASP:CG	25:Z:545:MET:H	2.26	0.42
26:1:163:LYS:HD2	26:1:166:ARG:NH1	2.35	0.42
26:1:641:ILE:HD11	26:1:675:MET:HE2	2.01	0.42
33:6:54:PRO:HA	33:6:57:ARG:HB2	2.01	0.42
34:7:37:VAL:HB	34:7:38:ARG:HG3	2.00	0.42
34:7:58:CYS:HB3	34:7:62:GLY:N	2.23	0.42
37:8:44:ASN:C	37:8:44:ASN:OD1	2.63	0.42
1:A:75:ASP:HB3	1:A:498:ARG:HH12	1.85	0.42
1:A:366:LYS:HE2	1:A:366:LYS:HB2	1.77	0.42
1:A:1516:LYS:H	1:A:1516:LYS:HG2	1.60	0.42
1:A:1639:VAL:HG11	1:A:1699:THR:CG2	2.50	0.42
1:A:2007:ILE:O	1:A:2011:ILE:HG13	2.19	0.42
1:A:2315:LEU:HA	1:A:2317:PHE:CE1	2.54	0.42
3:C:335:ASN:HD22	3:C:338:GLU:HB2	1.83	0.42
4:D:1350:ALA:HB1	4:D:1354:SER:CB	2.49	0.42
5:E:262:TRP:HA	5:E:272:ARG:O	2.20	0.42
7:G:112:U:H2'	7:G:113:U:O4'	2.20	0.42
8:H:52:G:H2'	8:H:53:U:C6	2.55	0.42
10:J:423:GLU:HB3	10:J:432:VAL:HG23	2.01	0.42
13:N:19:GLU:HG3	13:N:23:ASP:OD2	2.19	0.42
26:1:122:HIS:CE1	26:1:125:THR:HG1	2.37	0.42
26:1:1132:LEU:HD23	26:1:1132:LEU:HA	1.84	0.42
26:1:1174:GLU:O	26:1:1178:MET:HG3	2.20	0.42
27:3:875:ASN:N	27:3:875:ASN:ND2	2.65	0.42
27:3:1055:VAL:HG23	27:3:1093:MET:HG2	2.01	0.42
37:8:34:LEU:HG	37:8:82:SER:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:z:133:VAL:HG21	48:z:141:MET:SD	2.59	0.42
1:A:462:ARG:HA	1:A:462:ARG:HE	1.85	0.42
1:A:781:ARG:NH2	8:H:24:A:H5"	2.34	0.42
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	2.02	0.42
1:A:1939:ILE:HG23	1:A:1954:LEU:HD11	2.01	0.42
1:A:2129:TYR:CG	1:A:2169:LEU:HD22	2.54	0.42
1:A:2252:LEU:H	1:A:2255:HIS:CE1	2.38	0.42
3:C:491:HIS:CD2	3:C:551:LEU:HD13	2.55	0.42
3:C:658:PRO:HB2	3:C:881:PHE:CZ	2.55	0.42
3:C:872:LYS:HE3	3:C:872:LYS:HB2	1.92	0.42
12:L:62:GLU:OE2	12:L:62:GLU:N	2.53	0.42
17:R:253:ASN:HB3	17:R:254:TRP:CZ3	2.54	0.42
19:T:245:HIS:HE2	19:T:263:SER:HG	1.58	0.42
19:T:351:ASP:OD1	19:T:351:ASP:N	2.47	0.42
21:V:286:THR:H	21:V:289:SER:CB	2.33	0.42
21:V:519:LYS:HA	21:V:522:MET:HG3	2.01	0.42
23:X:315:ARG:NH2	23:X:321:GLY:HA3	2.35	0.42
26:1:141:LYS:HG2	26:1:142:THR:O	2.19	0.42
27:3:811:THR:O	27:3:815:ARG:HG3	2.20	0.42
28:p:178:LYS:N	28:p:193:GLU:O	2.52	0.42
34:7:46:CYS:H	34:7:85:CYS:HB2	1.84	0.42
37:8:70:PHE:HZ	37:8:88:ASN:ND2	2.18	0.42
1:A:62:PRO:HB2	1:A:64:GLU:OE1	2.19	0.42
1:A:2237:TRP:CZ2	1:A:2248:PRO:HB2	2.55	0.42
1:A:2330:ARG:NH1	4:D:546:SER:H	2.17	0.42
5:E:202:ASN:ND2	5:E:207:GLN:OE1	2.53	0.42
5:E:251:LEU:HD23	5:E:291:CYS:HB2	2.01	0.42
5:E:282:HIS:H	5:E:282:HIS:CD2	2.38	0.42
6:F:87:C:C2	6:F:88:G:C8	3.08	0.42
7:G:101:U:O4	34:7:102:ARG:HD2	2.19	0.42
9:I:428:GLN:CB	9:I:470:PHE:H	2.33	0.42
10:J:385:PHE:CE1	10:J:389:HIS:HD2	2.37	0.42
15:P:206:LYS:C	15:P:208:LYS:H	2.26	0.42
17:R:314:GLN:OE1	17:R:315:LYS:N	2.52	0.42
24:Y:69:ARG:HE	24:Y:69:ARG:HB3	1.47	0.42
26:1:747:LEU:HD12	26:1:747:LEU:HA	1.67	0.42
26:1:833:LEU:O	26:1:837:THR:OG1	2.29	0.42
26:1:1028:HIS:HB3	26:1:1031:VAL:HG13	2.02	0.42
27:3:187:MET:CE	27:3:206:GLN:HG2	2.49	0.42
27:3:805:ASN:N	27:3:861:GLN:O	2.50	0.42
36:9:336:THR:HG21	36:9:341:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:GLU:HB2	1:A:591:MET:HG3	2.02	0.42
1:A:693:ILE:HG22	1:A:694:LEU:CD2	2.50	0.42
1:A:825:ILE:HD13	1:A:825:ILE:HG21	1.89	0.42
1:A:981:PHE:O	1:A:1166:THR:OG1	2.38	0.42
1:A:1093:ASP:OD1	1:A:1093:ASP:N	2.51	0.42
1:A:1923:TRP:O	1:A:1927:ILE:HG12	2.20	0.42
3:C:600:LEU:N	3:C:601:PRO:HD2	2.34	0.42
3:C:610:VAL:HG12	3:C:648:TYR:HD2	1.85	0.42
3:C:850:LEU:HD23	3:C:850:LEU:HA	1.73	0.42
10:J:411:MET:O	10:J:443:ILE:HD12	2.20	0.42
13:N:28:LYS:NZ	13:N:28:LYS:HB2	2.35	0.42
21:V:520:GLU:H	21:V:520:GLU:CD	2.28	0.42
27:3:1:MET:HE1	27:3:1055:VAL:HG11	2.00	0.42
27:3:614:VAL:HG12	27:3:631:GLN:CD	2.45	0.42
27:3:982:GLU:OE2	27:3:984:LYS:HE3	2.20	0.42
36:9:269:ASP:OD2	36:9:269:ASP:N	2.43	0.42
37:8:102:MET:HB3	37:8:102:MET:HE2	1.75	0.42
40:o:46:ALA:HA	40:o:68:THR:O	2.20	0.42
1:A:150:MET:HG3	1:A:193:LEU:HB2	2.02	0.42
1:A:175:PRO:HD3	1:A:520:TYR:CD1	2.55	0.42
1:A:312:TYR:CD1	1:A:312:TYR:N	2.88	0.42
1:A:988:ILE:HG21	1:A:1030:ILE:HD12	2.02	0.42
1:A:1020:LYS:H	1:A:1020:LYS:HG3	1.68	0.42
1:A:1179:SER:HB3	1:A:1181:ASP:H	1.85	0.42
1:A:1220:VAL:HG12	1:A:1221:THR:HG22	2.02	0.42
1:A:1284:LEU:HD23	1:A:1284:LEU:HA	1.86	0.42
1:A:1426:ASP:OD2	1:A:1426:ASP:N	2.53	0.42
1:A:1808:PHE:C	1:A:1808:PHE:CD2	2.98	0.42
1:A:1921:ASP:HB3	1:A:1966:HIS:CE1	2.55	0.42
1:A:2115:ILE:HG23	1:A:2218:PHE:CE1	2.54	0.42
3:C:244:LYS:HB2	3:C:292:TYR:CE2	2.55	0.42
3:C:286:ASN:CG	3:C:300:LEU:H	2.21	0.42
3:C:519:GLU:O	3:C:522:SER:HB3	2.19	0.42
14:O:32:PRO:HA	17:R:195:ARG:NH1	2.34	0.42
17:R:332:ARG:HH12	23:X:267:ASP:HA	1.85	0.42
19:T:209:CYS:SG	19:T:252:VAL:HG22	2.60	0.42
21:V:615:LEU:HA	21:V:615:LEU:HD23	1.76	0.42
24:Y:53:ILE:O	24:Y:57:SER:HB2	2.20	0.42
26:1:1088:ILE:HG22	26:1:1089:GLY:H	1.85	0.42
27:3:305:THR:CG2	27:3:309:ASP:HB2	2.50	0.42
27:3:507:SER:O	27:3:518:GLN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:563:LEU:HB3	27:3:581:LYS:H	1.84	0.42
27:3:889:PHE:HE2	27:3:913:LEU:HD12	1.84	0.42
27:3:1049:LYS:HB2	27:3:1049:LYS:HE3	1.64	0.42
29:w:384:PRO:HG3	29:w:402:LEU:HD13	2.01	0.42
29:w:479:TYR:O	29:w:487:VAL:N	2.29	0.42
34:7:102:ARG:O	34:7:105:TYR:N	2.53	0.42
36:9:273:TYR:CD2	36:9:301:PRO:HB2	2.53	0.42
36:9:397:PHE:CD1	36:9:397:PHE:N	2.74	0.42
37:8:55:ARG:O	37:8:59:ILE:HG13	2.20	0.42
37:8:85:MET:HE2	37:8:85:MET:HB2	1.75	0.42
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.83	0.41
1:A:534:GLU:O	1:A:538:SER:OG	2.28	0.41
1:A:1818:PHE:CE1	1:A:1916:LEU:HD13	2.55	0.41
1:A:2102:TYR:CD2	1:A:2140:LYS:HG2	2.55	0.41
2:B:9:G:H2'	2:B:10:U:C6	2.55	0.41
3:C:313:GLN:HB2	50:C:1500:GTP:C6	2.54	0.41
3:C:801:LEU:O	3:C:803:ARG:N	2.52	0.41
6:F:58:G:O2'	6:F:59:G:H5'	2.19	0.41
8:H:11:G:N1	8:H:12:G:N7	2.68	0.41
8:H:121:A:N3	8:H:121:A:H2'	2.35	0.41
17:R:282:GLU:HA	36:9:221:LEU:HD13	2.01	0.41
19:T:207:VAL:CG1	19:T:480:ALA:HB1	2.49	0.41
21:V:604:LYS:HD3	21:V:604:LYS:HA	1.89	0.41
24:Y:94:VAL:HG22	24:Y:109:VAL:HG12	2.02	0.41
26:1:832:GLN:O	26:1:836:THR:HG23	2.20	0.41
26:1:871:THR:OG1	26:1:872:ILE:N	2.53	0.41
26:1:962:MET:HE3	26:1:974:LEU:HD11	2.02	0.41
26:1:1018:PRO:HG3	26:1:1054:GLU:OE2	2.18	0.41
27:3:202:ALA:O	27:3:203:ASN:ND2	2.53	0.41
27:3:506:LEU:HD23	27:3:547:CYS:SG	2.59	0.41
27:3:957:GLY:C	27:3:958:ARG:HG2	2.42	0.41
1:A:119:LEU:HD12	1:A:483:GLN:O	2.20	0.41
1:A:338:VAL:O	3:C:266:GLU:HG2	2.19	0.41
1:A:376:GLU:O	1:A:377:GLU:HB3	2.20	0.41
1:A:723:ASN:ND2	36:9:253:THR:OG1	2.42	0.41
1:A:1658:GLN:HB2	11:K:98:VAL:HG11	2.02	0.41
1:A:2109:ASN:HA	1:A:2112:LYS:HD3	2.01	0.41
1:A:2213:ILE:N	1:A:2213:ILE:HD12	2.35	0.41
1:A:2264:SER:HA	1:A:2266:ARG:NH1	2.35	0.41
1:A:2327:SER:O	1:A:2327:SER:OG	2.33	0.41
3:C:137:HIS:HB3	3:C:140:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:556:ASP:OD1	3:C:557:GLN:N	2.51	0.41
3:C:674:CYS:CB	3:C:818:SER:HB2	2.46	0.41
4:D:584:GLN:O	4:D:585:ILE:C	2.63	0.41
4:D:884:ASN:C	4:D:886:GLN:H	2.21	0.41
5:E:136:TRP:HA	5:E:142:GLU:O	2.20	0.41
11:K:126:LYS:HD3	11:K:187:GLU:OE2	2.19	0.41
12:L:94:ALA:O	12:L:98:GLU:HG2	2.20	0.41
13:N:32:ALA:HA	13:N:35:GLU:HG3	2.01	0.41
21:V:216:ALA:HB2	21:V:262:HIS:CB	2.51	0.41
21:V:452:LEU:HD23	21:V:452:LEU:HA	1.72	0.41
27:3:544:ILE:CD1	27:3:556:ILE:HB	2.49	0.41
27:3:604:PHE:CD1	27:3:628:LEU:HD23	2.50	0.41
27:3:641:CYS:HB3	27:3:703:ARG:NE	2.35	0.41
27:3:715:MET:HG3	27:3:739:LEU:HB2	2.02	0.41
39:v:28:GLU:O	39:v:32:GLN:HG2	2.21	0.41
48:z:53:ILE:HD12	48:z:55:HIS:HB3	2.02	0.41
1:A:228:TRP:CD1	1:A:228:TRP:H	2.38	0.41
1:A:261:LYS:NZ	1:A:261:LYS:H	2.19	0.41
1:A:719:CYS:HG	17:R:254:TRP:HZ3	1.64	0.41
1:A:1275:ARG:O	1:A:1369:TYR:HE1	2.03	0.41
1:A:1778:TRP:CE2	1:A:1858:PRO:HG3	2.56	0.41
2:B:97:G:H2'	2:B:98:G:H8	1.82	0.41
3:C:590:ILE:HG13	3:C:637:LEU:HD13	2.02	0.41
5:E:73:LYS:NZ	5:E:73:LYS:HB2	2.33	0.41
5:E:113:MET:HE3	5:E:129:THR:CG2	2.50	0.41
5:E:126:SER:OG	5:E:136:TRP:NE1	2.53	0.41
5:E:240:GLY:O	5:E:252:SER:HA	2.20	0.41
6:F:85:U:C2	6:F:86:U:C4	3.08	0.41
6:F:90:G:H2'	6:F:91:A:C8	2.54	0.41
8:H:118:G:N1	8:H:140:A:C6	2.88	0.41
10:J:269:LEU:HD12	10:J:269:LEU:HA	1.72	0.41
13:N:38:GLU:OE2	13:N:40:LYS:HD2	2.20	0.41
17:R:289:GLU:OE2	36:9:215:PHE:CD1	2.73	0.41
19:T:309:ASP:OD1	19:T:309:ASP:N	2.39	0.41
19:T:343:PRO:HD3	19:T:365:ARG:HH22	1.85	0.41
19:T:385:TYR:HE2	19:T:401:PRO:HD3	1.85	0.41
21:V:496:CYS:HB3	21:V:507:PHE:CE1	2.55	0.41
26:1:982:LEU:HA	26:1:982:LEU:HD12	1.79	0.41
26:1:1226:VAL:O	26:1:1230:VAL:HG23	2.20	0.41
27:3:174:ASP:HB3	27:3:240:GLY:H	1.85	0.41
27:3:674:LEU:C	27:3:675:LEU:HD12	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:747:SER:N	27:3:750:CYS:O	2.53	0.41
27:3:791:HIS:CD2	27:3:791:HIS:C	2.99	0.41
27:3:967:LEU:HD22	27:3:1002:VAL:HG21	2.02	0.41
27:3:1015:LYS:NZ	27:3:1067:ASP:HB2	2.35	0.41
31:2:469:VAL:HG11	31:2:489:VAL:HG11	2.03	0.41
35:5:15:GLN:O	35:5:18:TYR:O	2.39	0.41
36:9:282:VAL:O	36:9:293:LEU:HB3	2.21	0.41
1:A:380:LEU:HD12	3:C:349:PHE:CE1	2.55	0.41
1:A:407:ALA:O	1:A:412:ASN:ND2	2.54	0.41
1:A:464:PRO:HG2	2:B:20:G:C4	2.54	0.41
1:A:1194:CYS:HB3	1:A:1228:CYS:SG	2.60	0.41
1:A:1872:LEU:O	1:A:1873:GLU:C	2.63	0.41
1:A:1952:VAL:HA	25:Z:517:GLU:OE1	2.21	0.41
1:A:2143:ARG:O	1:A:2269:GLY:HA2	2.21	0.41
1:A:2178:ILE:HG13	1:A:2214:ILE:HB	2.02	0.41
3:C:83:GLU:HB2	3:C:84:GLU:H	1.71	0.41
3:C:491:HIS:HD2	3:C:551:LEU:HD13	1.85	0.41
3:C:687:MET:HB3	3:C:815:VAL:CG1	2.50	0.41
3:C:941:LYS:HG2	3:C:942:GLY:N	2.36	0.41
6:F:41:A:C2	7:G:6:A:N1	2.88	0.41
6:F:43:A:OP2	31:2:560:LYS:HE3	2.21	0.41
8:H:139:C:N4	8:H:140:A:H62	2.18	0.41
13:N:21:THR:O	13:N:24:GLU:HG3	2.19	0.41
14:O:188:ASP:O	14:O:190:ASP:N	2.53	0.41
16:Q:745:PRO:HG2	16:Q:781:PRO:HA	2.03	0.41
16:Q:817:GLY:O	16:Q:1090:ARG:HA	2.20	0.41
16:Q:1334:PRO:HD2	16:Q:1351:GLU:O	2.20	0.41
17:R:394:LEU:HD11	23:X:246:TYR:HA	2.03	0.41
19:T:325:THR:O	19:T:325:THR:OG1	2.38	0.41
21:V:600:ASN:OD1	21:V:604:LYS:HE3	2.20	0.41
23:X:338:PHE:HB2	23:X:359:LYS:HB3	2.01	0.41
26:1:1206:ASP:OD1	26:1:1207:SER:N	2.52	0.41
26:1:1227:ILE:HD12	26:1:1227:ILE:HA	1.79	0.41
26:1:1241:ILE:HD12	26:1:1241:ILE:HG23	1.67	0.41
27:3:472:ALA:O	27:3:487:ILE:N	2.54	0.41
27:3:667:ILE:HD12	27:3:675:LEU:O	2.21	0.41
27:3:672:GLY:O	27:3:690:ARG:HD3	2.20	0.41
27:3:720:TRP:HB3	27:3:731:LEU:HD11	2.02	0.41
27:3:1165:SER:HB3	27:3:1169:PRO:HA	2.02	0.41
31:2:452:LYS:C	31:2:452:LYS:HD3	2.45	0.41
36:9:287:ASN:ND2	36:9:426:ILE:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:297:CYS:HA	36:9:304:CYS:SG	2.61	0.41
37:8:94:ASN:OD1	37:8:94:ASN:N	2.54	0.41
1:A:227:ARG:HA	1:A:416:GLY:O	2.20	0.41
1:A:361:HIS:HB2	3:C:280:HIS:ND1	2.35	0.41
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	2.01	0.41
1:A:1537:TRP:CE3	1:A:1751:LEU:HD13	2.56	0.41
1:A:1639:VAL:HG11	1:A:1699:THR:HG21	2.02	0.41
1:A:1781:ASP:OD2	1:A:1893:PHE:HB2	2.20	0.41
1:A:2249:LYS:HD2	1:A:2249:LYS:N	2.34	0.41
1:A:2320:LEU:HD13	1:A:2320:LEU:HA	1.77	0.41
2:B:62:G:H2'	2:B:63:A:C8	2.55	0.41
3:C:364:SER:OG	3:C:364:SER:O	2.37	0.41
4:D:1345:ASN:HA	4:D:1487:ILE:O	2.21	0.41
5:E:196:VAL:HG11	5:E:210:SER:OG	2.21	0.41
5:E:269:PRO:C	5:E:271:GLU:H	2.29	0.41
10:J:283:ALA:O	10:J:287:MET:HG2	2.20	0.41
10:J:377:LYS:HE3	10:J:377:LYS:HB3	1.89	0.41
10:J:408:ASP:HA	10:J:443:ILE:HG22	2.03	0.41
12:L:19:LEU:O	12:L:20:LYS:C	2.62	0.41
12:L:70:LYS:O	12:L:71:LEU:C	2.63	0.41
12:L:86:ALA:HB1	12:L:91:ARG:O	2.21	0.41
13:N:23:ASP:O	13:N:26:ASP:N	2.52	0.41
19:T:203:HIS:CD2	19:T:207:VAL:HG22	2.56	0.41
19:T:351:ASP:O	19:T:352:THR:OG1	2.28	0.41
21:V:536:ILE:C	21:V:538:ARG:H	2.29	0.41
23:X:264:PHE:CD1	23:X:269:VAL:HG22	2.55	0.41
26:1:758:ASP:OD1	26:1:758:ASP:N	2.41	0.41
26:1:1227:ILE:O	26:1:1231:MET:HG2	2.20	0.41
27:3:275:ARG:HA	27:3:386:PHE:HD2	1.85	0.41
27:3:590:MET:SD	27:3:607:VAL:HG22	2.60	0.41
33:6:14:PRO:HA	33:6:15:PRO:HD3	1.92	0.41
1:A:610:HIS:NE2	49:A:2401:IHP:O31	2.47	0.41
1:A:1838:LYS:HB3	1:A:1871:PRO:HG2	2.02	0.41
3:C:855:GLY:O	3:C:874:PHE:O	2.38	0.41
4:D:2033:GLY:O	4:D:2096:ALA:N	2.48	0.41
5:E:125:PHE:HE2	5:E:135:VAL:HG13	1.85	0.41
5:E:253:ASN:CG	5:E:291:CYS:HB3	2.46	0.41
7:G:7:G:C6	7:G:8:C:N4	2.89	0.41
8:H:48:A:H2'	8:H:49:U:C6	2.55	0.41
12:L:44:LYS:HB3	12:L:44:LYS:HE3	1.54	0.41
12:L:73:HIS:NE2	36:9:218:ASP:OD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:561:SER:O	18:S:566:ASP:N	2.48	0.41
25:Z:592:GLY:O	25:Z:596:LYS:HG3	2.21	0.41
26:1:151:THR:OG1	26:1:154:ASP:OD2	2.32	0.41
26:1:1062:LEU:O	26:1:1064:GLU:N	2.53	0.41
29:w:435:MET:HE3	29:w:435:MET:HB3	1.78	0.41
33:6:113:LEU:HA	33:6:113:LEU:HD13	1.89	0.41
37:8:96:LYS:HE2	37:8:96:LYS:HB3	1.55	0.41
39:v:39:ASP:O	39:v:42:LYS:N	2.40	0.41
1:A:47:GLU:OE1	1:A:47:GLU:N	2.40	0.41
1:A:1454:TRP:CD1	1:A:1454:TRP:H	2.37	0.41
1:A:1526:LEU:H	1:A:1526:LEU:HD12	1.86	0.41
3:C:442:LYS:HA	3:C:442:LYS:HD3	1.63	0.41
5:E:137:ASP:O	5:E:141:GLY:N	2.48	0.41
5:E:258:THR:HG22	5:E:260:ARG:HE	1.85	0.41
10:J:437:LYS:HA	10:J:437:LYS:HD2	1.62	0.41
12:L:98:GLU:HG3	12:L:99:HIS:N	2.36	0.41
17:R:234:SER:HB3	17:R:236:LYS:NZ	2.36	0.41
19:T:205:GLY:O	19:T:206:TRP:C	2.63	0.41
26:1:489:PRO:HB3	26:1:491:GLU:HG3	2.02	0.41
26:1:641:ILE:N	26:1:642:PRO:HD2	2.36	0.41
26:1:888:LEU:HA	26:1:888:LEU:HD12	1.76	0.41
26:1:911:LEU:HG	26:1:957:ARG:HD2	2.02	0.41
26:1:969:LYS:H	26:1:969:LYS:HD2	1.86	0.41
27:3:329:TYR:OH	27:3:332:THR:HG22	2.21	0.41
27:3:511:LEU:HD13	27:3:517:VAL:HG21	2.02	0.41
27:3:580:ARG:HH11	27:3:580:ARG:HG3	1.85	0.41
27:3:679:LEU:HD13	27:3:679:LEU:HA	1.86	0.41
27:3:979:ARG:H	29:w:478:GLU:HG2	1.85	0.41
36:9:287:ASN:HD21	36:9:426:ILE:HA	1.86	0.41
36:9:413:VAL:HG21	36:9:424:GLU:CD	2.46	0.41
48:z:155:PRO:HD2	48:z:158:PRO:HG3	2.01	0.41
1:A:559:ASP:N	1:A:559:ASP:OD1	2.52	0.41
1:A:701:ILE:HD13	17:R:237:MET:SD	2.61	0.41
1:A:2012:LEU:HD13	1:A:2012:LEU:HA	1.79	0.41
2:B:91:U:O4	47:b:62:GLY:N	2.53	0.41
3:C:323:PHE:CZ	3:C:373:ILE:HG23	2.56	0.41
3:C:394:ARG:O	3:C:397:ASP:HB2	2.21	0.41
5:E:119:THR:HG21	5:E:162:ARG:NH1	2.35	0.41
7:G:83:A:N3	7:G:84:U:C5	2.88	0.41
7:G:91:A:H2'	7:G:92:U:C6	2.55	0.41
7:G:93:A:H2'	7:G:94:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:307:GLN:HG3	17:R:308:VAL:N	2.36	0.41
21:V:631:PHE:HD1	21:V:634:ILE:HD11	1.84	0.41
26:1:102:ASP:HA	26:1:103:PRO:HD3	1.86	0.41
26:1:1124:SER:HB2	26:1:1126:PHE:CE1	2.55	0.41
27:3:18:ILE:HD12	27:3:67:ALA:HB2	2.02	0.41
27:3:610:VAL:C	27:3:612:ASN:H	2.29	0.41
27:3:753:GLY:O	27:3:754:ILE:HD13	2.20	0.41
27:3:833:GLU:OE1	27:3:833:GLU:N	2.47	0.41
27:3:1053:ILE:HD13	27:3:1053:ILE:HG21	1.83	0.41
27:3:1190:GLN:O	27:3:1194:SER:OG	2.31	0.41
34:7:23:CYS:N	34:7:58:CYS:SG	2.73	0.41
35:5:50:LEU:HA	35:5:50:LEU:HD12	1.73	0.41
1:A:407:ALA:HB3	1:A:412:ASN:HB3	2.03	0.41
1:A:482:PHE:HZ	17:R:207:MET:HE2	1.86	0.41
1:A:1189:MET:HE3	1:A:1189:MET:HB2	1.79	0.41
1:A:1399:GLN:C	1:A:1401:ARG:H	2.29	0.41
1:A:1455:TRP:H	1:A:1455:TRP:CD1	2.39	0.41
1:A:1817:LEU:HD22	1:A:1902:PHE:HE1	1.86	0.41
1:A:1924:LEU:HD23	1:A:1924:LEU:HA	1.67	0.41
1:A:2179:HIS:HD2	1:A:2214:ILE:O	2.03	0.41
2:B:64:G:C2	2:B:65:G:C4	3.09	0.41
3:C:278:LEU:HD23	3:C:278:LEU:HA	1.86	0.41
3:C:350:ASN:HD21	3:C:352:LYS:HB2	1.86	0.41
3:C:379:LYS:O	3:C:383:GLN:HG2	2.20	0.41
3:C:467:ASP:O	3:C:468:CYS:HB2	2.20	0.41
3:C:666:VAL:HG12	3:C:667:VAL:N	2.35	0.41
3:C:745:LEU:HD22	3:C:770:PHE:CG	2.56	0.41
4:D:503:ALA:O	4:D:653:ALA:HA	2.20	0.41
5:E:316:SER:C	5:E:318:ARG:H	2.29	0.41
6:F:5:U:H2'	6:F:7:G:H5'	2.02	0.41
6:F:5:U:H4'	6:F:6:C:OP2	2.20	0.41
6:F:78:A:H3'	6:F:79:C:H6	1.85	0.41
9:I:619:ALA:O	9:I:623:VAL:HA	2.21	0.41
11:K:231:GLN:HG2	11:K:234:ARG:HH21	1.85	0.41
12:L:24:MET:HE3	12:L:24:MET:HB3	1.69	0.41
12:L:37:LEU:HD12	12:L:37:LEU:HA	1.87	0.41
17:R:126:ASN:HD22	19:T:442:ARG:HD2	1.86	0.41
17:R:280:ILE:HG22	17:R:281:ASN:O	2.21	0.41
19:T:393:ASP:HB2	19:T:394:ASN:OD1	2.20	0.41
25:Z:543:ASP:OD2	25:Z:546:ALA:N	2.50	0.41
26:1:477:LYS:HB3	26:1:499:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:781:ASP:OD1	26:1:781:ASP:C	2.63	0.41
26:1:1088:ILE:HG22	26:1:1089:GLY:N	2.36	0.41
27:3:206:GLN:HE21	27:3:231:HIS:CA	2.32	0.41
27:3:219:HIS:CE1	27:3:221:VAL:HG12	2.56	0.41
27:3:334:PRO:HG3	27:3:357:TYR:HE2	1.86	0.41
27:3:438:LEU:HB3	27:3:774:PHE:HB3	2.02	0.41
27:3:552:ARG:HH12	27:3:601:ARG:HH22	1.68	0.41
27:3:638:GLU:HB3	27:3:668:GLY:O	2.21	0.41
33:6:57:ARG:HD3	33:6:57:ARG:HA	1.82	0.41
33:6:85:ARG:HE	33:6:85:ARG:HB3	1.61	0.41
35:5:51:ASN:O	35:5:52:TYR:C	2.62	0.41
36:9:327:ASN:HD22	36:9:385:ARG:CD	2.34	0.41
37:8:21:GLN:HA	37:8:24:LEU:HD12	2.03	0.41
37:8:121:SER:HA	37:8:124:LEU:HD12	2.03	0.41
48:z:120:ALA:HB1	48:z:123:LEU:HD12	2.03	0.41
1:A:108:MET:HG3	1:A:110:TRP:CZ2	2.56	0.41
1:A:284:ARG:HH11	1:A:284:ARG:HG2	1.86	0.41
1:A:317:PRO:HB2	1:A:327:VAL:HG11	2.03	0.41
1:A:641:MET:HB3	1:A:641:MET:HE2	1.79	0.41
1:A:694:LEU:HD22	1:A:709:ILE:HD12	2.02	0.41
1:A:762:ARG:HH12	15:P:226:LYS:HZ1	1.69	0.41
1:A:1012:LYS:HG2	1:A:1036:PHE:HZ	1.85	0.41
1:A:2226:THR:HB	1:A:2228:TYR:CE1	2.56	0.41
3:C:259:LYS:HG2	50:C:1500:GTP:C6	2.56	0.41
3:C:731:SER:HB2	3:C:746:VAL:CG1	2.47	0.41
5:E:71:CYS:SG	5:E:114:GLU:HA	2.61	0.41
16:Q:1101:PRO:HD3	16:Q:1288:ARG:CB	2.51	0.41
21:V:553:HIS:O	21:V:557:THR:HG23	2.21	0.41
23:X:230:GLY:O	23:X:234:GLU:CB	2.68	0.41
26:1:117:ASP:CG	26:1:119:TYR:H	2.29	0.41
26:1:405:ASP:O	33:6:99:GLN:NE2	2.53	0.41
27:3:275:ARG:O	27:3:275:ARG:HG3	2.20	0.41
27:3:455:ASN:HB2	27:3:479:VAL:CG2	2.51	0.41
27:3:553:GLN:CD	27:3:601:ARG:HA	2.46	0.41
36:9:309:ARG:N	36:9:309:ARG:HD2	2.34	0.41
40:o:37:LEU:H	40:o:61:PRO:HG3	1.85	0.41
1:A:184:ASP:OD2	48:z:31:LYS:HD2	2.21	0.40
1:A:1000:ILE:HD12	1:A:1000:ILE:HA	1.51	0.40
1:A:1367:ASN:HD22	1:A:1367:ASN:HA	1.53	0.40
1:A:1956:PRO:HD2	1:A:1960:THR:HG21	2.03	0.40
3:C:83:GLU:H	3:C:83:GLU:HG2	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:VAL:HA	3:C:198:TYR:O	2.21	0.40
3:C:506:PRO:HG3	3:C:569:ARG:HH12	1.86	0.40
3:C:617:LEU:HD11	3:C:629:ILE:HG23	2.02	0.40
3:C:664:GLU:HB2	3:C:784:ILE:HG22	2.03	0.40
6:F:86:U:C4	8:H:12:G:O6	2.74	0.40
8:H:118:G:H2'	8:H:119:G:C8	2.56	0.40
21:V:565:LEU:HD12	21:V:612:PHE:CE1	2.56	0.40
25:Z:529:GLU:O	25:Z:533:ARG:HG3	2.21	0.40
26:1:396:ASN:HB2	33:6:67:ILE:CG2	2.50	0.40
26:1:827:ARG:HE	26:1:827:ARG:HB2	1.67	0.40
26:1:1025:LYS:HB3	26:1:1025:LYS:HE3	1.61	0.40
26:1:1136:TYR:HB2	26:1:1147:VAL:HG21	2.02	0.40
27:3:474:ILE:HD12	27:3:485:LEU:O	2.21	0.40
36:9:276:VAL:HG13	36:9:437:PRO:HB2	2.02	0.40
37:8:38:VAL:HG22	37:8:113:GLN:NE2	2.29	0.40
45:k:17:LEU:O	45:k:28:GLN:HA	2.21	0.40
1:A:1237:MET:HE2	1:A:1281:THR:HG21	2.03	0.40
1:A:1762:TYR:O	1:A:1768:TYR:CZ	2.74	0.40
1:A:2261:MET:O	1:A:2262:LEU:HD23	2.21	0.40
3:C:516:LEU:HB3	3:C:517:GLU:OE2	2.20	0.40
3:C:534:VAL:O	3:C:535:ALA:C	2.64	0.40
3:C:727:LEU:CD2	20:U:71:LEU:CB	2.90	0.40
4:D:1204:ILE:O	4:D:1249:GLU:HA	2.21	0.40
5:E:313:ASP:O	5:E:317:ARG:HA	2.20	0.40
7:G:98:U:H3'	7:G:99:C:H5''	2.03	0.40
8:H:63:G:H1	8:H:64:A:H62	1.58	0.40
10:J:244:ASN:HA	10:J:247:LYS:HZ2	1.86	0.40
10:J:411:MET:HG2	10:J:412:ASP:N	2.35	0.40
13:N:58:ARG:HA	13:N:58:ARG:HD3	1.91	0.40
21:V:444:ILE:H	21:V:444:ILE:HD12	1.86	0.40
26:1:134:ASP:HA	26:1:135:PRO:HD3	1.90	0.40
26:1:172:LEU:HA	26:1:175:LYS:HG3	2.03	0.40
26:1:885:ASP:OD1	26:1:887:LYS:N	2.53	0.40
27:3:609:LEU:HG	27:3:613:THR:O	2.21	0.40
27:3:680:ASP:O	27:3:682:VAL:N	2.54	0.40
27:3:942:LYS:HE3	27:3:942:LYS:HB2	1.92	0.40
29:w:335:GLY:O	29:w:339:HIS:N	2.54	0.40
29:w:445:HIS:CD2	29:w:445:HIS:N	2.88	0.40
31:2:512:GLN:OE1	31:2:512:GLN:N	2.54	0.40
33:6:71:LYS:HG3	33:6:72:ASN:N	2.35	0.40
48:z:20:THR:HG23	48:z:160:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MET:O	1:A:110:TRP:N	2.54	0.40
1:A:1336:PRO:HB3	1:A:1350:ILE:HD13	2.02	0.40
1:A:1633:ALA:HB2	1:A:1637:TRP:CZ3	2.56	0.40
1:A:2188:LEU:HD13	1:A:2228:TYR:CD2	2.56	0.40
2:B:103:G:N1	2:B:111:A:C6	2.89	0.40
5:E:90:ILE:CD1	5:E:112:VAL:HG11	2.48	0.40
5:E:323:LEU:HD23	5:E:323:LEU:HA	1.88	0.40
7:G:103:U:O2'	7:G:104:C:H5''	2.22	0.40
10:J:314:TYR:HD1	10:J:314:TYR:HA	1.67	0.40
11:K:114:MET:HE3	11:K:114:MET:HB3	1.73	0.40
23:X:225:SER:O	23:X:226:PHE:HD2	2.04	0.40
23:X:330:ASP:OD1	23:X:337:THR:OG1	2.40	0.40
26:1:618:ASP:OD1	26:1:618:ASP:N	2.53	0.40
27:3:1107:THR:OG1	27:3:1108:THR:N	2.54	0.40
34:7:58:CYS:CB	34:7:61:CYS:HB3	2.50	0.40
1:A:422:LEU:HD23	1:A:422:LEU:N	2.36	0.40
1:A:693:ILE:HG13	1:A:738:MET:CB	2.50	0.40
1:A:901:LEU:HD12	1:A:904:HIS:CE1	2.57	0.40
1:A:1339:ASP:O	1:A:1340:LEU:C	2.63	0.40
1:A:1362:ASP:CG	1:A:1363:GLN:H	2.27	0.40
3:C:237:LEU:HB2	3:C:835:GLU:OE1	2.22	0.40
3:C:325:LYS:O	3:C:329:ASP:HB2	2.20	0.40
3:C:514:TYR:CD1	3:C:514:TYR:C	3.00	0.40
4:D:2030:ARG:O	4:D:2096:ALA:HB3	2.22	0.40
5:E:321:TYR:HB3	5:E:323:LEU:HG	2.02	0.40
6:F:15:A:C6	6:F:16:G:C6	3.08	0.40
6:F:85:U:O2	6:F:86:U:N3	2.55	0.40
6:F:88:G:N3	8:H:11:G:C2	2.89	0.40
8:H:18:U:O2'	8:H:19:G:O5'	2.38	0.40
10:J:415:LEU:O	10:J:415:LEU:HD12	2.22	0.40
11:K:227:LYS:HD2	11:K:227:LYS:HA	1.74	0.40
18:S:642:LEU:HA	18:S:668:ARG:O	2.21	0.40
21:V:447:LYS:HE2	21:V:447:LYS:HB3	1.48	0.40
23:X:276:HIS:CD2	23:X:276:HIS:H	2.39	0.40
26:1:564:ASP:O	26:1:603:ALA:HB1	2.22	0.40
26:1:736:ARG:HH21	26:1:736:ARG:HG2	1.86	0.40
27:3:95:SER:OG	27:3:96:LYS:HG3	2.22	0.40
36:9:444:GLN:O	36:9:447:GLN:HB3	2.21	0.40
37:8:56:VAL:O	37:8:59:ILE:N	2.54	0.40
47:b:33:ASP:H	47:b:37:ASN:N	2.20	0.40
1:A:26:SER:O	1:A:30:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLU:HG3	1:A:33:LYS:N	2.36	0.40
1:A:121:HIS:ND1	1:A:123:THR:HG23	2.37	0.40
1:A:625:PRO:O	1:A:627:CYS:N	2.51	0.40
1:A:940:ILE:HG21	1:A:940:ILE:HD13	1.86	0.40
1:A:941:LYS:HG2	1:A:951:LEU:HD11	2.04	0.40
1:A:1179:SER:O	1:A:1201:ARG:NH1	2.47	0.40
1:A:1247:ILE:O	1:A:1251:SER:HB3	2.21	0.40
1:A:2228:TYR:CG	1:A:2258:ARG:HG3	2.57	0.40
1:A:2247:ASN:HD22	1:A:2247:ASN:C	2.29	0.40
2:B:97:G:C2	2:B:98:G:C5	3.09	0.40
3:C:461:LEU:HD11	3:C:573:GLU:O	2.21	0.40
3:C:519:GLU:N	3:C:519:GLU:OE1	2.55	0.40
5:E:65:HIS:NE2	5:E:91:LEU:HD23	2.36	0.40
5:E:197:LEU:HD11	5:E:213:ILE:HD13	2.03	0.40
5:E:315:THR:OG1	5:E:316:SER:N	2.54	0.40
8:H:139:C:H5"	43:m:56:SER:H	1.86	0.40
17:R:128:ASP:HB3	17:R:131:ASP:HB3	2.04	0.40
17:R:239:VAL:O	17:R:243:GLN:HG3	2.21	0.40
17:R:391:VAL:O	17:R:392:ILE:HD13	2.22	0.40
26:1:554:LYS:NZ	34:7:97:ASP:OD1	2.49	0.40
26:1:729:LYS:HA	26:1:729:LYS:HD3	1.57	0.40
26:1:781:ASP:OD1	26:1:782:GLU:N	2.55	0.40
26:1:823:MET:HE3	26:1:829:ASN:HB3	2.04	0.40
27:3:159:GLU:OE2	34:7:14:GLN:HB2	2.21	0.40
27:3:459:VAL:HG22	27:3:476:VAL:HA	2.03	0.40
27:3:592:LEU:HD13	27:3:605:LEU:HD13	2.03	0.40
27:3:791:HIS:HD2	27:3:794:SER:H	1.67	0.40
27:3:926:TYR:HB3	27:3:928:TYR:CE2	2.57	0.40
28:p:181:ARG:O	28:p:190:ALA:HA	2.21	0.40
35:5:8:HIS:CD2	35:5:11:LEU:HD11	2.57	0.40
39:v:36:GLU:OE2	39:v:36:GLU:HA	2.22	0.40
46:j:58:LEU:O	46:j:76:ARG:HA	2.21	0.40
48:z:39:ASN:HA	48:z:78:ILE:CD1	2.51	0.40
48:z:56:ARG:HB3	48:z:64:GLN:HB3	2.04	0.40
45:f:14:ASP:N	45:f:31:LEU:O	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	2232/2335 (96%)	2012 (90%)	205 (9%)	15 (1%)	18	53
3	C	854/972 (88%)	748 (88%)	99 (12%)	7 (1%)	16	50
4	D	1720/2136 (80%)	1598 (93%)	118 (7%)	4 (0%)	43	76
5	E	297/357 (83%)	268 (90%)	28 (9%)	1 (0%)	36	70
9	I	591/855 (69%)	492 (83%)	98 (17%)	1 (0%)	43	76
10	J	245/848 (29%)	229 (94%)	15 (6%)	1 (0%)	30	65
11	K	124/343 (36%)	115 (93%)	9 (7%)	0	100	100
12	L	97/802 (12%)	89 (92%)	8 (8%)	0	100	100
13	N	141/144 (98%)	119 (84%)	20 (14%)	2 (1%)	9	36
14	O	288/420 (69%)	271 (94%)	17 (6%)	0	100	100
15	P	40/229 (18%)	30 (75%)	9 (22%)	1 (2%)	4	23
16	Q	1319/1485 (89%)	1237 (94%)	82 (6%)	0	100	100
17	R	227/536 (42%)	208 (92%)	18 (8%)	1 (0%)	30	65
18	S	639/1041 (61%)	600 (94%)	39 (6%)	0	100	100
19	T	318/514 (62%)	295 (93%)	23 (7%)	0	100	100
20	U	68/2752 (2%)	59 (87%)	9 (13%)	0	100	100
21	V	464/908 (51%)	438 (94%)	26 (6%)	0	100	100
22	W	4/122 (3%)	4 (100%)	0	0	100	100
23	X	152/396 (38%)	136 (90%)	16 (10%)	0	100	100
24	Y	116/322 (36%)	111 (96%)	5 (4%)	0	100	100
25	Z	135/619 (22%)	126 (93%)	8 (6%)	1 (1%)	18	53
26	1	984/1304 (76%)	910 (92%)	68 (7%)	6 (1%)	21	56
27	3	1165/1217 (96%)	1058 (91%)	104 (9%)	3 (0%)	36	70
28	p	165/225 (73%)	155 (94%)	10 (6%)	0	100	100
29	w	428/501 (85%)	393 (92%)	35 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	u	183/793 (23%)	175 (96%)	8 (4%)	0	100	100
31	2	246/895 (28%)	221 (90%)	25 (10%)	0	100	100
32	4	157/424 (37%)	143 (91%)	14 (9%)	0	100	100
33	6	107/125 (86%)	99 (92%)	8 (8%)	0	100	100
34	7	103/110 (94%)	95 (92%)	8 (8%)	0	100	100
35	5	79/86 (92%)	69 (87%)	10 (13%)	0	100	100
36	9	373/520 (72%)	336 (90%)	35 (9%)	2 (0%)	24	60
37	8	113/904 (12%)	106 (94%)	7 (6%)	0	100	100
38	y	77/301 (26%)	73 (95%)	4 (5%)	0	100	100
39	v	165/464 (36%)	156 (94%)	9 (6%)	0	100	100
40	o	160/255 (63%)	145 (91%)	15 (9%)	0	100	100
41	c	95/118 (80%)	84 (88%)	11 (12%)	0	100	100
41	h	91/118 (77%)	85 (93%)	6 (7%)	0	100	100
42	d	72/86 (84%)	66 (92%)	6 (8%)	0	100	100
42	i	70/86 (81%)	66 (94%)	4 (6%)	0	100	100
43	a	84/240 (35%)	78 (93%)	6 (7%)	0	100	100
43	m	80/240 (33%)	74 (92%)	6 (8%)	0	100	100
44	g	77/126 (61%)	70 (91%)	7 (9%)	0	100	100
44	l	81/126 (64%)	74 (91%)	7 (9%)	0	100	100
45	f	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
45	k	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
46	e	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
46	j	79/92 (86%)	71 (90%)	8 (10%)	0	100	100
47	b	80/119 (67%)	75 (94%)	5 (6%)	0	100	100
47	n	78/119 (66%)	70 (90%)	8 (10%)	0	100	100
48	z	176/472 (37%)	163 (93%)	13 (7%)	0	100	100
All	All	15859/28446 (56%)	14501 (91%)	1313 (8%)	45 (0%)	37	70

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	THR
1	A	856	LEU

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Mol	Chain	Res	Type
3	C	801	LEU
3	C	824	THR
13	N	40	LYS
36	9	269	ASP
1	A	189	GLU
1	A	1764	SER
1	A	1765	SER
3	C	802	HIS
4	D	531	ILE
4	D	1584	ILE
4	D	2098	ALA
4	D	2099	THR
1	A	377	GLU
1	A	855	ARG
1	A	1202	THR
1	A	570	ASP
1	A	699	GLU
3	C	440	SER
15	P	205	LYS
26	1	436	THR
26	1	1063	LEU
27	3	672	GLY
1	A	108	MET
1	A	857	ASN
25	Z	500	GLY
26	1	430	LYS
26	1	435	PRO
1	A	698	PRO
1	A	942	PRO
1	A	1761	PRO
3	C	444	GLY
3	C	472	GLY
5	E	317	ARG
26	1	417	PRO
27	3	1008	SER
17	R	185	GLY
27	3	997	GLY
9	I	371	PRO
3	C	93	ILE
10	J	241	VAL
26	1	1103	VAL
36	9	349	PRO

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Mol	Chain	Res	Type
13	N	36	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	2012/2108 (95%)	1687 (84%)	325 (16%)	2	12
3	C	747/866 (86%)	619 (83%)	128 (17%)	2	11
5	E	256/300 (85%)	214 (84%)	42 (16%)	2	12
9	I	23/749 (3%)	23 (100%)	0	100	100
10	J	205/751 (27%)	178 (87%)	27 (13%)	4	18
11	K	111/294 (38%)	93 (84%)	18 (16%)	2	12
12	L	86/709 (12%)	74 (86%)	12 (14%)	3	16
13	N	130/130 (100%)	110 (85%)	20 (15%)	2	13
15	P	40/203 (20%)	36 (90%)	4 (10%)	7	29
16	Q	71/1336 (5%)	71 (100%)	0	100	100
17	R	200/459 (44%)	166 (83%)	34 (17%)	2	11
19	T	273/441 (62%)	232 (85%)	41 (15%)	3	14
20	U	21/2432 (1%)	20 (95%)	1 (5%)	23	57
21	V	194/838 (23%)	167 (86%)	27 (14%)	3	17
22	W	4/4 (100%)	4 (100%)	0	100	100
23	X	139/349 (40%)	119 (86%)	20 (14%)	3	15
24	Y	105/291 (36%)	90 (86%)	15 (14%)	3	16
25	Z	118/545 (22%)	101 (86%)	17 (14%)	3	15
26	1	840/1103 (76%)	674 (80%)	166 (20%)	1	8
27	3	1018/1051 (97%)	838 (82%)	180 (18%)	2	10
28	p	8/195 (4%)	8 (100%)	0	100	100
29	w	112/446 (25%)	101 (90%)	11 (10%)	7	30
30	u	10/709 (1%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	2	152/776 (20%)	130 (86%)	22 (14%)	3	15
33	6	97/109 (89%)	80 (82%)	17 (18%)	2	10
34	7	90/95 (95%)	76 (84%)	14 (16%)	2	13
35	5	72/77 (94%)	64 (89%)	8 (11%)	6	25
36	9	218/456 (48%)	180 (83%)	38 (17%)	2	10
37	8	104/831 (12%)	92 (88%)	12 (12%)	5	24
39	v	78/382 (20%)	66 (85%)	12 (15%)	2	13
40	o	6/218 (3%)	6 (100%)	0	100	100
41	h	5/110 (4%)	5 (100%)	0	100	100
42	i	4/74 (5%)	4 (100%)	0	100	100
43	m	4/177 (2%)	4 (100%)	0	100	100
44	l	3/101 (3%)	3 (100%)	0	100	100
45	k	3/66 (4%)	3 (100%)	0	100	100
46	j	1/84 (1%)	1 (100%)	0	100	100
47	n	3/101 (3%)	3 (100%)	0	100	100
48	z	152/416 (36%)	132 (87%)	20 (13%)	4	18
All	All	7715/20382 (38%)	6484 (84%)	1231 (16%)	4	12

All (1231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	31	GLN
1	A	35	ARG
1	A	59	GLU
1	A	60	ASP
1	A	71	ARG
1	A	88	TYR
1	A	89	LEU
1	A	97	HIS
1	A	106	MET
1	A	108	MET
1	A	122	ILE
1	A	123	THR
1	A	127	SER
1	A	153	ARG

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Mol	Chain	Res	Type
1	A	158	ARG
1	A	164	MET
1	A	165	ARG
1	A	184	ASP
1	A	189	GLU
1	A	193	LEU
1	A	194	GLU
1	A	195	LEU
1	A	203	VAL
1	A	216	SER
1	A	221	ASN
1	A	223	SER
1	A	226	GLN
1	A	250	VAL
1	A	258	PHE
1	A	261	LYS
1	A	273	ILE
1	A	283	VAL
1	A	284	ARG
1	A	300	ASN
1	A	322	ASN
1	A	327	VAL
1	A	329	LEU
1	A	330	THR
1	A	331	TRP
1	A	334	THR
1	A	337	VAL
1	A	340	ILE
1	A	342	THR
1	A	343	GLU
1	A	346	ASP
1	A	347	LEU
1	A	363	HIS
1	A	366	LYS
1	A	367	SER
1	A	382	GLU
1	A	387	PHE
1	A	390	ASP
1	A	409	ARG
1	A	414	ARG
1	A	418	THR
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	426	LEU
1	A	433	GLU
1	A	434	HIS
1	A	442	LYS
1	A	443	VAL
1	A	465	LYS
1	A	467	GLN
1	A	468	LYS
1	A	470	ARG
1	A	479	THR
1	A	480	LYS
1	A	486	LYS
1	A	492	VAL
1	A	498	ARG
1	A	510	ARG
1	A	511	LYS
1	A	512	ASN
1	A	514	ASN
1	A	523	ASN
1	A	527	VAL
1	A	529	THR
1	A	533	LYS
1	A	539	ARG
1	A	554	THR
1	A	555	LYS
1	A	569	VAL
1	A	576	ASP
1	A	579	GLN
1	A	587	GLN
1	A	595	LYS
1	A	598	LEU
1	A	604	MET
1	A	606	LYS
1	A	615	ARG
1	A	617	ASN
1	A	627	CYS
1	A	644	ILE
1	A	663	ARG
1	A	670	LYS
1	A	674	LYS
1	A	677	VAL
1	A	686	ARG

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Mol	Chain	Res	Type
1	A	690	MET
1	A	695	ASP
1	A	708	THR
1	A	738	MET
1	A	770	THR
1	A	773	LYS
1	A	788	GLN
1	A	796	LYS
1	A	797	ASP
1	A	801	ILE
1	A	802	THR
1	A	804	GLU
1	A	812	THR
1	A	819	SER
1	A	824	PRO
1	A	830	LEU
1	A	833	LYS
1	A	835	ASP
1	A	836	THR
1	A	845	ARG
1	A	855	ARG
1	A	856	LEU
1	A	864	LEU
1	A	868	GLU
1	A	879	SER
1	A	931	ASP
1	A	933	ARG
1	A	941	LYS
1	A	945	THR
1	A	946	GLU
1	A	976	MET
1	A	979	SER
1	A	985	TYR
1	A	995	ARG
1	A	1000	ILE
1	A	1001	VAL
1	A	1010	THR
1	A	1015	VAL
1	A	1017	ILE
1	A	1021	ASP
1	A	1027	SER
1	A	1030	ILE

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Mol	Chain	Res	Type
1	A	1032	ARG
1	A	1038	SER
1	A	1048	MET
1	A	1066	GLN
1	A	1070	ASP
1	A	1079	THR
1	A	1083	HIS
1	A	1089	CYS
1	A	1094	ARG
1	A	1102	THR
1	A	1104	ASP
1	A	1125	ILE
1	A	1129	ASN
1	A	1130	ASN
1	A	1136	ARG
1	A	1139	ARG
1	A	1147	VAL
1	A	1165	VAL
1	A	1168	VAL
1	A	1171	GLU
1	A	1173	SER
1	A	1180	LYS
1	A	1186	LEU
1	A	1203	SER
1	A	1219	GLU
1	A	1221	THR
1	A	1229	PHE
1	A	1257	THR
1	A	1268	ILE
1	A	1276	GLU
1	A	1279	VAL
1	A	1284	LEU
1	A	1295	ILE
1	A	1301	ILE
1	A	1315	VAL
1	A	1318	THR
1	A	1321	GLU
1	A	1328	LEU
1	A	1329	SER
1	A	1330	MET
1	A	1338	SER
1	A	1339	ASP

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Mol	Chain	Res	Type
1	A	1344	LYS
1	A	1359	HIS
1	A	1361	GLU
1	A	1367	ASN
1	A	1368	LEU
1	A	1370	ARG
1	A	1376	GLU
1	A	1381	ASP
1	A	1382	SER
1	A	1385	VAL
1	A	1404	THR
1	A	1405	LEU
1	A	1407	ASP
1	A	1414	ARG
1	A	1416	ILE
1	A	1419	ILE
1	A	1429	THR
1	A	1438	VAL
1	A	1441	ASP
1	A	1449	LYS
1	A	1458	GLN
1	A	1463	LYS
1	A	1475	ILE
1	A	1497	THR
1	A	1501	LEU
1	A	1504	GLU
1	A	1516	LYS
1	A	1519	THR
1	A	1523	ARG
1	A	1526	LEU
1	A	1536	LEU
1	A	1544	ARG
1	A	1548	TYR
1	A	1556	ASP
1	A	1558	THR
1	A	1566	ILE
1	A	1568	THR
1	A	1572	SER
1	A	1574	ILE
1	A	1575	GLN
1	A	1583	GLN
1	A	1588	SER

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Mol	Chain	Res	Type
1	A	1602	ASP
1	A	1613	THR
1	A	1619	SER
1	A	1623	ASN
1	A	1630	LEU
1	A	1639	VAL
1	A	1640	SER
1	A	1655	THR
1	A	1656	THR
1	A	1658	GLN
1	A	1681	ARG
1	A	1683	LYS
1	A	1702	LEU
1	A	1711	LEU
1	A	1730	MET
1	A	1749	LYS
1	A	1756	SER
1	A	1759	THR
1	A	1760	GLU
1	A	1770	GLU
1	A	1771	LEU
1	A	1773	SER
1	A	1777	ILE
1	A	1789	THR
1	A	1790	ILE
1	A	1793	THR
1	A	1795	GLU
1	A	1808	PHE
1	A	1814	THR
1	A	1819	LEU
1	A	1824	THR
1	A	1833	LEU
1	A	1851	SER
1	A	1852	LEU
1	A	1863	VAL
1	A	1865	ARG
1	A	1868	MET
1	A	1870	ASP
1	A	1876	LEU
1	A	1878	ASP
1	A	1883	VAL
1	A	1898	LYS

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Mol	Chain	Res	Type
1	A	1915	VAL
1	A	1924	LEU
1	A	1926	THR
1	A	1928	SER
1	A	1929	SER
1	A	1937	ILE
1	A	1943	LEU
1	A	1945	VAL
1	A	1962	THR
1	A	1970	THR
1	A	1972	THR
1	A	1981	VAL
1	A	1995	ASN
1	A	1997	VAL
1	A	2012	LEU
1	A	2070	LYS
1	A	2072	GLU
1	A	2074	ARG
1	A	2078	ILE
1	A	2084	HIS
1	A	2090	ILE
1	A	2103	THR
1	A	2110	VAL
1	A	2115	ILE
1	A	2118	SER
1	A	2120	LEU
1	A	2123	GLN
1	A	2124	ILE
1	A	2135	ASP
1	A	2136	ASN
1	A	2145	ILE
1	A	2147	MET
1	A	2153	THR
1	A	2159	LEU
1	A	2165	GLN
1	A	2184	GLU
1	A	2191	GLN
1	A	2193	VAL
1	A	2212	ILE
1	A	2219	THR
1	A	2225	LEU
1	A	2226	THR

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Mol	Chain	Res	Type
1	A	2228	TYR
1	A	2230	LEU
1	A	2231	THR
1	A	2239	ARG
1	A	2242	THR
1	A	2254	SER
1	A	2266	ARG
1	A	2272	MET
1	A	2273	VAL
1	A	2293	LYS
1	A	2295	GLU
1	A	2298	LEU
1	A	2309	HIS
1	A	2321	GLN
1	A	2325	VAL
1	A	2330	ARG
3	C	57	VAL
3	C	58	VAL
3	C	63	LYS
3	C	65	TYR
3	C	71	GLU
3	C	72	VAL
3	C	77	VAL
3	C	83	GLU
3	C	86	THR
3	C	89	LEU
3	C	97	VAL
3	C	99	THR
3	C	117	ASP
3	C	132	VAL
3	C	133	THR
3	C	134	LEU
3	C	173	THR
3	C	187	THR
3	C	202	ILE
3	C	203	MET
3	C	213	ASP
3	C	223	ASP
3	C	226	VAL
3	C	229	ILE
3	C	243	ILE
3	C	249	GLU

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Mol	Chain	Res	Type
3	C	256	CYS
3	C	263	LEU
3	C	282	VAL
3	C	288	LEU
3	C	289	ILE
3	C	311	SER
3	C	312	SER
3	C	320	LEU
3	C	322	SER
3	C	326	ILE
3	C	327	TYR
3	C	329	ASP
3	C	334	ILE
3	C	357	THR
3	C	363	SER
3	C	366	GLN
3	C	374	LEU
3	C	377	LEU
3	C	387	ASP
3	C	388	VAL
3	C	389	ASP
3	C	390	THR
3	C	391	SER
3	C	404	THR
3	C	406	GLU
3	C	412	ILE
3	C	416	LEU
3	C	417	ARG
3	C	431	VAL
3	C	435	VAL
3	C	438	ILE
3	C	448	LYS
3	C	451	HIS
3	C	452	THR
3	C	454	THR
3	C	457	VAL
3	C	458	ASP
3	C	469	ASP
3	C	495	ARG
3	C	497	LEU
3	C	498	SER
3	C	507	VAL

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Mol	Chain	Res	Type
3	C	510	LEU
3	C	532	ILE
3	C	540	GLU
3	C	541	VAL
3	C	543	ARG
3	C	551	LEU
3	C	559	ILE
3	C	562	THR
3	C	564	THR
3	C	572	GLU
3	C	585	THR
3	C	587	VAL
3	C	590	ILE
3	C	596	ASN
3	C	623	GLU
3	C	632	THR
3	C	641	MET
3	C	650	GLU
3	C	653	ILE
3	C	659	VAL
3	C	660	VAL
3	C	664	GLU
3	C	668	GLU
3	C	670	SER
3	C	673	LYS
3	C	674	CYS
3	C	683	ASN
3	C	687	MET
3	C	694	LYS
3	C	696	LEU
3	C	707	ILE
3	C	708	THR
3	C	713	LYS
3	C	714	LEU
3	C	731	SER
3	C	740	THR
3	C	747	ASP
3	C	749	THR
3	C	759	LEU
3	C	767	VAL
3	C	779	LEU
3	C	780	CYS

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Mol	Chain	Res	Type
3	C	785	ARG
3	C	787	VAL
3	C	791	ILE
3	C	811	THR
3	C	834	VAL
3	C	841	ASP
3	C	843	VAL
3	C	871	ILE
3	C	875	ILE
3	C	878	ILE
3	C	914	LYS
3	C	915	SER
3	C	916	ILE
3	C	922	GLU
3	C	928	HIS
3	C	937	THR
3	C	941	LYS
3	C	943	LEU
5	E	61	LEU
5	E	73	LYS
5	E	81	LEU
5	E	98	ASP
5	E	100	ASP
5	E	106	LYS
5	E	120	ASP
5	E	143	ARG
5	E	144	VAL
5	E	150	HIS
5	E	157	CYS
5	E	162	ARG
5	E	167	VAL
5	E	173	ASP
5	E	175	THR
5	E	176	VAL
5	E	181	ILE
5	E	188	GLN
5	E	189	THR
5	E	192	ASN
5	E	197	LEU
5	E	209	ILE
5	E	210	SER
5	E	213	ILE

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Mol	Chain	Res	Type
5	E	214	ASP
5	E	215	ASN
5	E	218	LYS
5	E	222	LEU
5	E	225	ASN
5	E	231	MET
5	E	234	HIS
5	E	237	SER
5	E	241	LEU
5	E	260	ARG
5	E	263	ASP
5	E	284	PHE
5	E	289	LEU
5	E	300	ILE
5	E	329	SER
5	E	338	ASP
5	E	342	ILE
5	E	343	ILE
10	J	216	ASP
10	J	220	LEU
10	J	222	ASP
10	J	244	ASN
10	J	254	SER
10	J	280	LEU
10	J	286	GLU
10	J	288	LYS
10	J	290	ARG
10	J	299	TRP
10	J	314	TYR
10	J	321	GLU
10	J	347	HIS
10	J	350	ILE
10	J	360	ASP
10	J	365	ILE
10	J	376	VAL
10	J	377	LYS
10	J	380	ILE
10	J	406	PHE
10	J	411	MET
10	J	415	LEU
10	J	419	PHE
10	J	431	ARG

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Mol	Chain	Res	Type
10	J	432	VAL
10	J	438	TYR
10	J	440	LEU
11	K	99	VAL
11	K	102	SER
11	K	103	THR
11	K	121	GLU
11	K	126	LYS
11	K	133	ILE
11	K	140	ILE
11	K	152	ILE
11	K	154	ARG
11	K	158	ASN
11	K	163	MET
11	K	189	LEU
11	K	192	THR
11	K	201	ILE
11	K	206	LYS
11	K	218	LYS
11	K	224	SER
11	K	225	ASP
12	L	14	THR
12	L	25	LYS
12	L	29	ASN
12	L	32	SER
12	L	44	LYS
12	L	54	LEU
12	L	59	LYS
12	L	70	LYS
12	L	83	ARG
12	L	89	ILE
12	L	91	ARG
12	L	104	LEU
13	N	1	MET
13	N	4	VAL
13	N	6	ARG
13	N	9	LYS
13	N	13	ASP
13	N	17	LEU
13	N	21	THR
13	N	34	THR
13	N	41	ARG

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Mol	Chain	Res	Type
13	N	44	GLU
13	N	56	LYS
13	N	60	ILE
13	N	71	SER
13	N	102	CYS
13	N	104	ARG
13	N	115	THR
13	N	119	CYS
13	N	123	LYS
13	N	134	CYS
13	N	136	HIS
15	P	192	VAL
15	P	224	MET
15	P	225	GLU
15	P	229	LYS
17	R	133	GLN
17	R	147	THR
17	R	148	ARG
17	R	151	LEU
17	R	182	SER
17	R	196	VAL
17	R	200	VAL
17	R	208	GLU
17	R	212	PHE
17	R	213	LYS
17	R	214	ILE
17	R	218	ILE
17	R	224	SER
17	R	232	SER
17	R	236	LYS
17	R	237	MET
17	R	238	THR
17	R	239	VAL
17	R	241	GLU
17	R	242	GLN
17	R	252	SER
17	R	256	ASN
17	R	278	VAL
17	R	282	GLU
17	R	283	ASN
17	R	295	ASP
17	R	332	ARG

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Mol	Chain	Res	Type
17	R	386	ARG
17	R	388	ILE
17	R	391	VAL
17	R	404	GLU
17	R	408	ASP
17	R	414	GLN
17	R	420	SER
19	T	196	LEU
19	T	198	ARG
19	T	201	SER
19	T	208	ARG
19	T	230	ILE
19	T	241	SER
19	T	243	THR
19	T	250	ARG
19	T	254	VAL
19	T	256	THR
19	T	263	SER
19	T	267	ASP
19	T	294	LEU
19	T	302	VAL
19	T	303	LEU
19	T	304	VAL
19	T	309	ASP
19	T	314	ILE
19	T	319	THR
19	T	323	VAL
19	T	325	THR
19	T	338	CYS
19	T	366	VAL
19	T	369	THR
19	T	374	SER
19	T	384	HIS
19	T	386	THR
19	T	389	SER
19	T	393	ASP
19	T	397	GLN
19	T	398	TRP
19	T	399	LYS
19	T	402	ASP
19	T	413	ASN
19	T	418	THR

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Mol	Chain	Res	Type
19	T	424	ASP
19	T	427	LEU
19	T	432	ASP
19	T	438	LEU
19	T	443	THR
19	T	459	LEU
20	U	5	ILE
21	V	442	VAL
21	V	450	ILE
21	V	454	SER
21	V	457	ARG
21	V	458	THR
21	V	464	GLN
21	V	483	GLU
21	V	494	LEU
21	V	496	CYS
21	V	516	MET
21	V	517	LEU
21	V	528	ILE
21	V	540	GLU
21	V	543	LYS
21	V	555	LEU
21	V	556	TYR
21	V	559	SER
21	V	563	SER
21	V	568	ILE
21	V	571	SER
21	V	588	GLN
21	V	591	CYS
21	V	628	ILE
21	V	632	THR
21	V	639	LEU
21	V	644	ARG
21	V	648	LYS
23	X	221	LYS
23	X	225	SER
23	X	228	LEU
23	X	229	SER
23	X	245	LYS
23	X	247	SER
23	X	251	GLU
23	X	260	ARG

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Mol	Chain	Res	Type
23	X	279	SER
23	X	291	ASP
23	X	292	ILE
23	X	298	SER
23	X	309	ARG
23	X	311	VAL
23	X	339	LEU
23	X	343	ARG
23	X	344	ILE
23	X	352	LEU
23	X	364	SER
23	X	373	SER
24	Y	2	ASN
24	Y	16	ARG
24	Y	25	LYS
24	Y	26	VAL
24	Y	34	ASP
24	Y	35	SER
24	Y	40	LEU
24	Y	48	THR
24	Y	57	SER
24	Y	69	ARG
24	Y	73	THR
24	Y	86	ASP
24	Y	89	SER
24	Y	106	THR
24	Y	107	ILE
25	Z	488	SER
25	Z	490	ARG
25	Z	520	LYS
25	Z	522	LEU
25	Z	526	ILE
25	Z	532	ASP
25	Z	543	ASP
25	Z	547	ASN
25	Z	549	ILE
25	Z	563	ARG
25	Z	567	SER
25	Z	575	ARG
25	Z	583	ARG
25	Z	610	LEU
25	Z	615	SER

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Mol	Chain	Res	Type
25	Z	617	GLU
25	Z	619	MET
26	1	88	VAL
26	1	106	GLU
26	1	111	LYS
26	1	121	LYS
26	1	127	ILE
26	1	128	ILE
26	1	134	ASP
26	1	142	THR
26	1	151	THR
26	1	154	ASP
26	1	161	LEU
26	1	162	THR
26	1	163	LYS
26	1	165	GLU
26	1	169	ARG
26	1	172	LEU
26	1	396	ASN
26	1	407	MET
26	1	415	LEU
26	1	442	THR
26	1	448	THR
26	1	449	GLU
26	1	452	THR
26	1	453	MET
26	1	471	ASP
26	1	479	LEU
26	1	486	THR
26	1	488	SER
26	1	491	GLU
26	1	497	ILE
26	1	498	MET
26	1	500	LEU
26	1	502	LEU
26	1	503	LYS
26	1	506	ASN
26	1	516	LEU
26	1	518	GLN
26	1	519	ILE
26	1	534	GLN
26	1	544	LEU

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Mol	Chain	Res	Type
26	1	551	LEU
26	1	577	VAL
26	1	581	LEU
26	1	582	LEU
26	1	583	ILE
26	1	591	VAL
26	1	592	GLU
26	1	596	ILE
26	1	598	SER
26	1	611	SER
26	1	612	THR
26	1	613	MET
26	1	620	MET
26	1	621	ASP
26	1	628	THR
26	1	632	PHE
26	1	635	VAL
26	1	637	SER
26	1	652	CYS
26	1	654	SER
26	1	655	LYS
26	1	666	LYS
26	1	675	MET
26	1	677	CYS
26	1	680	LEU
26	1	685	SER
26	1	689	ILE
26	1	695	VAL
26	1	697	GLU
26	1	701	VAL
26	1	703	THR
26	1	717	THR
26	1	726	SER
26	1	727	VAL
26	1	739	ARG
26	1	757	MET
26	1	760	GLU
26	1	761	TYR
26	1	769	VAL
26	1	782	GLU
26	1	787	ILE
26	1	788	VAL

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Mol	Chain	Res	Type
26	1	789	LEU
26	1	795	CYS
26	1	798	THR
26	1	801	VAL
26	1	802	GLU
26	1	808	THR
26	1	816	LYS
26	1	836	THR
26	1	837	THR
26	1	839	GLU
26	1	843	LYS
26	1	844	VAL
26	1	851	SER
26	1	854	VAL
26	1	859	ASP
26	1	866	LYS
26	1	868	VAL
26	1	871	THR
26	1	873	GLU
26	1	883	ASP
26	1	885	ASP
26	1	887	LYS
26	1	905	THR
26	1	924	ARG
26	1	932	ILE
26	1	936	VAL
26	1	940	LEU
26	1	942	ASN
26	1	946	LYS
26	1	947	VAL
26	1	960	VAL
26	1	962	MET
26	1	969	LYS
26	1	973	HIS
26	1	980	GLU
26	1	998	LYS
26	1	1003	VAL
26	1	1004	ILE
26	1	1013	ILE
26	1	1021	THR
26	1	1031	VAL
26	1	1036	ILE

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Mol	Chain	Res	Type
26	1	1048	GLU
26	1	1050	VAL
26	1	1057	ARG
26	1	1059	CYS
26	1	1061	GLU
26	1	1065	LEU
26	1	1080	THR
26	1	1086	LYS
26	1	1093	VAL
26	1	1094	LEU
26	1	1099	ASN
26	1	1100	ASN
26	1	1102	LYS
26	1	1103	VAL
26	1	1105	GLU
26	1	1112	THR
26	1	1113	THR
26	1	1121	GLU
26	1	1128	VAL
26	1	1138	VAL
26	1	1143	VAL
26	1	1147	VAL
26	1	1150	SER
26	1	1152	SER
26	1	1158	ILE
26	1	1161	MET
26	1	1164	ASP
26	1	1169	VAL
26	1	1170	THR
26	1	1178	MET
26	1	1179	ASP
26	1	1182	LEU
26	1	1219	VAL
26	1	1235	GLU
26	1	1239	VAL
26	1	1251	LEU
26	1	1261	VAL
26	1	1277	GLN
26	1	1289	ASN
26	1	1293	ASN
26	1	1301	ASP
26	1	1304	LEU

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Mol	Chain	Res	Type
27	3	8	LEU
27	3	9	GLN
27	3	23	SER
27	3	27	GLN
27	3	30	ILE
27	3	33	SER
27	3	36	LYS
27	3	44	ASP
27	3	46	ASN
27	3	47	THR
27	3	50	VAL
27	3	54	LEU
27	3	57	GLU
27	3	68	PHE
27	3	71	THR
27	3	79	VAL
27	3	82	SER
27	3	86	ARG
27	3	87	ILE
27	3	88	VAL
27	3	89	ILE
27	3	90	LEU
27	3	110	SER
27	3	114	ARG
27	3	124	ASP
27	3	126	LYS
27	3	135	ILE
27	3	139	LYS
27	3	152	LEU
27	3	153	THR
27	3	155	SER
27	3	186	GLU
27	3	191	GLU
27	3	197	THR
27	3	204	THR
27	3	209	THR
27	3	215	LEU
27	3	221	VAL
27	3	225	SER
27	3	226	GLU
27	3	235	LEU
27	3	237	THR

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Mol	Chain	Res	Type
27	3	252	SER
27	3	253	GLU
27	3	256	ILE
27	3	266	ASP
27	3	290	SER
27	3	295	THR
27	3	305	THR
27	3	314	THR
27	3	317	THR
27	3	318	ASP
27	3	323	THR
27	3	332	THR
27	3	335	VAL
27	3	342	LEU
27	3	347	LEU
27	3	351	SER
27	3	370	GLU
27	3	379	LEU
27	3	384	THR
27	3	390	ARG
27	3	393	LYS
27	3	394	ASN
27	3	404	LEU
27	3	408	LEU
27	3	410	CYS
27	3	411	GLN
27	3	412	ILE
27	3	417	ASN
27	3	434	SER
27	3	442	LEU
27	3	443	GLU
27	3	447	MET
27	3	451	GLU
27	3	459	VAL
27	3	462	VAL
27	3	466	ILE
27	3	477	SER
27	3	482	THR
27	3	489	GLU
27	3	491	VAL
27	3	507	SER
27	3	511	LEU

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Mol	Chain	Res	Type
27	3	518	GLN
27	3	519	VAL
27	3	520	TYR
27	3	524	ILE
27	3	525	ARG
27	3	549	VAL
27	3	555	VAL
27	3	558	LEU
27	3	574	LEU
27	3	584	SER
27	3	588	VAL
27	3	589	CYS
27	3	591	SER
27	3	595	VAL
27	3	604	PHE
27	3	609	LEU
27	3	611	ASP
27	3	614	VAL
27	3	617	ILE
27	3	622	SER
27	3	625	LEU
27	3	633	LEU
27	3	639	SER
27	3	640	LEU
27	3	665	LEU
27	3	674	LEU
27	3	677	THR
27	3	678	VAL
27	3	679	LEU
27	3	683	THR
27	3	689	THR
27	3	690	ARG
27	3	704	VAL
27	3	707	GLN
27	3	712	VAL
27	3	713	LEU
27	3	729	PHE
27	3	732	THR
27	3	734	LEU
27	3	736	TYR
27	3	743	SER
27	3	748	GLU

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Mol	Chain	Res	Type
27	3	768	GLU
27	3	777	VAL
27	3	823	MET
27	3	824	VAL
27	3	837	GLU
27	3	865	VAL
27	3	875	ASN
27	3	876	THR
27	3	883	GLU
27	3	890	SER
27	3	899	THR
27	3	909	VAL
27	3	913	LEU
27	3	915	LEU
27	3	919	SER
27	3	920	VAL
27	3	927	THR
27	3	931	VAL
27	3	933	ASN
27	3	936	LYS
27	3	943	THR
27	3	948	VAL
27	3	958	ARG
27	3	959	VAL
27	3	961	ILE
27	3	982	GLU
27	3	991	SER
27	3	995	THR
27	3	996	ILE
27	3	998	HIS
27	3	1001	ILE
27	3	1003	SER
27	3	1028	THR
27	3	1035	THR
27	3	1037	SER
27	3	1056	VAL
27	3	1066	VAL
27	3	1088	LYS
27	3	1093	MET
27	3	1102	LEU
27	3	1114	SER
27	3	1120	THR

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Mol	Chain	Res	Type
27	3	1121	THR
27	3	1128	ILE
27	3	1133	THR
27	3	1134	SER
27	3	1135	HIS
27	3	1137	ASP
27	3	1145	GLU
27	3	1170	VAL
27	3	1174	ILE
27	3	1194	SER
27	3	1203	GLU
27	3	1210	ASP
29	w	396	LEU
29	w	400	HIS
29	w	425	HIS
29	w	438	LEU
29	w	443	THR
29	w	468	SER
29	w	480	GLU
29	w	486	VAL
29	w	489	LYS
29	w	497	ARG
29	w	500	LEU
31	2	465	LEU
31	2	467	GLN
31	2	473	ASP
31	2	474	VAL
31	2	478	HIS
31	2	481	THR
31	2	488	LEU
31	2	495	ARG
31	2	508	ARG
31	2	517	ILE
31	2	531	THR
31	2	542	GLU
31	2	546	GLN
31	2	548	THR
31	2	557	VAL
31	2	564	ILE
31	2	565	ASP
31	2	585	THR
31	2	589	ASP

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Mol	Chain	Res	Type
31	2	599	THR
31	2	706	THR
31	2	711	LEU
33	6	26	LEU
33	6	31	THR
33	6	59	THR
33	6	65	GLU
33	6	69	ASP
33	6	77	LEU
33	6	78	SER
33	6	82	VAL
33	6	84	ASN
33	6	85	ARG
33	6	87	LEU
33	6	89	VAL
33	6	99	GLN
33	6	100	LYS
33	6	105	LYS
33	6	108	GLU
33	6	113	LEU
34	7	7	ASP
34	7	9	ILE
34	7	12	ARG
34	7	23	CYS
34	7	29	LYS
34	7	33	CYS
34	7	35	SER
34	7	40	CYS
34	7	46	CYS
34	7	48	GLU
34	7	59	VAL
34	7	60	ILE
34	7	76	THR
34	7	89	VAL
35	5	5	TYR
35	5	13	HIS
35	5	23	HIS
35	5	27	THR
35	5	30	GLU
35	5	33	VAL
35	5	36	HIS
35	5	69	MET

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Mol	Chain	Res	Type
36	9	220	ILE
36	9	221	LEU
36	9	224	THR
36	9	225	MET
36	9	230	LYS
36	9	232	LYS
36	9	243	THR
36	9	249	SER
36	9	256	VAL
36	9	260	THR
36	9	266	ILE
36	9	269	ASP
36	9	271	LEU
36	9	284	LEU
36	9	286	THR
36	9	293	LEU
36	9	295	LEU
36	9	296	HIS
36	9	298	ASP
36	9	299	LEU
36	9	300	THR
36	9	330	ILE
36	9	336	THR
36	9	338	THR
36	9	340	THR
36	9	344	SER
36	9	359	SER
36	9	365	ILE
36	9	367	SER
36	9	380	PHE
36	9	386	SER
36	9	389	TYR
36	9	395	THR
36	9	396	ILE
36	9	397	PHE
36	9	424	GLU
36	9	426	ILE
36	9	435	VAL
37	8	24	LEU
37	8	25	LEU
37	8	29	LYS
37	8	43	VAL

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Mol	Chain	Res	Type
37	8	45	LEU
37	8	55	ARG
37	8	58	GLU
37	8	85	MET
37	8	90	THR
37	8	102	MET
37	8	111	SER
37	8	116	ILE
39	v	11	THR
39	v	16	VAL
39	v	33	LEU
39	v	37	THR
39	v	38	ILE
39	v	46	PHE
39	v	47	MET
39	v	51	LEU
39	v	59	CYS
39	v	65	ASN
39	v	82	LEU
39	v	85	ARG
48	z	4	ILE
48	z	8	GLU
48	z	18	LYS
48	z	23	ASP
48	z	28	LEU
48	z	41	ILE
48	z	63	VAL
48	z	71	THR
48	z	77	SER
48	z	95	ARG
48	z	117	LEU
48	z	121	ASP
48	z	133	VAL
48	z	134	THR
48	z	136[A]	ASP
48	z	136[B]	ASP
48	z	137	THR
48	z	149	ILE
48	z	175	ILE
48	z	177	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	160	HIS
1	A	181	ASN
1	A	210	HIS
1	A	244	GLN
1	A	270	ASN
1	A	300	ASN
1	A	321	ASN
1	A	325	HIS
1	A	326	HIS
1	A	328	HIS
1	A	439	GLN
1	A	483	GLN
1	A	514	ASN
1	A	563	GLN
1	A	584	HIS
1	A	675	GLN
1	A	755	HIS
1	A	775	ASN
1	A	788	GLN
1	A	793	ASN
1	A	815	HIS
1	A	1014	ASN
1	A	1096	HIS
1	A	1111	GLN
1	A	1117	HIS
1	A	1424	GLN
1	A	1460	HIS
1	A	1487	HIS
1	A	1527	ASN
1	A	1543	ASN
1	A	1552	GLN
1	A	1586	HIS
1	A	1623	ASN
1	A	1717	ASN
1	A	1804	ASN
1	A	1894	GLN
1	A	1944	HIS
1	A	1966	HIS
1	A	2082	ASN
1	A	2155	GLN
1	A	2158	HIS
1	A	2162	GLN

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Mol	Chain	Res	Type
1	A	2179	HIS
1	A	2191	GLN
1	A	2240	GLN
1	A	2247	ASN
1	A	2297	GLN
1	A	2306	HIS
1	A	2316	ASN
3	C	82	GLN
3	C	87	GLN
3	C	139	HIS
3	C	140	HIS
3	C	154	HIS
3	C	245	HIS
3	C	248	GLN
3	C	335	ASN
3	C	505	GLN
3	C	513	ASN
3	C	548	ASN
3	C	575	GLN
3	C	596	ASN
3	C	859	GLN
5	E	94	ASN
5	E	101	ASN
5	E	165	GLN
10	J	234	ASN
10	J	297	ASN
10	J	331	GLN
10	J	351	ASN
10	J	373	HIS
11	K	131	GLN
11	K	160	GLN
11	K	188	HIS
12	L	29	ASN
12	L	45	GLN
15	P	212	ASN
17	R	157	GLN
17	R	215	ASN
17	R	279	HIS
17	R	320	HIS
17	R	385	ASN
19	T	269	GLN
19	T	285	HIS

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Mol	Chain	Res	Type
19	T	407	GLN
19	T	413	ASN
19	T	500	HIS
20	U	20	GLN
21	V	474	HIS
21	V	588	GLN
21	V	646	HIS
23	X	286	HIS
23	X	302	GLN
23	X	303	HIS
24	Y	2	ASN
24	Y	19	GLN
24	Y	29	HIS
24	Y	66	ASN
24	Y	87	GLN
24	Y	98	ASN
25	Z	538	GLN
25	Z	559	ASN
25	Z	595	GLN
26	1	159	GLN
26	1	447	GLN
26	1	463	ASN
26	1	670	GLN
26	1	692	HIS
26	1	738	HIS
26	1	949	GLN
26	1	966	GLN
26	1	1100	ASN
26	1	1104	GLN
26	1	1142	ASN
26	1	1218	ASN
27	3	19	HIS
27	3	138	GLN
27	3	203	ASN
27	3	206	GLN
27	3	218	ASN
27	3	276	ASN
27	3	304	GLN
27	3	411	GLN
27	3	417	ASN
27	3	480	ASN
27	3	518	GLN

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Mol	Chain	Res	Type
27	3	666	ASN
27	3	796	ASN
27	3	817	GLN
27	3	861	GLN
27	3	870	ASN
27	3	875	ASN
27	3	932	ASN
27	3	985	HIS
27	3	1105	GLN
27	3	1142	GLN
29	w	445	HIS
31	2	458	ASN
33	6	47	GLN
33	6	52	ASN
33	6	84	ASN
33	6	99	GLN
33	6	109	GLN
34	7	4	HIS
34	7	78	GLN
35	5	10	GLN
35	5	23	HIS
36	9	199	ASN
36	9	296	HIS
36	9	327	ASN
36	9	394	HIS
36	9	412	ASN
37	8	88	ASN
37	8	113	GLN
48	z	3	ASN
48	z	107	HIS
48	z	112	GLN
48	z	125	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	27 (28%)	3 (3%)
6	F	96/107 (89%)	49 (51%)	6 (6%)
7	G	69/220 (31%)	43 (62%)	9 (13%)
8	H	163/188 (86%)	73 (44%)	7 (4%)
All	All	424/632 (67%)	192 (45%)	25 (5%)

All (192) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	26	A
2	B	27	U
2	B	32	C
2	B	40	U
2	B	57	G
2	B	70	A
2	B	71	C
2	B	85	C
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	9	U
6	F	10	U
6	F	12	G
6	F	22	A
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	30	A
6	F	31	U
6	F	33	G
6	F	34	G

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Mol	Chain	Res	Type
6	F	36	A
6	F	37	C
6	F	38	G
6	F	40	U
6	F	41	A
6	F	44	G
6	F	46	G
6	F	47	A
6	F	48	A
6	F	49	G
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	66	C
6	F	68	C
6	F	69	A
6	F	73	A
6	F	74	U
6	F	78	A
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	88	G
6	F	89	U
6	F	91	A
6	F	93	G
6	F	95	G
7	G	-11	G
7	G	-10	G
7	G	-7	U
7	G	-4	G
7	G	1	G
7	G	3	A
7	G	4	A
7	G	5	G

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Mol	Chain	Res	Type
7	G	7	G
7	G	8	C
7	G	11	A
7	G	12	G
7	G	13	C
7	G	14	A
7	G	17	U
7	G	22	C
7	G	23	U
7	G	24	G
7	G	84	U
7	G	88	G
7	G	89	U
7	G	90	C
7	G	91	A
7	G	92	U
7	G	94	C
7	G	97	A
7	G	98	U
7	G	99	C
7	G	100	C
7	G	101	U
7	G	102	G
7	G	103	U
7	G	104	C
7	G	105	C
7	G	106	C
7	G	107	U
7	G	109	U
7	G	110	U
7	G	111	U
7	G	112	U
7	G	114	U
7	G	115	C
7	G	116	C
8	H	2	U
8	H	4	G
8	H	13	C
8	H	14	C
8	H	15	U
8	H	16	U
8	H	17	U

Continued on next page...

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Mol	Chain	Res	Type
8	H	18	U
8	H	19	G
8	H	22	U
8	H	23	A
8	H	24	A
8	H	25	G
8	H	28	C
8	H	29	A
8	H	30	A
8	H	31	G
8	H	35	A
8	H	44	U
8	H	45	C
8	H	46	U
8	H	47	U
8	H	48	A
8	H	49	U
8	H	50	C
8	H	56	A
8	H	60	U
8	H	62	U
8	H	63	G
8	H	64	A
8	H	81	G
8	H	82	G
8	H	83	A
8	H	84	C
8	H	98	G
8	H	101	U
8	H	103	U
8	H	104	U
8	H	112	G
8	H	116	A
8	H	117	U
8	H	118	G
8	H	119	G
8	H	120	A
8	H	121	A
8	H	122	U
8	H	124	G
8	H	128	C
8	H	129	U

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Mol	Chain	Res	Type
8	H	130	U
8	H	136	G
8	H	137	U
8	H	138	C
8	H	142	U
8	H	145	A
8	H	146	C
8	H	147	G
8	H	153	A
8	H	156	U
8	H	157	G
8	H	161	U
8	H	162	U
8	H	163	G
8	H	164	C
8	H	166	G
8	H	168	A
8	H	169	C
8	H	170	C
8	H	174	A
8	H	177	A
8	H	178	A
8	H	179	C
8	H	180	G

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	20	G
2	B	39	C
2	B	94	U
6	F	5	U
6	F	35	A
6	F	37	C
6	F	47	A
6	F	58	G
6	F	84	A
7	G	-11	G
7	G	21	A
7	G	22	C
7	G	88	G
7	G	89	U

Continued on next page...

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Mol	Chain	Res	Type
7	G	101	U
7	G	104	C
7	G	106	C
7	G	108	U
8	H	12	G
8	H	13	C
8	H	18	U
8	H	22	U
8	H	24	A
8	H	28	C
8	H	47	U

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
26	SEP	1	129	26	8,9,10	1.52	1 (12%)	7,12,14	1.08	0

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
26	SEP	1	129	26	-	2/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	129	SEP	P-O1P	3.27	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	1	129	SEP	N-CA-CB-OG
26	1	129	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 13 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	$\# Z > 2$
49	IHP	A	2401	-	36,36,36	1.47	8 (22%)	60,60,60	1.90	15 (25%)
50	GTP	C	1500	51	33,34,34	0.93	1 (3%)	50,54,54	1.73	10 (20%)

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
49	IHP	A	2401	-	-	3/30/54/54	0/1/1/1
50	GTP	C	1500	51	-	6/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	A	2401	IHP	P1-O31	-2.91	1.44	1.54
49	A	2401	IHP	P5-O35	-2.62	1.45	1.54
49	A	2401	IHP	P5-O45	-2.40	1.45	1.54
50	C	1500	GTP	C5-N7	-2.27	1.34	1.39
49	A	2401	IHP	P6-O46	-2.18	1.46	1.54
49	A	2401	IHP	P4-O44	-2.17	1.46	1.54
49	A	2401	IHP	P1-O41	-2.12	1.46	1.54
49	A	2401	IHP	P6-O16	-2.01	1.56	1.59
49	A	2401	IHP	P4-O34	-2.01	1.47	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C	1500	GTP	C5-C4-N3	-5.29	119.97	128.39
49	A	2401	IHP	O15-C5-C4	5.19	119.81	108.76
50	C	1500	GTP	C2-N3-C4	4.81	120.59	112.30
49	A	2401	IHP	C5-C4-C3	4.47	120.24	110.43
49	A	2401	IHP	O14-C4-C5	4.25	117.80	108.76
49	A	2401	IHP	C5-C6-C1	3.83	118.84	110.43
49	A	2401	IHP	O44-P4-O34	3.48	120.85	107.80
49	A	2401	IHP	O15-C5-C6	3.41	116.01	108.76
50	C	1500	GTP	N9-C4-N3	3.35	132.66	125.95
50	C	1500	GTP	C2-N1-C6	-3.29	119.14	125.11
49	A	2401	IHP	O11-C1-C6	2.93	114.99	108.76
49	A	2401	IHP	O13-C3-C4	2.90	114.93	108.76
49	A	2401	IHP	P4-O14-C4	-2.88	115.73	123.43
50	C	1500	GTP	N9-C8-N7	-2.87	108.07	113.40
49	A	2401	IHP	O43-P3-O33	2.87	118.55	107.80
50	C	1500	GTP	C5-C6-N1	2.76	120.27	113.25
50	C	1500	GTP	C8-N7-C5	2.74	109.15	104.26
49	A	2401	IHP	C4-C3-C2	2.62	116.17	110.43
50	C	1500	GTP	O6-C6-C5	-2.57	119.75	126.53
49	A	2401	IHP	P6-O16-C6	-2.53	116.68	123.43
49	A	2401	IHP	O13-C3-C2	2.33	113.72	108.76
49	A	2401	IHP	O43-P3-O13	-2.32	96.82	105.85
50	C	1500	GTP	O2G-PG-O3B	2.17	111.93	104.64
49	A	2401	IHP	P3-O13-C3	-2.17	117.64	123.43
50	C	1500	GTP	C3'-C2'-C1'	2.12	105.48	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

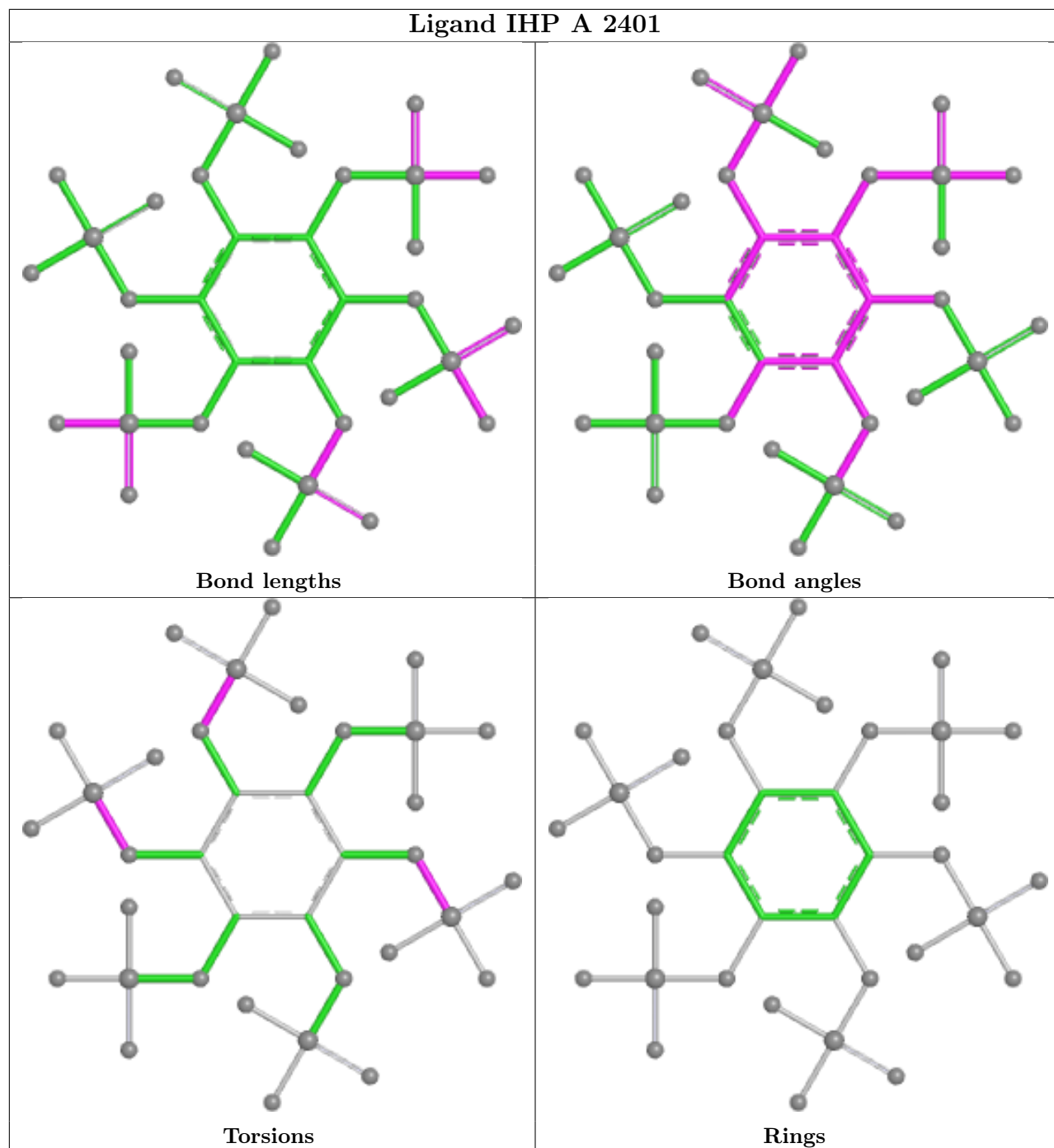
Mol	Chain	Res	Type	Atoms
50	C	1500	GTP	C5'-O5'-PA-O1A
50	C	1500	GTP	O4'-C4'-C5'-O5'
50	C	1500	GTP	C3'-C4'-C5'-O5'
49	A	2401	IHP	C2-O12-P2-O22
50	C	1500	GTP	C5'-O5'-PA-O3A
49	A	2401	IHP	C3-O13-P3-O43
49	A	2401	IHP	C5-O15-P5-O35
50	C	1500	GTP	PB-O3A-PA-O2A
50	C	1500	GTP	PB-O3A-PA-O1A

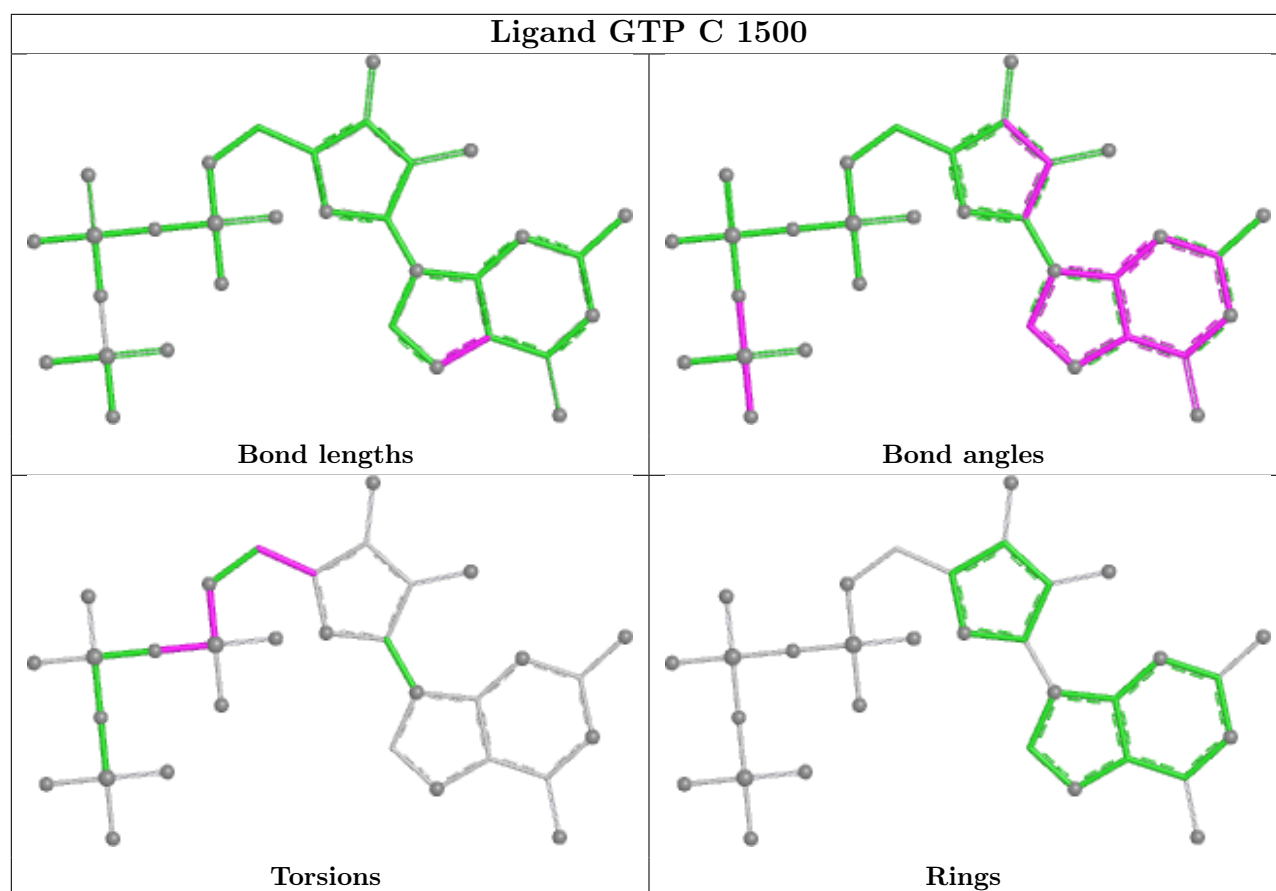
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	A	2401	IHP	2	0
50	C	1500	GTP	3	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.

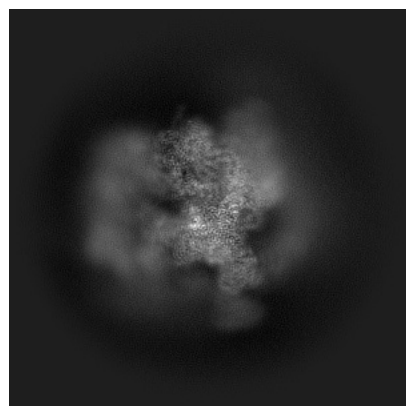
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35107. These allow visual inspection of the internal detail of the map and identification of artifacts.

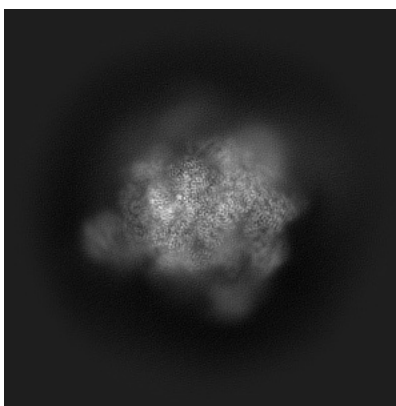
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

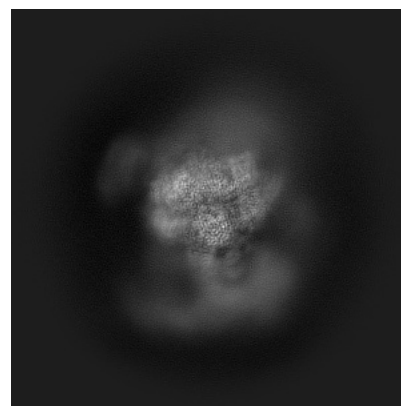
6.1.1 Primary map



X

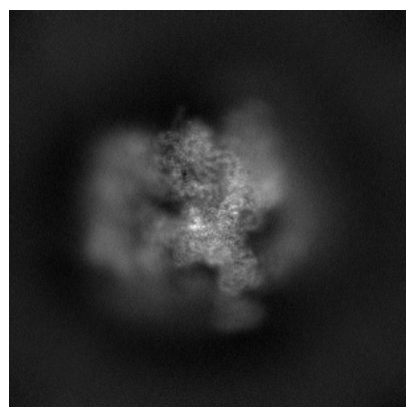


Y

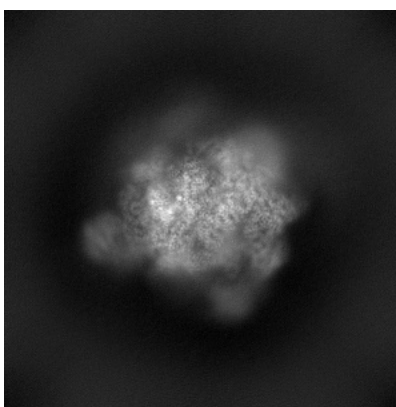


Z

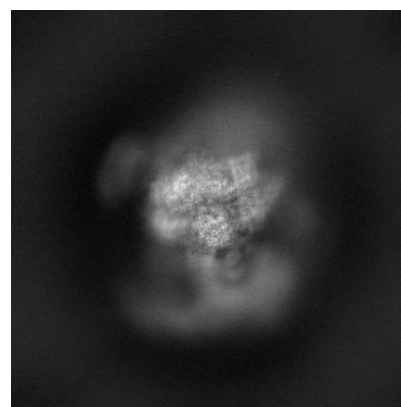
6.1.2 Raw map



X



Y

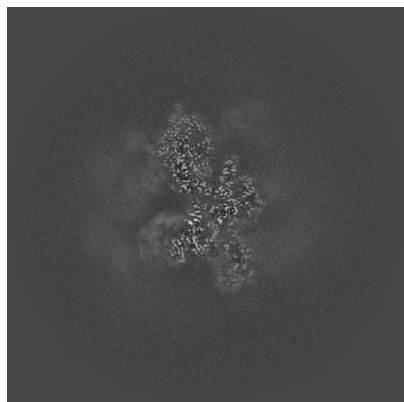


Z

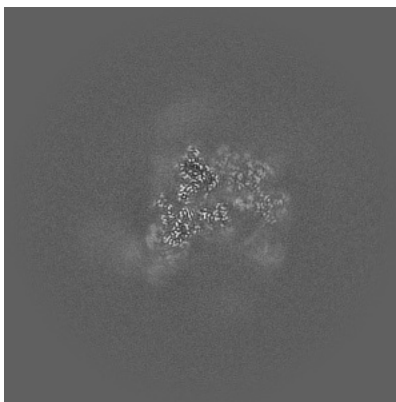
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

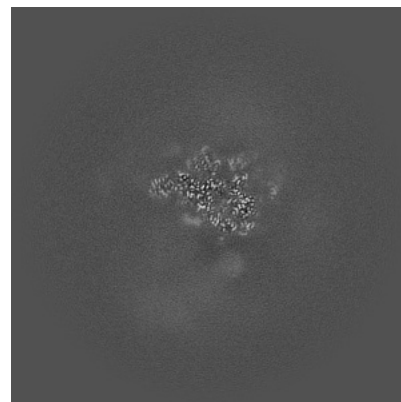
6.2.1 Primary map



X Index: 240

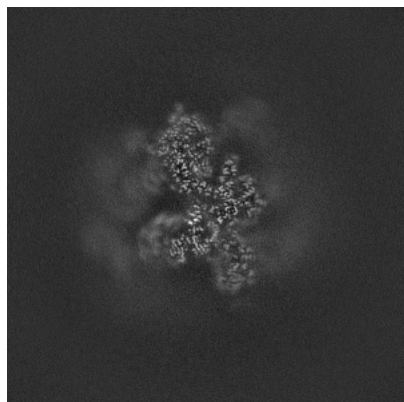


Y Index: 240

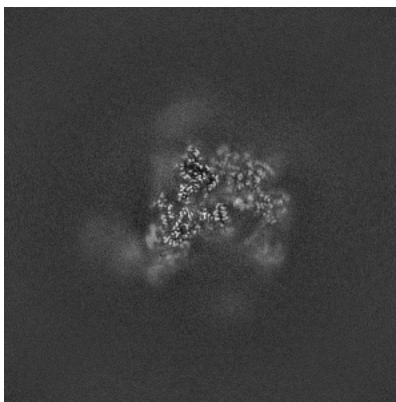


Z Index: 240

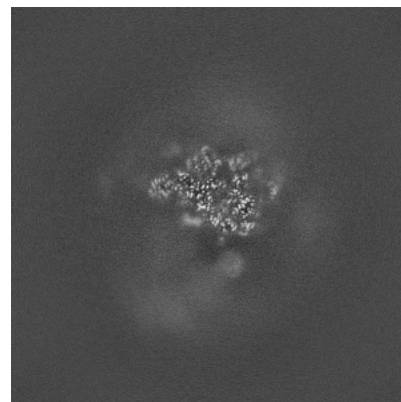
6.2.2 Raw map



X Index: 240



Y Index: 240

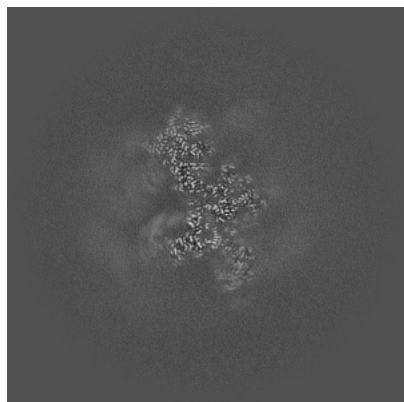


Z Index: 240

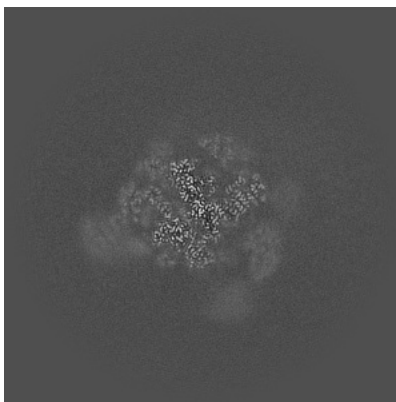
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

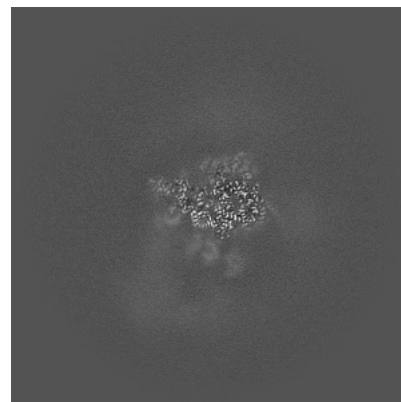
6.3.1 Primary map



X Index: 237

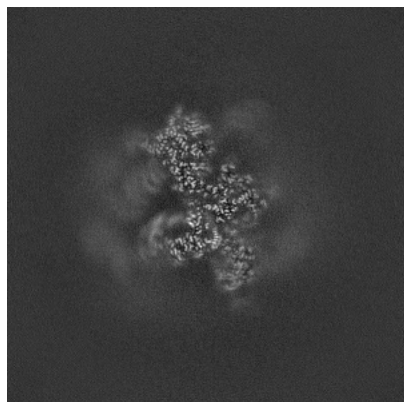


Y Index: 262

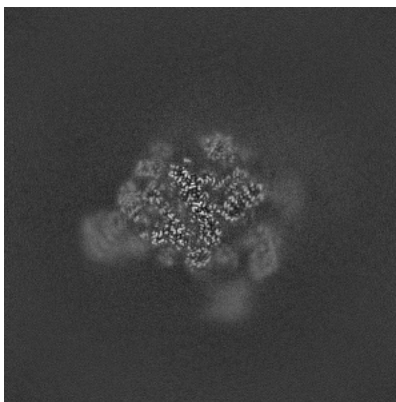


Z Index: 220

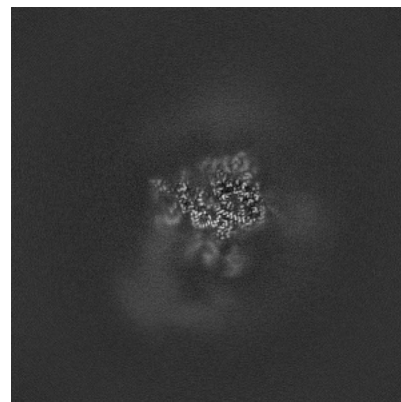
6.3.2 Raw map



X Index: 237



Y Index: 266

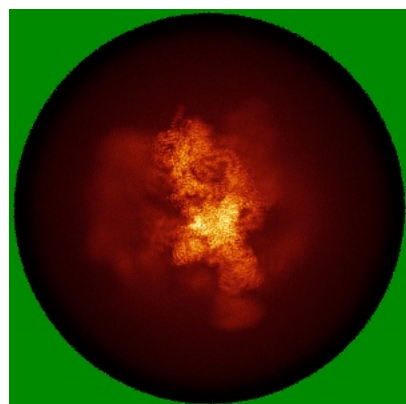


Z Index: 219

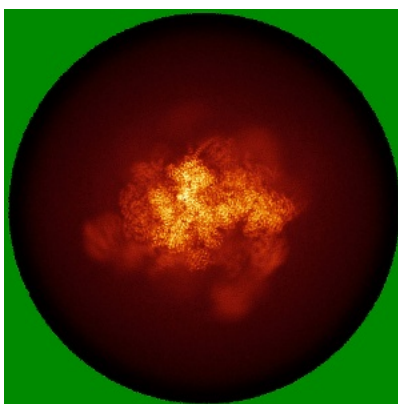
The images above show the largest variance slices of the map in three orthogonal directions.

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

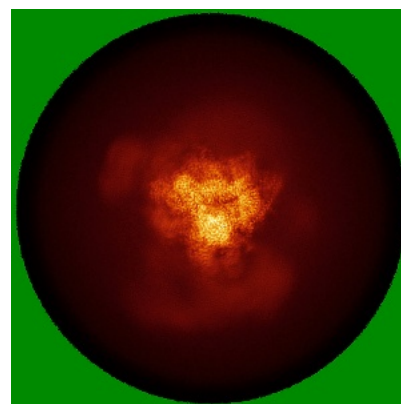
6.4.1 Primary map



X

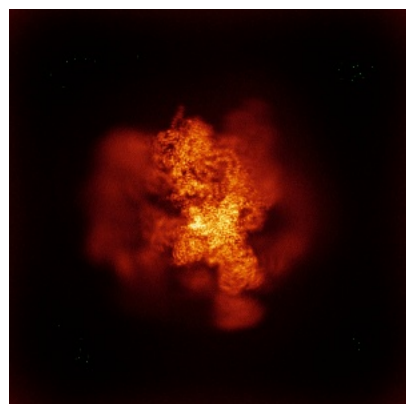


Y

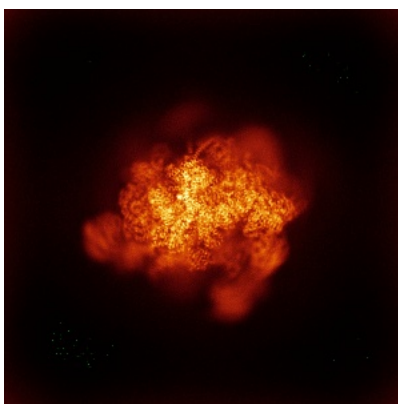


Z

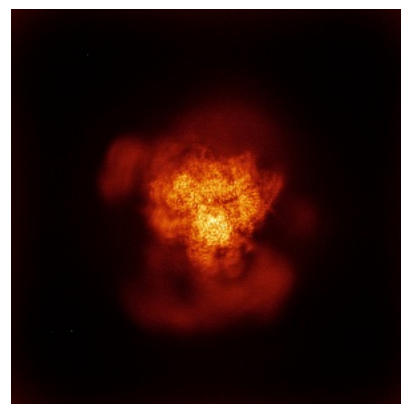
6.4.2 Raw map



X



Y

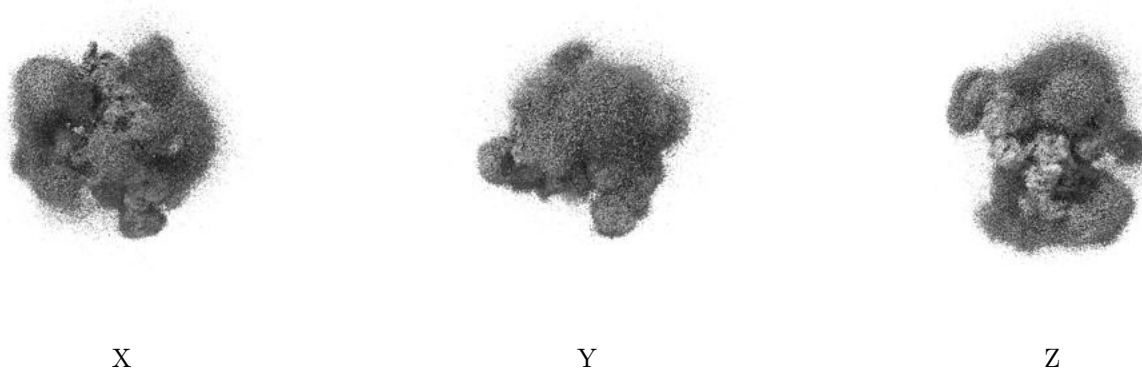


Z

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.

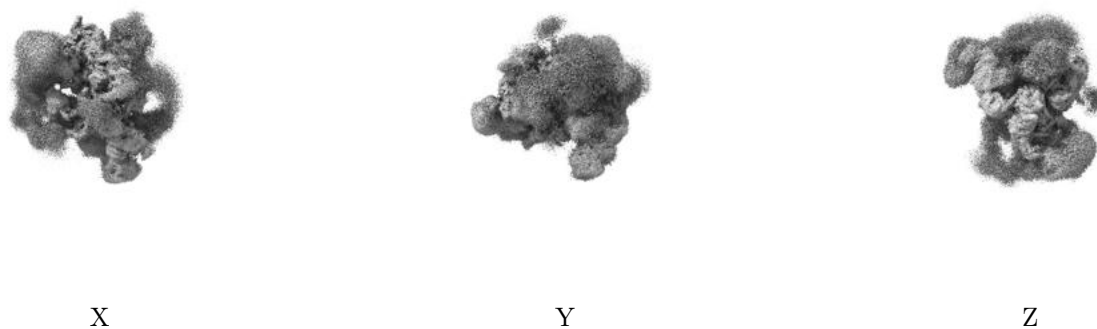
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

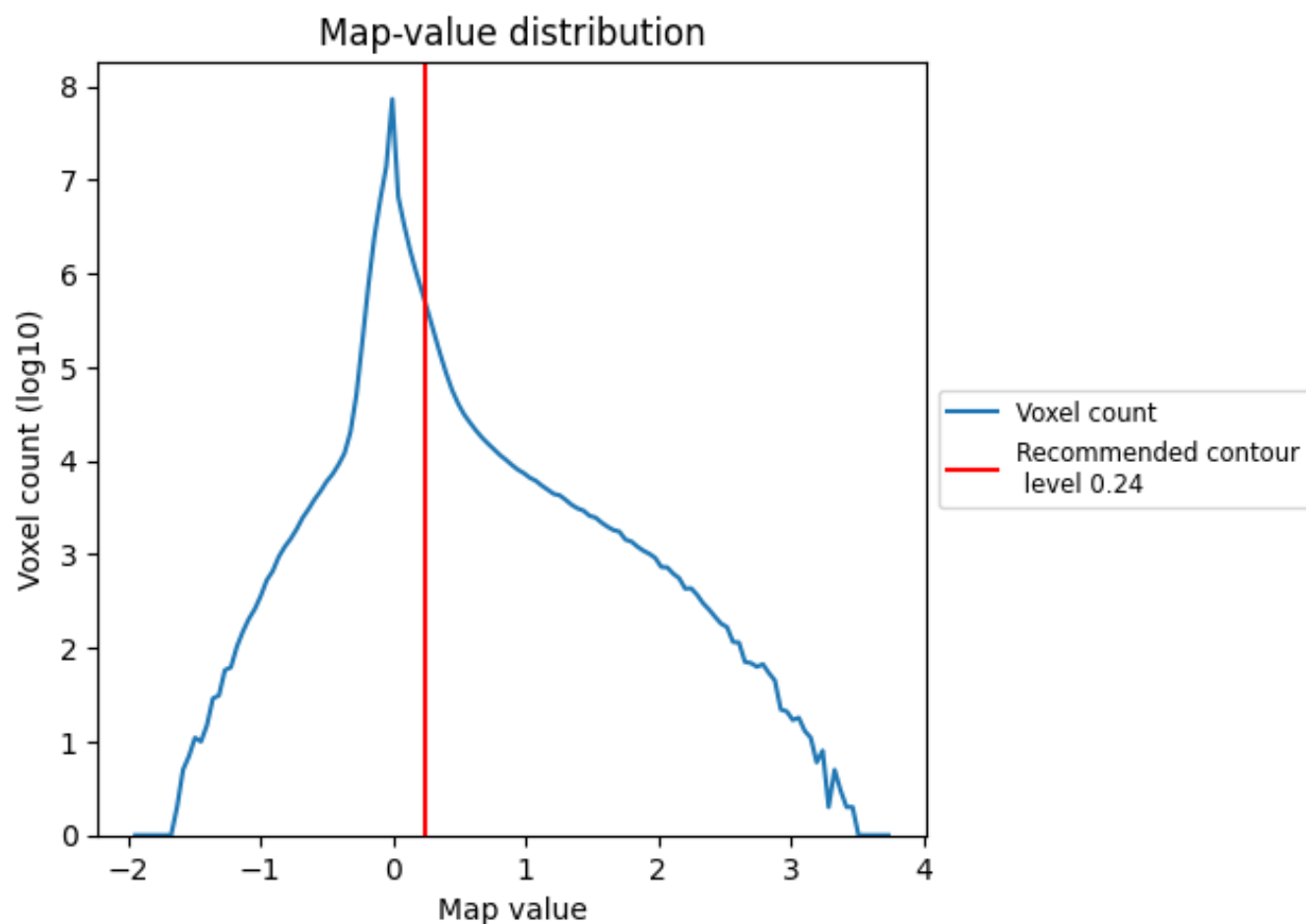
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

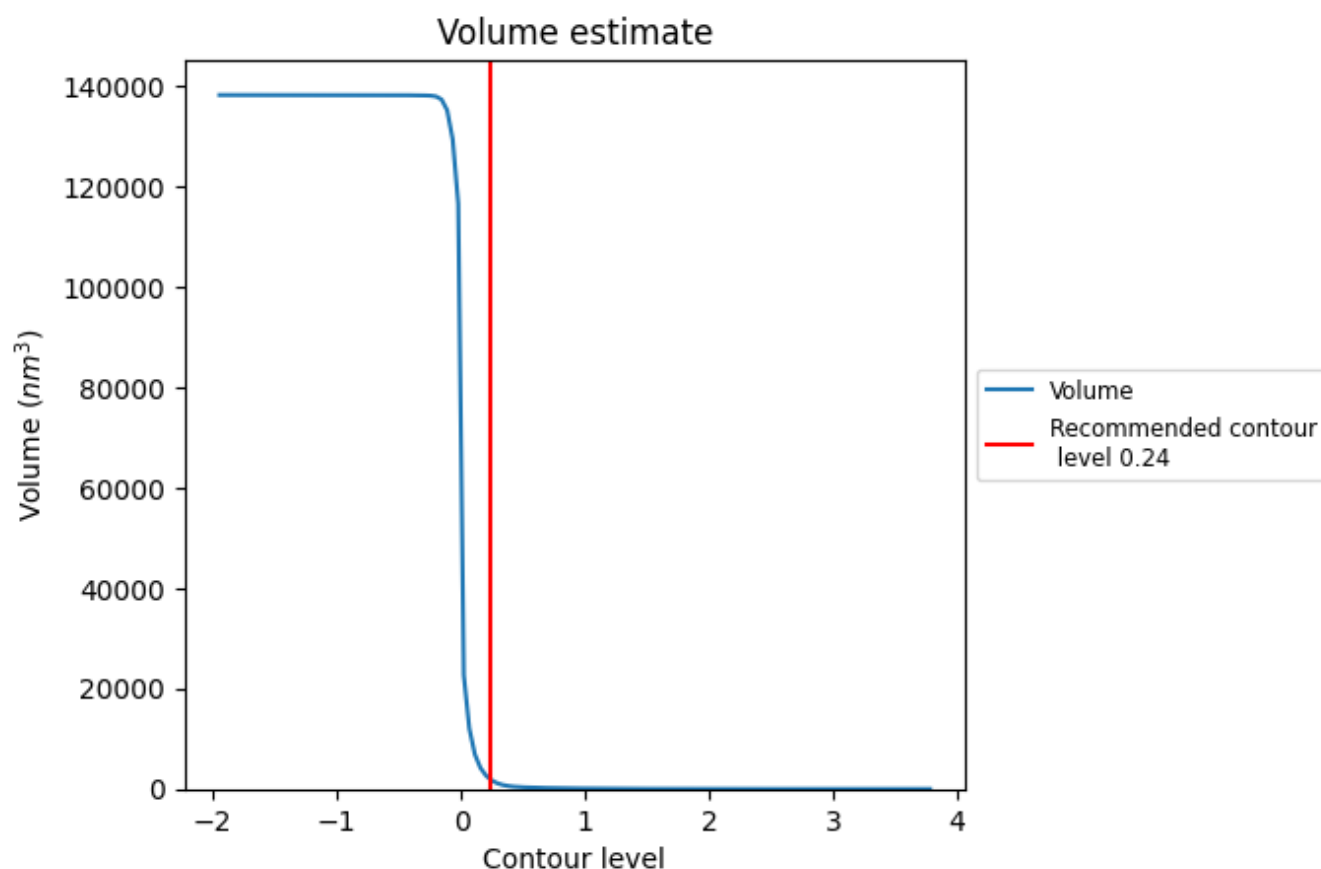
This section contains the results of statistical analysis of the map.

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.

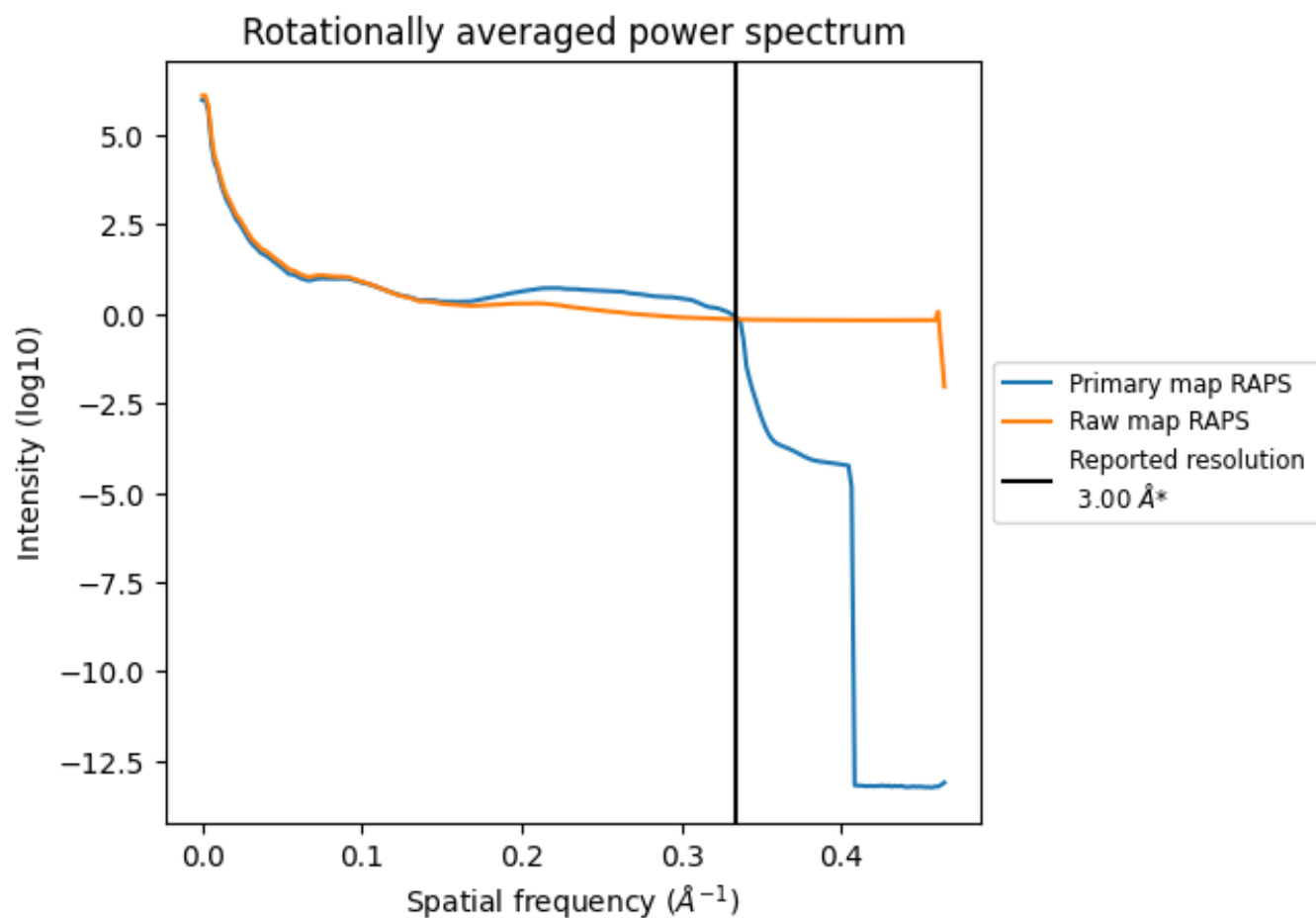
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1878 nm^3 ; this corresponds to an approximate mass of 1697 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

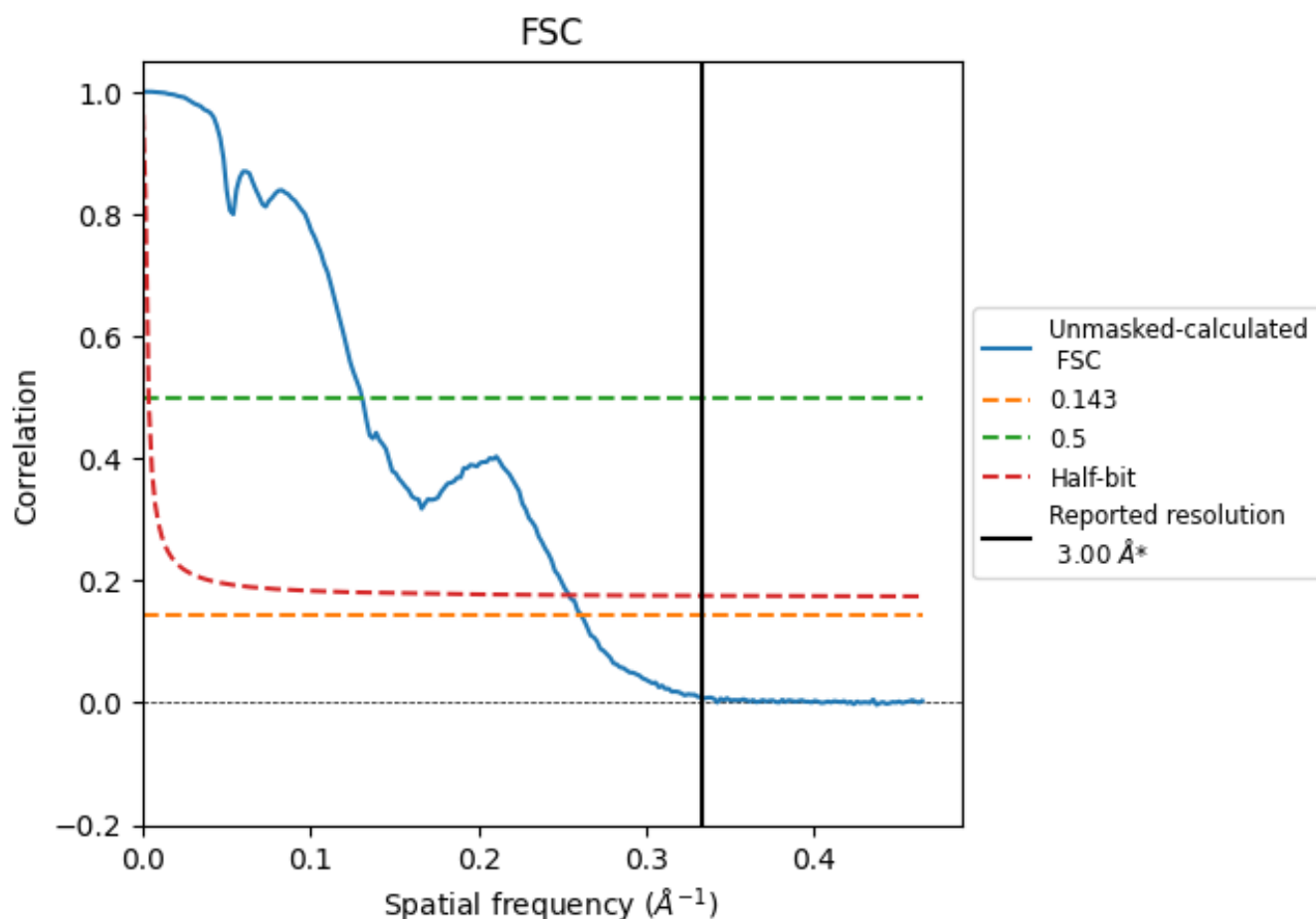


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

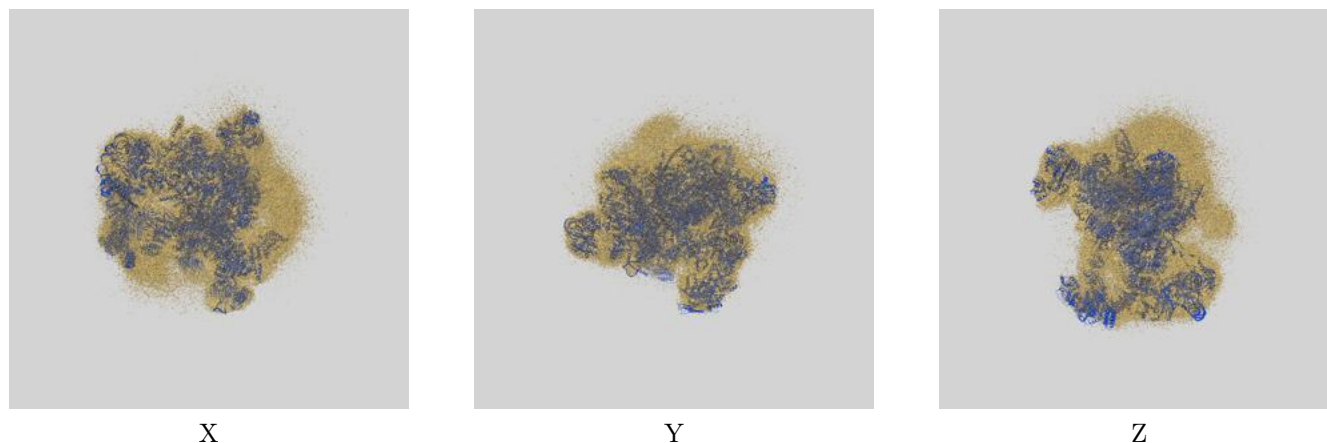
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	7.65	3.94

*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 3.83 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

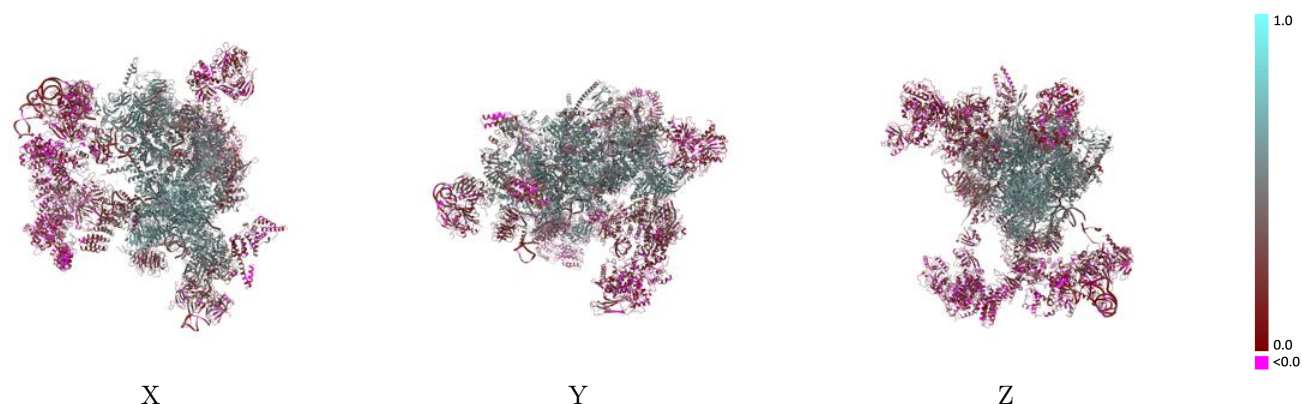
This section contains information regarding the fit between EMDB map EMD-35107 and PDB model 8I0R. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



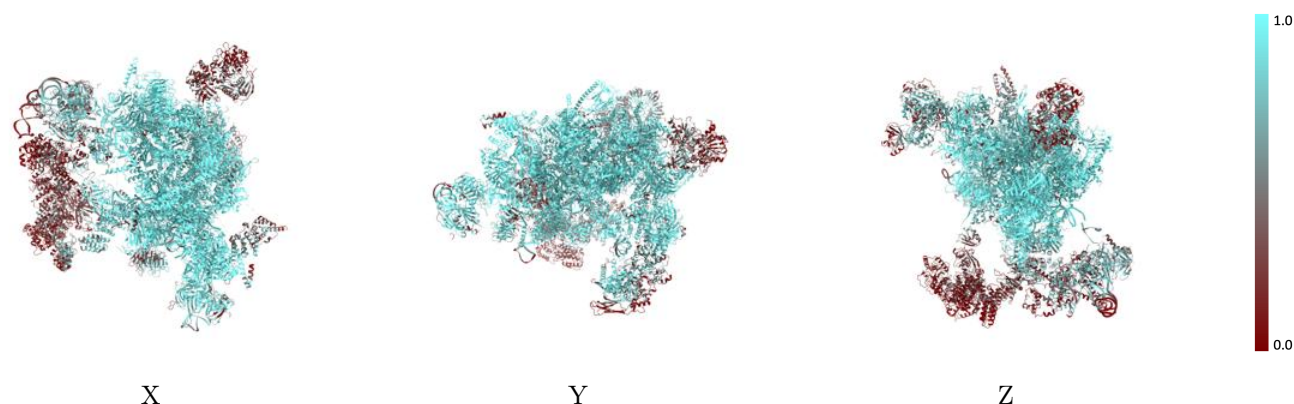
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



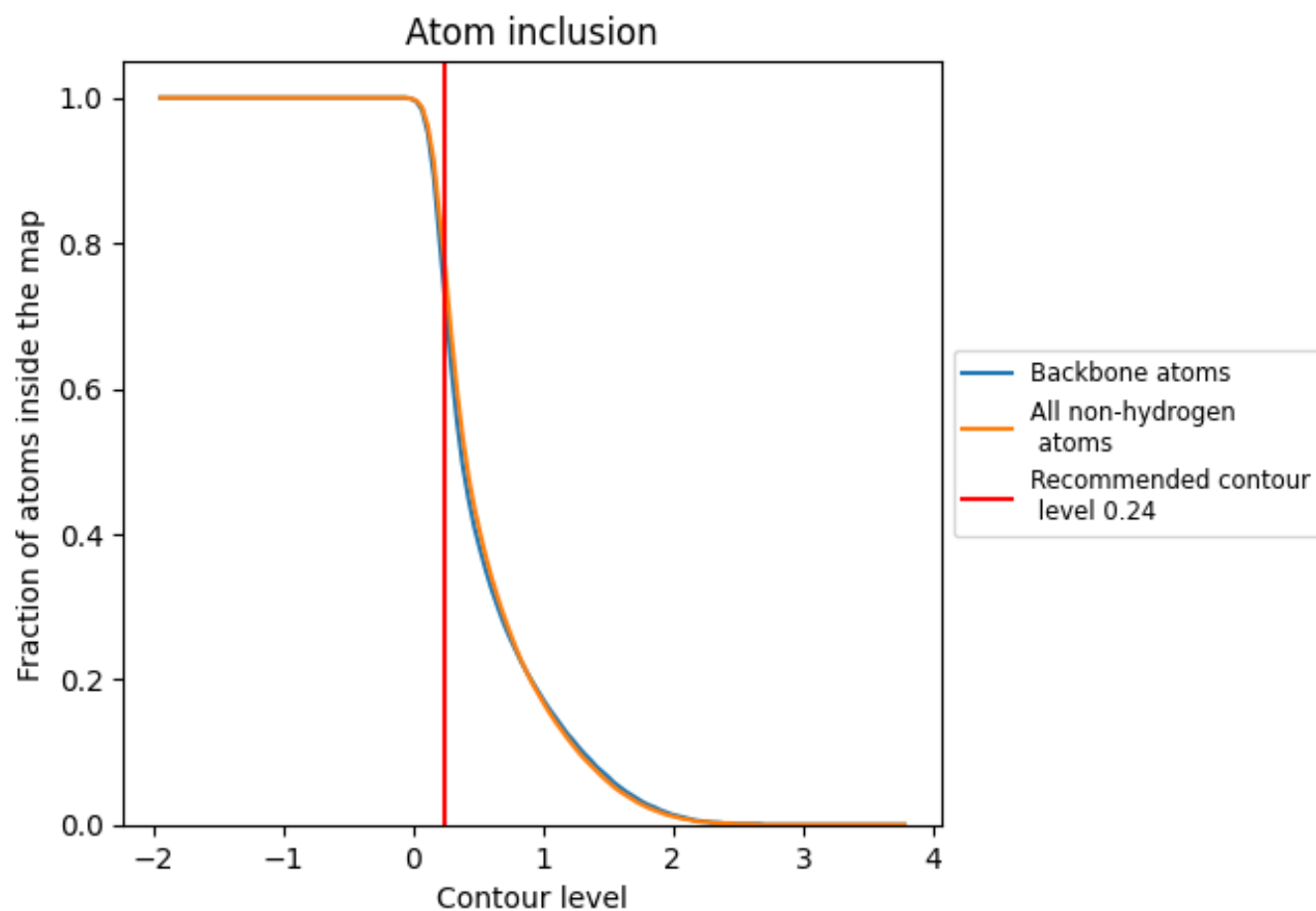
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.24).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 78% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.3880
1	 0.9580	 0.5450
2	 0.8750	 0.4670
3	 0.9680	 0.4970
4	 0.7370	 0.2210
5	 0.9130	 0.5330
6	 0.9390	 0.4230
7	 0.9170	 0.5070
8	 0.9470	 0.4500
9	 0.8880	 0.3600
A	 0.9370	 0.5370
B	 0.9000	 0.3820
C	 0.9660	 0.4770
D	 0.6980	 0.2090
E	 0.5950	 0.2590
F	 0.8920	 0.3750
G	 0.9370	 0.3900
H	 0.6720	 0.2550
I	 0.3100	 0.1380
J	 0.8480	 0.2900
K	 0.9090	 0.5550
L	 0.9780	 0.5670
N	 0.9300	 0.4500
O	 0.6680	 0.2620
P	 0.9550	 0.5210
Q	 0.1020	 0.1460
R	 0.9300	 0.4930
S	 0.2830	 0.1640
T	 0.9920	 0.6000
U	 0.6610	 0.2900
V	 0.7560	 0.3430
W	 0.8680	 0.4140
X	 0.9540	 0.4960
Y	 0.9690	 0.5740
Z	 0.8500	 0.4850



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Chain	Atom inclusion	Q-score
a	 0.7670	 0.2450
b	 0.8720	 0.2450
c	 0.7420	 0.2020
d	 0.8040	 0.2300
e	 0.8130	 0.2130
f	 0.7330	 0.3120
g	 0.8980	 0.3170
h	 0.6140	 0.1890
i	 0.6680	 0.1730
j	 0.6650	 0.2140
k	 0.5880	 0.1740
l	 0.5570	 0.1680
m	 0.6370	 0.2450
n	 0.5450	 0.1990
o	 0.4720	 0.1700
p	 0.6100	 0.1980
u	 0.2810	 0.1830
v	 0.7100	 0.4520
w	 0.5330	 0.2690
y	 0.2800	 0.1760
z	 0.9840	 0.5600