Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:49 AM JST

PDB ID	:	7ENC / pdb_00007enc
EMDB ID	:	EMD-31207
Title	:	TFIID-based PIC-Mediator holo-complex in fully-assembled state (hPIC-MED)
Authors	:	Chen, X.; Qi, Y.; Wang, X.; Wu, Z.; Yin, X.; Li, J.; Liu, W.; Xu, Y.
Deposited on	:	2021-04-16
Resolution	:	4.13 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

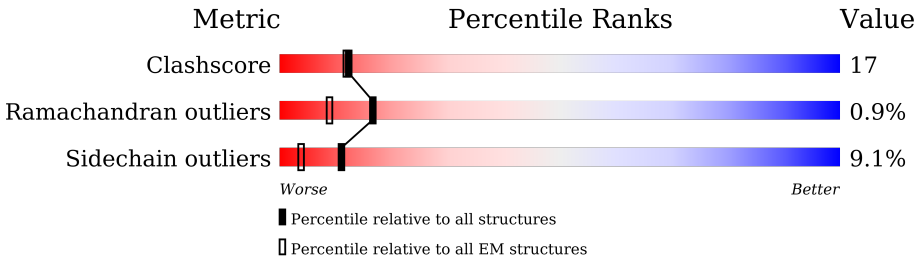
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

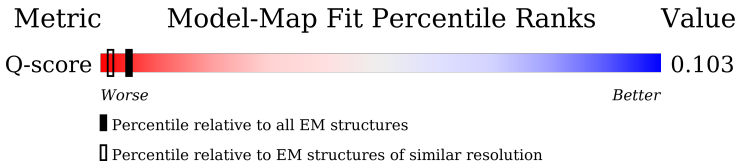
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.13 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.





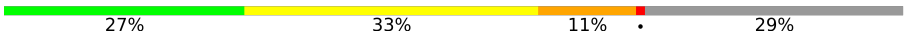
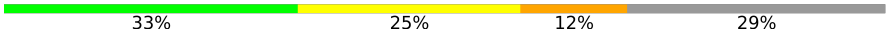
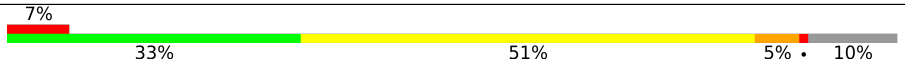
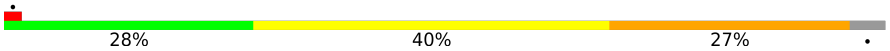
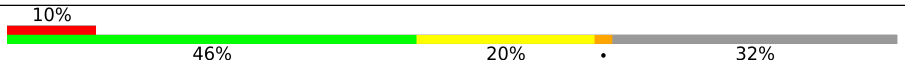
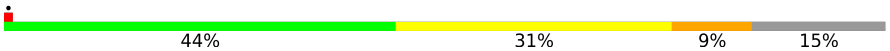
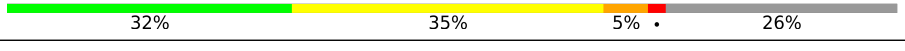
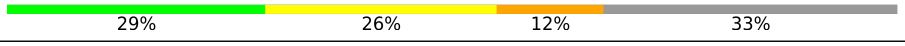
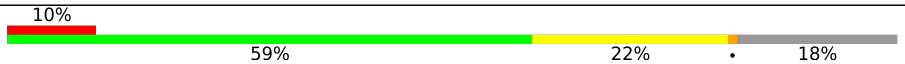
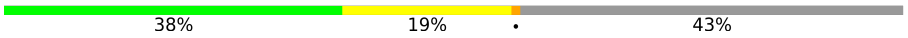
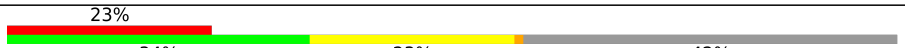
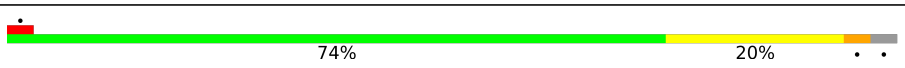
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5607 (3.63 - 4.63)

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 <=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	1581	30% 17% 9% • 70%
2	m	131	47% 38% 15%
3	d	270	14% 24% 24% 10% 41%
4	f	246	32% 28% 6% • 32%

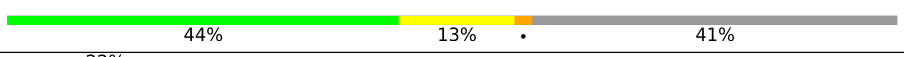
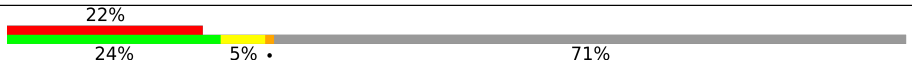
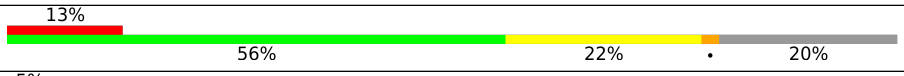
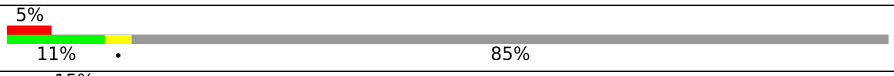
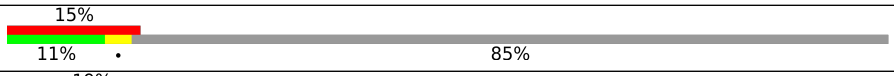
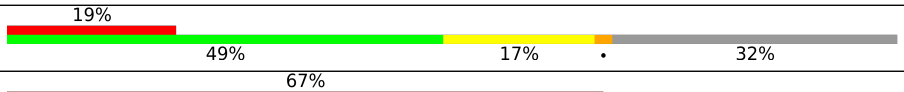
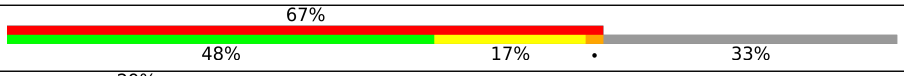
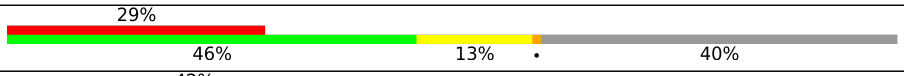
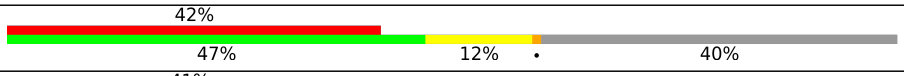
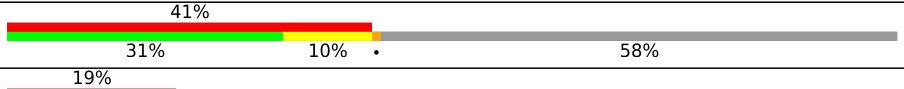
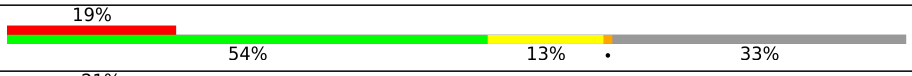
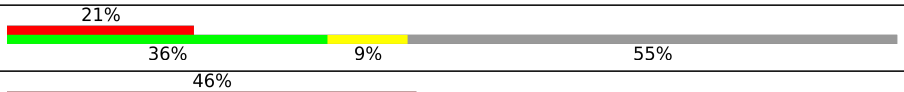
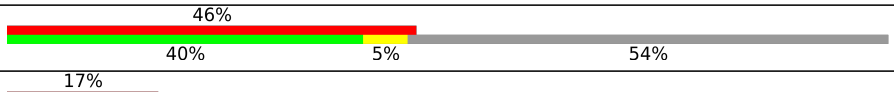
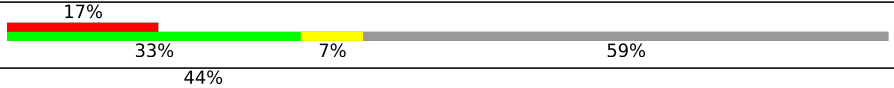
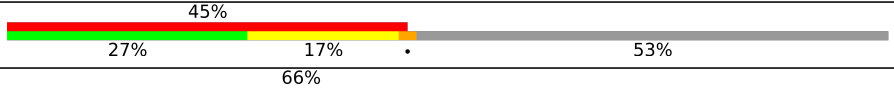
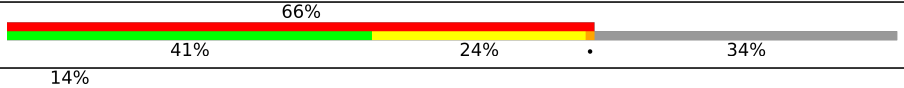
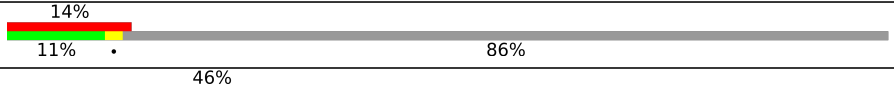
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Mol	Chain	Length	Quality of chain
5	g	233	
6	h	268	
7	r	208	
8	t	212	
9	j	135	
10	k	117	
11	n	1454	
12	q	651	
13	s	244	
14	u	144	
15	v	200	
16	z	600	
17	c	311	
18	e	178	
19	b	200	
20	l	178	
21	o	788	
22	i	146	
23	0	309	
24	8	346	
25	9	323	
26	1	548	
27	2	395	
28	3	308	
29	4	462	

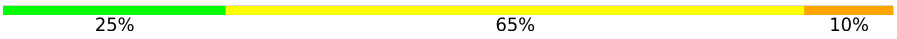
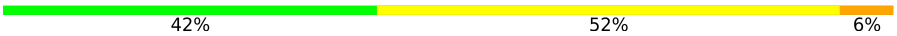
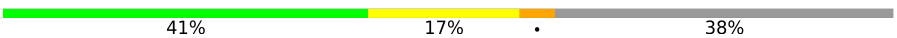
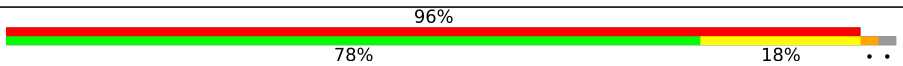
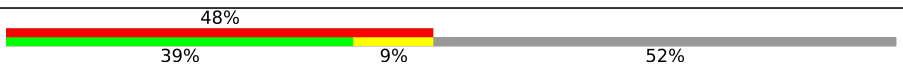
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Mol	Chain	Length	Quality of chain
30	5	71	
31	6	782	
32	7	760	
33	EA	439	
34	EB	291	
35	DA	1872	
36	DB	1199	
37	DD	1085	
37	Dd	1085	
38	DE	800	
38	De	800	
39	DF	677	
39	Df	677	
40	DG	349	
41	DH	310	
42	DI	264	
42	Di	264	
43	DJ	218	
43	Dj	218	
44	DL	161	
44	Dl	161	
45	Dc	929	
46	Dk	211	
47	Dm	124	
48	DO	109	

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Mol	Chain	Length	Quality of chain
49	DP	339	
50	DQ	307	
51	BA	316	
52	FB	249	
53	X	69	
54	Y	69	
55	PA	1970	
56	PB	1174	
57	PC	275	
58	PD	142	
59	PE	210	
60	PF	127	
61	PG	172	
62	PH	150	
63	PI	125	
64	PJ	67	
65	PK	117	
66	PL	58	
67	FA	517	
68	w	1368	
69	x	989	
70	p	841	

2 Entry composition (i)

There are 73 unique types of molecules in this entry. The entry contains 171177 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 Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	469	3570	2271	614	661	24	0	0

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	m	112	983	641	172	165	5	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	158	1264	788	227	243	6	0	0

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	167	1329	851	231	242	5	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	g	166	1382	880	244	248	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	10	ALA	LEU	conflict	UNP O43513
g	11	LEU	PRO	conflict	UNP O43513

- Molecule 6 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	190	Total	C	N	O	S	0	0
			1486	925	262	295	4		

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	191	Total	C	N	O	S	0	0
			1528	969	270	274	15		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	t	193	Total	C	N	O	S	0	0
			1499	955	247	280	17		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	122	Total	C	N	O	S	0	0
			1001	636	174	187	4		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	112	Total	C	N	O	S	0	0
			879	537	163	175	4		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	994	Total	C	N	O	S	0	0
			7241	4576	1293	1334	38		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	133	LEU	ALA	conflict	UNP O60244

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	552	Total	C	N	O	S	0	0
			4261	2691	764	789	17		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	77	Total	C	N	O	S	0	0
			485	300	87	96	2		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	u	107	Total	C	N	O	S	0	0
			792	492	132	165	3		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	v	134	Total	C	N	O	S	0	0
			1083	668	185	226	4		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	z	97	Total	C	N	O	S	0	0
			765	472	136	154	3		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	255	Total	C	N	O	S	0	0
			2069	1314	370	374	11		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	102	Total	C	N	O	S	0	0
			832	520	146	163	3		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	126	Total	C	N	O	S	0	0
			1040	649	191	193	7		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	o	156	Total	C	N	O	S	0	0
			1221	780	212	222	7		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	62	Total	C	N	O	S	0	0
			520	329	92	94	5		

- Molecule 23 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	306	Total	C	N	O	S	0	0
			2255	1404	399	441	11		

- Molecule 24 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	8	299	Total	C	N	O	S	0	0
			2378	1535	406	426	11		

- Molecule 25 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	9	287	Total	C	N	O	S	0	0
			2307	1477	398	417	15		

- Molecule 26 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	405	Total	C	N	O	S	0	0
			2634	1640	486	501	7		

- Molecule 27 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	331	Total	C	N	O	S	0	0
			2534	1597	441	470	26		

- Molecule 28 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	263	Total	C	N	O	S	0	0
			2065	1323	344	379	19		

- Molecule 29 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	449	Total	C	N	O	S	0	0
			3579	2303	624	638	14		

- Molecule 30 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	54	Total	C	N	O	S	0	0
			428	277	67	82	2		

- Molecule 31 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	606	Total	C	N	O	S	0	0
			4880	3117	849	884	30		

- Molecule 32 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	734	Total	C	N	O	S	0	0
			5833	3727	1022	1055	29		

- Molecule 33 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	EA	179	Total	C	N	O	S	0	0
			1476	932	261	272	11		

- Molecule 34 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	EB	172	Total	C	N	O	S	0	0
			1404	893	243	264	4		

- Molecule 35 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	DA	550	Total	C	N	O	S	0	0
			4511	2882	782	820	27		

- Molecule 36 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	DB	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 37 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	DD	159	Total	C	N	O	S	0	0
			1330	830	248	249	3		
37	Dd	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 38 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	DE	546	Total	C	N	O	S	0	0
			4364	2766	757	820	21		
38	De	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 39 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	DF	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
39	Df	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	DG	145	Total	C	N	O	S	0	0
			1180	748	217	211	4		

- Molecule 41 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	DH	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 42 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	DI	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
42	Di	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 43 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	DJ	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
43	Dj	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 44 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	DL	75	Total	C	N	O	S	0	0
			614	384	107	120	3		
44	Dl	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 45 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Dc	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 46 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Dk	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 47 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Dm	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 48 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	DO	97	Total	C	N	O	S	0	0
			771	491	133	145	2		

- Molecule 49 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DP	177	Total	C	N	O	S	0	0
			1412	918	249	238	7		

- Molecule 50 is a protein called TFIIA-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	DQ	122	Total	C	N	O	S	0	0
			996	623	162	207	4		

- Molecule 51 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BA	251	Total	C	N	O	S	0	0
			1939	1214	344	364	17		

- Molecule 52 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	FB	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 53 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	69	Total	C	N	O	P	0	0
			1429	672	279	409	69		

- Molecule 54 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	69	Total	C	N	O	P	0	0
			1400	664	248	419	69		

- Molecule 55 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	PA	1474	Total	C	N	O	S	0	0
			11655	7333	2070	2180	72		

- Molecule 56 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	PB	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 57 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	PC	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 58 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	PD	129	Total	C	N	O	S	0	0
			1021	643	174	200	4		

- Molecule 59 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	PE	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 60 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	PF	79	Total	C	N	O	S	0	0
			635	406	108	116	5		

- Molecule 61 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	PG	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 62 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	PH	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 63 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	PI	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 64 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	PJ	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 65 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	PK	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 66 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PL	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 67 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	FA	134	Total	C	N	O	S	0	0
			1101	698	199	202	2		

- Molecule 68 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	w	1334	Total	C	N	O	S	0	0
			10772	6965	1827	1909	71		

- Molecule 69 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	x	896	Total	C	N	O	S	0	0
			7050	4516	1188	1292	54		

- Molecule 70 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	p	406	Total	C	N	O	S	0	0
			3124	1982	536	585	21		

- Molecule 71 is ZINC ION (CCD ID: ZN) (formula: Zn).

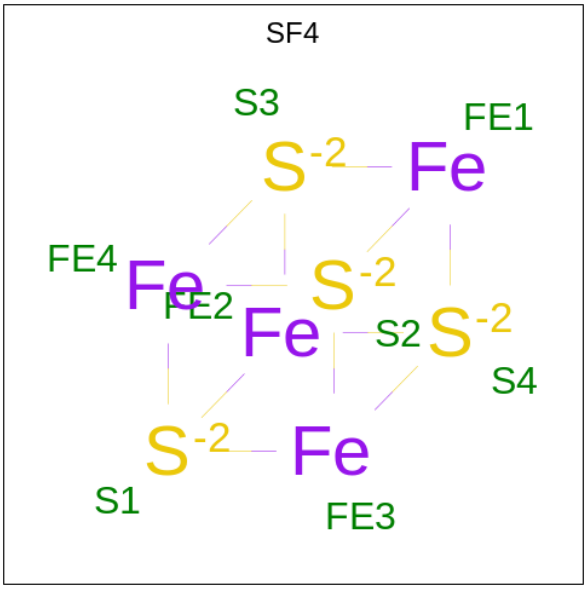
Mol	Chain	Residues	Atoms		AltConf
71	0	2	Total	Zn	0
			2	2	
71	2	3	Total	Zn	0
			3	3	
71	3	1	Total	Zn	0
			1	1	
71	EA	1	Total	Zn	0
			1	1	
71	BA	1	Total	Zn	0
			1	1	
71	PA	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
71	PB	1	Total Zn 1 1	0
71	PC	1	Total Zn 1 1	0
71	PI	2	Total Zn 2 2	0
71	PJ	1	Total Zn 1 1	0
71	PL	1	Total Zn 1 1	0

- Molecule 72 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
72	7	1	Total Fe S 8 4 4	0

- Molecule 73 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
73	PA	1	Total Mg 1 1	0

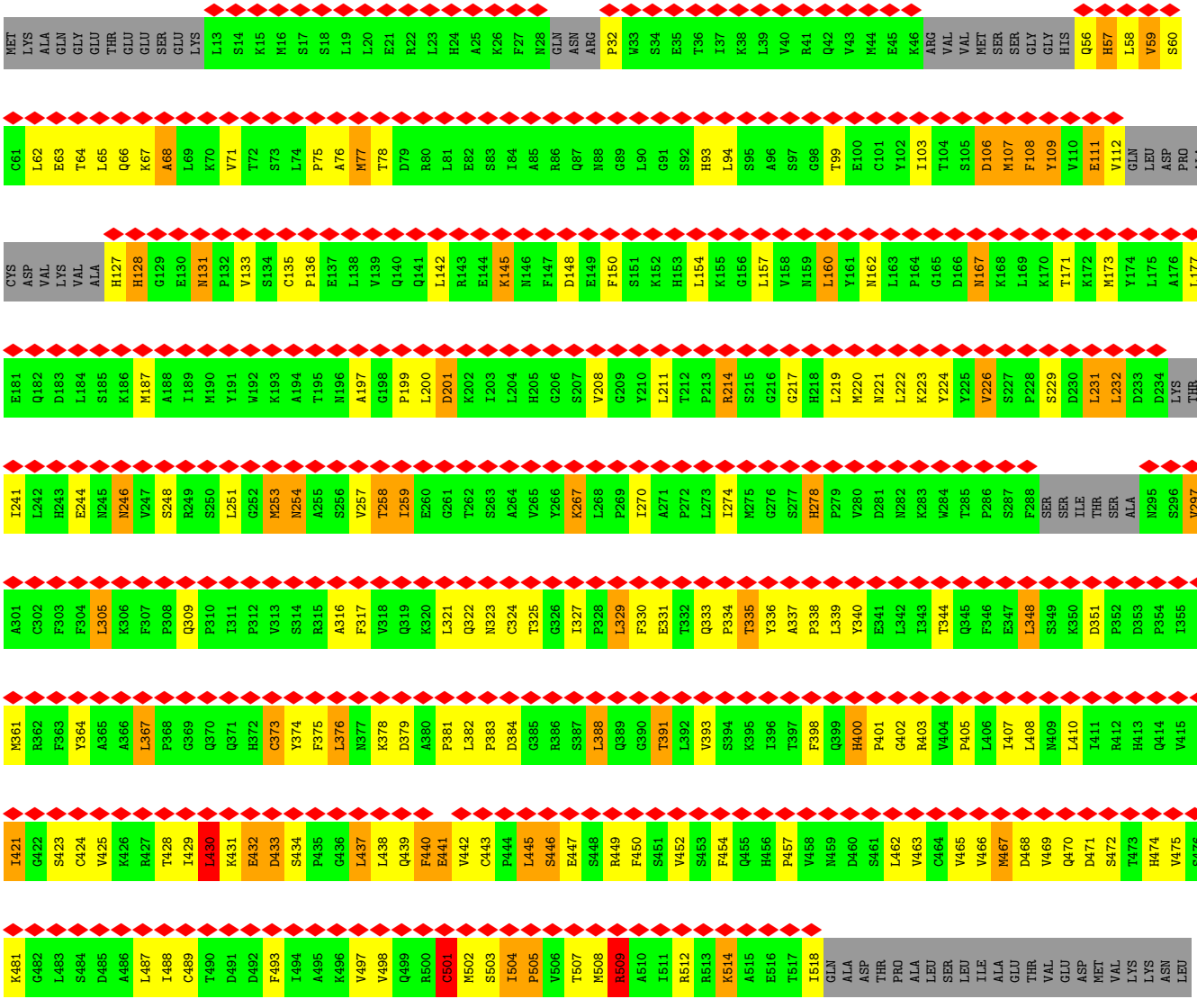
3 Residue-property plots (i)

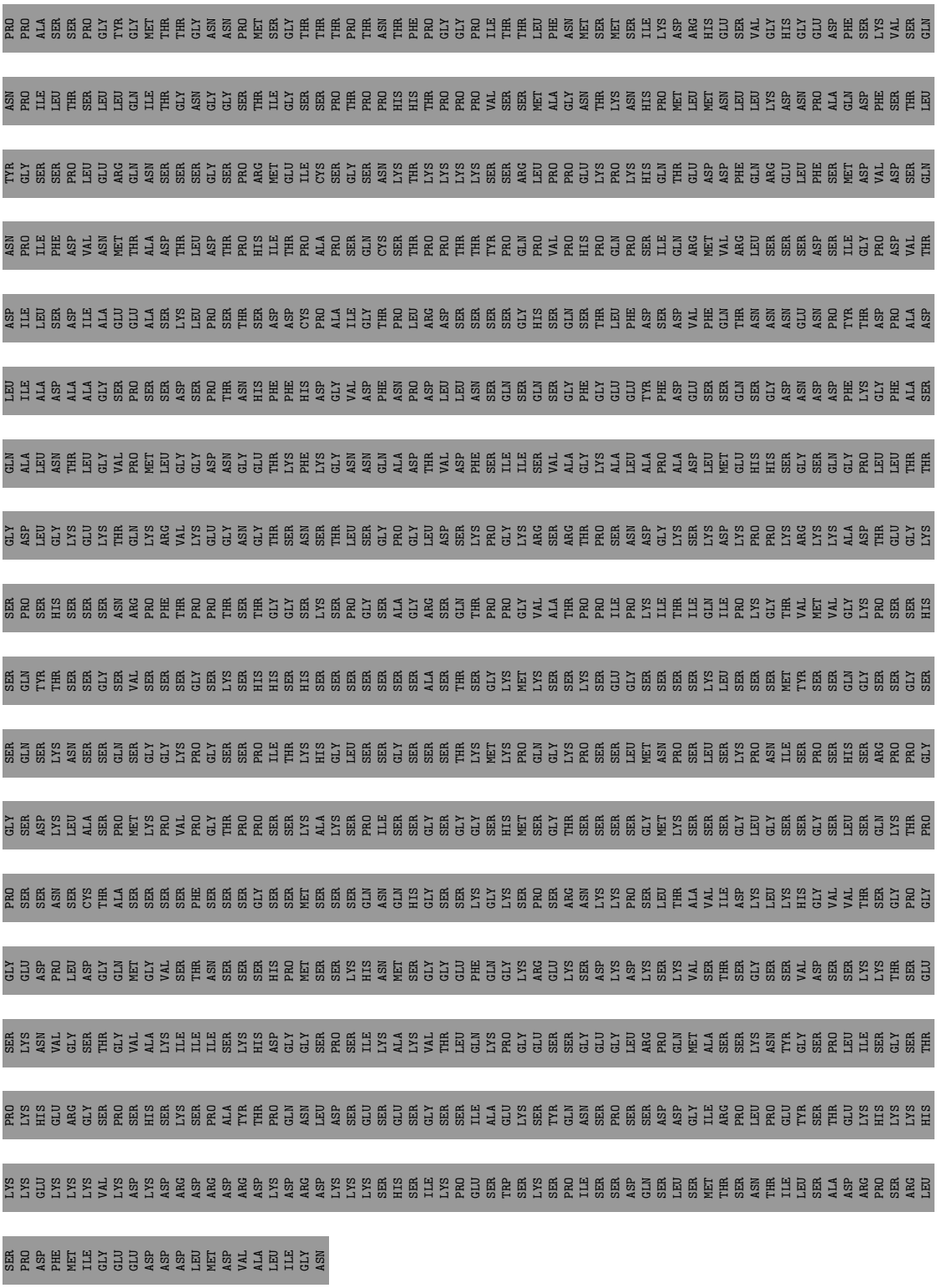
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mediator of RNA polymerase II transcription subunit 1

Chain a:



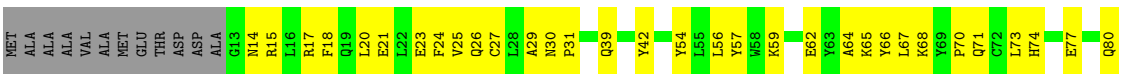


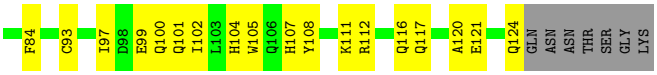


• Molecule 2: Mediator of RNA polymerase II transcription subunit 31

Chain m:

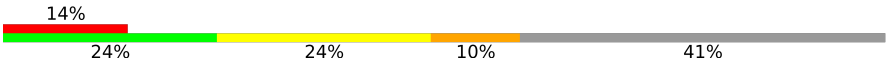


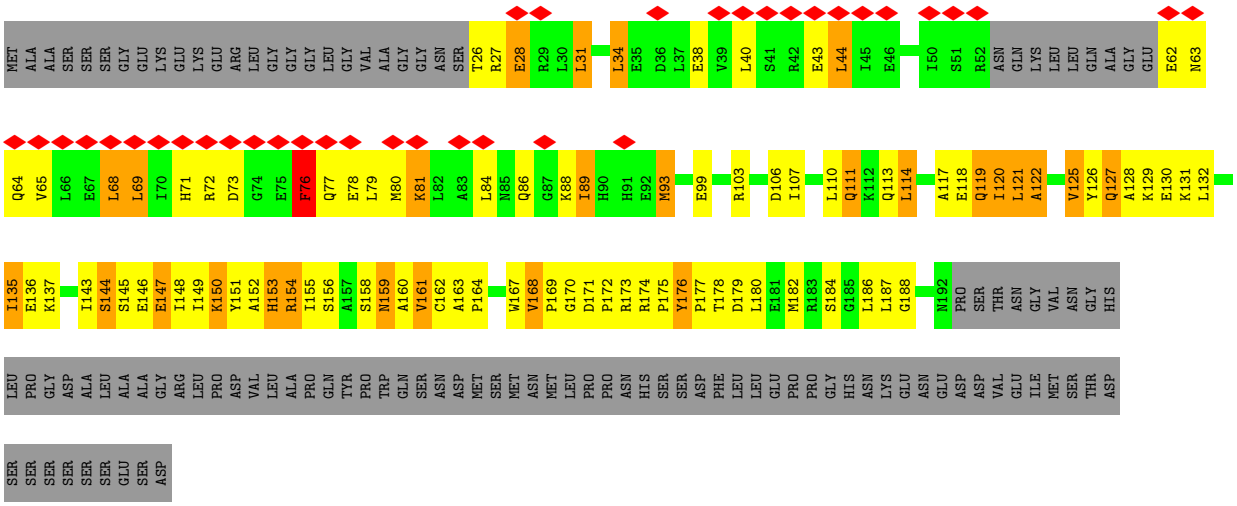




• Molecule 3: Mediator of RNA polymerase II transcription subunit 4

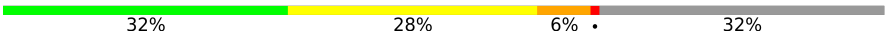
Chain d:

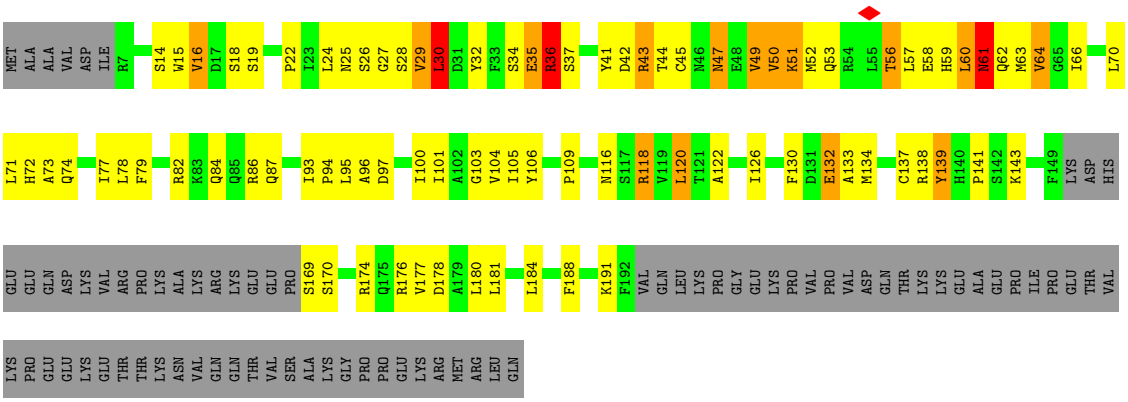




• Molecule 4: Mediator of RNA polymerase II transcription subunit 6

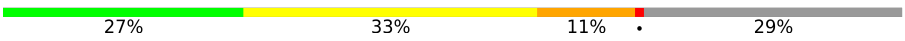
Chain f:

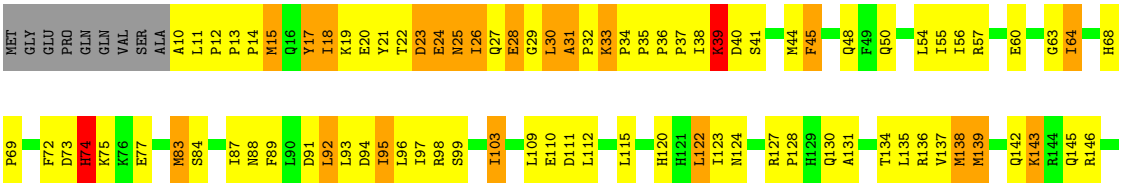


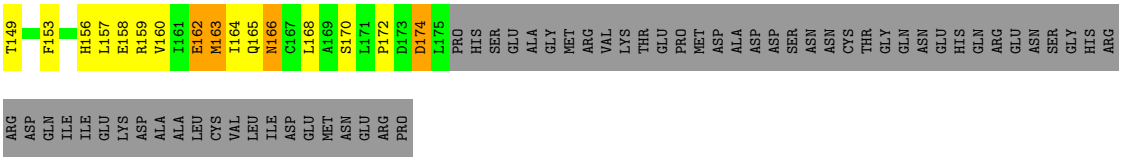


• Molecule 5: Mediator of RNA polymerase II transcription subunit 7

Chain g:

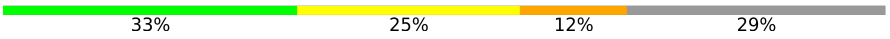


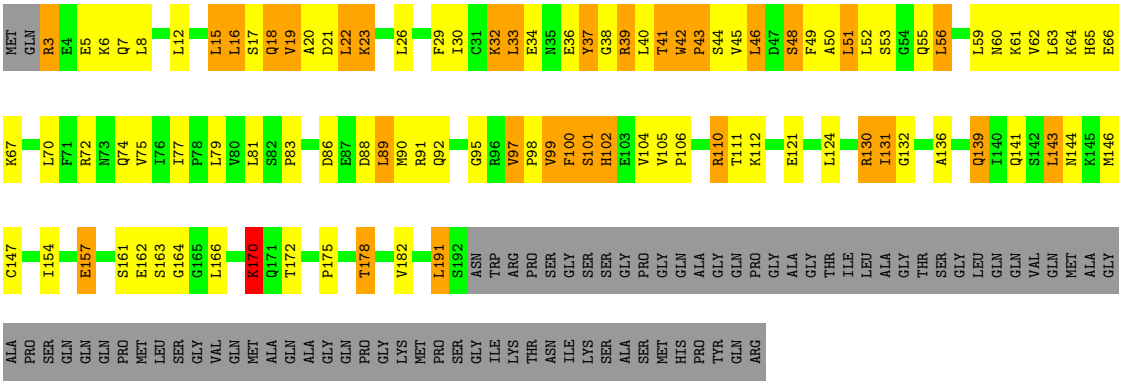




• Molecule 6: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

Chain h:

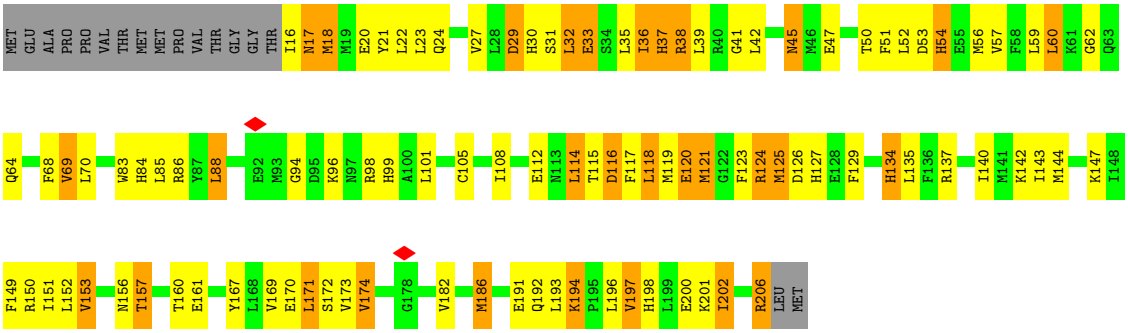




• Molecule 7: Mediator of RNA polymerase II transcription subunit 18

Chain r:

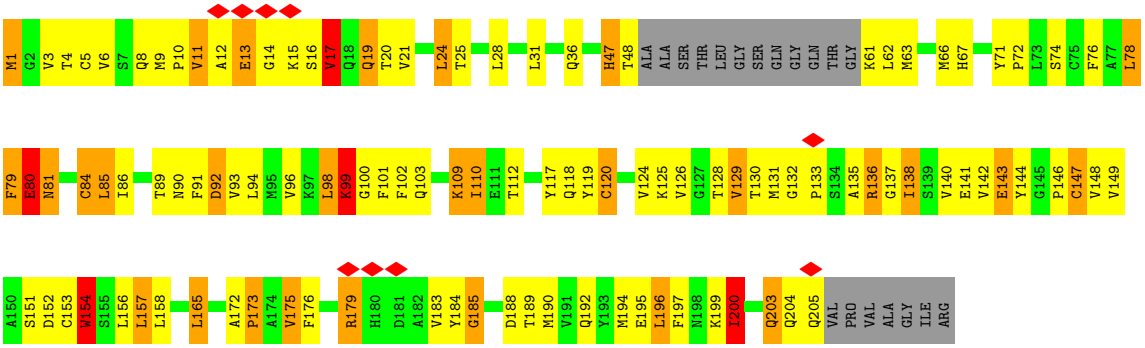




• Molecule 8: Mediator of RNA polymerase II transcription subunit 20

Chain t:

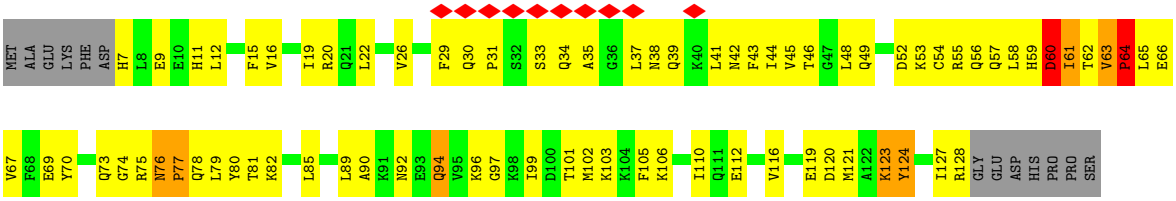




• Molecule 9: Mediator of RNA polymerase II transcription subunit 10

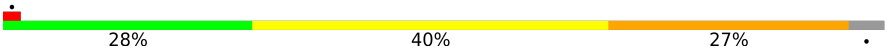
Chain j:

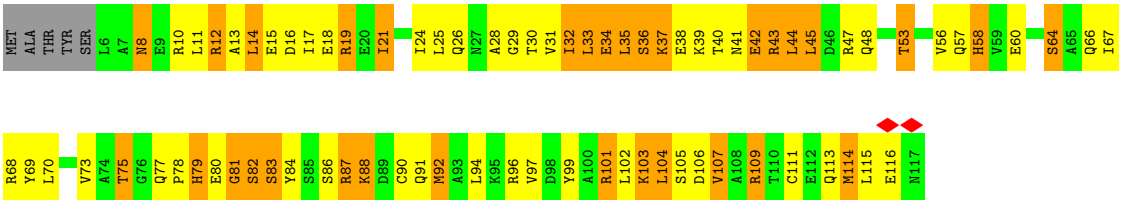




• Molecule 10: Mediator of RNA polymerase II transcription subunit 11

Chain k:

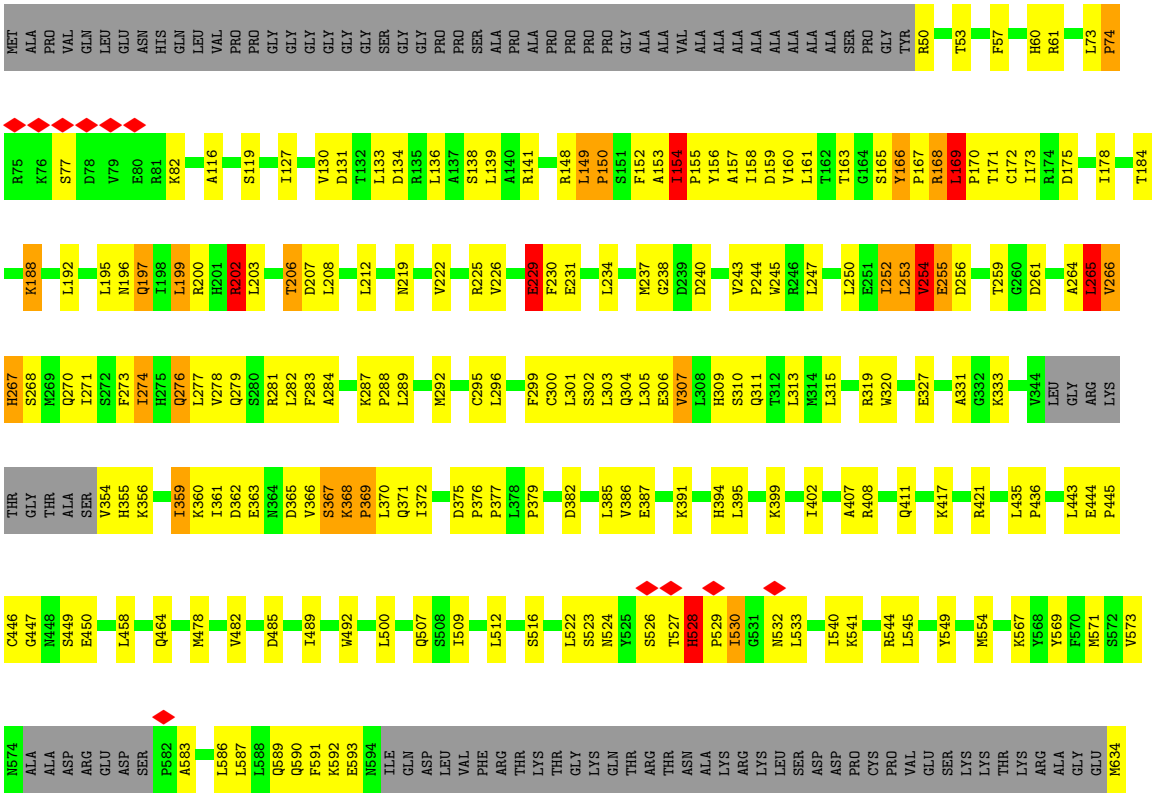


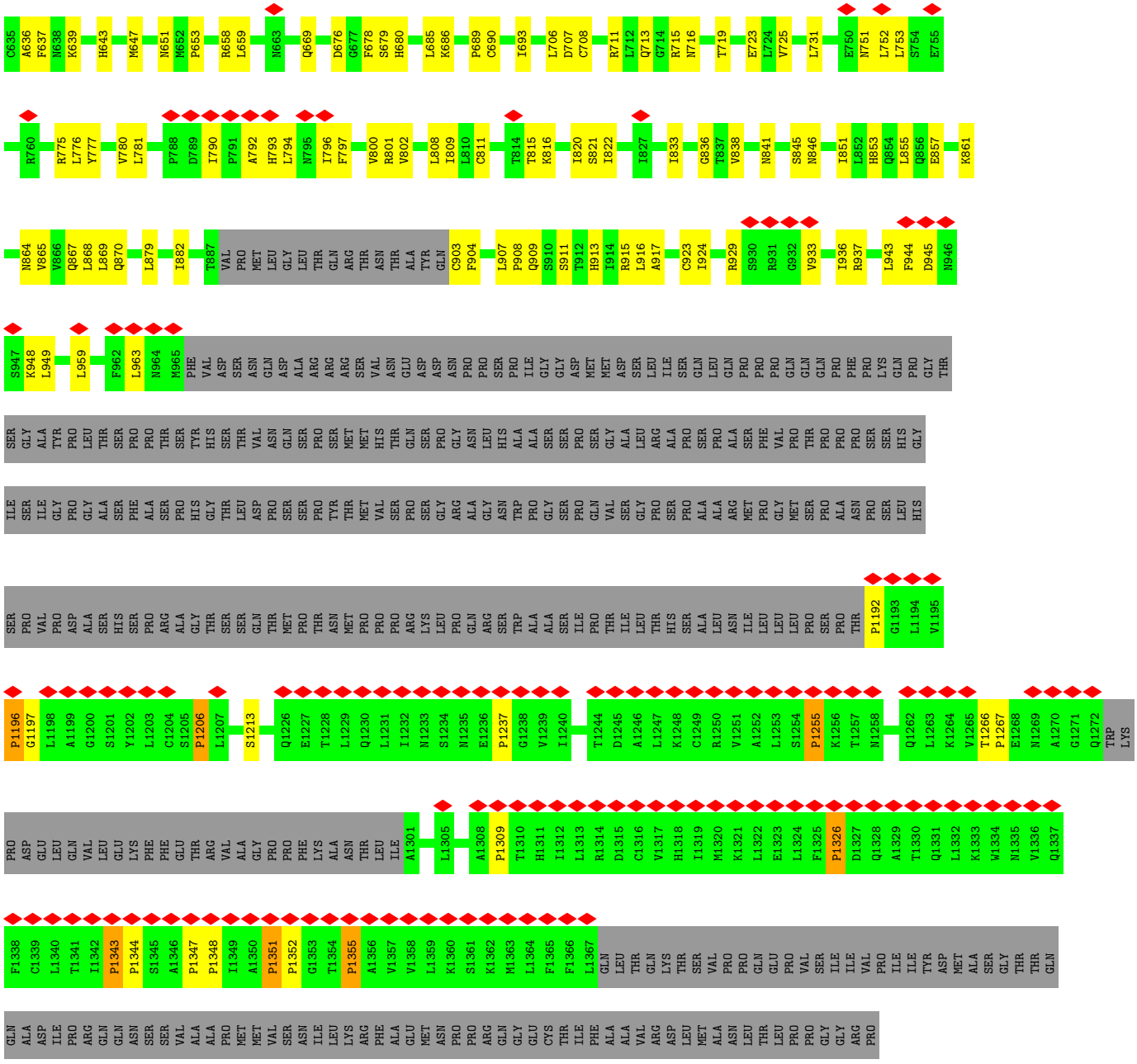


• Molecule 11: Mediator of RNA polymerase II transcription subunit 14

Chain n:



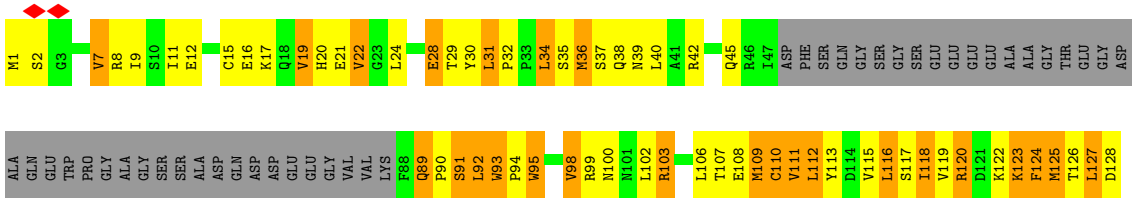


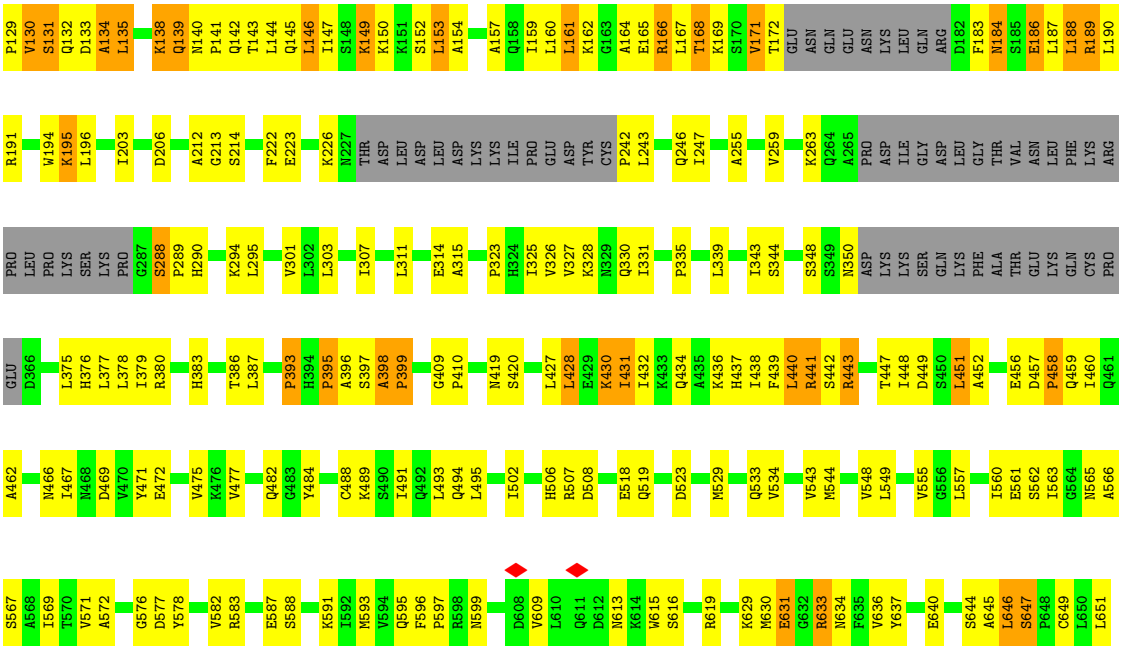


• Molecule 12: Mediator of RNA polymerase II transcription subunit 17

Chain q:



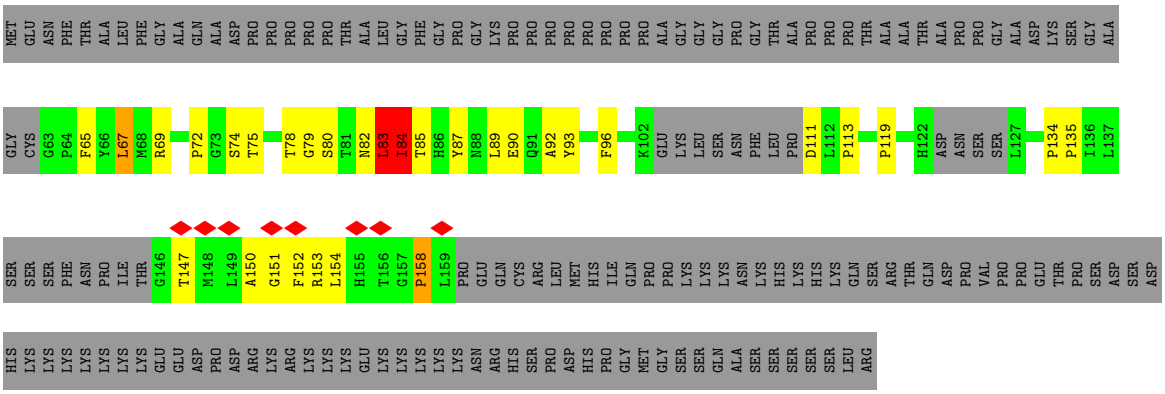




• Molecule 13: Mediator of RNA polymerase II transcription subunit 19

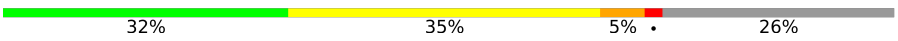
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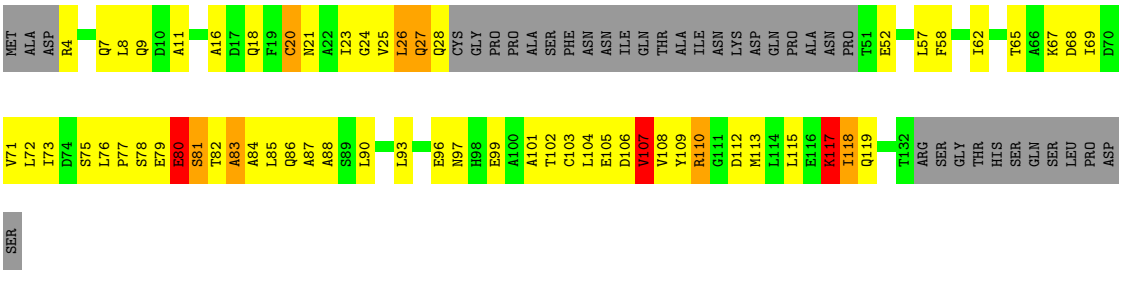




• Molecule 14: Mediator of RNA polymerase II transcription subunit 21

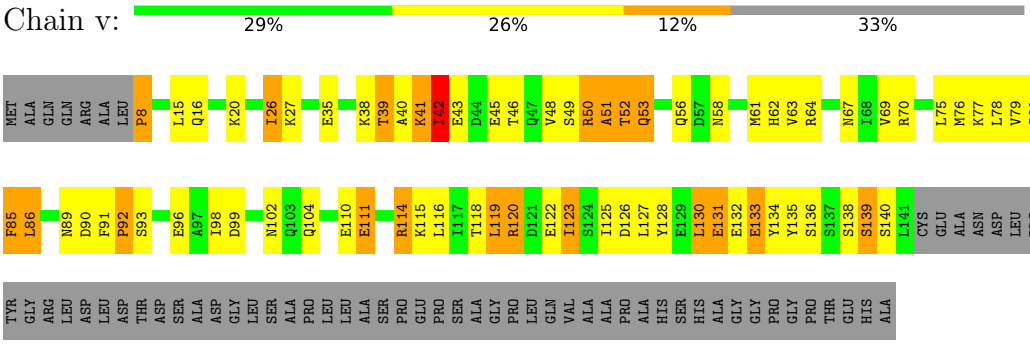
Chain u:





• Molecule 15: Mediator of RNA polymerase II transcription subunit 22

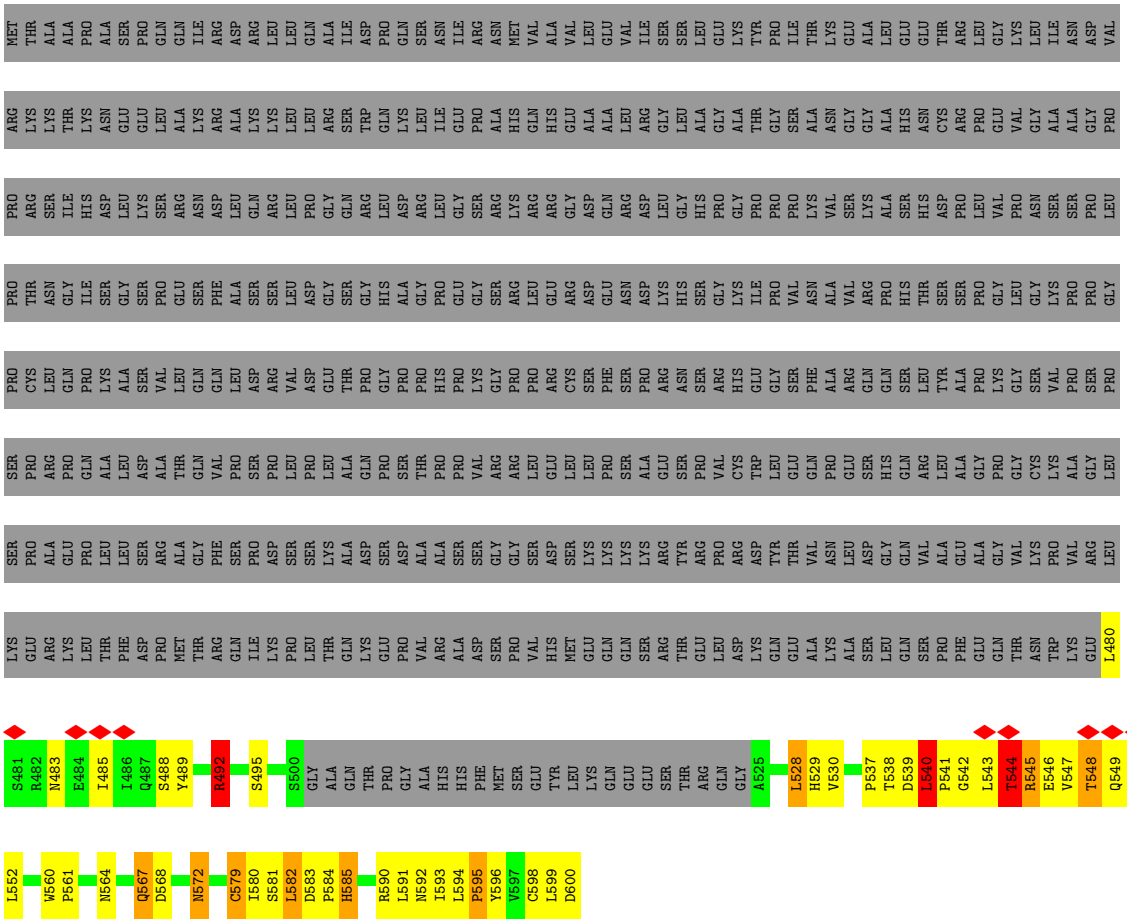
Chain v:



• Molecule 16: Mediator of RNA polymerase II transcription subunit 26

Chain z:

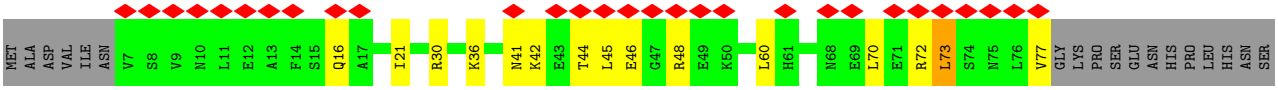


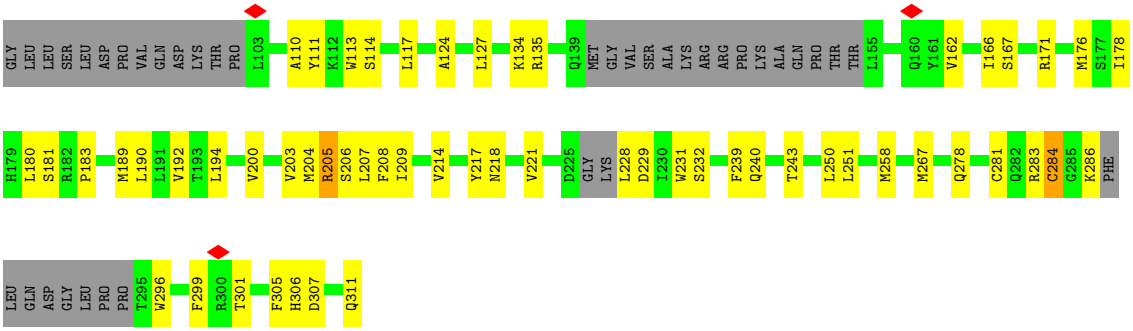


• Molecule 17: Mediator of RNA polymerase II transcription subunit 27

Chain c:

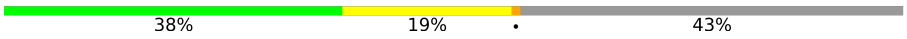


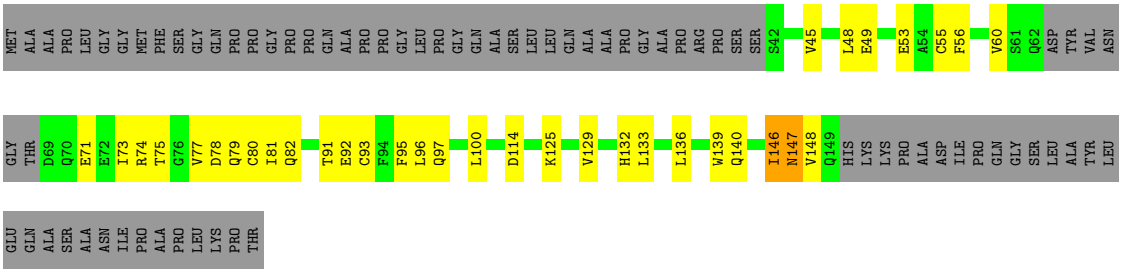




• Molecule 18: Mediator of RNA polymerase II transcription subunit 28

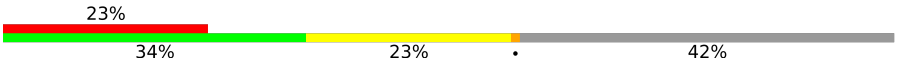
Chain e:

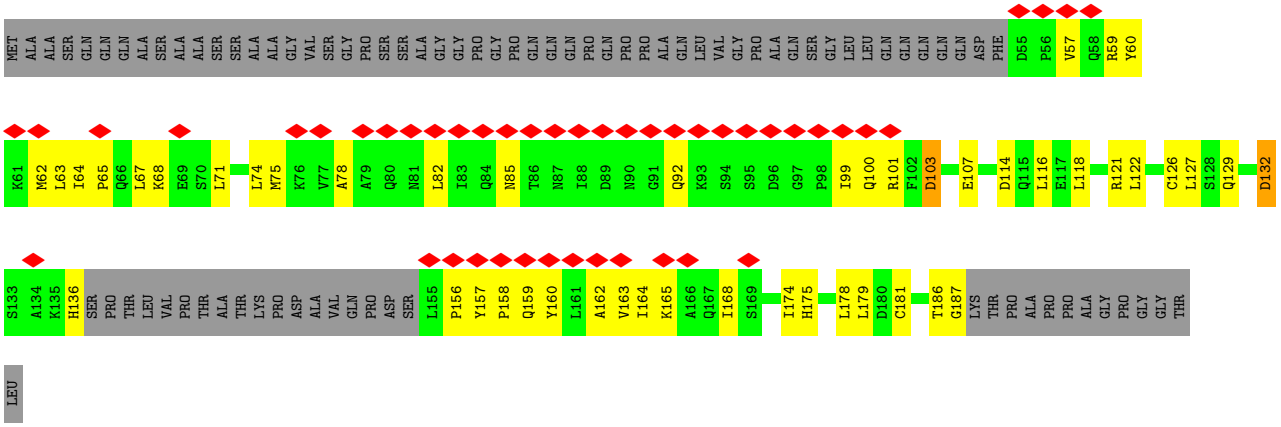




• Molecule 19: Mediator of RNA polymerase II transcription subunit 29

Chain b:

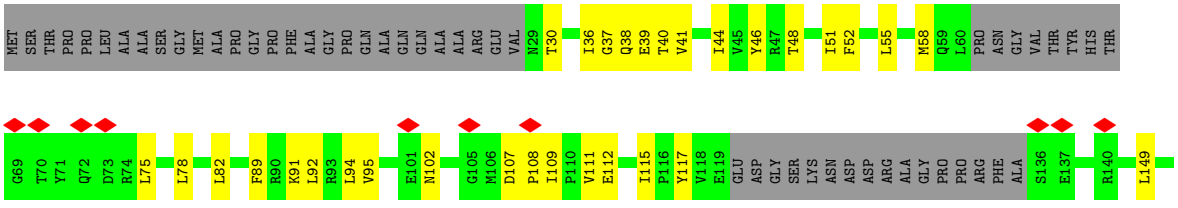




• Molecule 20: Mediator of RNA polymerase II transcription subunit 30

Chain l:



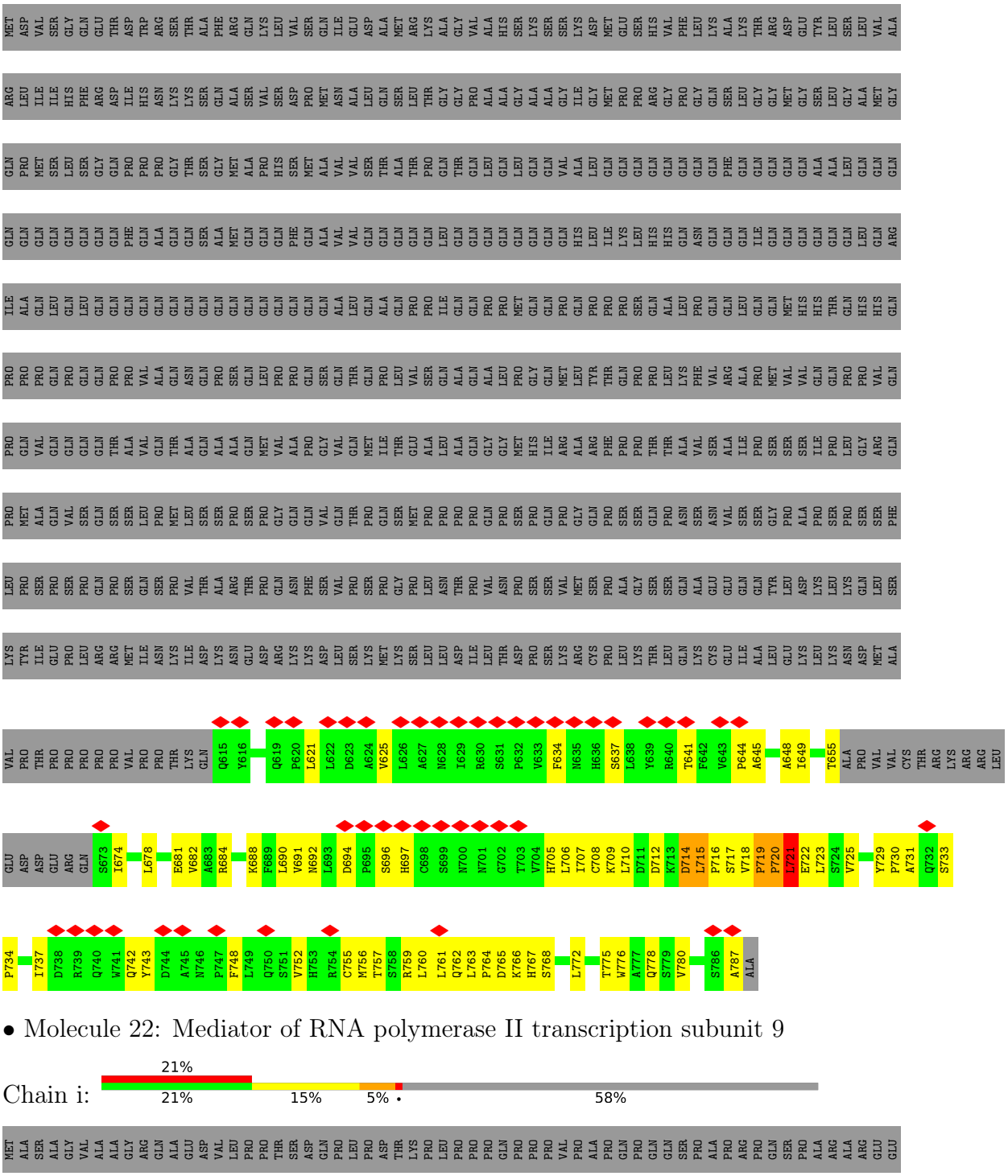




• Molecule 21: Mediator of RNA polymerase II transcription subunit 15

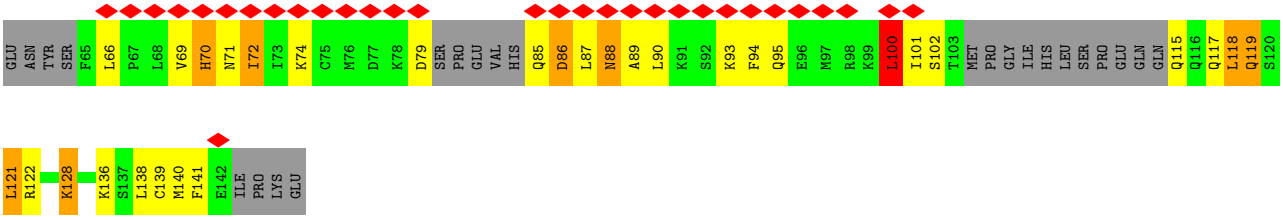
Chain o:





• Molecule 22: Mediator of RNA polymerase II transcription subunit 9

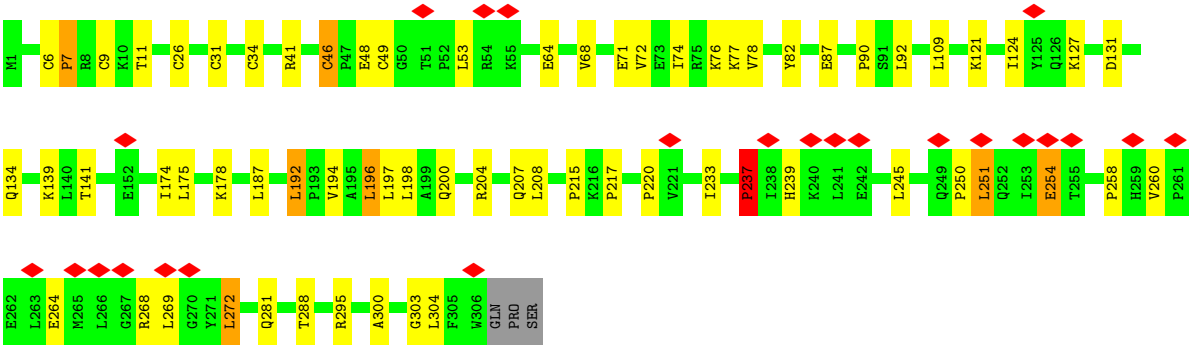
Chain i:



• Molecule 23: CDK-activating kinase assembly factor MAT1

Chain 0:

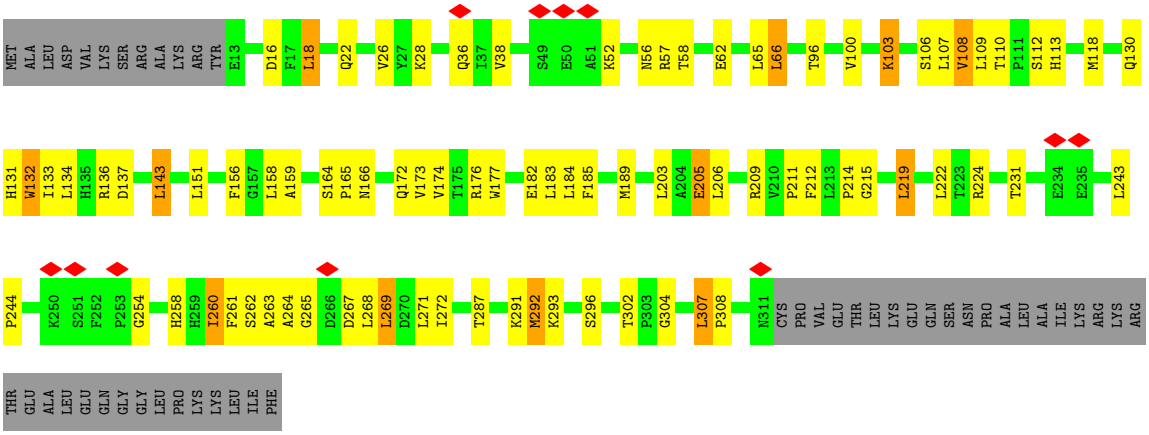




• Molecule 24: Cyclin-dependent kinase 7

Chain 8:

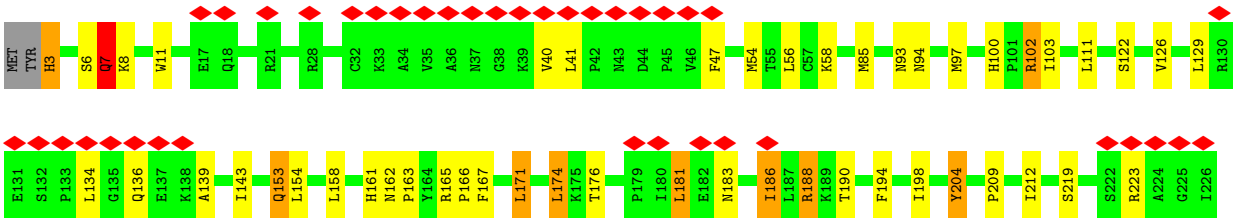


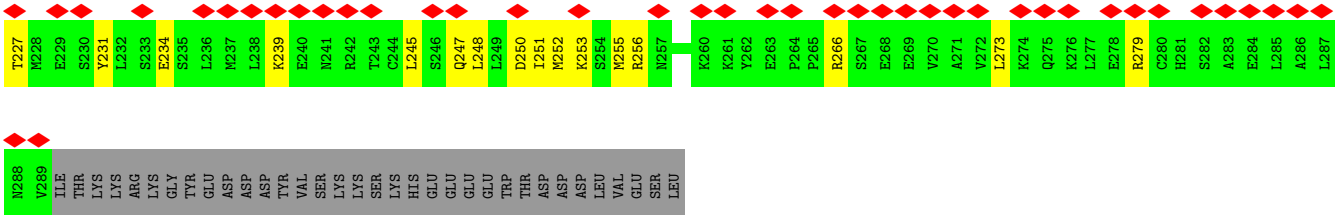


• Molecule 25: Cyclin-H

Chain 9:



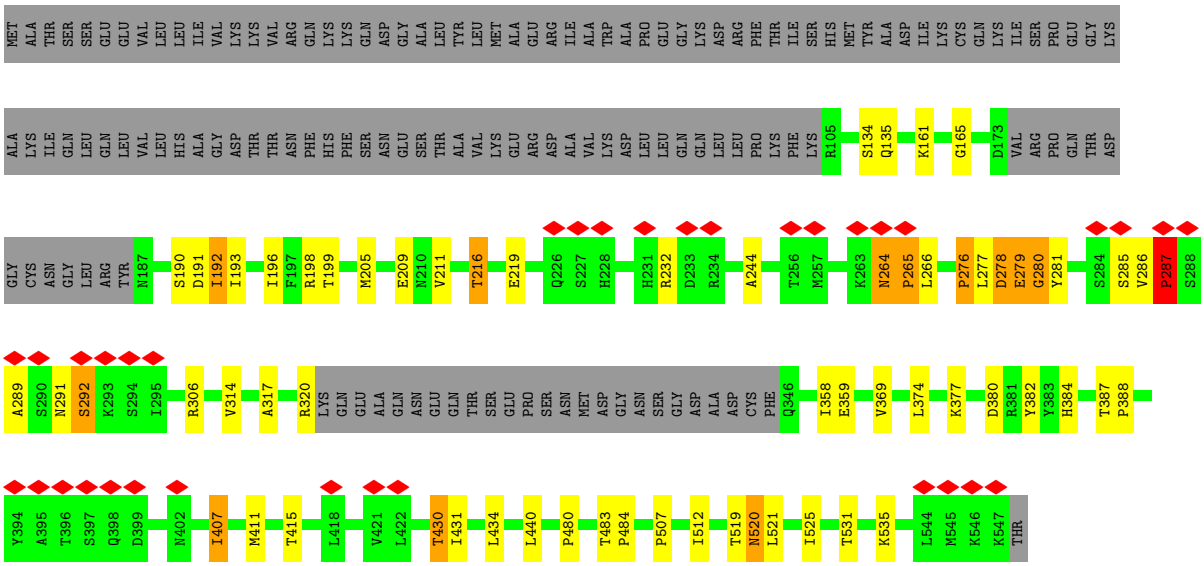




• Molecule 26: General transcription factor IIH subunit 1

Chain 1:

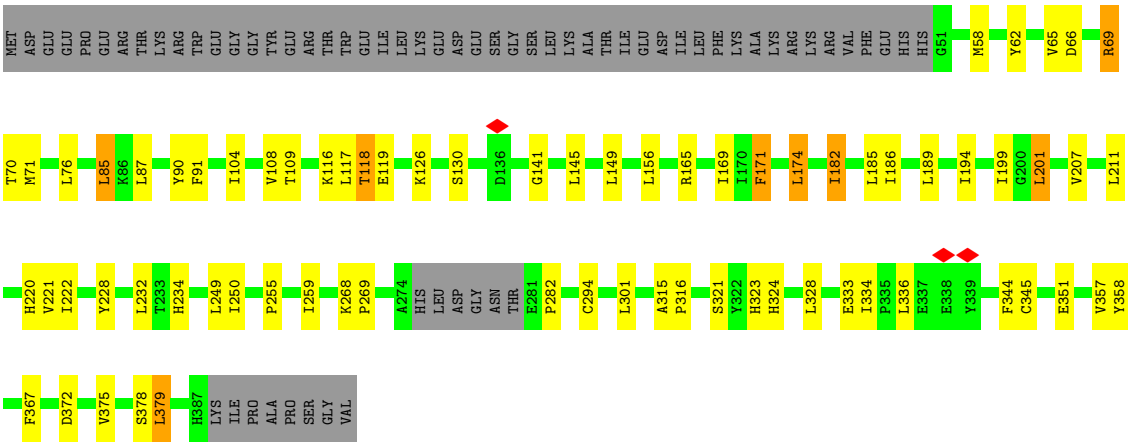




• Molecule 27: General transcription factor IIH subunit 2

Chain 2:

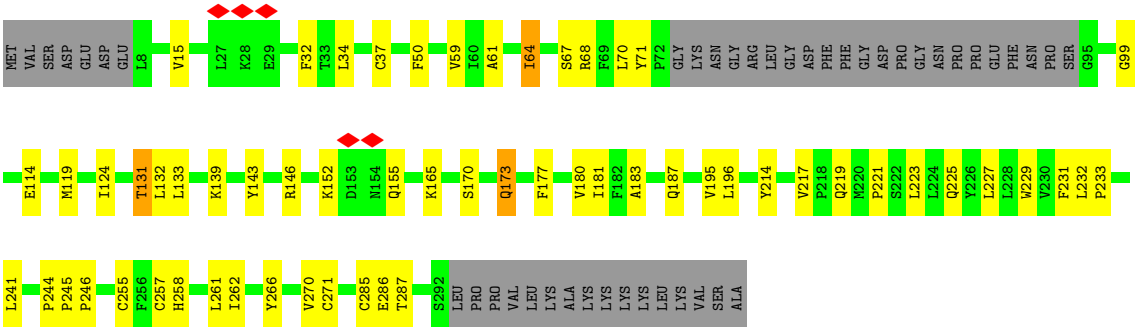




• Molecule 28: General transcription factor IIH subunit 3

Chain 3:

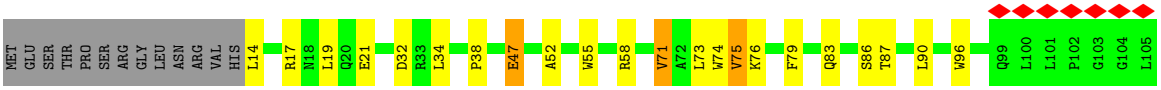


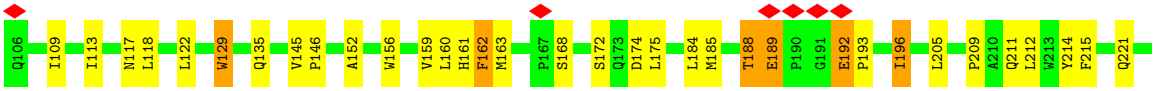


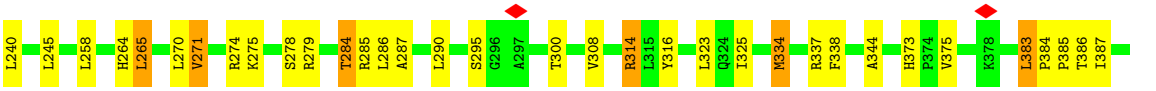
• Molecule 29: General transcription factor IIH subunit 4

Chain 4:







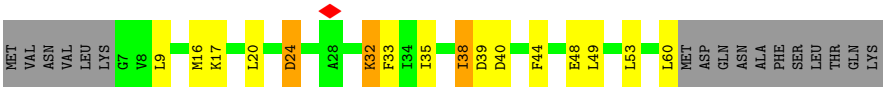




• Molecule 30: General transcription factor IIH subunit 5

Chain 5:





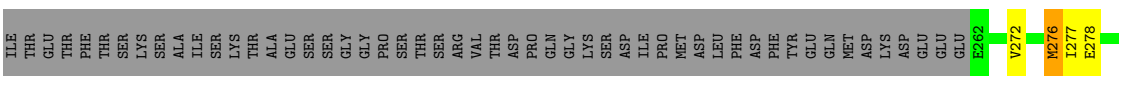
• Molecule 31: General transcription and DNA repair factor IIH helicase subunit XPB

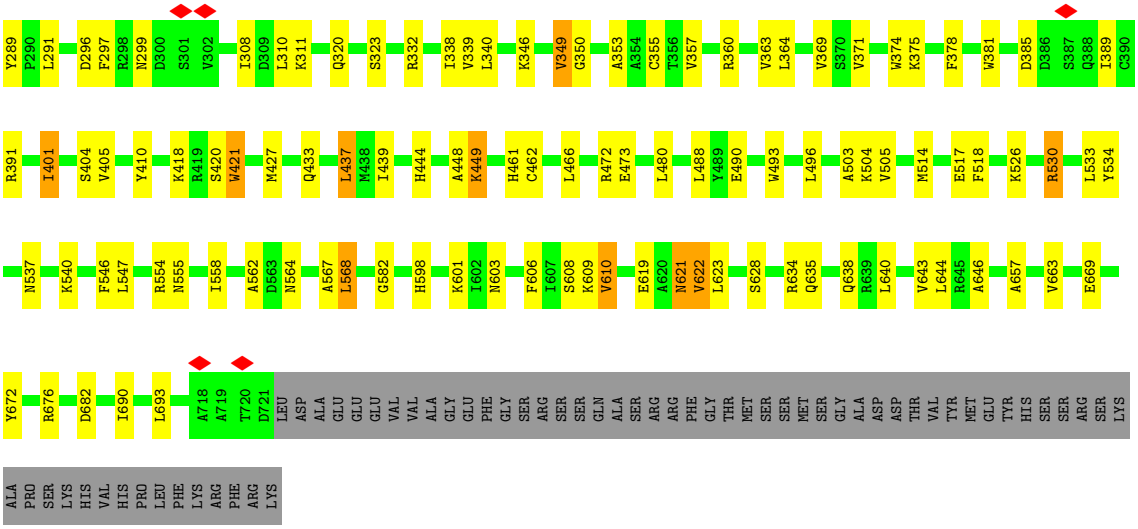
Chain 6:







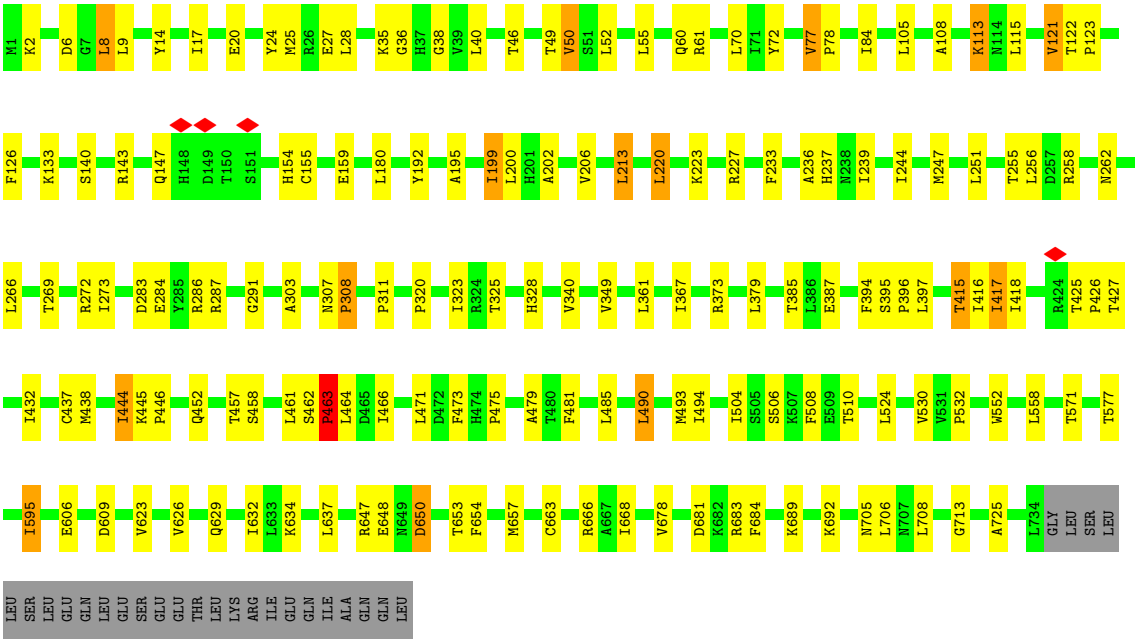




• Molecule 32: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 7:

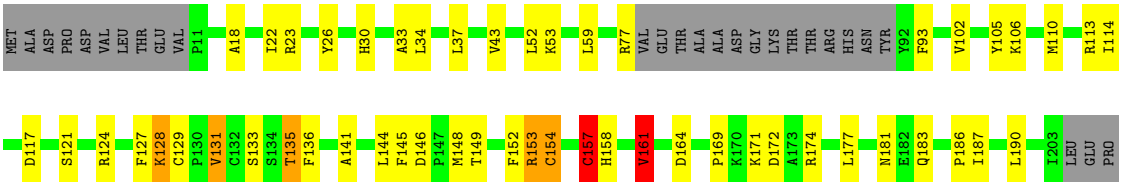


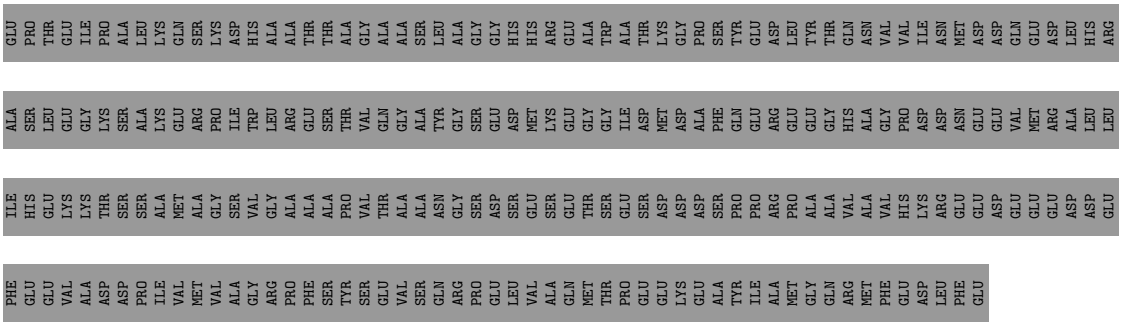


• Molecule 33: General transcription factor IIE subunit 1

Chain EA:

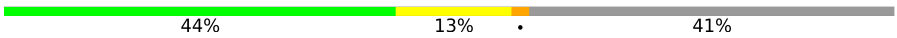


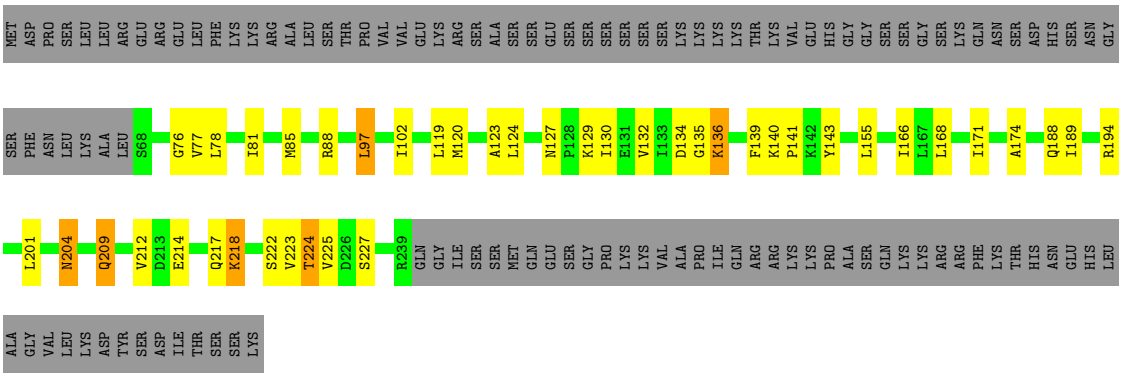




• Molecule 34: Transcription initiation factor IIE subunit beta

Chain EB:

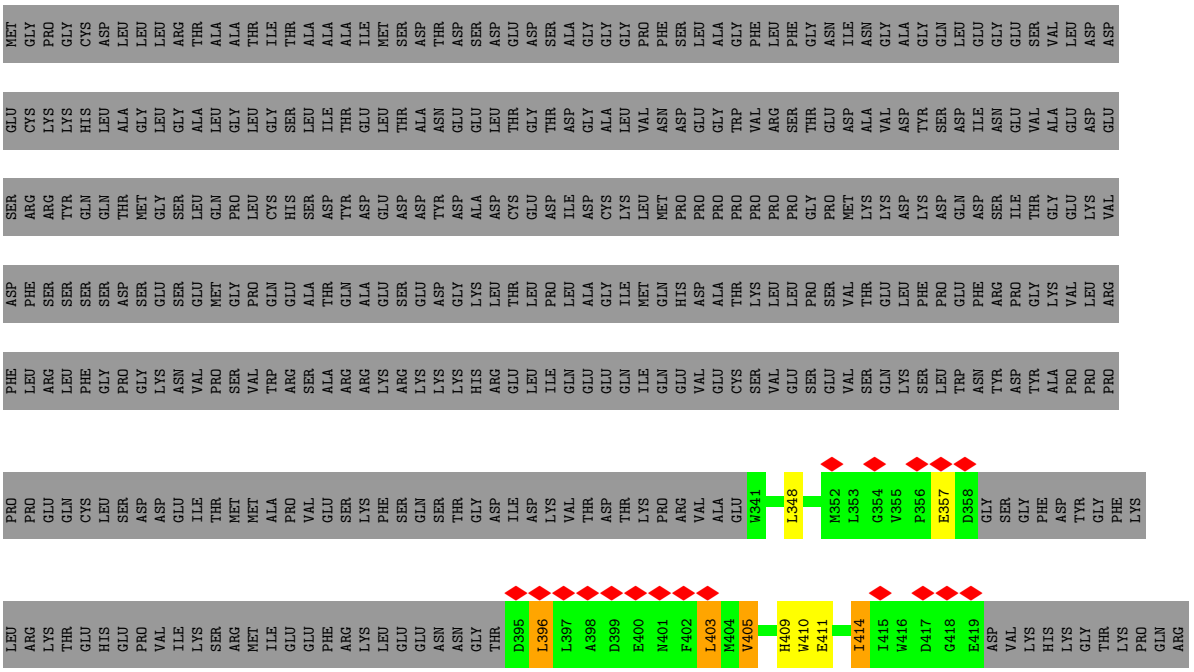


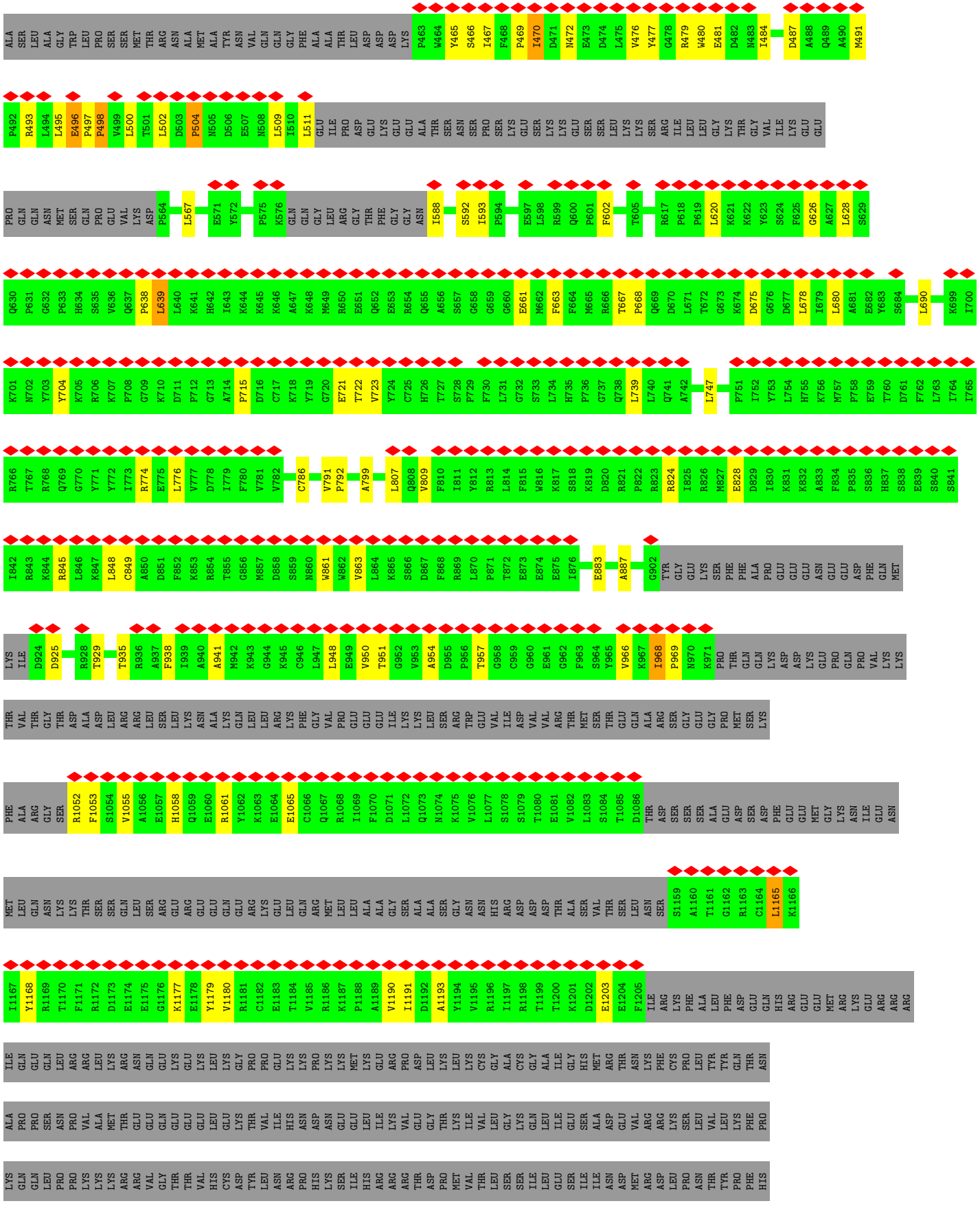


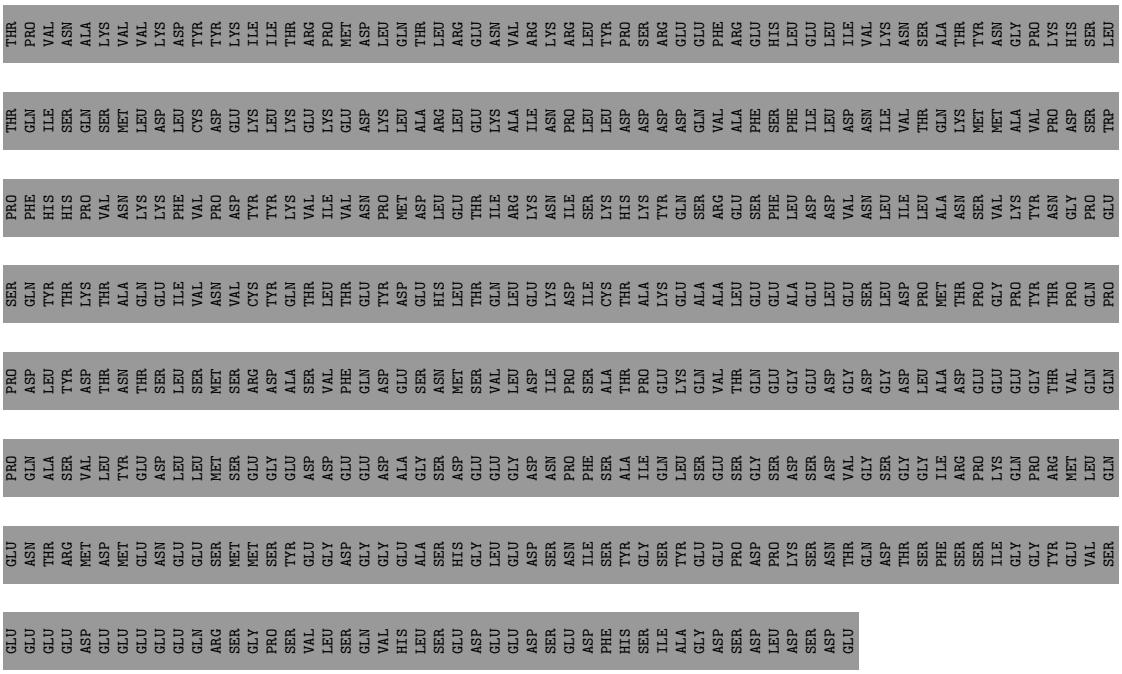
• Molecule 35: Transcription initiation factor TFIID subunit 1

Chain DA:





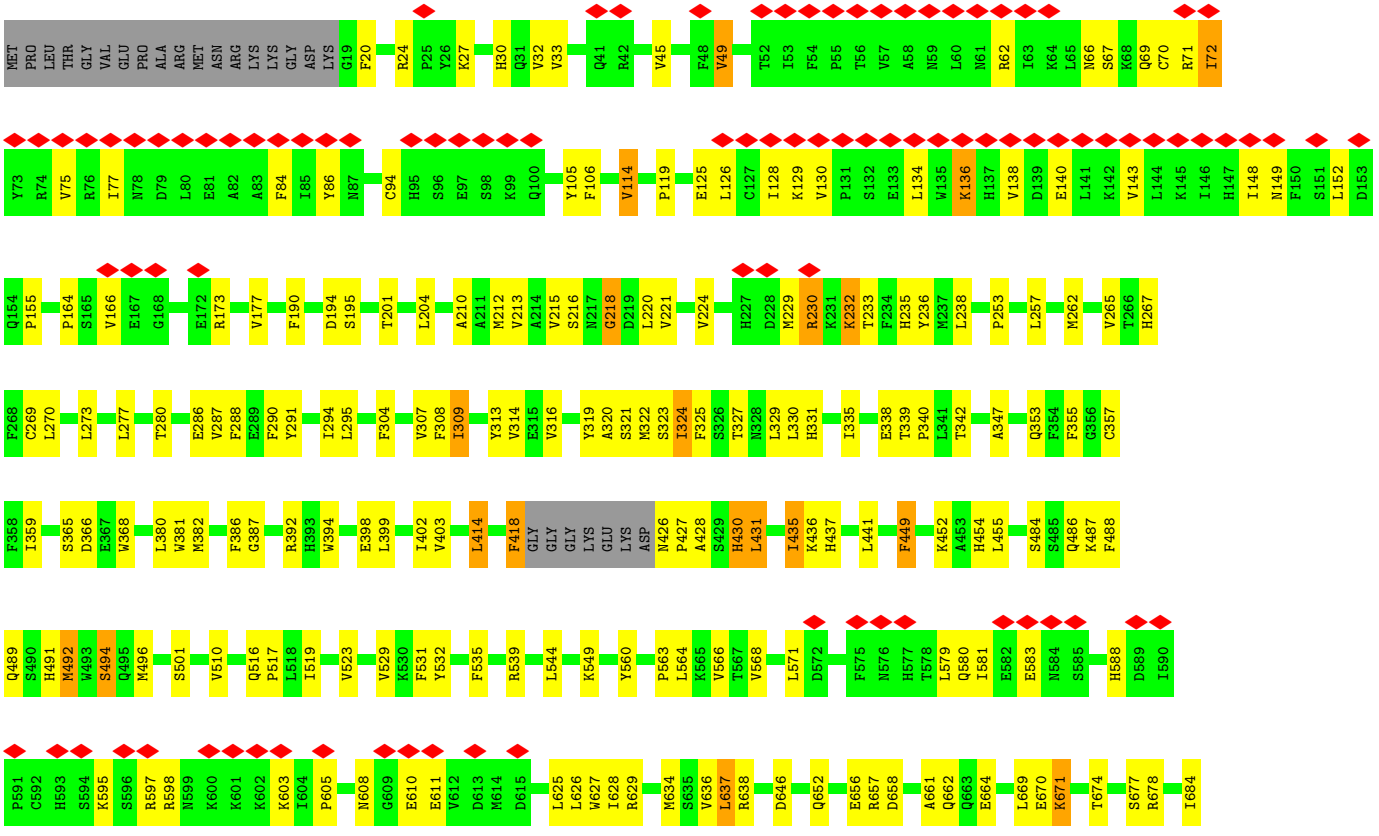


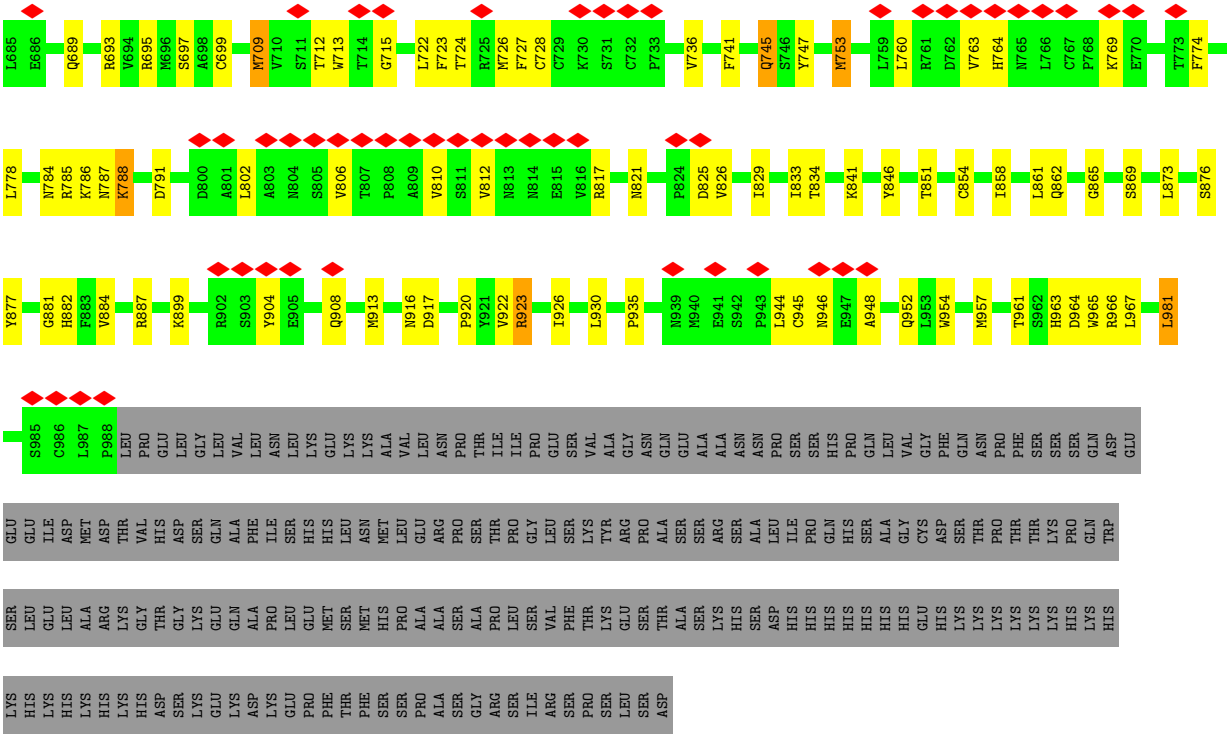


• Molecule 36: Transcription initiation factor TFIID subunit 2

Chain DB:

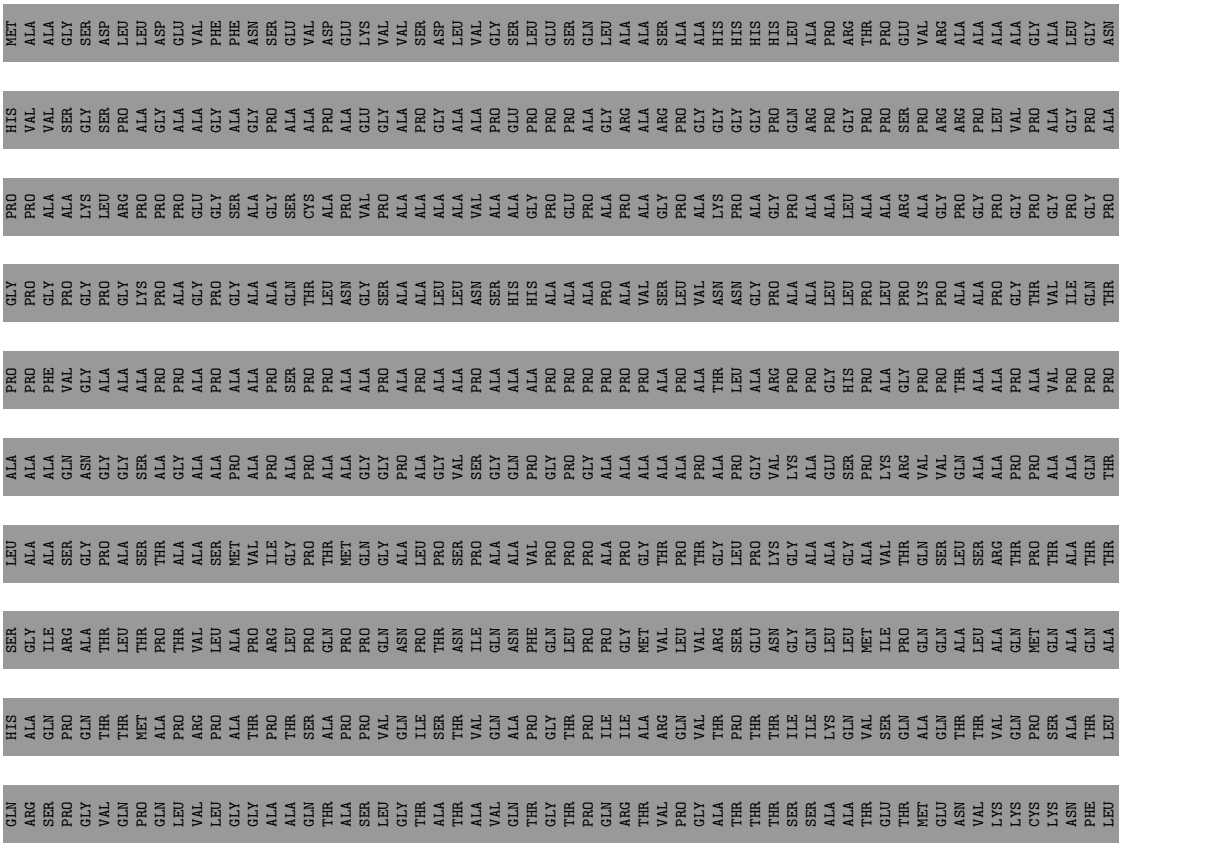


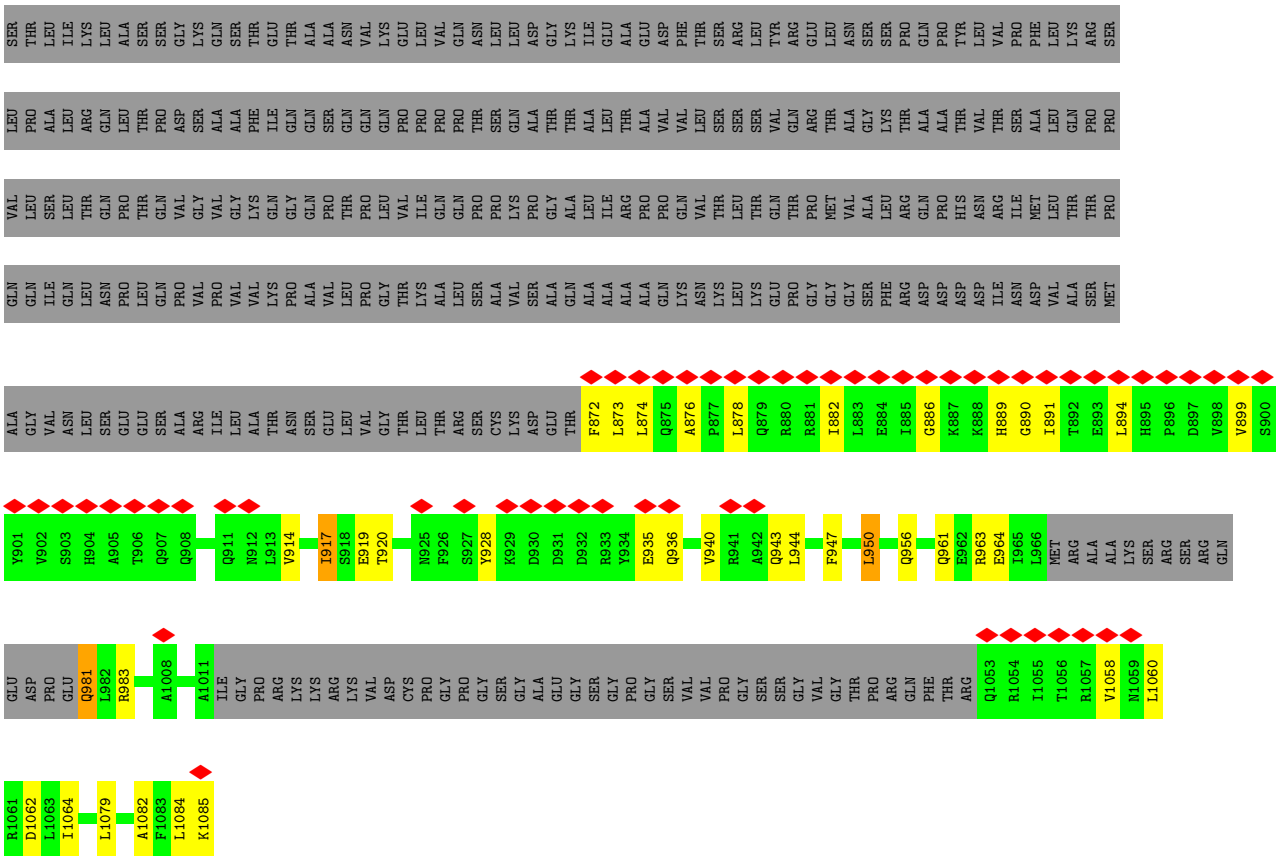




• Molecule 37: Transcription initiation factor TFIID subunit 4



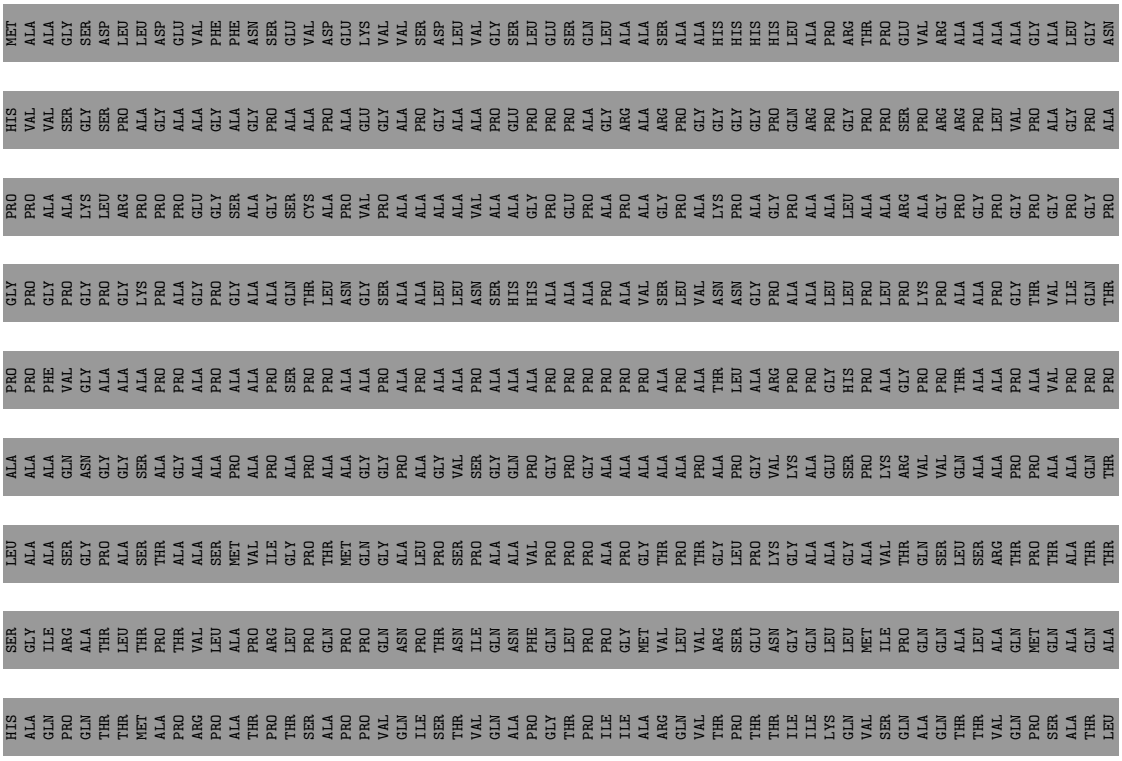


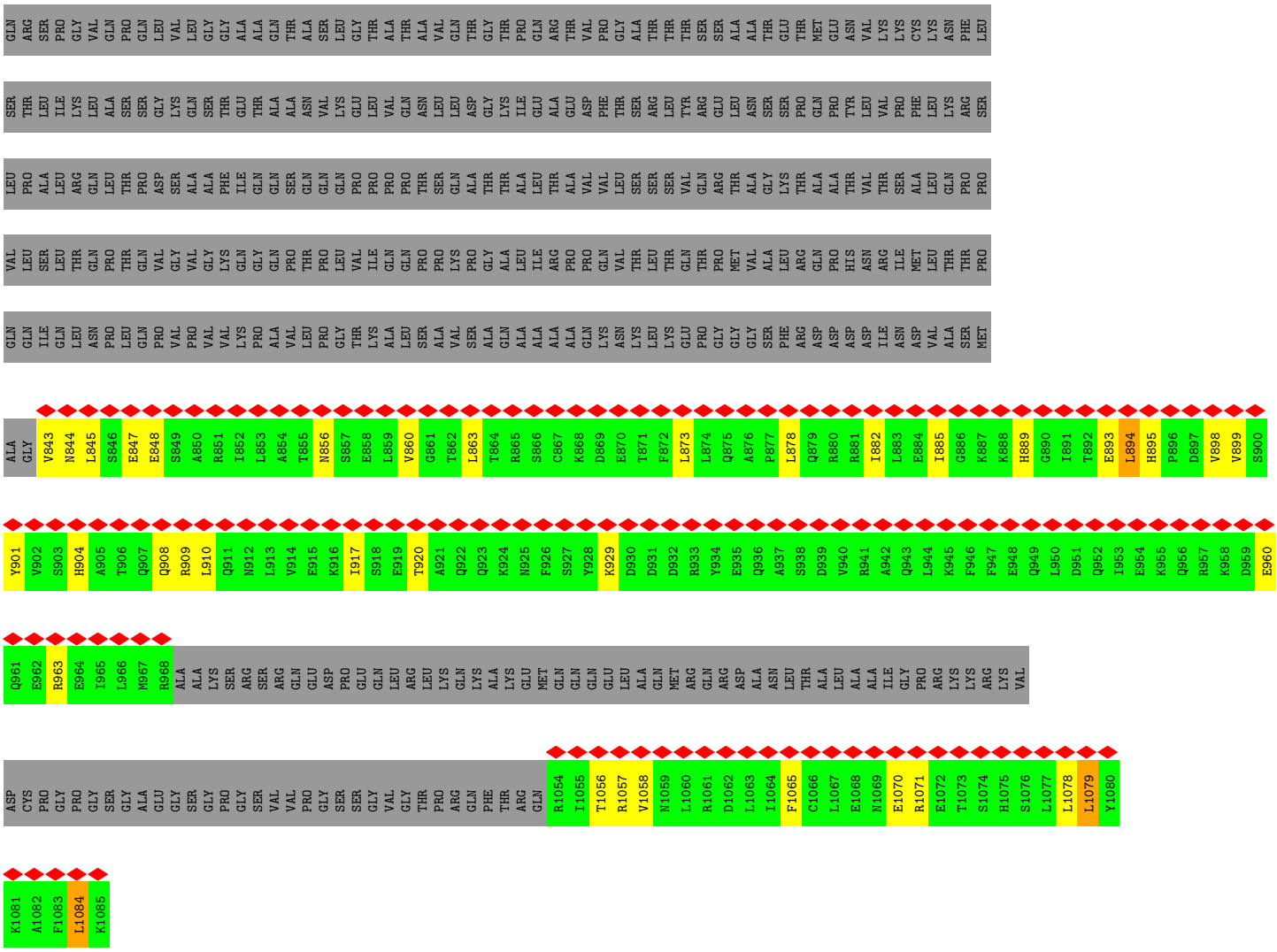


• Molecule 37: Transcription initiation factor TFIID subunit 4

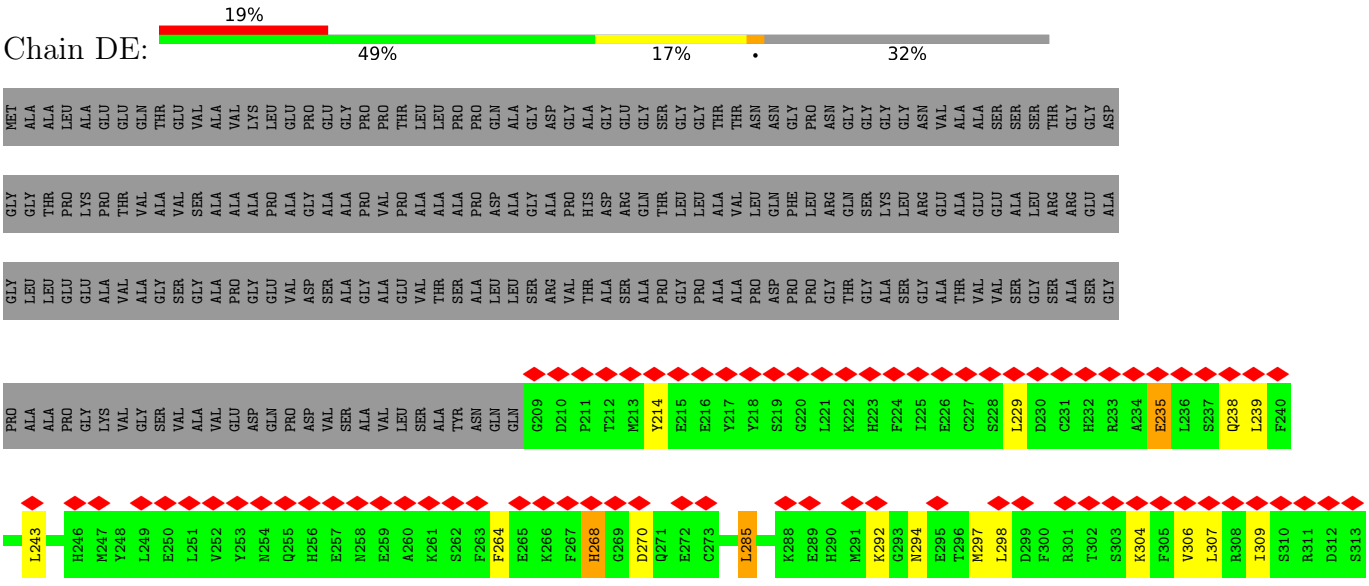
Chain Dd:

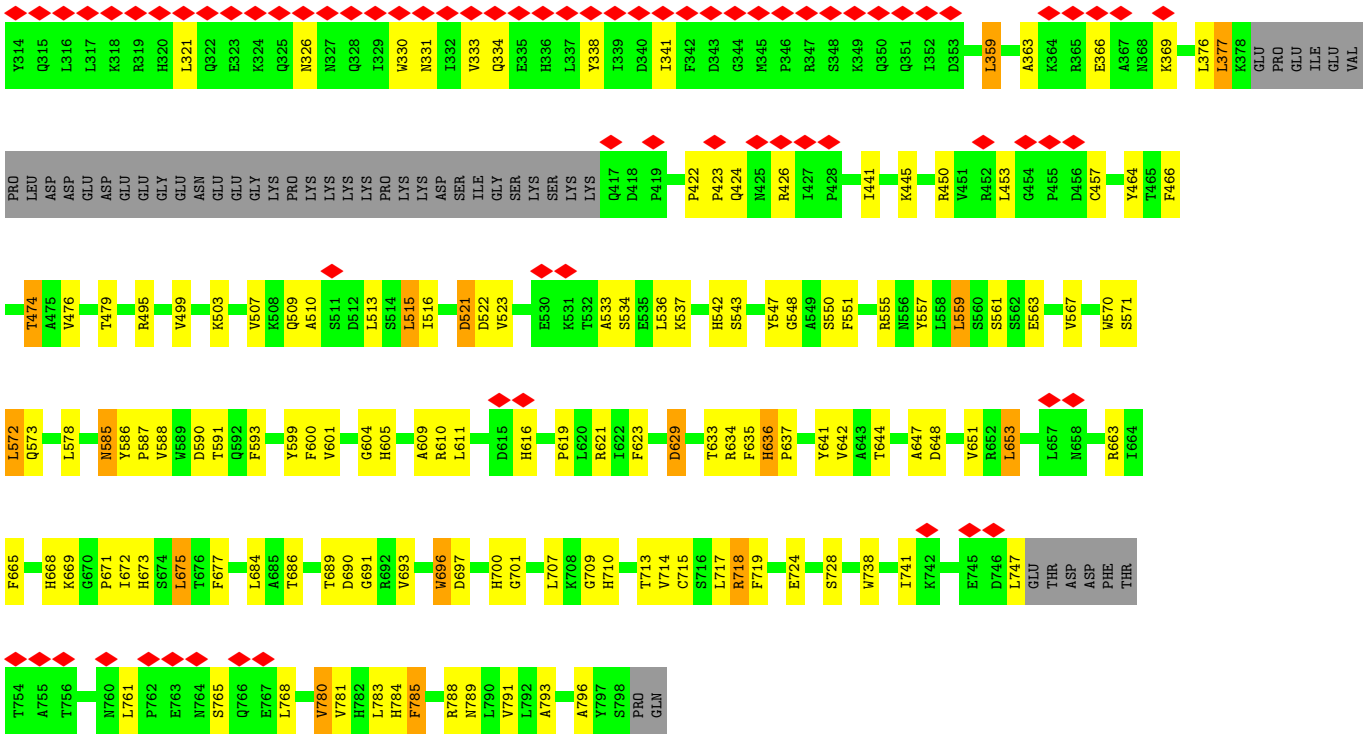






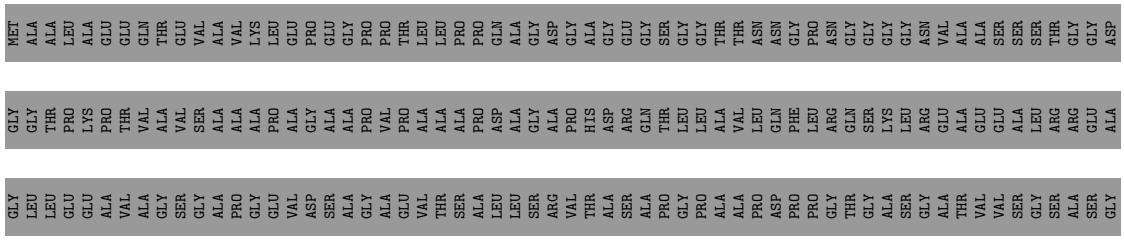
• Molecule 38: Transcription initiation factor TFIID subunit 5

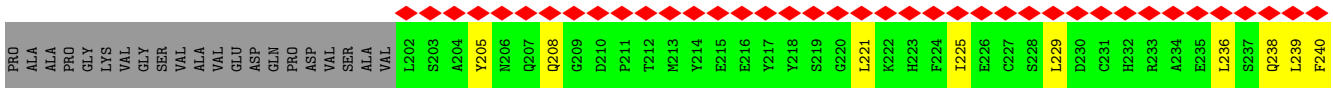


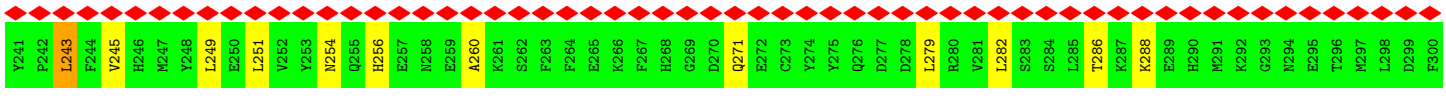


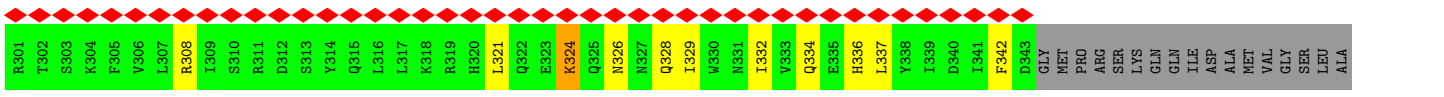
• Molecule 38: Transcription initiation factor TFIID subunit 5

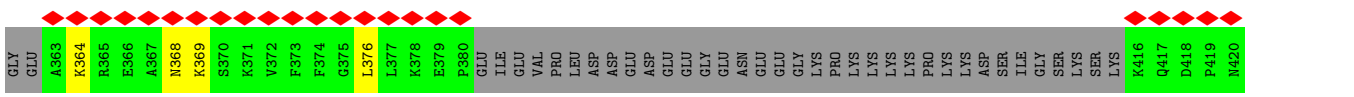




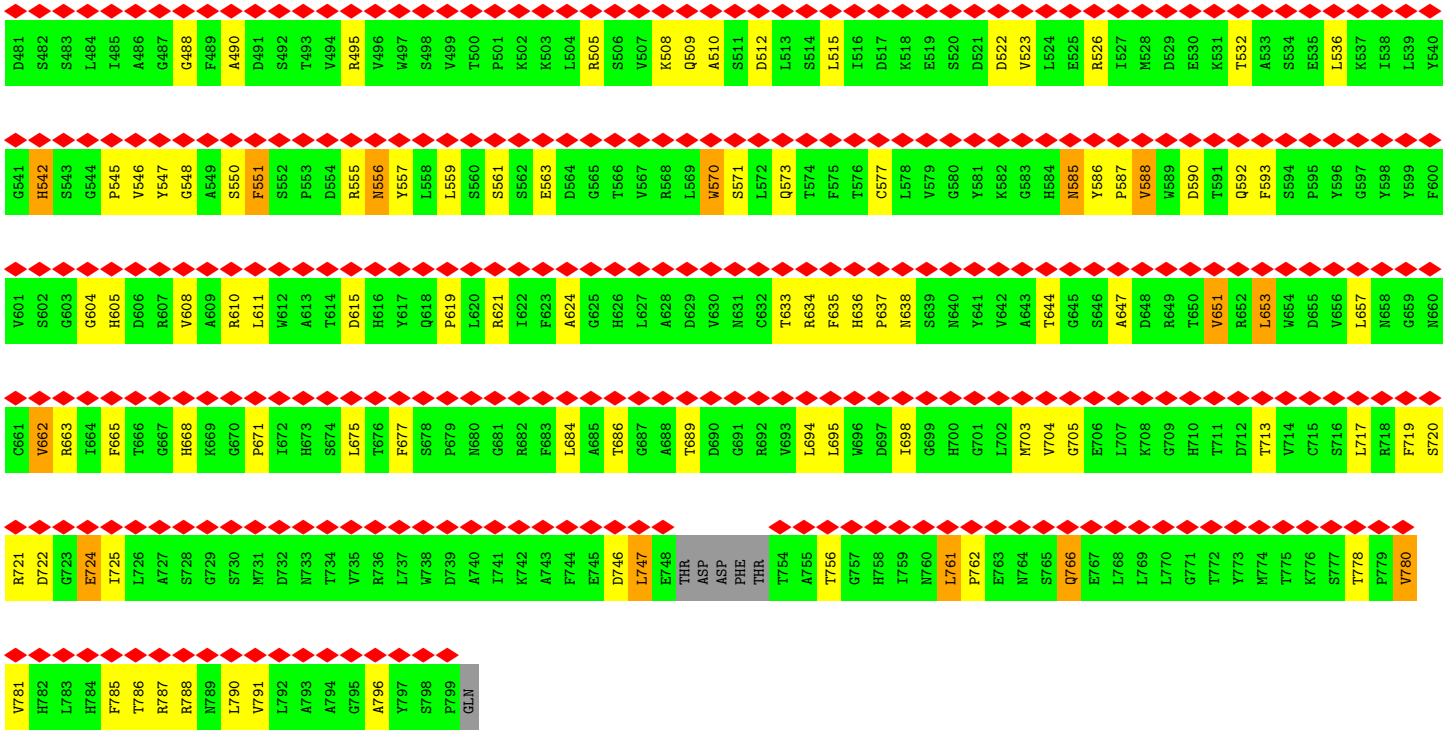






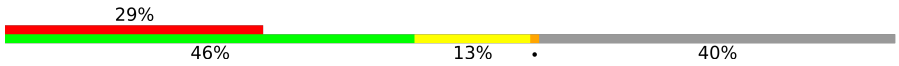


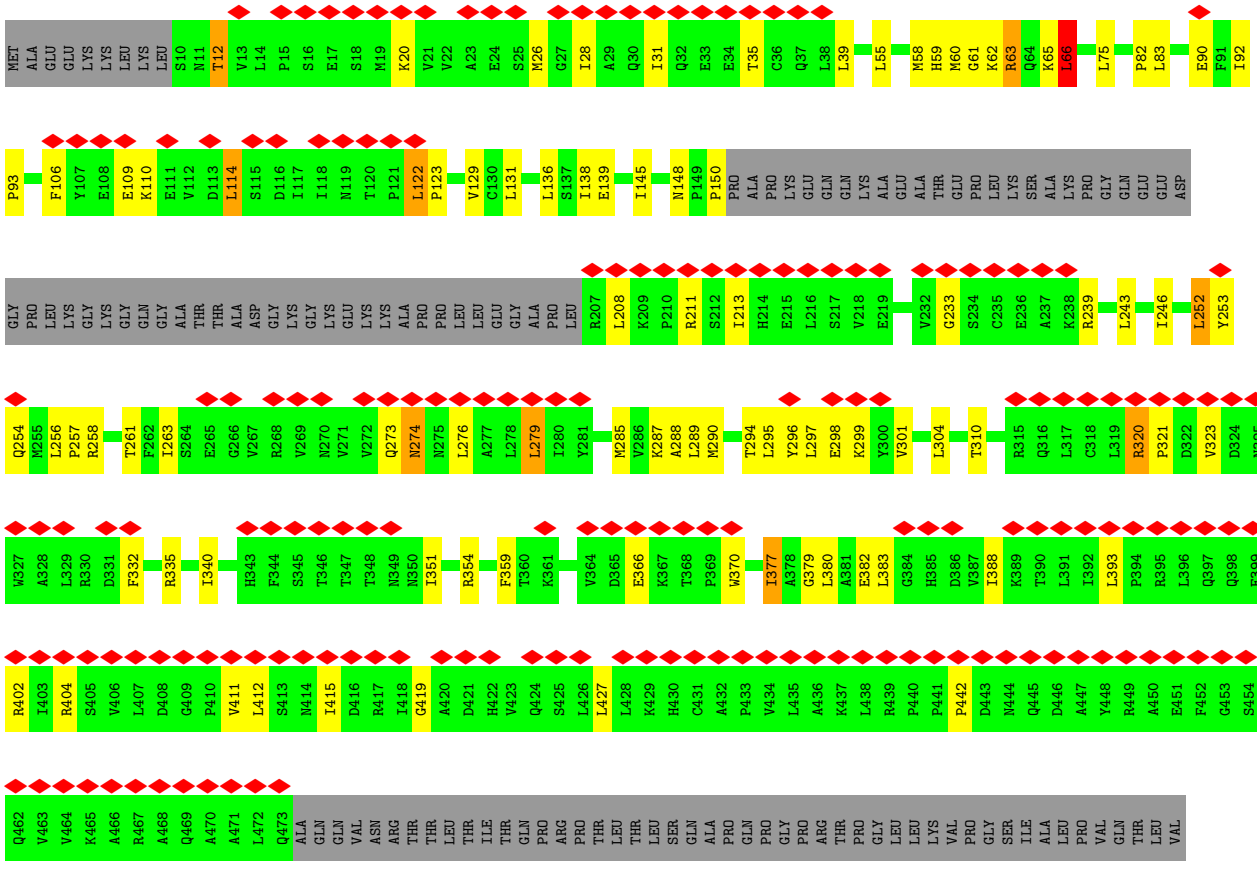


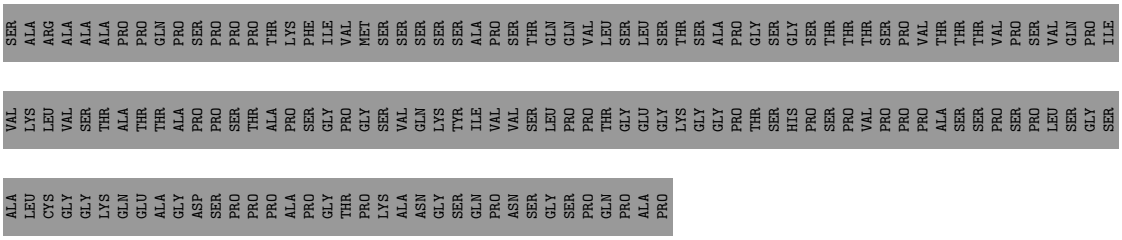


• Molecule 39: Transcription initiation factor TFIID subunit 6

Chain DF:

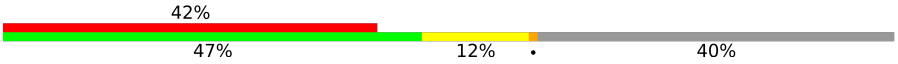


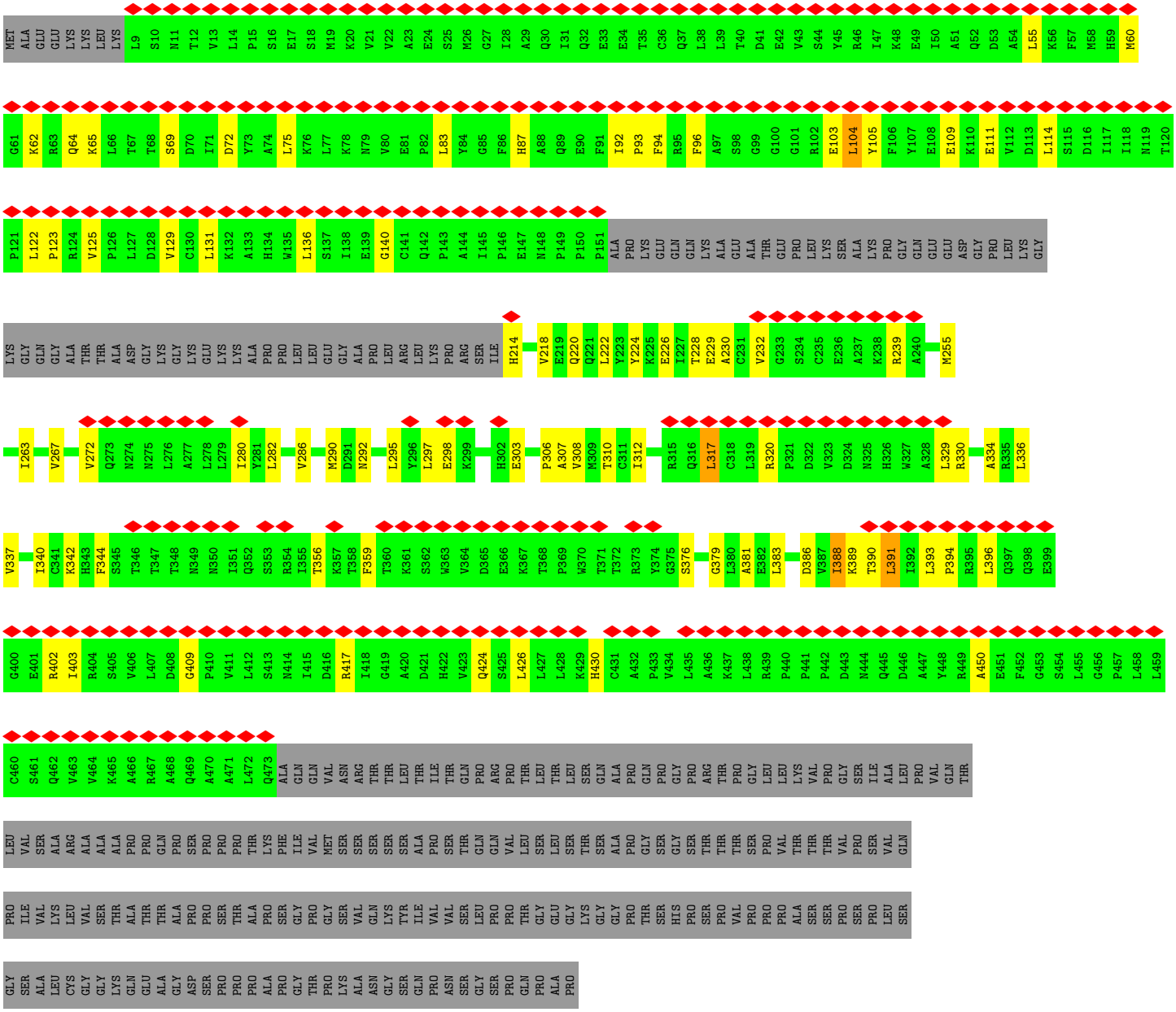




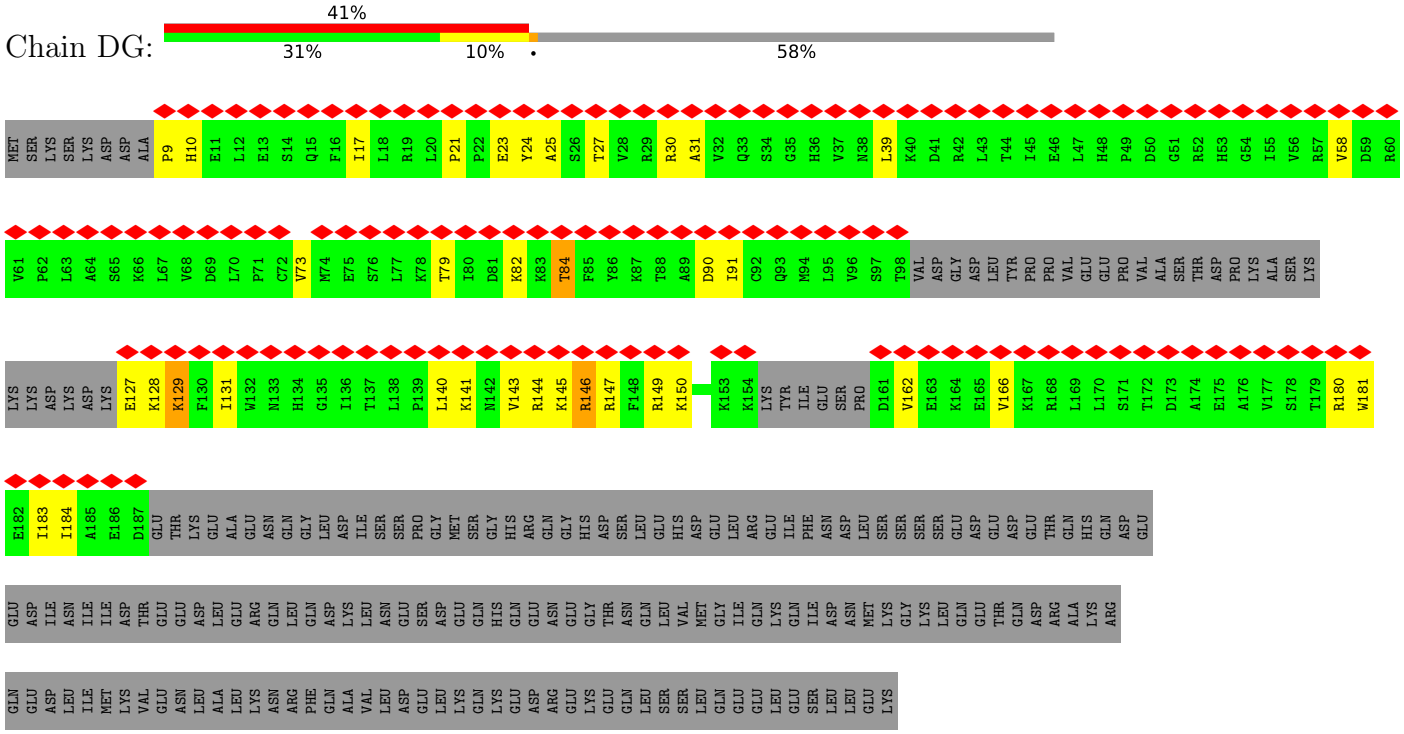
• Molecule 39: Transcription initiation factor TFIID subunit 6

Chain Df:

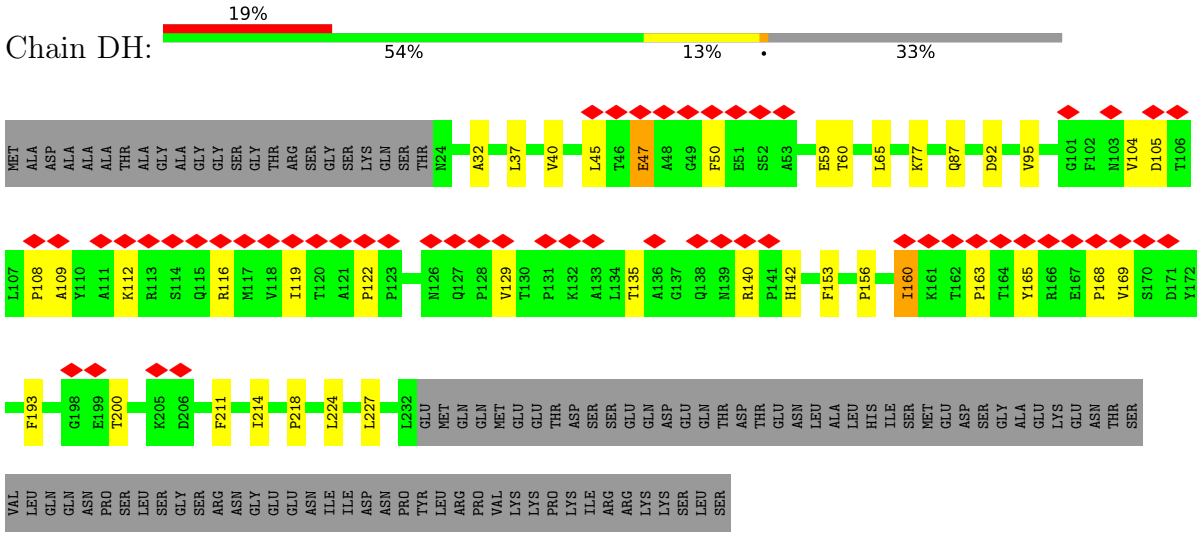




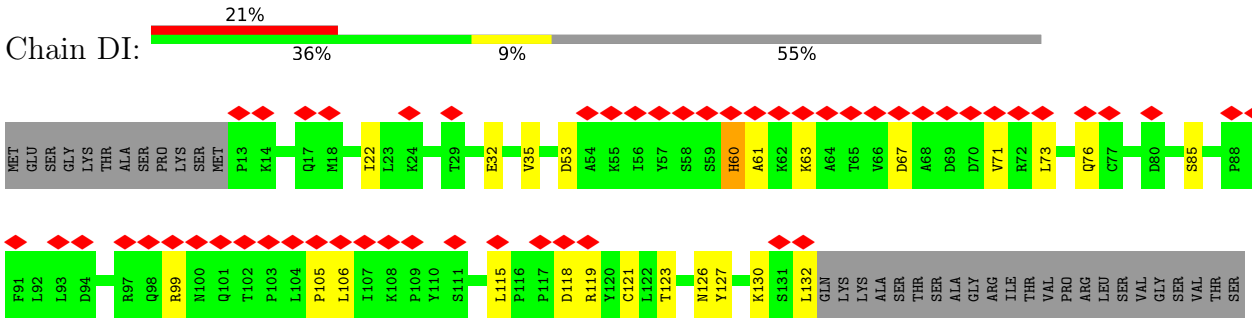
• Molecule 40: Transcription initiation factor TFIID subunit 7

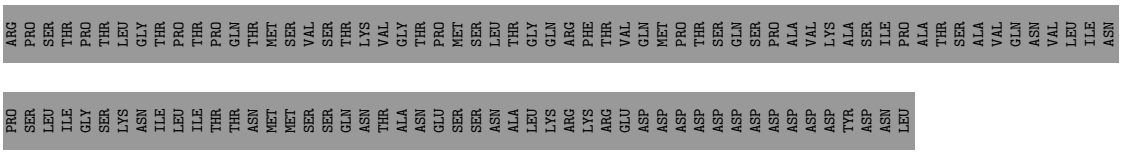


• Molecule 41: Transcription initiation factor TFIID subunit 8



• Molecule 42: Transcription initiation factor TFIID subunit 9

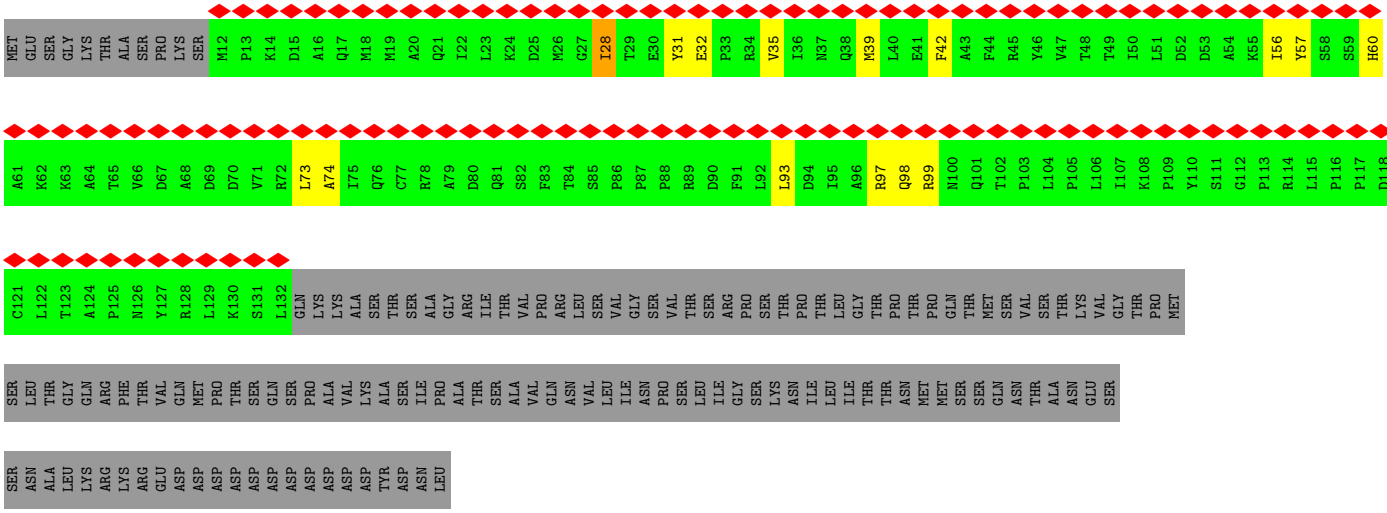




• Molecule 42: Transcription initiation factor TFIID subunit 9

Chain Di:

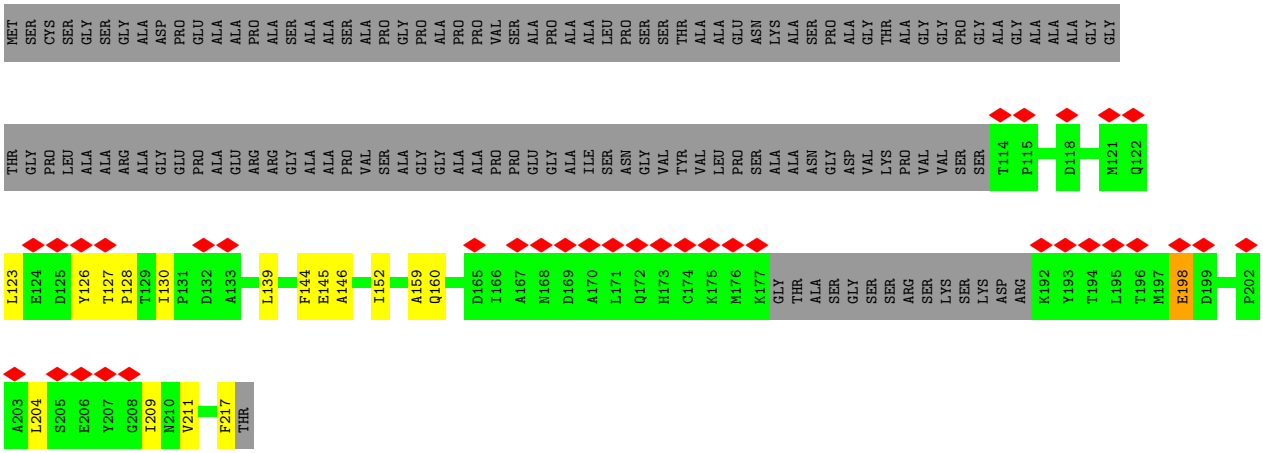




• Molecule 43: Transcription initiation factor TFIID subunit 10

Chain DJ:



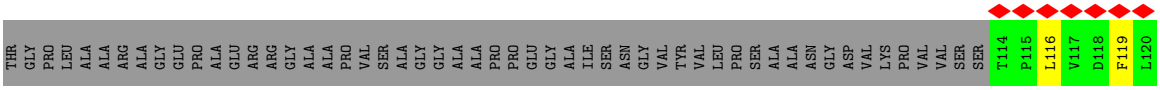


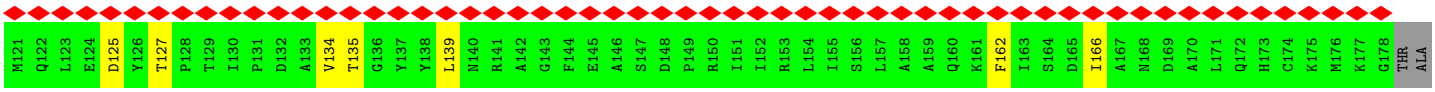
• Molecule 43: Transcription initiation factor TFIID subunit 10

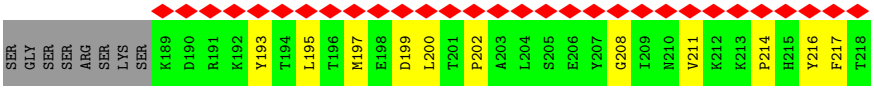
Chain Dj:







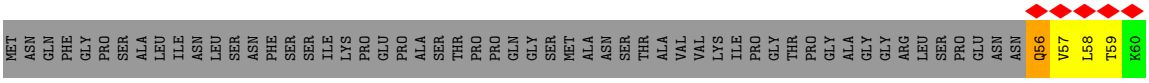


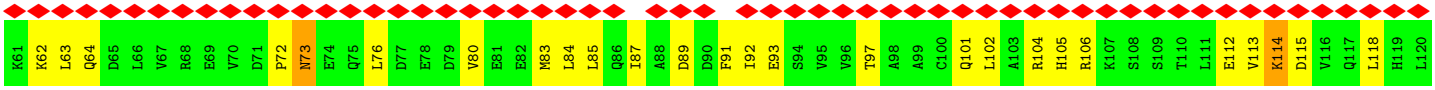


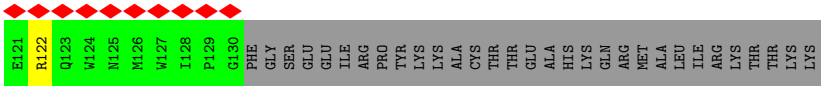
• Molecule 44: Transcription initiation factor TFIID subunit 12

Chain DL:





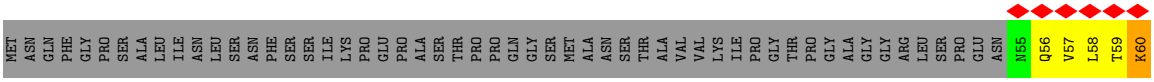


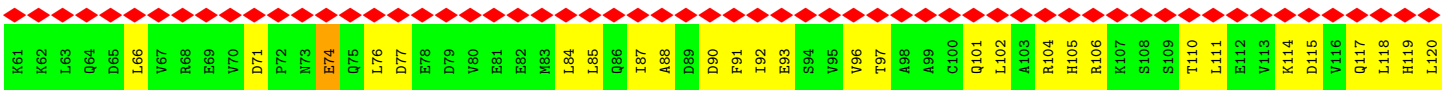


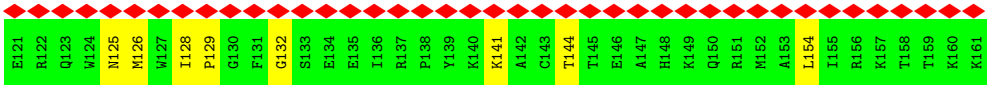
• Molecule 44: Transcription initiation factor TFIID subunit 12

Chain Dl:





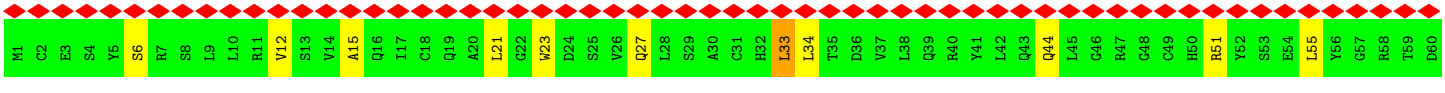


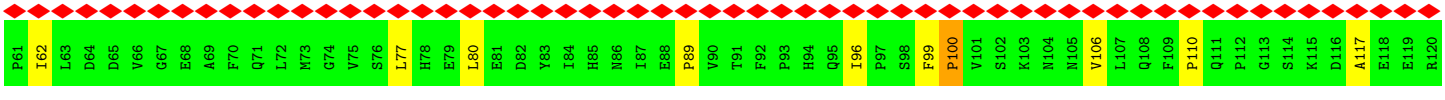


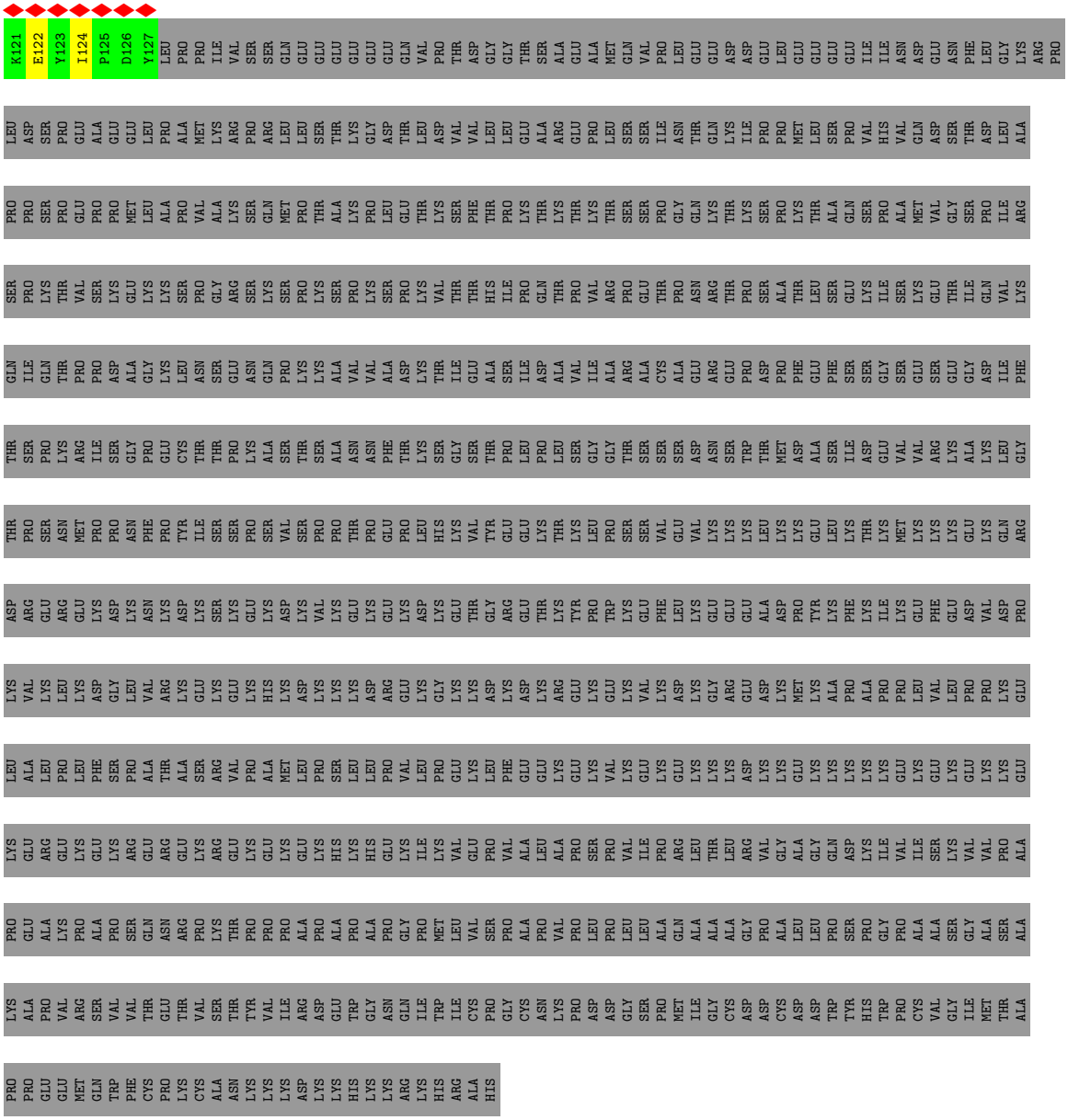
• Molecule 45: Transcription initiation factor TFIID subunit 3

Chain Dc:





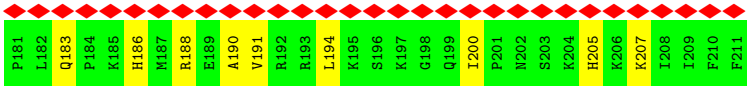




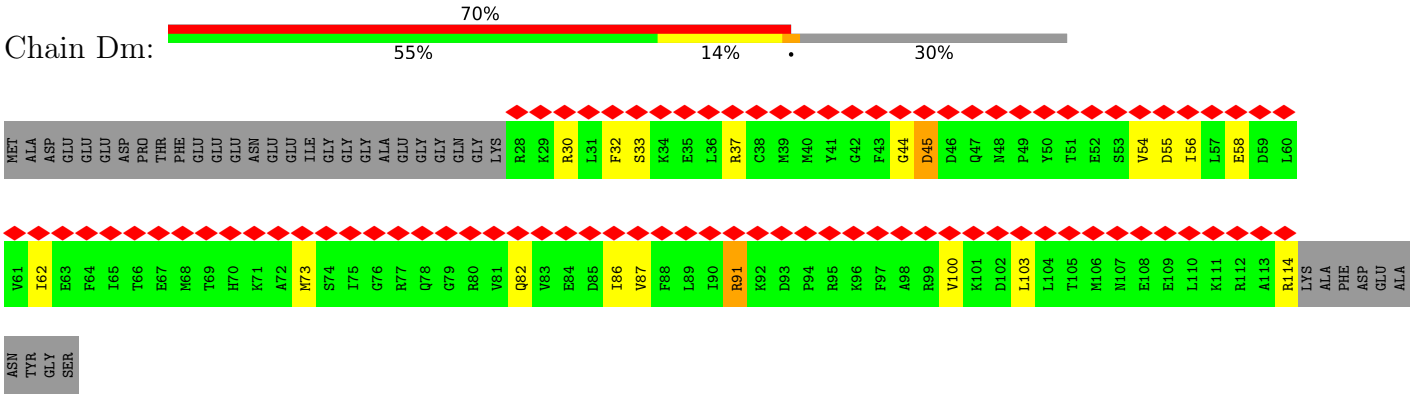
• Molecule 46: Transcription initiation factor TFIID subunit 11

Chain Dk:

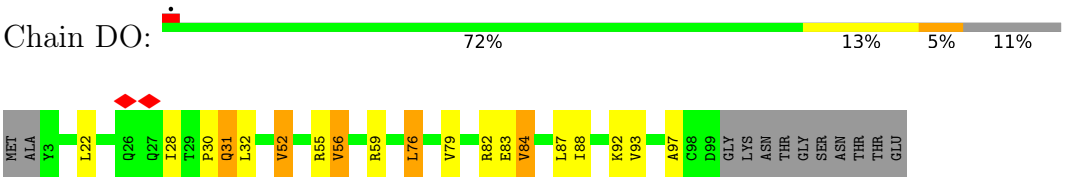




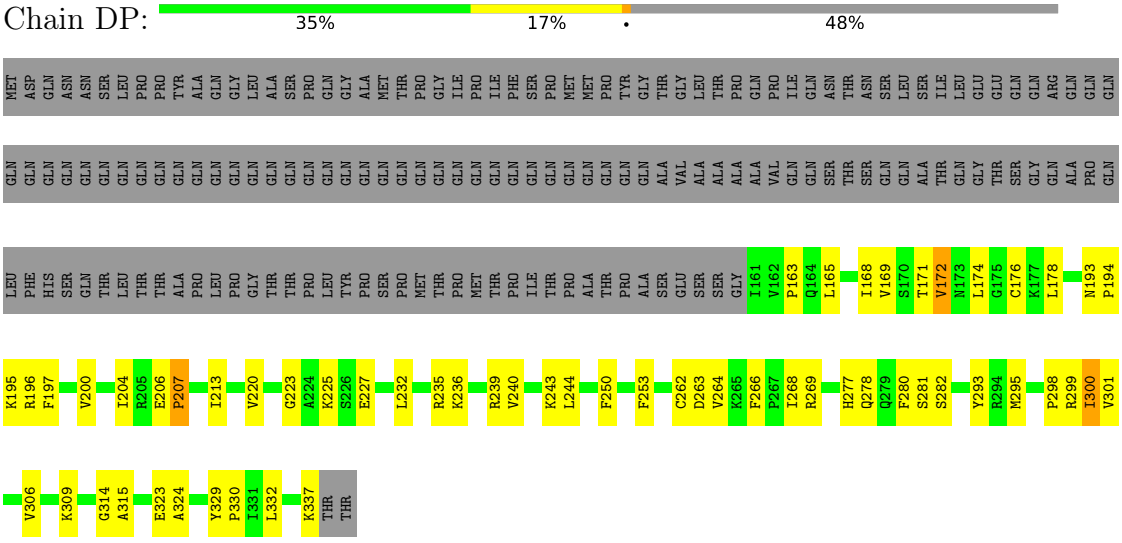
• Molecule 47: Transcription initiation factor TFIID subunit 13

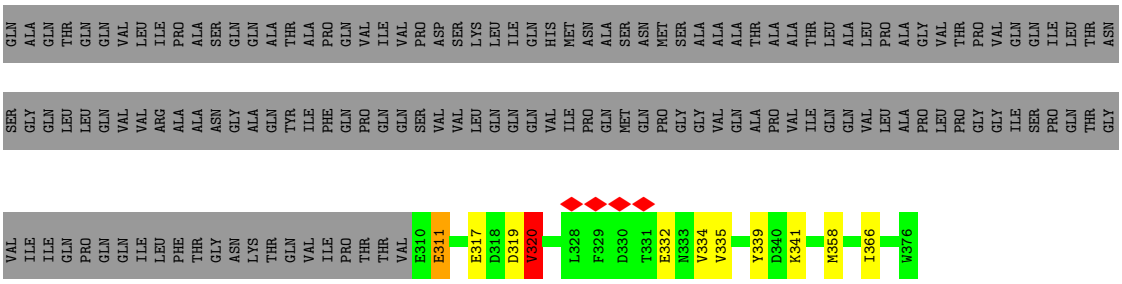


• Molecule 48: Transcription initiation factor IIA subunit 2



• Molecule 49: TATA-box-binding protein

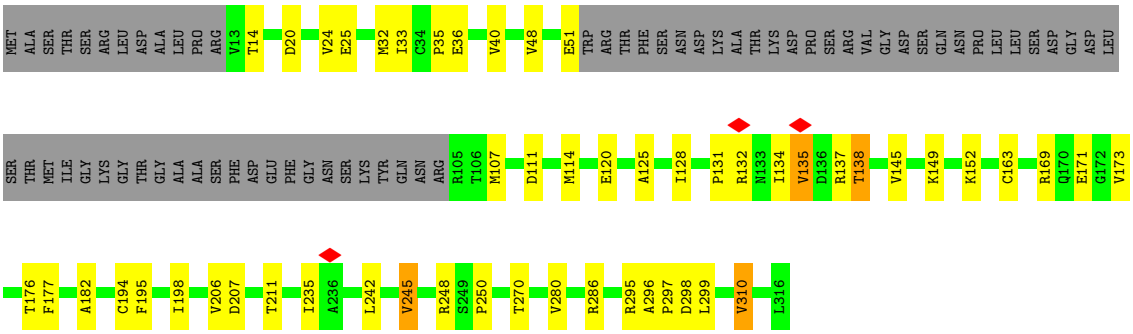

Chain DP:
35%
17%
48%
MET ASP GLN ASN SER LEU PRO PRO TYR ALA GLN GLY LEU ALA SER PRO GLN GLY ALA MET THR PRO GLY ILE PRO ILE PHE SER PRO MET MET PRO TYR GLY THR GLY LEU THR PRO GLN PRO ILE GLN ASN THR ASN SER LEU SER ILE LEU GLU GLU GLN GLN ARG GLN GLN
GLN GLN GLN



• Molecule 51: Transcription initiation factor IIB

Chain BA:

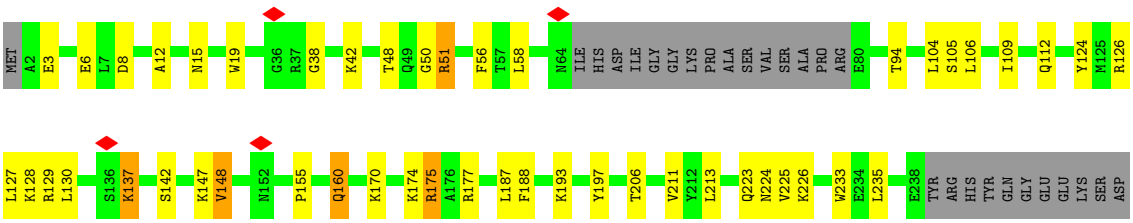




• Molecule 52: General transcription factor IIF subunit 2

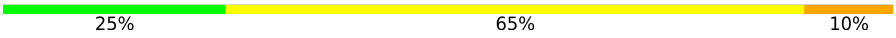
Chain FB:

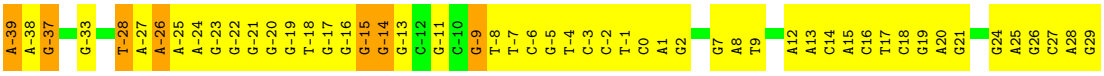




• Molecule 53: DNA (69-MER)

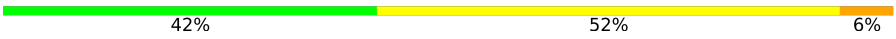
Chain X:

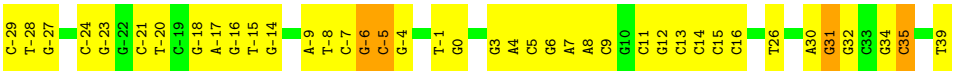




• Molecule 54: DNA (69-MER)

Chain Y:

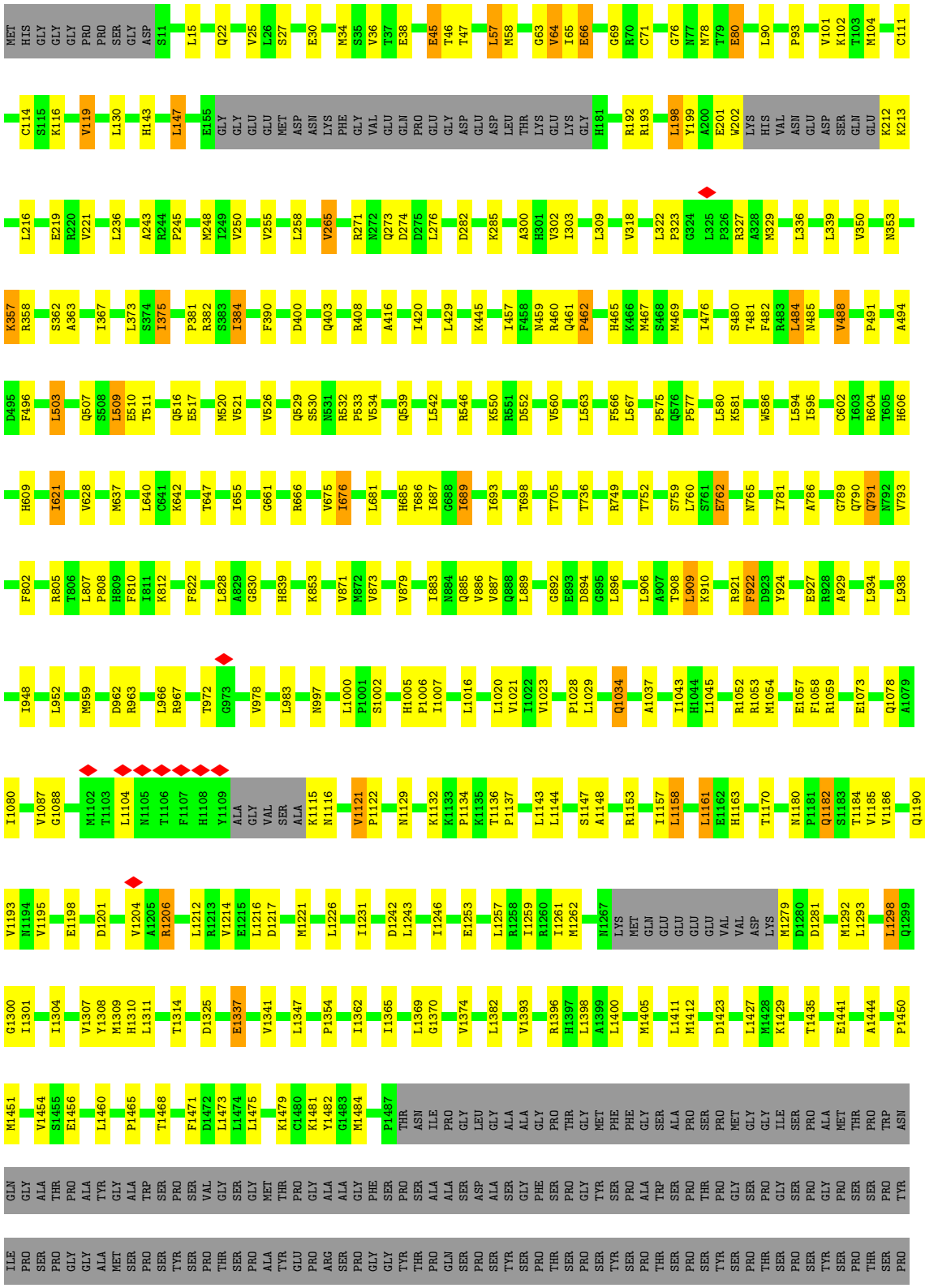


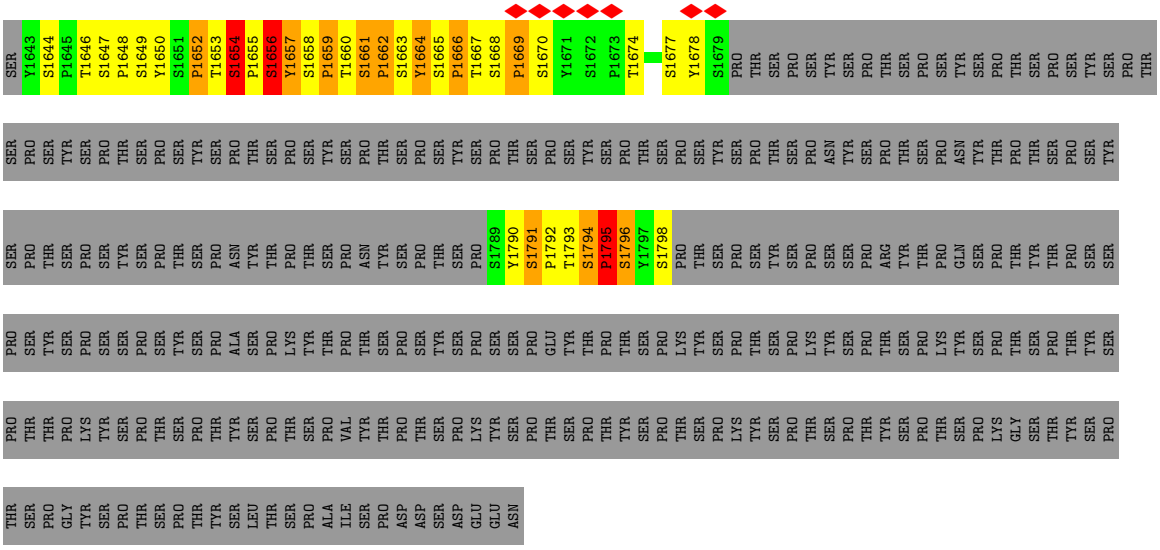


• Molecule 55: RPB1

Chain PA:



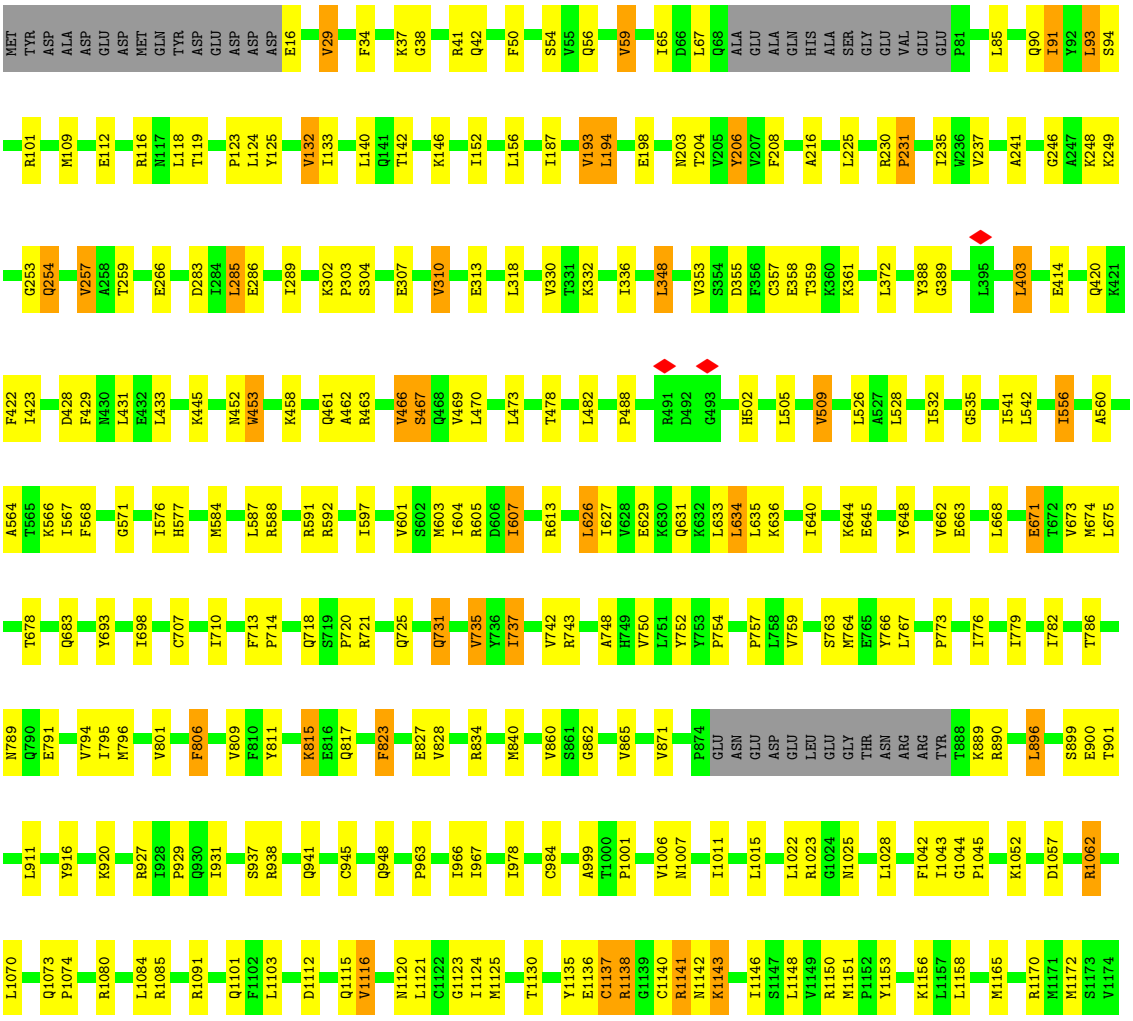

MET HIS GLY GLY GLY PRO PRO SER GLY ASP S11 L15 Q22 V25 L26 S27 E30 M34 S35 V36 T37 E38 E45 T46 T47 L57 M58 G63 V64 I65 E66 G69 R70 C71 G76 N77 N78 T79 E80 L90 P93 V101 K102 T103 M104 C111
C114 S115 K116 V119 L130 H143 L147 E155 GLY GLY GLU GLU MET ASP ASN LYS PHE GLY VAL GLU GLN PRO GLU GLY ASP GLU ASP LEU THR LYS GLU LYS GLY H181 R192 R193 L198 Y199 A200 E201 W202 LYS HIS VAL ASN GLU ASP SER GLN GLU K212 K213
L216 E219 R220 V221 L236 A243 R244 P245 M248 T249 V250 V255 L258 V265 R271 N272 Q273 D274 D275 L276 D282 K285 A300 H301 V302 I303 L309 V318 L322 P323 G324 L325 P326 R327 A328 M329 L336 L339 V350 N353
K357 B358 S362 A363 I367 L373 S374 I375 P381 R382 S383 I384 F390 D400 Q403 R408 A416 I420 L429 K445 I457 F458 N459 R460 Q461 P462 H465 K466 M467 S468 M469 I476 S480 T481 F482 R483 L484 N485 V488 P491 A494
D495 F496 L503 Q507 S508 L509 E510 T511 Q516 E517 M520 V521 V526 Q529 S530 N531 R532 P533 V534 Q539 L542 R546 K550 R551 D552 V560 L563 F566 L567 P575 Q576 P577 L580 K581 W586 L594 I595 C602 I603 R604 T605 H606
H609 I621 V628 M637 L640 C641 K642 T647 I655 G661 R666 V675 I676 L681 H685 T686 I687 G688 I689 I693 T698 T705 T736 R749 T752 S759 L760 S761 E762 N765 I781 A786 G789 Q790 Q791 N792 V793
F802 R805 T806 L807 P808 H809 F810 I811 K812 F822 L828 A829 G830 H839 K853 V871 M872 V873 V879 I883 N884 Q885 V886 V887 Q888 L889 G892 E893 D894 G895 L896 L906 A907 T908 L909 K910 R921 F922 D923 Y924 E927 R928 A929 L934 L938
I948 L952 M959 D962 R963 L966 R967 T972 G973 V978 L983 N997 L1000 P1001 S1002 H1005 P1006 I1007 L1016 L1020 V1021 I1022 V1023 P1028 L1029 Q1034 A1037 I1043 H1044 L1045 R1052 R1053 M1054 E1057 F1058 R1059 E1073 Q1078 A1079
I1080 V1087 G1088 M1102 T1103 L1104 N1105 T1106 F1107 H1108 Y1109 ALA GLY VAL SER ALA K1115 N1116 V1121 P1122 N1129 K1132 K1133 P1134 K1135 T1136 P1137 L1143 L1144 S1147 A1148 R1153 I1157 L1158 L1161 E1162 H1163 T1170 N1180 P1181 Q1182 S1183 T1184 V1185 V1186 Q1190
V1193 N1194 V1195 E1198 D1201 V1204 A1205 R1206 L1212 R1213 V1214 E1215 L1216 D1217 M1221 L1226 I1231 D1242 L1243 I1246 E1253 L1257 R1258 I1259 R1260 I1261 M1262 N1267 LYS MET GLN GLU GLU GLU GLU VAL VAL ASP LYS M1279 D1280 D1281 M1292 L1293 L1298 Q1299
G1300 I1301 I1304 V1307 Y1308 M1309 H1310 L1311 T1314 D1325 E1337 V1341 L1347 P1354 I1362 I1365 L1369 G1370 V1374 L1382 V1393 R1396 H1397 L1398 A1399 L1400 M1405 L1411 M1412 D1423 L1427 M1428 K1429 T1435 E1441 A1444 P1450
M1451 V1454 S1455 E1456 L1460 P1465 T1468 F1471 D1472 L1473 L1474 L1475 K1479 C1480 K1481 Y1482 G1483 M1484 P1487 THR ASN ILE PRO GLY LEU GLY ALA ILE PRO GLN SER PRO ASP ALA SER GLY PHE SER PRO GLY TYR SER PRO ALA TRP SER PRO THR PRO GLY SER PRO THR SER PRO SER PRO SER PRO PRO SER PRO SER PRO SER



• Molecule 56: DNA-directed RNA polymerase subunit beta

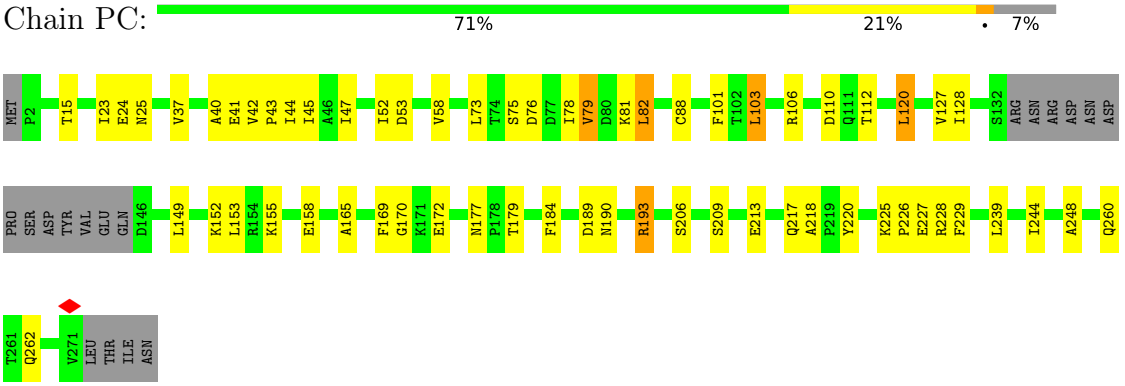
Chain PB:





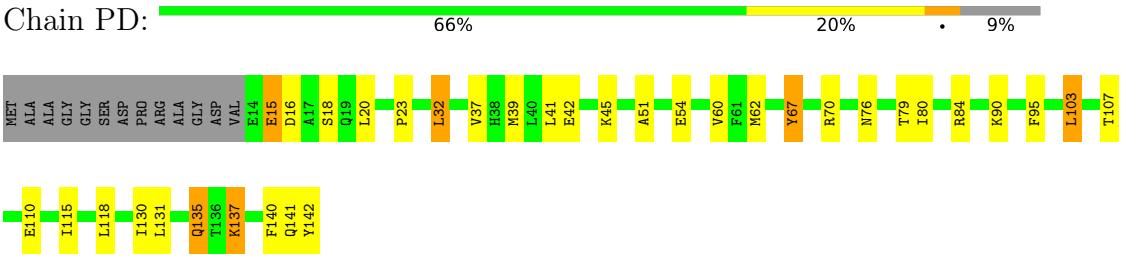
• Molecule 57: DNA-directed RNA polymerase II subunit RPB3

Chain PC:



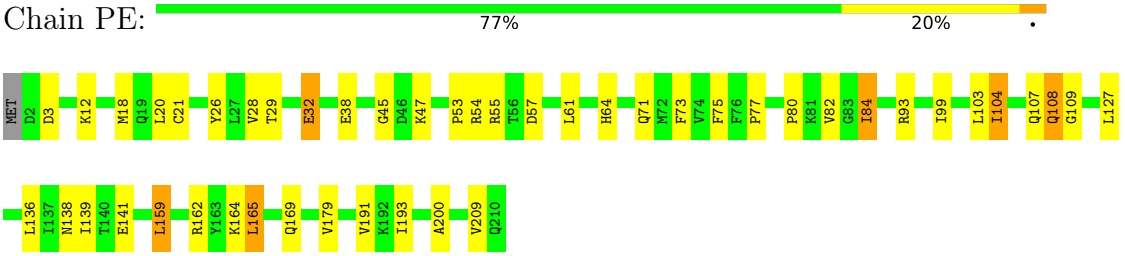
• Molecule 58: DNA-directed RNA polymerase II subunit RPB4

Chain PD:



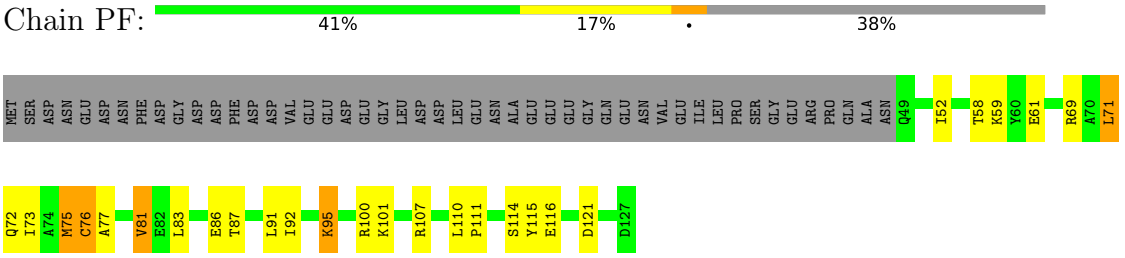
• Molecule 59: DNA-directed RNA polymerase II subunit E

Chain PE:



• Molecule 60: DNA-directed RNA polymerase II subunit F

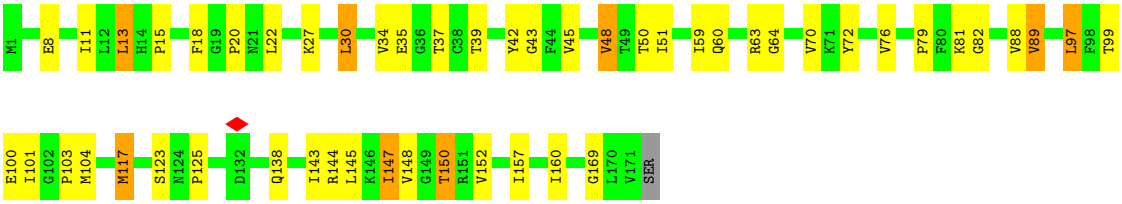
Chain PF:



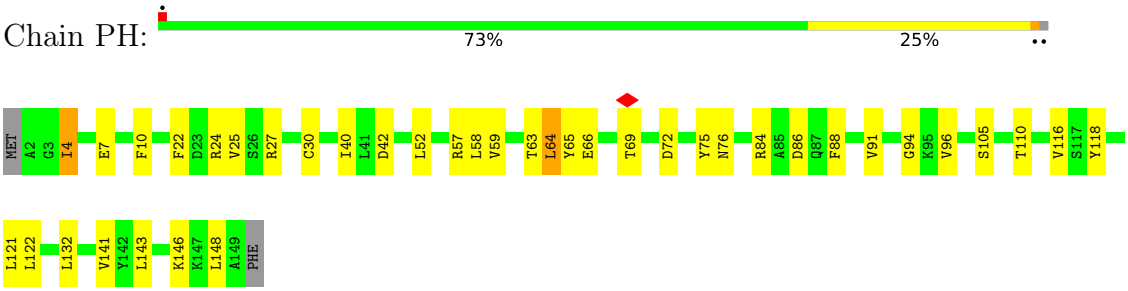
• Molecule 61: DNA-directed RNA polymerase II subunit RPB7

Chain PG:

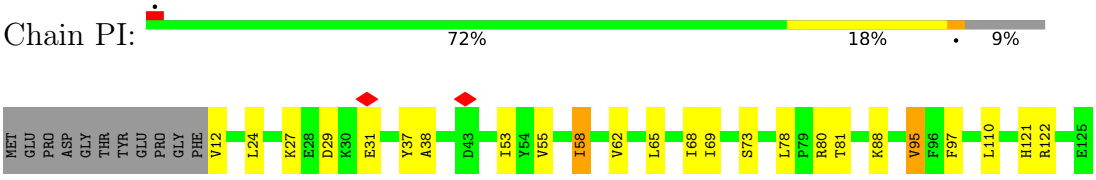




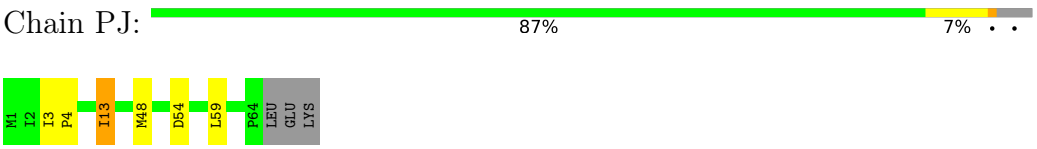
• Molecule 62: DNA-directed RNA polymerases I, II, and III subunit RPABC3



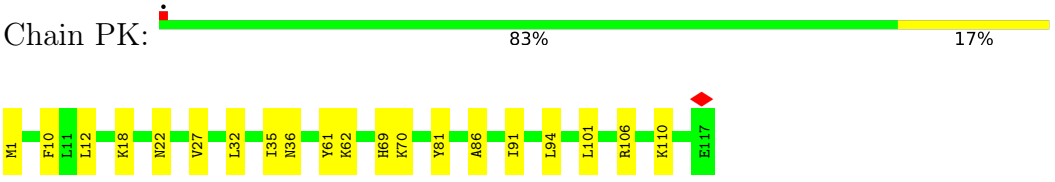
• Molecule 63: DNA-directed RNA polymerase II subunit RPB9



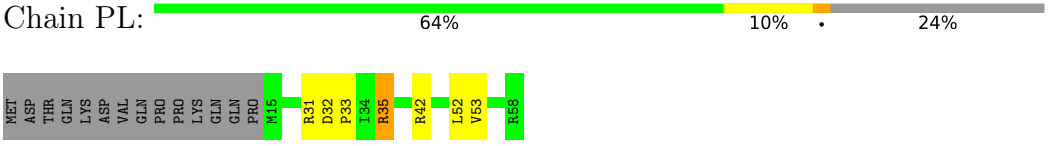
• Molecule 64: RPB10



• Molecule 65: RNA_pol_L_2 domain-containing protein

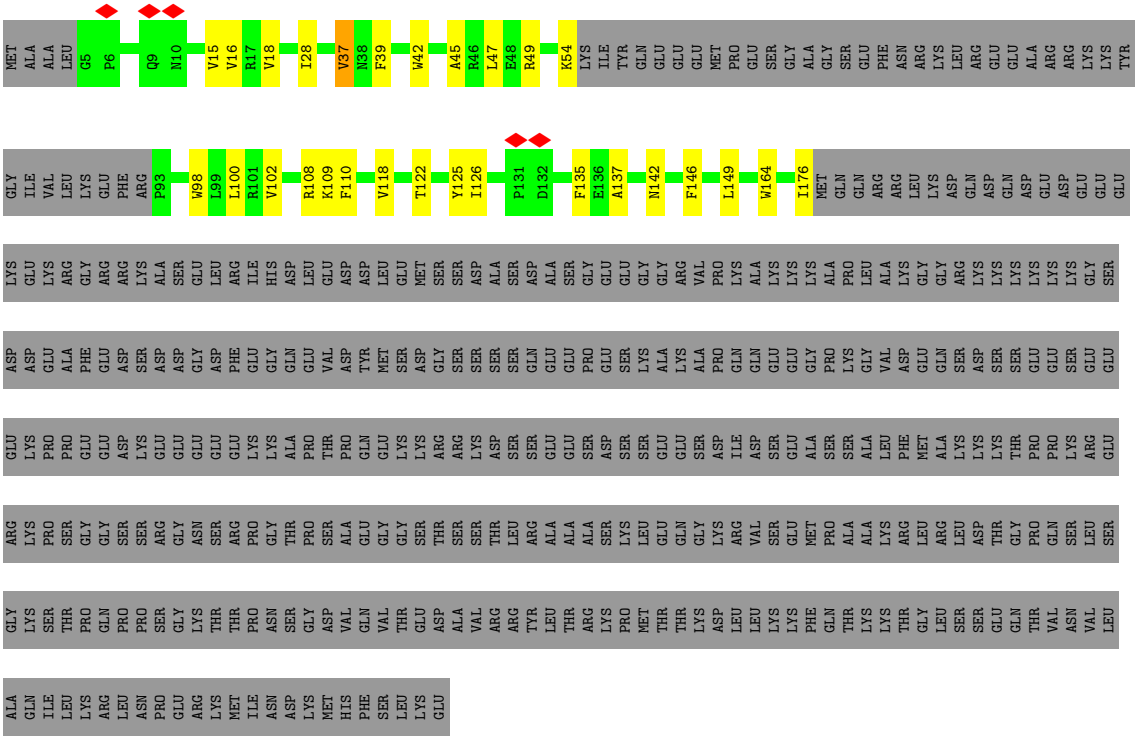


• Molecule 66: RPB12



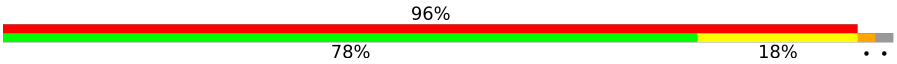
• Molecule 67: General transcription factor IIF subunit 1

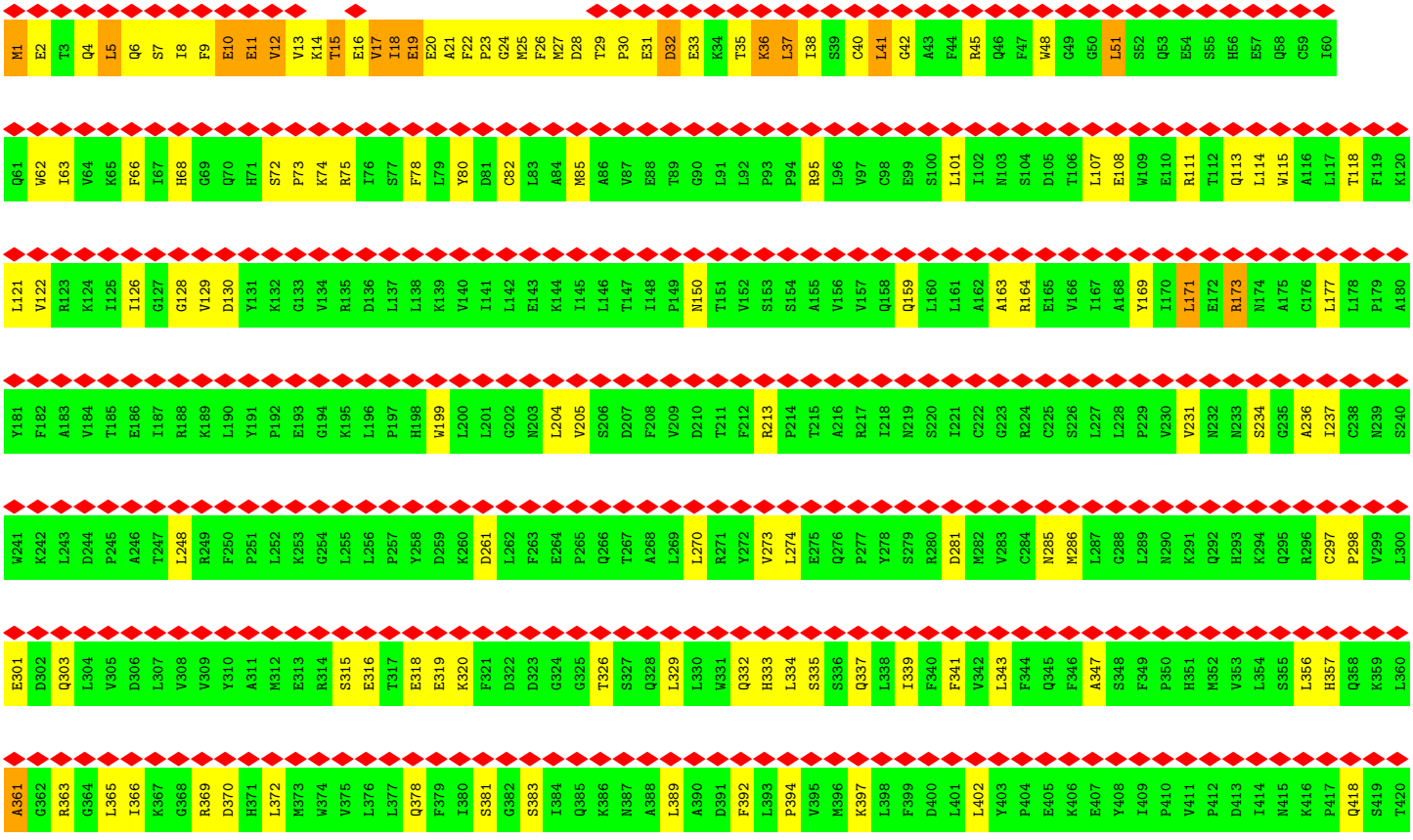


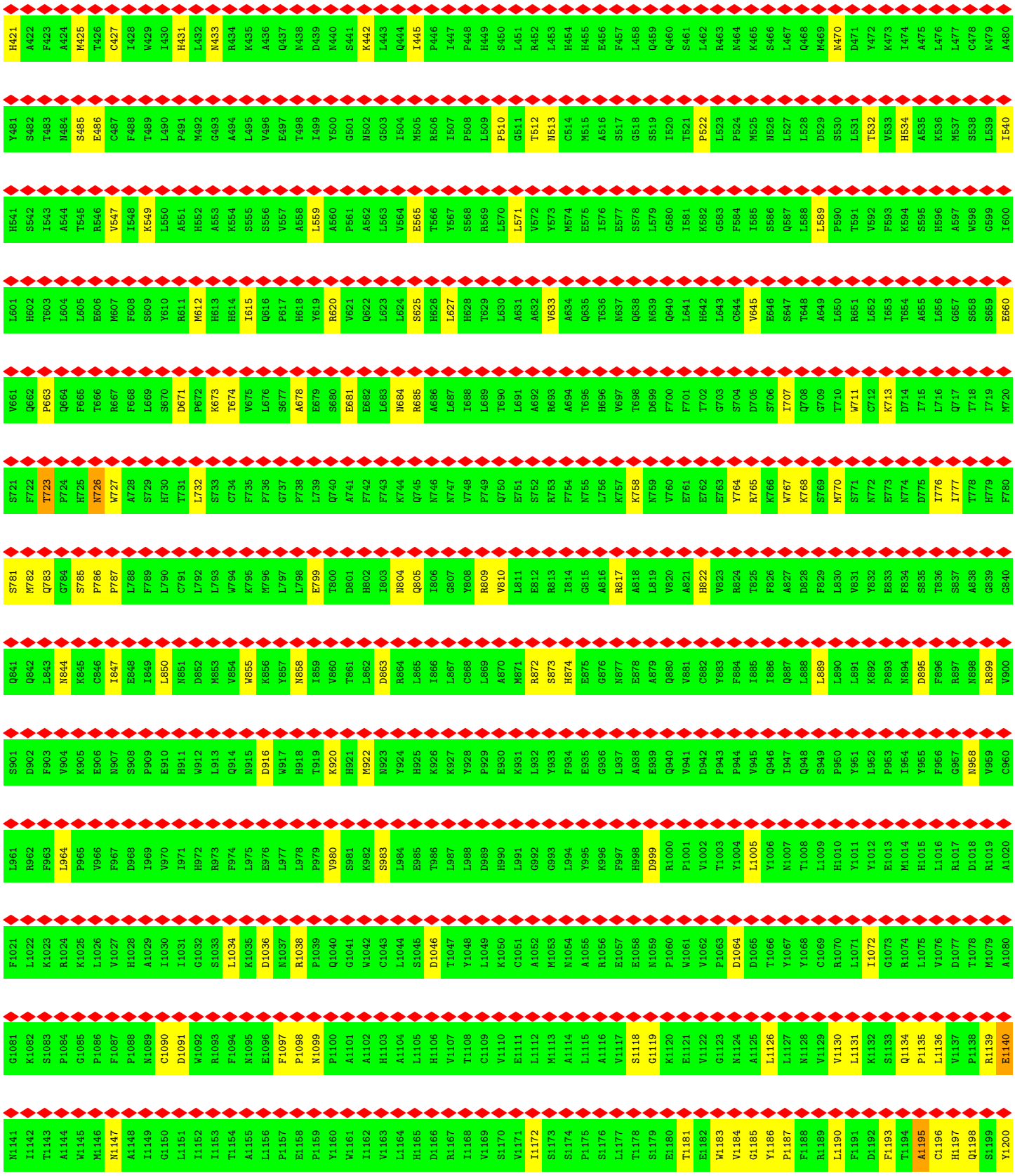


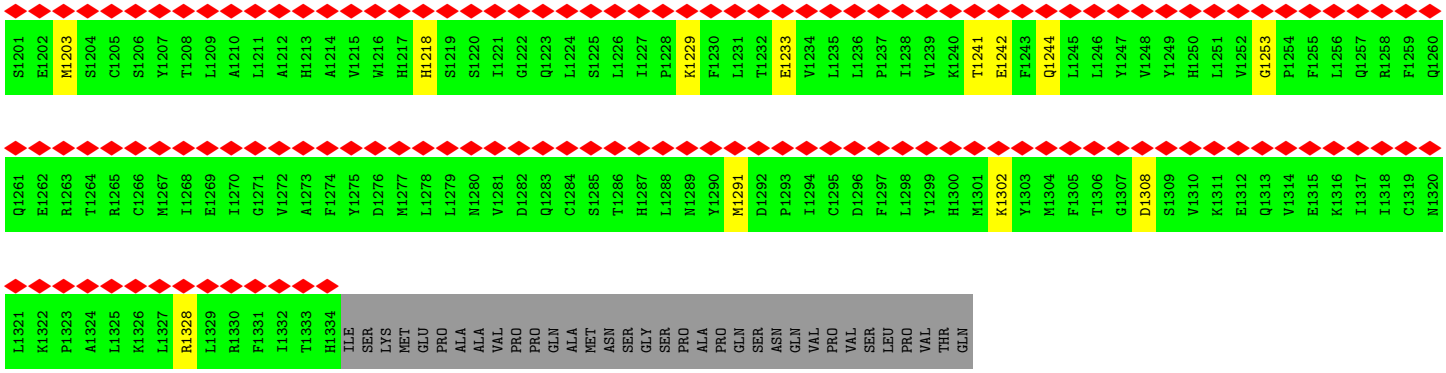
• Molecule 68: Mediator of RNA polymerase II transcription subunit 23

Chain w:

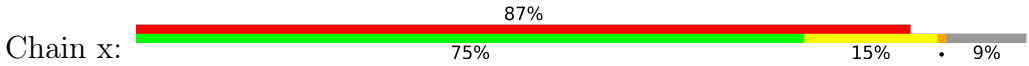


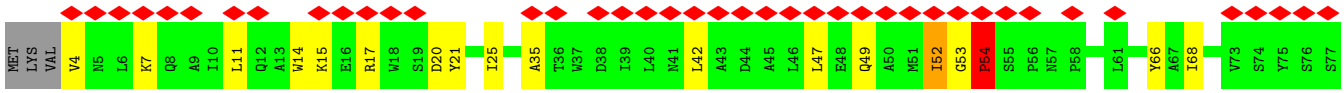


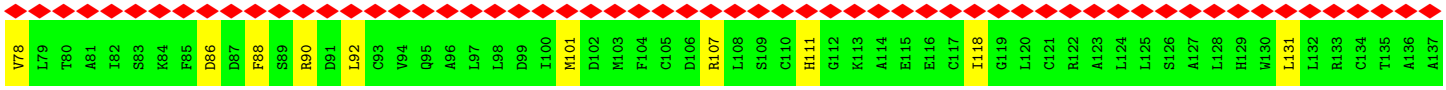

H421 A422 F423 A424 M425 T426 C427 I428 W429 I430 H431 L432 N433 R434 K435 A436 Q437 N438 D439 N440 S441 K442 L443 Q444 I445 P446 I447 P448 H449 S450 L451 R452 L453 H454 H455 E456 F457 L458 Q459 Q460 S461 L462 R463 N464 K465 S466 L467 Q468 M469 N470 D471 Y472 K473 I474 A475 L476 L477 C478 N479 A480
Y481 S482 T483 N484 S485 E486 C487 F488 T489 L490 P491 M492 G493 A494 L495 V496 E497 T498 I499 Y500 G501 N502 G503 I504 M505 R506 I507 P508 L509 P510 G511 T512 N513 C514 M515 A516 S517 G518 S519 I520 T521 P522 L523 P524 M525 N526 L527 L528 D529 S530 L531 T532 V533 H534 A535 K536 M537 S538 L539 I540
H541 S542 I543 A544 T545 R546 V547 I548 K549 L550 A551 H552 A553 K554 S555 S556 V557 A558 L559 A560 P561 A562 L563 V564 E565 T566 Y567 S568 R569 L570 L571 V572 Y573 M574 E575 I576 E577 S578 L579 G580 I581 K582 G583 F584 I585 S586 Q587 L588 L589 P590 T591 V592 F593 K594 S595 H596 A597 W598 G599 I600
L601 H602 T603 L604 L605 E606 M607 F608 S609 Y610 R611 M612 H613 H614 I615 Q616 P617 H618 Y619 R620 V621 Q622 L623 L624 S625 H626 L627 H628 T629 L630 A631 A632 V633 A634 Q635 T636 N637 Q638 N639 Q640 L641 H642 L643 C644 V645 E646 S647 T648 A649 L650 R651 L652 I653 T654 A655 L656 G657 S658 S659 E660
V661 Q662 P663 Q664 F665 T666 R667 F668 L669 S670 D671 P672 K673 T674 V675 L676 S677 A678 E679 S680 E681 E682 L683 N684 R685 A686 L687 I688 L689 T690 L691 A692 R693 A694 T695 H696 V697 T698 D699 F700 F701 T702 G703 S704 D705 S706 I707 Q708 G709 T710 W711 C712 K713 D714 I715 L716 Q717 T718 I719 M720
S721 F722 T723 P724 H725 N726 W727 A728 S729 H730 T731 L732 S733 C734 F735 P736 G737 P738 L739 Q740 A741 F742 F743 K744 Q745 N746 N747 V748 P749 Q750 E751 S752 R753 F754 N755 L756 K757 K758 N759 V760 E761 E762 E763 Y764 R765 K766 W767 K768 S769 M770 S771 N772 E773 N774 D775 I776 I777 T778 H779 F780
S781 M782 Q783 G784 S785 P786 P787 L788 F789 L790 C791 L792 L793 W794 K795 M796 L797 L798 E799 T800 D801 H802 I803 N804 Q805 I806 G807 Y808 R809 V810 L811 E812 R813 I814 G815 A816 R817 A818 L819 V820 A821 H822 V823 R824 T825 F826 A827 D828 F829 L830 V831 Y832 E833 F834 S835 T836 S837 A838 G839 G840
Q841 Q842 L843 N844 K845 C846 I847 E848 I849 L850 N851 D852 M853 V854 W855 K856 Y857 N858 I859 V860 T861 L862 D863 R864 L865 I866 L867 C868 L869 A870 M871 R872 S873 H874 E875 G876 N877 E878 A879 Q880 V881 C882 Y883 F884 I885 I886 Q887 L888 L889 L890 L891 K892 P893 N894 D895 F896 R897 N898 R899 V900
S901 D902 F903 V904 K905 E906 N907 S908 P909 E910 H911 W912 L913 Q914 N915 D916 W917 H918 T919 K920 H921 M922 N923 Y924 H925 K926 K927 Y928 P929 E930 K931 L932 Y933 F934 E935 G936 L937 A938 E939 Q940 V941 D942 P943 P944 V945 Q946 I947 Q948 S949 P950 Y951 L952 P953 I954 Y955 F956 G957 N958 V959 C960
L961 R962 F963 L964 P965 V966 F967 D968 I969 V970 I971 H972 R973 F974 L975 E976 L977 L978 P979 V980 S981 K982 S983 L984 E985 T986 L987 L988 D989 H990 L991 G992 G993 L994 Y995 K996 F997 H998 D999 R1000 P1001 V1002 T1003 Y1004 L1005 Y1006 N1007 T1008 L1009 H1010 Y1011 Y1012 E1013 M1014 H1015 L1016 R1017 D1018 R1019 A1020
F1021 L1022 K1023 R1024 K1025 L1026 V1027 H1028 A1029 I1030 I1031 G1032 S1033 L1034 K1035 D1036 N1037 R1038 P1039 Q1040 G1041 W1042 C1043 L1044 S1045 D1046 T1047 Y1048 L1049 K1050 C1051 A1052 M1053 N1054 A1055 R1056 E1057 E1058 N1059 P1060 W1061 V1062 P1063 D1064 D1065 T1066 Y1067 Y1068 C1069 R1070 L1071 I1072 G1073 R1074 L1075 V1076 D1077 T1078 M1079 A1080
G1081 K1082 S1083 P1084 G1085 P1086 F1087 P1088 N1089 C1090 D1091 W1092 R1093 F1094 N1095 E1096 F1097 P1098 N1099 P1100 A1101 A1102 H1103 A1104 L1105 H1106 V1107 T1108 C1109 V1110 E1111 L1112 M1113 A1114 L1115 A1116 V1117 S1118 G1119 K1120 E1121 V1122 G1123 N1124 A1125 L1126 L1127 N1128 V1129 V1130 L1131 K1132 S1133 Q1134 P1135 L1136 V1137 P1138 R1139 E1140
N1141 I1142 T1143 A1144 W1145 M1146 N1147 A1148 I1149 G1150 L1151 L1152 I1153 T1154 A1155 L1156 P1157 E1158 P1159 Y1160 W1161 I1162 V1163 L1164 H1165 D1166 R1167 I1168 V1169 S1170 V1171 I1172 S1173 S1174 P1175 S1176 L1177 T1178 S1179 E1180 T1181 E1182 W1183 V1184 G1185 Y1186 P1187 F1188 R1189 L1190 F1191 D1192 F1193 T1194 A1195 C1196 H1197 Q1198 S1199 Y1200

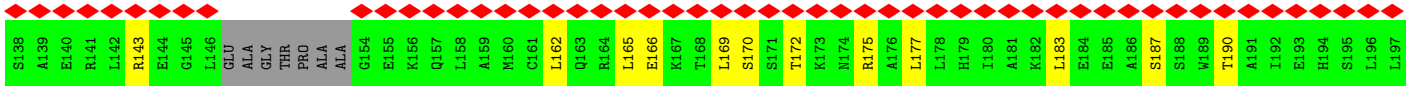


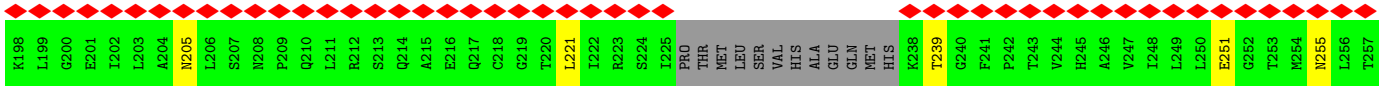
• Molecule 69: Mediator of RNA polymerase II transcription subunit 24

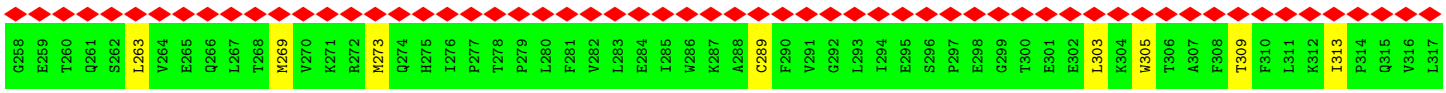


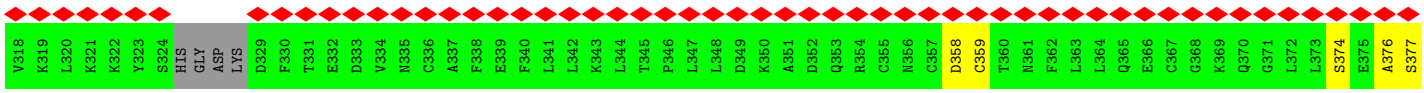


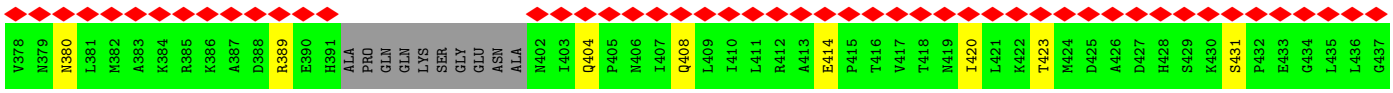


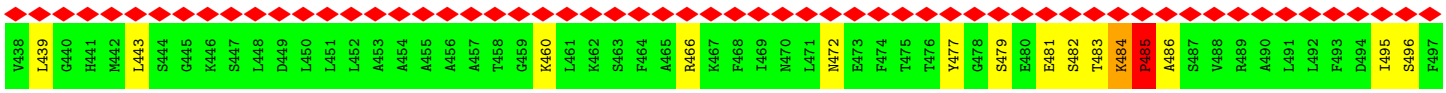


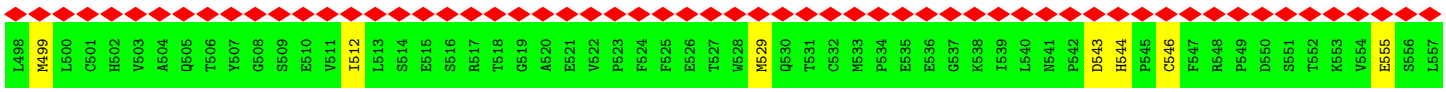


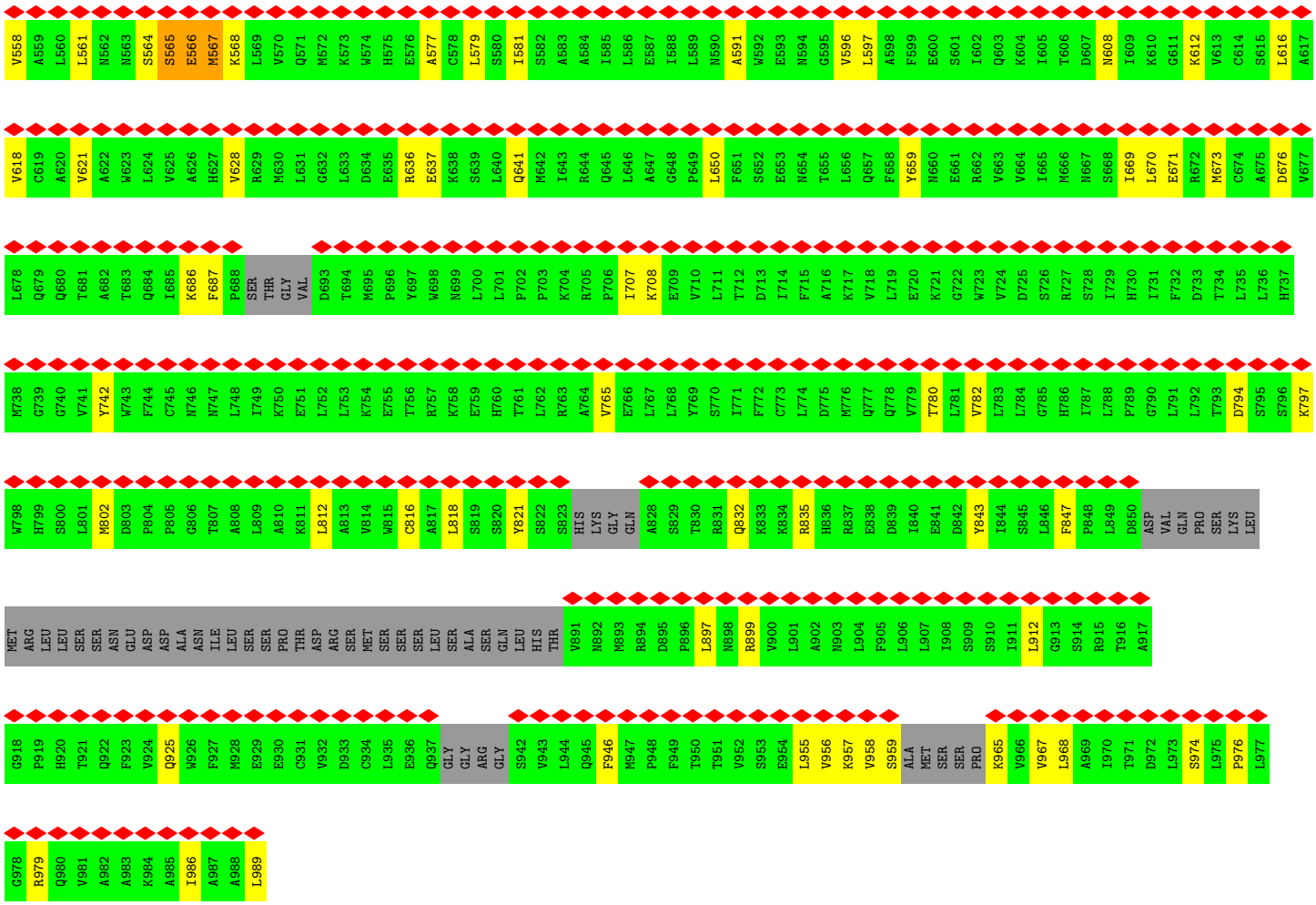








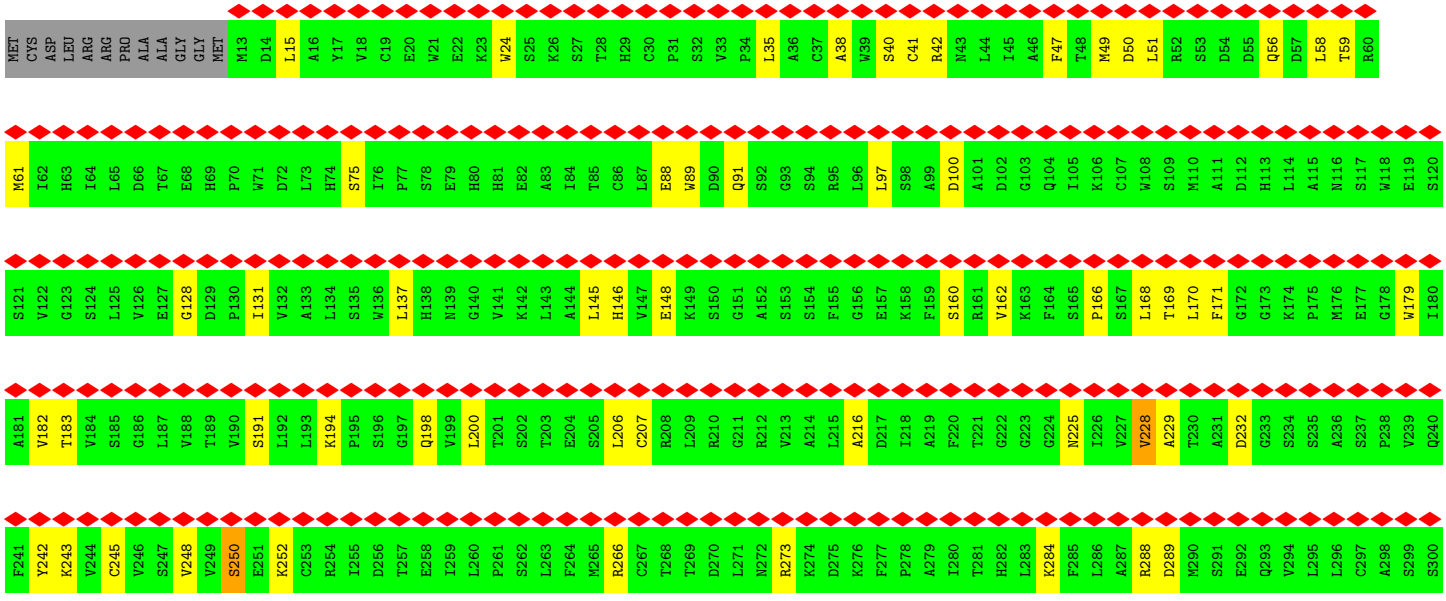


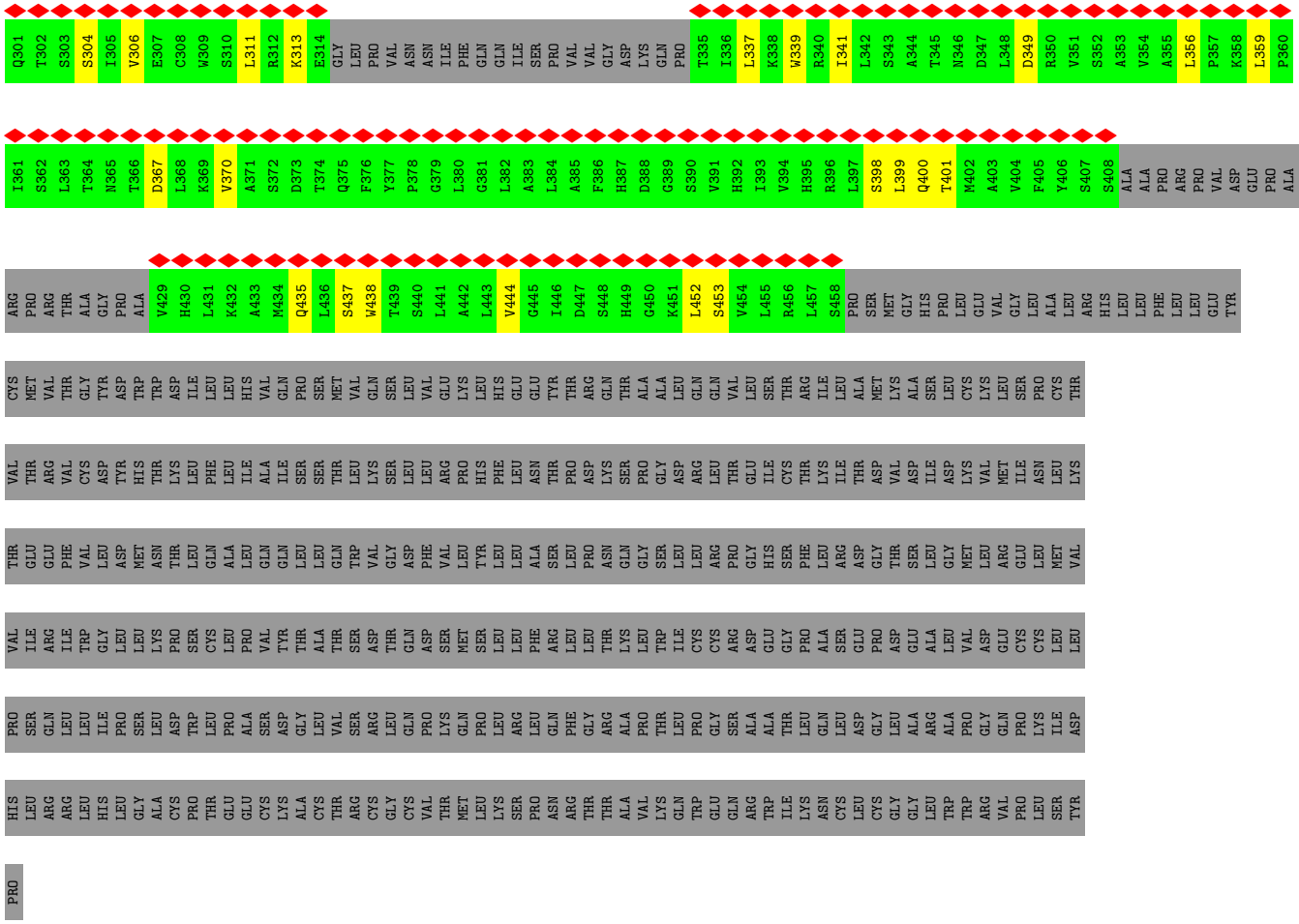


• Molecule 70: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

Chain p:






Q301 T302 S303 S304 I305 V306 E307 C308 W309 S310 L311 R312 K313 E314 GLY LEU PRO VAL ASN ASN ILE PHE GLN GLN ILE SER PRO VAL VAL GLY ASP LYS GLN PRO T335 I336 L337 K338 W339 R340 I341 L342 S343 A344 T345 N346 D347 L348 D349 R350 V351 S352 A353 V354 A355 L356 P357 K358 L359 P360
I361 S362 L363 T364 N365 T366 D367 L368 K369 V370 A371 S372 D373 T374 Q375 F376 Y377 P378 G379 L380 G381 L382 A383 L384 A385 F386 H387 D388 G389 S390 V391 H392 I393 V394 H395 R396 L397 S398 L399 Q400 T401 M402 A403 V404 F405 Y406 S407 S408 ALA ALA PRO ARG PRO VAL ASP GLU PRO ALA MET LYS
ARG PRO ARG THR ALA GLY PRO ALA V429 H430 L431 K432 A433 M434 Q435 L436 S437 W438 T439 S440 L441 A442 L443 V444 G445 I446 D447 S448 H449 G450 K451 L452 S453 V454 L455 R456 L457 S458 PRO SER MET GLY HIS PRO LEU GLU VAL GLY LEU ALA LEU ARG HIS LEU LEU PHE LEU LEU GLU TYR
CYS MET VAL THR GLY TYR ASP TRP TRP ASP ILE LEU LEU HIS VAL GLN PRO SER MET VAL GLN SER LEU VAL GLU LYS LEU HIS GLU GLU TYR THR ARG GLN THR ALA ALA LEU GLN GLN VAL LEU SER THR ARG ILE LEU ALA MET LYS ALA SER LEU CYS LYS LEU SER PRO CYS THR
VAL THR ARG VAL CYS ASP TYR HIS THR LYS LEU PHE LEU ILE ALA ILE SER SER THR LEU LYS SER LEU LEU ARG PRO HIS PHE LEU ASN THR PRO ASP LYS SER PRO GLY ASP ARG LEU THR GLU ILE CYS THR LYS ILE THR ASP VAL ASP ILE ASP LYS VAL MET ILE ASN LEU LYS
THR GLU GLU PHE VAL LEU ASP MET ASN THR LEU GLN ALA LEU GLN GLN LEU LEU GLN TRP VAL GLY ASP PHE VAL LEU TYR LEU LEU ALA SER LEU PRO ASN GLN GLY SER LEU LEU ARG PRO GLY HIS SER PHE LEU ARG ASP GLY THR SER LEU GLY MET LEU ARG GLU LEU MET VAL
VAL ILE ARG ILE TRP GLY LEU LEU LYS PRO SER CYS LEU PRO VAL TYR THR ALA THR SER ASP THR GLN ASP SER MET SER LEU LEU PHE ARG LEU LEU THR LYS LEU TRP ILE CYS CYS ARG ASP GLU GLY PRO ALA SER GLU PRO ASP GLU ALA LEU VAL ASP GLU CYS CYS LEU LEU
PRO SER GLN LEU LEU ILE PRO SER LEU ASP TRP LEU PRO ALA SER ASP GLY LEU VAL SER ARG LEU GLN PRO LYS GLN PRO LEU ARG LEU GLN PHE GLY ARG ALA PRO THR LEU PRO GLY SER ALA ALA THR LEU GLN LEU ASP GLY LEU ALA ARG ALA LEU PRO GLY GLN PRO LYS LEU ILE ASP
HIS LEU ARG ARG LEU HIS LEU GLY ALA CYS PRO THR GLU GLU CYS LYS ALA CYS THR ARG CYS GLY CYS VAL THR MET LEU LYS SER PRO ASN ARG THR THR ALA VAL LYS GLN TRP GLU GLN ARG TRP ILE LYS ASN CYS LEU CYS GLY GLY LEU TRP TRP ARG VAL PRO LEU SER TYR
PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67732	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.867	Depositor
Minimum map value	-3.734	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.41	Depositor
Map size (Å)	674.39996, 674.39996, 674.39996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.405, 1.405, 1.405	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.98	3/3645 (0.1%)	1.37	15/4952 (0.3%)
2	m	0.19	0/1010	0.38	0/1359
3	d	0.97	0/1277	1.50	11/1714 (0.6%)
4	f	0.76	0/1359	1.04	4/1845 (0.2%)
5	g	0.94	0/1411	1.38	2/1901 (0.1%)
6	h	0.94	1/1507 (0.1%)	1.31	2/2036 (0.1%)
7	r	0.94	1/1558 (0.1%)	1.27	5/2096 (0.2%)
8	t	1.05	2/1530 (0.1%)	1.54	20/2066 (1.0%)
9	j	0.55	1/1016 (0.1%)	0.91	6/1363 (0.4%)
10	k	0.96	0/885	1.26	0/1190
11	n	0.45	2/7371 (0.0%)	0.73	20/10037 (0.2%)
12	q	0.67	2/4336 (0.0%)	0.89	4/5865 (0.1%)
13	s	0.73	0/489	1.27	8/663 (1.2%)
14	u	0.68	0/797	1.12	5/1082 (0.5%)
15	v	1.00	2/1092 (0.2%)	1.58	8/1468 (0.5%)
16	z	0.92	0/781	1.39	5/1067 (0.5%)
17	c	0.51	0/2106	0.79	3/2842 (0.1%)
18	e	0.18	0/840	0.34	0/1128
19	b	0.75	0/911	1.08	0/1229
20	l	0.18	0/1048	0.36	0/1405
21	o	0.39	0/1256	0.76	2/1724 (0.1%)
22	i	0.98	1/523 (0.2%)	1.25	0/692
23	0	0.99	0/2288	1.27	4/3101 (0.1%)
24	8	0.97	0/2437	1.19	1/3306 (0.0%)
25	9	0.95	0/2356	1.23	1/3185 (0.0%)
26	1	1.06	0/2674	1.28	7/3660 (0.2%)
27	2	1.00	0/2588	1.18	2/3509 (0.1%)
28	3	0.99	0/2102	1.17	0/2844
29	4	0.97	0/3663	1.18	2/4965 (0.0%)
30	5	0.99	0/433	1.22	0/585
31	6	0.97	0/4983	1.18	1/6731 (0.0%)
32	7	0.97	0/5957	1.19	3/8071 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	EA	0.95	1/1499 (0.1%)	1.21	2/2012 (0.1%)
34	EB	0.96	0/1428	1.21	0/1917
35	DA	0.96	0/4627	1.17	3/6248 (0.0%)
36	DB	0.97	0/7993	1.16	5/10836 (0.0%)
37	DD	0.94	0/1343	1.22	2/1795 (0.1%)
37	Dd	0.95	0/1321	1.17	0/1772
38	DE	0.98	0/4469	1.19	3/6050 (0.0%)
38	De	0.98	0/4433	1.18	2/6004 (0.0%)
39	DF	1.00	0/3167	1.22	1/4303 (0.0%)
39	Df	1.00	0/3140	1.21	1/4268 (0.0%)
40	DG	1.00	0/1199	1.15	0/1612
41	DH	0.99	0/1673	1.18	0/2285
42	DI	0.98	0/981	1.20	0/1332
42	Di	0.95	0/989	1.18	0/1343
43	DJ	0.94	0/736	1.18	0/998
43	Dj	0.93	0/775	1.19	0/1049
44	DL	0.94	0/622	1.23	0/841
44	Dl	0.95	0/888	1.22	1/1194 (0.1%)
45	Dc	0.98	0/1035	1.16	0/1406
46	Dk	0.96	0/799	1.19	1/1070 (0.1%)
47	Dm	0.94	0/733	1.20	0/977
48	DO	1.00	0/781	1.20	0/1061
49	DP	0.98	0/1438	1.14	0/1935
50	DQ	0.96	0/1013	1.19	0/1366
51	BA	0.98	0/1967	1.21	0/2656
52	FB	0.98	0/1817	1.17	1/2445 (0.0%)
53	X	0.73	4/1607 (0.2%)	0.69	6/2481 (0.2%)
54	Y	0.57	0/1565	0.73	5/2410 (0.2%)
55	PA	0.99	0/11881	1.21	8/16057 (0.0%)
56	PB	0.99	0/9243	1.17	4/12475 (0.0%)
57	PC	1.00	0/2102	1.17	0/2857
58	PD	0.97	0/1036	1.20	0/1397
59	PE	0.97	0/1751	1.18	0/2366
60	PF	0.95	0/645	1.20	1/871 (0.1%)
61	PG	1.02	0/1365	1.18	1/1853 (0.1%)
62	PH	0.99	0/1207	1.14	0/1628
63	PI	0.99	0/948	1.15	1/1284 (0.1%)
64	PJ	0.96	0/516	1.19	0/696
65	PK	0.96	0/956	1.16	0/1294
66	PL	0.98	0/377	1.07	0/500
67	FA	0.96	0/1130	1.13	0/1528
68	w	0.56	0/11053	0.73	8/15018 (0.1%)
69	x	0.57	0/7179	0.72	5/9712 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
70	p	0.72	0/3191	0.78	0/4333
All	All	0.89	20/174847 (0.0%)	1.11	202/237216 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	X	-39	DA	O3'-P	-13.42	1.41	1.61
12	q	452	ALA	C-N	9.04	1.46	1.33
7	r	174	VAL	C-O	-8.00	1.15	1.24
9	j	94	GLN	C-N	-7.89	1.24	1.33
1	a	57	HIS	C-O	7.62	1.32	1.24
8	t	136	ARG	C-O	-6.98	1.15	1.23
15	v	38	LYS	C-O	6.92	1.32	1.24
1	a	64	THR	C-O	6.26	1.31	1.24
22	i	100	LEU	C-O	6.23	1.31	1.24
15	v	42	ILE	N-CA	6.20	1.54	1.46
1	a	501	CYS	N-CA	6.09	1.50	1.46
12	q	189	ARG	C-O	5.73	1.30	1.24
11	n	206	THR	N-CA	5.41	1.53	1.46
53	X	-37	DG	C1'-N9	-5.14	1.36	1.46
53	X	-9	DG	C1'-N9	-5.13	1.36	1.46
8	t	185	GLY	C-O	5.12	1.30	1.24
11	n	202	ARG	C-O	5.11	1.30	1.24
53	X	-26	DA	C1'-N9	-5.09	1.36	1.46
6	h	43	PRO	C-O	-5.04	1.17	1.24
33	EA	157	CYS	N-CA	5.02	1.49	1.46

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	d	161	VAL	N-CA-C	-12.81	100.00	112.17
3	d	130	GLU	N-CA-C	-11.44	98.89	111.36
54	Y	35	DC	C2'-C3'-O3'	-10.79	95.32	111.50
8	t	11	VAL	N-CA-C	-9.86	100.96	110.42
9	j	77	PRO	CA-N-CD	-9.34	98.92	112.00
69	x	54	PRO	N-CA-CB	-9.30	93.49	103.25
8	t	154	TRP	N-CA-C	-8.89	101.55	111.07
1	a	505	PRO	N-CA-C	-8.85	101.71	113.65
68	w	19	GLU	N-CA-C	-8.84	101.57	111.82
1	a	505	PRO	CA-C-N	8.81	132.53	120.46
1	a	505	PRO	C-N-CA	8.81	132.53	120.46
69	x	485	PRO	CA-N-CD	-8.79	99.70	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	v	39	THR	CA-C-O	-8.70	111.69	120.82
11	n	369	PRO	N-CA-C	-8.65	97.16	111.26
11	n	1343	PRO	N-CA-CB	8.62	111.44	103.08
11	n	1351	PRO	N-CA-CB	8.50	111.33	103.08
8	t	80	GLU	CB-CA-C	-8.32	106.97	116.54
3	d	119	GLN	N-CA-C	-8.21	102.41	111.36
11	n	1347	PRO	N-CA-CB	7.90	110.74	103.08
15	v	41	LYS	N-CA-C	-7.89	101.64	111.11
11	n	1355	PRO	N-CA-CB	7.87	111.51	103.25
16	z	595	PRO	CB-CA-C	-7.82	101.38	111.46
6	h	43	PRO	CB-CA-C	-7.75	100.75	113.06
35	DA	467	ILE	N-CA-C	-7.68	105.22	112.83
27	2	269	PRO	N-CA-CB	7.61	109.94	103.17
1	a	68	ALA	N-CA-C	-7.59	103.08	111.36
15	v	41	LYS	CA-C-O	-7.58	112.80	120.90
11	n	1237	PRO	N-CA-CB	7.51	111.14	103.25
38	DE	521	ASP	CB-CA-C	7.47	117.22	109.83
11	n	1196	PRO	N-CA-CB	7.43	111.06	103.25
16	z	545	ARG	N-CA-C	-7.40	104.13	113.01
13	s	134	PRO	N-CA-CB	7.19	110.05	103.08
11	n	1255	PRO	N-CA-CB	7.17	110.78	103.25
16	z	546	GLU	CB-CA-C	-7.12	108.36	116.63
11	n	1326	PRO	N-CA-CB	7.02	110.62	103.25
32	7	311	PRO	N-CA-CB	7.00	109.49	103.19
11	n	1344	PRO	N-CA-CB	6.83	110.42	103.25
35	DA	498	PRO	N-CA-CB	6.81	110.40	103.25
3	d	114	LEU	N-CA-C	-6.81	103.86	111.28
8	t	137	GLY	CA-C-O	-6.79	114.90	122.24
55	PA	830	GLY	CA-C-O	-6.76	117.82	122.22
11	n	1352	PRO	N-CA-CB	6.75	110.34	103.25
55	PA	661	GLY	CA-C-O	-6.71	117.86	122.22
5	g	23	ASP	N-CA-C	-6.65	104.03	111.28
4	f	30	LEU	N-CA-C	-6.64	104.04	111.28
11	n	1192	PRO	N-CA-CB	6.63	110.30	103.00
21	o	719	PRO	N-CA-C	6.63	118.79	110.70
53	X	-14	DG	C4'-C3'-O3'	6.62	119.93	110.00
26	1	483	THR	O-C-N	6.58	124.56	121.53
11	n	1267	PRO	N-CA-CB	6.55	110.63	103.23
11	n	1206	PRO	N-CA-CB	6.53	110.11	103.25
68	w	30	PRO	N-CA-CB	6.52	110.51	103.33
1	a	231	LEU	N-CA-C	-6.51	104.18	111.28
12	q	393	PRO	N-CA-CB	6.51	110.08	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	s	158	PRO	N-CA-CB	6.51	110.08	103.25
26	1	276	PRO	N-CA-CB	6.49	110.07	103.25
13	s	119	PRO	N-CA-CB	6.43	110.00	103.25
53	X	-15	DG	C2'-C3'-O3'	-6.42	101.87	111.50
12	q	395	PRO	N-CA-CB	6.41	109.98	103.25
9	j	124	TYR	N-CA-C	-6.40	104.35	111.71
23	0	217	PRO	N-CA-CB	6.38	110.34	103.33
53	X	-9	DG	C2'-C3'-O3'	-6.38	101.94	111.50
23	0	237	PRO	N-CA-CB	6.36	109.93	103.25
1	a	59	VAL	CA-C-O	-6.33	114.82	121.41
26	1	265	PRO	N-CA-CB	6.32	109.88	103.25
27	2	282	PRO	N-CA-CB	6.32	109.88	103.25
55	PA	1370	GLY	CA-C-O	-6.32	117.76	122.37
61	PG	43	GLY	CA-C-O	-6.31	117.88	122.23
32	7	308	PRO	N-CA-CB	6.29	109.86	103.25
1	a	32	PRO	N-CA-CB	6.28	109.91	103.00
26	1	484	PRO	N-CA-CB	6.27	109.83	103.25
1	a	509	ARG	CB-CA-C	-6.24	101.08	110.88
26	1	287	PRO	N-CA-CB	6.24	109.80	103.25
26	1	480	PRO	N-CA-CB	6.24	109.95	103.15
8	t	173	PRO	N-CA-C	6.23	120.99	111.34
69	x	35	ALA	CA-C-N	6.21	133.41	121.54
69	x	35	ALA	C-N-CA	6.21	133.41	121.54
13	s	135	PRO	N-CA-CB	6.21	110.10	103.52
54	Y	-6	DG	P-O3'-C3'	6.17	129.46	120.20
53	X	-37	DG	C2'-C3'-O3'	6.16	120.74	111.50
33	EA	161	VAL	CA-C-N	-6.15	111.54	122.74
33	EA	161	VAL	C-N-CA	-6.15	111.54	122.74
3	d	153	HIS	N-CA-C	-6.12	104.60	111.28
13	s	113	PRO	N-CA-CB	6.11	110.05	103.33
12	q	399	PRO	N-CA-CB	6.09	109.65	103.25
15	v	39	THR	O-C-N	6.08	128.34	122.07
46	Dk	180	PRO	N-CA-C	6.08	118.11	110.70
11	n	74	PRO	N-CA-CB	6.04	109.91	103.39
32	7	6	ASP	CB-CA-C	6.03	115.80	109.83
11	n	363	GLU	CB-CA-C	-6.03	109.61	116.54
53	X	-28	DT	C2'-C3'-O3'	-6.02	102.47	111.50
9	j	60	ASP	CA-C-N	6.01	132.79	121.97
9	j	60	ASP	C-N-CA	6.01	132.79	121.97
53	X	-25	DA	C2'-C3'-O3'	6.00	120.50	111.50
9	j	94	GLN	O-C-N	-6.00	115.32	122.15
11	n	1348	PRO	N-CA-CB	5.98	109.91	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	t	133	PRO	CB-CA-C	-5.98	101.69	111.56
56	PB	535	GLY	CA-C-O	-5.95	118.13	122.23
23	0	215	PRO	N-CA-CB	5.94	109.87	103.33
3	d	125	VAL	N-CA-C	-5.93	104.73	110.72
14	u	80	GLU	CA-C-O	-5.92	115.10	121.38
26	1	507	PRO	N-CA-CB	5.92	110.07	103.44
8	t	14	GLY	N-CA-C	-5.90	105.35	115.61
1	a	278	HIS	CB-CA-C	5.87	118.79	109.52
14	u	78	SER	N-CA-C	-5.87	104.89	111.28
8	t	203	GLN	CA-C-N	-5.86	112.81	122.89
8	t	203	GLN	C-N-CA	-5.86	112.81	122.89
12	q	410	PRO	N-CA-CB	5.86	110.00	103.44
35	DA	626	GLY	CA-C-O	-5.85	118.10	122.37
1	a	442	VAL	N-CA-C	5.84	114.76	106.53
38	De	615	ASP	N-CA-C	-5.84	106.50	113.97
11	n	1309	PRO	N-CA-CB	5.81	109.95	103.44
13	s	83	LEU	N-CA-C	-5.80	105.30	112.38
15	v	98	ILE	N-CA-C	-5.80	104.70	110.62
8	t	72	PRO	N-CA-C	5.80	121.60	113.53
5	g	24	GLU	N-CA-C	-5.80	104.86	111.07
9	j	64	PRO	N-CA-C	5.80	124.42	112.47
4	f	118	ARG	CB-CA-C	5.80	120.71	110.85
3	d	127	GLN	N-CA-C	-5.76	105.00	111.28
14	u	106	ASP	N-CA-C	-5.76	105.00	111.28
24	8	254	GLY	CA-C-O	-5.73	118.27	122.23
63	PI	58	ILE	N-CA-C	-5.72	107.17	112.83
23	0	220	PRO	N-CA-CB	5.72	109.84	103.44
37	DD	947	PHE	CA-CB-CG	5.71	119.50	113.80
55	PA	789	GLY	CA-C-O	-5.70	118.21	122.37
3	d	120	ILE	N-CA-C	-5.68	104.83	110.62
3	d	107	ILE	N-CA-C	-5.67	104.84	110.62
56	PB	253	GLY	CA-C-O	-5.66	118.24	122.37
68	w	1198	GLN	N-CA-C	-5.63	102.19	110.52
7	r	174	VAL	CA-C-O	-5.59	114.50	120.59
7	r	173	VAL	CA-C-N	-5.57	115.77	122.90
7	r	173	VAL	C-N-CA	-5.57	115.77	122.90
55	PA	1652	PRO	N-CA-CB	-5.56	97.42	103.25
7	r	157	THR	N-CA-C	-5.55	105.32	111.71
8	t	71	TYR	CB-CA-C	5.55	115.44	110.44
4	f	64	VAL	N-CA-CB	-5.52	102.13	111.23
55	PA	887	VAL	N-CA-C	-5.51	106.43	111.67
17	c	205	ARG	N-CA-C	-5.51	106.72	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	t	92	ASP	CA-C-N	-5.50	112.93	120.46
8	t	92	ASP	C-N-CA	-5.50	112.93	120.46
16	z	492	ARG	CB-CA-C	-5.46	102.31	110.88
11	n	307	VAL	N-CA-C	-5.45	104.24	111.05
3	d	122	ALA	N-CA-C	-5.44	105.25	111.07
37	DD	947	PHE	CB-CA-C	5.42	120.74	109.95
14	u	117	LYS	CB-CA-C	5.41	119.13	110.09
14	u	107	VAL	N-CA-C	-5.41	105.23	110.42
1	a	136	PRO	N-CA-C	-5.40	106.02	113.53
52	FB	128	LYS	N-CA-C	-5.40	105.39	111.28
8	t	92	ASP	CB-CA-C	-5.40	102.41	110.88
13	s	79	GLY	N-CA-C	-5.39	107.97	114.66
38	De	780	VAL	CA-C-O	-5.39	117.94	122.63
17	c	284	CYS	CB-CA-C	-5.39	98.66	110.67
8	t	99	LYS	N-CA-C	5.38	122.27	110.80
15	v	8	PRO	N-CA-CB	5.38	108.92	103.00
38	DE	780	VAL	CA-C-O	-5.38	117.95	122.63
60	PF	75	MET	CA-C-O	-5.37	114.85	120.55
25	9	7	GLN	CB-CA-C	5.37	117.79	110.06
1	a	480	TYR	CB-CA-C	5.36	118.87	110.19
68	w	1195	ALA	N-CA-C	-5.35	105.56	111.71
13	s	84	ILE	N-CA-C	-5.34	105.29	110.42
7	r	174	VAL	N-CA-CB	-5.32	104.99	111.21
31	6	449	LYS	CB-CA-C	5.31	117.71	110.06
15	v	42	ILE	N-CA-C	5.30	120.38	109.34
36	DB	745	GLN	N-CA-C	-5.30	107.18	113.97
36	DB	966	ARG	N-CA-C	-5.30	107.46	114.04
68	w	48	TRP	N-CA-C	-5.30	105.58	111.36
54	Y	31	DG	C2'-C3'-O3'	-5.30	103.56	111.50
6	h	131	ILE	N-CA-C	5.28	115.91	108.36
36	DB	338	GLU	N-CA-C	-5.28	107.50	114.31
56	PB	1135	TYR	CB-CA-C	5.28	119.02	109.37
68	w	15	THR	N-CA-C	-5.27	105.59	112.23
39	DF	254	GLN	CB-CA-C	5.25	115.03	109.83
55	PA	1656	SER	N-CA-C	-5.25	102.71	111.37
21	o	720	PRO	N-CA-C	5.24	120.96	113.47
55	PA	250	VAL	CA-C-O	-5.23	118.08	122.63
69	x	565	SER	CA-C-O	-5.22	116.09	122.41
11	n	199	LEU	N-CA-C	-5.21	105.60	111.28
8	t	200	ILE	N-CA-CB	5.20	117.61	110.54
1	a	440	PHE	CA-C-O	-5.18	115.05	121.11
8	t	189	THR	CB-CA-C	-5.15	102.23	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	Dl	132	GLY	CA-C-O	-5.15	118.12	122.29
8	t	99	LYS	CA-C-O	-5.15	113.15	120.51
38	DE	522	ASP	N-CA-C	-5.15	106.31	112.59
54	Y	-5	DC	C4'-C3'-O3'	5.14	117.72	110.00
16	z	548	THR	N-CA-C	-5.14	100.35	108.73
36	DB	387	GLY	CA-C-O	-5.14	118.13	122.29
3	d	76	PHE	CA-CB-CG	5.13	118.94	113.80
17	c	221	VAL	N-CA-C	-5.13	106.90	112.80
29	4	192	GLU	CA-C-O	-5.12	116.94	120.47
56	PB	38	GLY	CA-C-O	-5.12	118.14	122.29
15	v	114	ARG	N-CA-C	-5.12	105.70	111.28
8	t	199	LYS	CA-C-O	-5.11	115.45	120.82
68	w	1140	GLU	CA-CB-CG	5.09	124.29	114.10
29	4	442	VAL	N-CA-C	-5.09	107.33	112.17
54	Y	-28	DT	C2'-C3'-O3'	-5.09	103.87	111.50
39	Df	255	MET	N-CA-C	-5.08	107.47	113.97
1	a	501	CYS	CB-CA-C	-5.07	109.77	117.07
1	a	57	HIS	N-CA-C	5.07	117.20	111.11
8	t	175	VAL	N-CA-C	-5.05	105.47	110.62
4	f	109	PRO	O-C-N	5.05	129.27	123.06
68	w	1253	GLY	N-CA-C	5.02	122.58	112.34
36	DB	218	GLY	CA-C-O	-5.01	117.96	122.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3570	0	3480	309	0
2	m	983	0	967	231	0
3	d	1264	0	1293	227	0
4	f	1329	0	1302	173	0
5	g	1382	0	1410	307	0
6	h	1486	0	1500	230	0
7	r	1528	0	1538	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	t	1499	0	1482	132	0
9	j	1001	0	1021	364	0
10	k	879	0	886	200	0
11	n	7241	0	6673	623	0
12	q	4261	0	4237	508	0
13	s	485	0	352	101	0
14	u	792	0	749	231	0
15	v	1083	0	1059	169	0
16	z	765	0	727	162	0
17	c	2069	0	2079	101	0
18	e	832	0	824	112	0
19	b	899	0	908	110	0
20	l	1040	0	1065	81	0
21	o	1221	0	1212	125	0
22	i	520	0	545	46	0
23	0	2255	0	2007	80	0
24	8	2378	0	2397	79	0
25	9	2307	0	2314	34	0
26	1	2634	0	2042	38	0
27	2	2534	0	2455	33	0
28	3	2065	0	2098	33	0
29	4	3579	0	3620	67	0
30	5	428	0	434	11	0
31	6	4880	0	4924	66	0
32	7	5833	0	5798	72	0
33	EA	1476	0	1489	41	0
34	EB	1404	0	1424	26	0
35	DA	4511	0	4429	44	0
36	DB	7796	0	7751	213	0
37	DD	1330	0	1351	27	0
37	Dd	1307	0	1318	51	0
38	DE	4364	0	4244	86	0
38	De	4327	0	4197	77	0
39	DF	3109	0	3045	57	0
39	Df	3081	0	3012	58	0
40	DG	1180	0	1235	19	0
41	DH	1633	0	1621	27	0
42	DI	959	0	969	28	0
42	Di	967	0	977	25	0
43	DJ	720	0	719	12	0
43	Dj	759	0	759	19	0
44	DL	614	0	614	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Dl	876	0	893	91	0
45	Dc	1011	0	975	19	0
46	Dk	785	0	818	18	0
47	Dm	724	0	744	14	0
48	DO	771	0	764	9	0
49	DP	1412	0	1506	42	0
50	DQ	996	0	926	8	0
51	BA	1939	0	1979	29	0
52	FB	1788	0	1819	27	0
53	X	1429	0	770	120	0
54	Y	1400	0	775	90	0
55	PA	11655	0	11726	248	0
56	PB	9062	0	9107	131	0
57	PC	2059	0	2008	33	0
58	PD	1021	0	979	33	0
59	PE	1720	0	1737	25	0
60	PF	635	0	665	16	0
61	PG	1334	0	1333	39	0
62	PH	1186	0	1147	19	0
63	PI	927	0	859	9	0
64	PJ	507	0	523	4	0
65	PK	937	0	959	13	0
66	PL	372	0	379	4	0
67	FA	1101	0	1065	20	0
68	w	10772	0	10832	335	0
69	x	7050	0	7203	154	0
70	p	3124	0	3133	62	0
71	0	2	0	0	1	0
71	2	3	0	0	0	0
71	3	1	0	0	0	0
71	BA	1	0	0	0	0
71	EA	1	0	0	0	0
71	PA	2	0	0	0	0
71	PB	1	0	0	0	0
71	PC	1	0	0	0	0
71	PI	2	0	0	0	0
71	PJ	1	0	0	0	0
71	PL	1	0	0	0	0
72	7	8	0	0	0	0
73	PA	1	0	0	0	0
All	All	171177	0	168176	5752	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 17.

All (5752) 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)
33:EA:129:CYS:SG	33:EA:131:VAL:HG23	1.29	1.73
3:d:121:LEU:CD1	5:g:160:VAL:HG21	1.18	1.64
68:w:394:PRO:HA	70:p:171:PHE:CZ	1.29	1.63
3:d:121:LEU:HD11	5:g:160:VAL:CG2	1.21	1.62
9:j:82:LYS:HG2	13:s:96:PHE:CD1	1.17	1.62
1:a:467:MET:CE	1:a:504:ILE:HD11	1.25	1.61
1:a:493:PHE:CE2	1:a:514:LYS:HG3	1.29	1.60
11:n:659:LEU:CD2	68:w:17:VAL:HG21	1.27	1.59
4:f:180:LEU:CD2	11:n:299:PHE:CD1	1.82	1.58
5:g:93:LEU:CD2	9:j:106:LYS:HE2	1.21	1.58
11:n:659:LEU:HD21	68:w:17:VAL:CG2	1.32	1.58
5:g:93:LEU:HD22	9:j:106:LYS:CE	1.29	1.58
3:d:131:LYS:CD	14:u:104:LEU:HD13	1.17	1.58
3:d:131:LYS:CE	14:u:104:LEU:HD22	1.09	1.57
7:r:62:GLY:HA3	8:t:101:PHE:CE2	1.40	1.57
9:j:75:ARG:CB	9:j:80:TYR:CE2	1.82	1.56
9:j:53:LYS:HE3	11:n:60:HIS:CB	1.12	1.55
19:b:174:ILE:CD1	20:l:75:LEU:HD21	1.23	1.55
5:g:97:ILE:HG23	9:j:103:LYS:CE	1.22	1.55
9:j:82:LYS:CG	13:s:96:PHE:HD1	1.17	1.55
9:j:75:ARG:HB2	9:j:80:TYR:CE2	1.02	1.54
5:g:93:LEU:CG	9:j:106:LYS:HE2	1.31	1.54
9:j:26:VAL:CG1	9:j:38:ASN:HD21	1.17	1.54
9:j:59:HIS:C	11:n:50:ARG:CB	1.74	1.54
6:h:166:LEU:HD11	61:PG:125:PRO:CB	1.36	1.54
10:k:24:ILE:HG21	12:q:164:ALA:CB	1.35	1.54
68:w:9:PHE:HD2	68:w:66:PHE:CD2	1.23	1.54
4:f:188:PHE:HB3	11:n:281:ARG:CD	1.34	1.53
12:q:92:LEU:HD11	12:q:99:ARG:CZ	1.34	1.53
3:d:131:LYS:HD3	14:u:104:LEU:CD1	1.08	1.52
69:x:955:LEU:CD2	69:x:967:VAL:HG21	1.32	1.52
4:f:180:LEU:HD23	11:n:299:PHE:CE1	1.43	1.51
10:k:24:ILE:CG2	12:q:164:ALA:HB2	1.08	1.50
17:c:110:ALA:CB	19:b:168:ILE:CG2	1.89	1.50
68:w:9:PHE:CD2	68:w:66:PHE:CD2	1.97	1.50
4:f:180:LEU:HD21	11:n:299:PHE:CD1	1.41	1.49
5:g:93:LEU:CA	9:j:106:LYS:HZ3	1.21	1.49
9:j:92:ASN:ND2	13:s:83:LEU:CD2	1.76	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:493:PHE:CD2	1:a:514:LYS:CD	1.95	1.49
10:k:28:ALA:CB	12:q:161:LEU:CD2	1.88	1.49
5:g:97:ILE:CG2	9:j:103:LYS:HE2	1.42	1.48
9:j:78:GLN:HB3	9:j:82:LYS:CE	1.44	1.48
9:j:78:GLN:CB	9:j:82:LYS:HE3	1.41	1.48
11:n:686:LYS:HZ3	21:o:730:PRO:CG	1.20	1.48
9:j:53:LYS:CE	11:n:60:HIS:CB	1.87	1.47
10:k:28:ALA:CB	12:q:161:LEU:HD23	1.44	1.47
10:k:28:ALA:HB1	12:q:161:LEU:CD2	1.40	1.46
3:d:131:LYS:HE2	14:u:104:LEU:CD2	1.46	1.46
69:x:955:LEU:HD22	69:x:967:VAL:CG2	0.99	1.46
14:u:85:LEU:CD1	16:z:552:LEU:CD2	1.94	1.45
44:DL:106:ARG:CD	44:DL:114:LYS:NZ	1.78	1.45
6:h:166:LEU:HD11	61:PG:125:PRO:CG	1.32	1.45
9:j:75:ARG:HD2	9:j:80:TYR:CZ	1.51	1.44
11:n:156:TYR:CE1	11:n:168:ARG:HG2	1.46	1.44
9:j:26:VAL:HG11	9:j:38:ASN:ND2	1.23	1.44
6:h:166:LEU:CD1	61:PG:125:PRO:HG2	1.15	1.44
11:n:278:VAL:HG12	11:n:281:ARG:NH2	1.25	1.44
12:q:92:LEU:HD11	12:q:99:ARG:NH2	1.15	1.44
3:d:170:GLY:HA2	55:PA:1793:THR:CG2	1.46	1.43
4:f:180:LEU:CD2	11:n:299:PHE:CE1	1.98	1.43
10:k:12:ARG:CB	10:k:66:GLN:HE22	1.27	1.43
11:n:587:LEU:HD13	68:w:15:THR:CB	1.45	1.43
3:d:126:TYR:OH	12:q:36:MET:CE	1.66	1.42
5:g:87:ILE:CG2	9:j:127:ILE:HD11	1.47	1.42
9:j:78:GLN:O	9:j:82:LYS:CG	1.67	1.42
44:DL:106:ARG:HD3	44:DL:114:LYS:NZ	1.27	1.41
10:k:24:ILE:CG2	12:q:164:ALA:CB	1.90	1.41
11:n:587:LEU:HD22	68:w:15:THR:CG2	1.50	1.41
5:g:93:LEU:HD13	9:j:106:LYS:CG	1.45	1.40
12:q:290:HIS:CE1	12:q:294:LYS:HE3	1.56	1.39
19:b:174:ILE:CG1	20:l:75:LEU:HD21	1.49	1.39
9:j:75:ARG:HB2	9:j:80:TYR:CD2	1.55	1.39
3:d:170:GLY:CA	55:PA:1793:THR:HG21	1.48	1.39
2:m:30:ASN:HA	3:d:176:TYR:CB	1.54	1.38
44:DL:106:ARG:NH1	44:DL:114:LYS:CG	1.86	1.37
3:d:128:ALA:HB1	14:u:108:VAL:CB	1.52	1.37
9:j:89:LEU:HD21	13:s:93:TYR:CZ	1.59	1.37
44:DL:106:ARG:CD	44:DL:114:LYS:HZ3	1.36	1.37
9:j:60:ASP:N	11:n:50:ARG:CB	1.84	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:u:85:LEU:CD1	16:z:552:LEU:HD23	1.51	1.35
6:h:67:LYS:CD	23:0:141:THR:CG2	2.03	1.35
5:g:87:ILE:HG23	9:j:127:ILE:CD1	1.56	1.35
12:q:92:LEU:CD1	12:q:99:ARG:NH2	1.90	1.35
1:a:417:TYR:HD1	1:a:469:VAL:CG2	1.39	1.34
21:o:715:LEU:CD1	69:x:21:TYR:HB2	1.55	1.34
33:EA:129:CYS:SG	33:EA:131:VAL:CG2	2.16	1.34
2:m:124:GLN:OE1	16:z:590:ARG:CB	1.75	1.33
5:g:164:ILE:HD13	22:i:141:PHE:CD2	1.62	1.33
2:m:27:CYS:CA	3:d:177:PRO:HG3	1.58	1.33
10:k:12:ARG:CG	10:k:66:GLN:NE2	1.92	1.33
1:a:360:ASN:HB3	69:x:17:ARG:NH1	1.45	1.32
4:f:180:LEU:CG	11:n:299:PHE:CD1	2.11	1.32
2:m:27:CYS:HA	3:d:177:PRO:CG	1.58	1.32
3:d:131:LYS:CE	14:u:104:LEU:CD2	2.02	1.32
11:n:127:ILE:O	14:u:27:GLN:NE2	1.61	1.32
19:b:174:ILE:CD1	20:l:75:LEU:CD2	2.08	1.32
14:u:85:LEU:HD12	16:z:552:LEU:CD2	1.53	1.32
5:g:93:LEU:HB3	9:j:106:LYS:CE	1.60	1.32
17:c:113:TRP:CH2	19:b:175:HIS:HB2	1.66	1.31
1:a:364:TYR:HB3	1:a:430:LEU:CD1	1.58	1.31
1:a:493:PHE:CE2	1:a:514:LYS:CG	2.12	1.31
2:m:104:HIS:CE1	11:n:168:ARG:HG3	1.64	1.31
24:8:177:TRP:CZ3	24:8:214:PRO:HA	1.65	1.31
6:h:170:LYS:CE	6:h:172:THR:HG22	1.61	1.30
5:g:93:LEU:CD1	9:j:106:LYS:HG2	1.61	1.30
9:j:19:ILE:HG21	9:j:45:VAL:CG2	1.60	1.30
19:b:181:CYS:SG	20:l:82:LEU:HD13	1.69	1.30
23:0:194:VAL:CG2	23:0:198:LEU:HD22	1.60	1.30
11:n:73:LEU:O	11:n:77:SER:CB	1.80	1.30
12:q:89:GLN:CG	12:q:90:PRO:HD2	1.60	1.30
15:v:133:GLU:OE2	18:e:125:LYS:HE2	1.26	1.30
53:X:-11:DG:N2	54:Y:11:DC:N3	1.75	1.30
69:x:955:LEU:CD2	69:x:967:VAL:CG2	1.93	1.30
1:a:439:GLN:CD	69:x:15:LYS:HD3	1.56	1.30
2:m:104:HIS:CG	11:n:169:LEU:HA	1.67	1.30
4:f:180:LEU:HD21	11:n:299:PHE:CG	1.66	1.29
1:a:439:GLN:OE1	69:x:15:LYS:HD3	1.32	1.29
6:h:166:LEU:CD1	61:PG:125:PRO:CG	1.78	1.29
11:n:278:VAL:CG1	11:n:281:ARG:NH2	1.94	1.29
5:g:164:ILE:HG21	22:i:141:PHE:CE2	1.66	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:12:ARG:HB3	10:k:66:GLN:NE2	1.45	1.28
5:g:136:ARG:HB2	14:u:86:GLN:OE1	1.26	1.28
21:o:761:LEU:O	68:w:74:LYS:HE3	1.25	1.28
5:g:93:LEU:HB3	9:j:106:LYS:CD	1.62	1.28
9:j:77:PRO:O	9:j:81:THR:CB	1.82	1.27
3:d:169:PRO:CA	55:PA:1795:PRO:HG2	1.64	1.27
11:n:545:LEU:HD11	11:n:653:PRO:CG	1.62	1.27
17:c:110:ALA:CB	19:b:168:ILE:HG23	1.56	1.27
42:Di:73:LEU:HD22	44:Dl:105:HIS:CE1	1.70	1.26
53:X:-5:DG:N2	54:Y:6:DG:C2	2.01	1.26
2:m:124:GLN:OE1	16:z:590:ARG:HB3	1.27	1.26
12:q:441:ARG:NH1	20:l:168:TRP:CD2	2.01	1.26
15:v:119:LEU:CD2	18:e:139:TRP:CD2	2.19	1.26
9:j:60:ASP:HB2	11:n:50:ARG:CB	1.66	1.26
1:a:493:PHE:CD2	1:a:514:LYS:HD2	1.57	1.26
10:k:17:ILE:CG2	12:q:171:VAL:HG21	1.64	1.25
1:a:417:TYR:CE1	1:a:450:PHE:CD1	2.23	1.25
9:j:96:LYS:CD	13:s:80:SER:HA	1.62	1.25
7:r:120:GLU:OE1	8:t:79:PHE:CD1	1.90	1.25
11:n:245:TRP:HB2	11:n:282:LEU:CD1	1.64	1.25
5:g:93:LEU:CB	9:j:106:LYS:CE	2.13	1.25
9:j:53:LYS:CG	11:n:57:PHE:HA	1.65	1.25
9:j:102:MET:CB	14:u:26:LEU:HD21	1.66	1.25
12:q:9:ILE:CD1	14:u:90:LEU:HD22	1.67	1.25
11:n:254:VAL:CG1	11:n:304:GLN:HE21	1.48	1.25
9:j:53:LYS:O	9:j:57:GLN:HG3	1.18	1.24
44:DL:106:ARG:NH1	44:DL:114:LYS:HG3	0.93	1.24
9:j:69:GLU:O	9:j:73:GLN:HG3	1.33	1.24
4:f:180:LEU:HD13	11:n:302:SER:OG	1.12	1.24
6:h:77:ILE:HG13	12:q:126:THR:CB	1.65	1.24
11:n:159:ASP:OD2	11:n:167:PRO:CD	1.85	1.24
49:DP:300:ILE:CG2	49:DP:315:ALA:HB2	1.68	1.24
6:h:166:LEU:CD1	61:PG:125:PRO:CB	2.04	1.24
11:n:659:LEU:CD1	68:w:14:LYS:HG2	1.67	1.24
44:Dl:76:LEU:CD1	44:Dl:84:LEU:CD1	2.16	1.24
4:f:177:VAL:CG2	11:n:266:VAL:HG22	1.67	1.23
11:n:587:LEU:CD1	68:w:15:THR:HB	1.66	1.23
3:d:99:GLU:OE2	3:d:103:ARG:NH2	1.69	1.23
13:s:92:ALA:O	13:s:96:PHE:CD2	1.92	1.23
3:d:113:GLN:NE2	5:g:163:MET:SD	2.12	1.22
11:n:527:THR:HG21	68:w:42:GLY:CA	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:647:SER:HB3	18:e:93:CYS:SG	1.78	1.22
1:a:383:PRO:CA	69:x:92:LEU:HD21	1.69	1.22
68:w:394:PRO:HA	70:p:171:PHE:CE1	1.74	1.22
9:j:70:TYR:CD1	9:j:80:TYR:HB3	1.75	1.22
1:a:467:MET:CE	1:a:504:ILE:CD1	2.18	1.21
9:j:53:LYS:CD	11:n:57:PHE:HA	1.70	1.21
23:0:194:VAL:HG22	23:0:198:LEU:CD2	1.70	1.21
42:DI:60:HIS:HE1	44:DL:106:ARG:CG	1.53	1.21
68:w:357:HIS:CE1	68:w:397:LYS:HE2	1.76	1.21
24:8:177:TRP:CE3	24:8:214:PRO:HA	1.75	1.21
2:m:14:ASN:C	5:g:39:LYS:HZ1	1.48	1.21
12:q:1:MET:N	16:z:540:LEU:HD13	1.53	1.21
2:m:124:GLN:OE1	16:z:590:ARG:CD	1.89	1.20
2:m:70:PRO:HB2	11:n:166:TYR:OH	1.41	1.20
7:r:120:GLU:OE1	8:t:79:PHE:CE1	1.94	1.20
19:b:174:ILE:HD11	20:l:75:LEU:HD21	1.22	1.20
3:d:169:PRO:HA	55:PA:1795:PRO:CG	1.72	1.20
10:k:12:ARG:HG2	10:k:66:GLN:NE2	1.51	1.20
12:q:138:LYS:HB3	12:q:140:ASN:OD1	1.42	1.20
2:m:104:HIS:CD2	11:n:169:LEU:HA	1.74	1.20
5:g:136:ARG:CA	14:u:86:GLN:HE22	1.52	1.20
9:j:53:LYS:HZ3	11:n:61:ARG:N	1.40	1.20
9:j:59:HIS:HB2	11:n:50:ARG:N	1.54	1.20
42:DI:60:HIS:HE1	44:DL:106:ARG:HG2	1.03	1.20
2:m:116:GLN:HG3	16:z:594:LEU:HG	1.20	1.20
53:X:29:DG:N2	54:Y:-29:DC:C2	2.10	1.20
2:m:121:GLU:HA	16:z:592:ASN:ND2	1.57	1.19
11:n:159:ASP:OD2	11:n:167:PRO:HD3	1.41	1.19
42:DI:60:HIS:CE1	44:DL:106:ARG:HG2	1.77	1.19
53:X:29:DG:N2	54:Y:-29:DC:N3	1.89	1.19
3:d:106:ASP:OD2	5:g:174:ASP:HB2	1.41	1.19
6:h:67:LYS:HD2	23:0:141:THR:CG2	1.65	1.19
44:DL:106:ARG:HH12	44:DL:114:LYS:CG	1.49	1.19
1:a:417:TYR:HE1	1:a:450:PHE:CD1	1.58	1.19
11:n:686:LYS:NZ	21:o:730:PRO:CG	2.05	1.19
21:o:696:SER:OG	69:x:111:HIS:CE1	1.96	1.19
3:d:121:LEU:CD1	5:g:160:VAL:CG2	1.88	1.19
3:d:128:ALA:CB	14:u:108:VAL:CG2	2.20	1.19
5:g:83:MET:SD	9:j:120:ASP:OD1	2.01	1.19
11:n:587:LEU:CD2	68:w:15:THR:HG22	1.72	1.19
11:n:686:LYS:HZ3	21:o:730:PRO:CD	1.56	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:67:LYS:CD	23:0:141:THR:HG23	1.65	1.19
68:w:394:PRO:CA	70:p:171:PHE:CZ	2.25	1.19
5:g:93:LEU:CA	9:j:106:LYS:NZ	2.05	1.18
11:n:169:LEU:HB3	11:n:170:PRO:CD	1.72	1.18
1:a:417:TYR:CD1	1:a:469:VAL:CG2	2.26	1.18
6:h:83:PRO:HG3	55:PA:1790:TYR:CE1	1.77	1.18
12:q:9:ILE:HG13	14:u:90:LEU:HD13	1.21	1.18
44:Dl:87:ILE:O	44:Dl:91:PHE:CD2	1.96	1.18
3:d:131:LYS:NZ	14:u:104:LEU:HD22	1.57	1.18
7:r:120:GLU:OE1	8:t:79:PHE:CG	1.95	1.18
2:m:14:ASN:O	5:g:39:LYS:NZ	1.75	1.18
2:m:124:GLN:HE21	16:z:581:SER:CB	1.54	1.18
4:f:180:LEU:HG	11:n:299:PHE:CD1	1.74	1.18
14:u:77:PRO:HG2	14:u:79:GLU:CG	1.73	1.17
53:X:15:DA:C2	54:Y:-14:DG:N2	2.11	1.17
11:n:686:LYS:NZ	21:o:730:PRO:HG3	1.60	1.17
12:q:596:PHE:HZ	20:l:117:TYR:OH	1.24	1.17
22:i:85:GLN:HG3	22:i:86:ASP:N	1.53	1.17
1:a:417:TYR:CD1	1:a:469:VAL:HG21	1.77	1.17
1:a:232:LEU:HD12	1:a:502:MET:HE1	1.24	1.17
3:d:125:VAL:HB	14:u:112:ASP:OD1	1.43	1.17
12:q:1:MET:HB2	16:z:541:PRO:CG	1.75	1.17
17:c:204:MET:CE	17:c:208:PHE:H	1.57	1.17
44:Dl:76:LEU:HD13	44:Dl:84:LEU:CD1	1.72	1.17
5:g:93:LEU:CG	9:j:106:LYS:CE	2.18	1.17
4:f:180:LEU:HG	11:n:299:PHE:HD1	1.01	1.16
9:j:78:GLN:O	9:j:82:LYS:CD	1.91	1.16
44:DL:106:ARG:CZ	44:DL:115:ASP:OD1	1.93	1.16
4:f:15:TRP:HH2	4:f:35:GLU:OE1	1.28	1.16
5:g:93:LEU:CB	9:j:106:LYS:HZ3	1.57	1.16
10:k:17:ILE:CG2	12:q:171:VAL:CG2	2.24	1.16
9:j:53:LYS:HG2	11:n:57:PHE:HA	1.18	1.16
9:j:75:ARG:CG	9:j:80:TYR:CE2	2.29	1.16
68:w:9:PHE:CD2	68:w:66:PHE:CE2	2.33	1.16
3:d:128:ALA:HB1	14:u:108:VAL:CG2	1.74	1.16
6:h:67:LYS:HD3	23:0:141:THR:CG2	1.70	1.16
10:k:28:ALA:CB	12:q:161:LEU:HD21	1.76	1.16
53:X:15:DA:N1	54:Y:-14:DG:N2	1.92	1.16
9:j:53:LYS:NZ	11:n:61:ARG:N	1.95	1.15
11:n:587:LEU:CD2	68:w:15:THR:CG2	2.25	1.15
68:w:357:HIS:HE1	68:w:397:LYS:HE2	0.99	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:83:PRO:HG3	55:PA:1790:TYR:CZ	1.81	1.15
9:j:60:ASP:CA	11:n:50:ARG:CB	2.25	1.15
2:m:116:GLN:CG	16:z:594:LEU:HG	1.75	1.15
11:n:587:LEU:HD13	68:w:15:THR:CG2	1.76	1.15
17:c:110:ALA:CB	19:b:168:ILE:HG21	1.63	1.15
44:Dl:102:LEU:CD1	44:Dl:118:LEU:HD11	1.74	1.15
5:g:27:GLN:OE1	5:g:32:PRO:HG3	1.01	1.15
21:o:762:GLN:HA	68:w:74:LYS:NZ	1.60	1.15
44:DL:106:ARG:HH11	44:DL:114:LYS:NZ	1.45	1.15
4:f:15:TRP:CH2	4:f:35:GLU:OE1	2.00	1.14
4:f:188:PHE:CB	11:n:281:ARG:CD	2.25	1.14
5:g:27:GLN:OE1	5:g:32:PRO:CG	1.93	1.14
9:j:49:GLN:O	9:j:52:ASP:OD1	1.65	1.14
15:v:119:LEU:CD2	18:e:139:TRP:CG	2.30	1.14
17:c:204:MET:HE1	17:c:208:PHE:N	1.59	1.14
1:a:417:TYR:CE1	1:a:450:PHE:CE1	2.35	1.14
1:a:493:PHE:CG	1:a:514:LYS:HD2	1.82	1.14
7:r:120:GLU:OE1	8:t:79:PHE:CD2	1.99	1.14
19:b:174:ILE:HG12	20:l:75:LEU:HD11	1.30	1.14
6:h:147:CYS:CB	15:v:41:LYS:HB2	1.77	1.14
9:j:92:ASN:ND2	13:s:83:LEU:HD21	0.81	1.14
58:PD:51:ALA:HB3	58:PD:54:GLU:HG3	1.26	1.14
6:h:67:LYS:CD	23:0:141:THR:HG21	1.70	1.13
3:d:44:LEU:CG	3:d:68:LEU:HD12	1.76	1.13
3:d:113:GLN:NE2	5:g:163:MET:CE	2.11	1.13
4:f:77:ILE:HG21	55:PA:1792:PRO:HG2	1.24	1.13
4:f:188:PHE:HB3	11:n:281:ARG:HD2	1.18	1.13
53:X:-2:DC:H2"	53:X:-1:DT:H71	1.28	1.13
2:m:124:GLN:OE1	16:z:590:ARG:HD3	1.47	1.13
5:g:87:ILE:CG2	9:j:127:ILE:CD1	2.20	1.13
10:k:21:ILE:HD12	12:q:168:THR:OG1	1.43	1.13
12:q:441:ARG:NH1	20:l:168:TRP:CE3	2.09	1.13
14:u:85:LEU:HD11	16:z:551:ASP:HB2	1.30	1.13
4:f:177:VAL:HG21	11:n:266:VAL:HG22	1.19	1.13
12:q:212:ALA:HA	12:q:387:LEU:HD11	1.18	1.13
2:m:120:ALA:C	16:z:592:ASN:ND2	2.06	1.12
4:f:180:LEU:HD11	11:n:299:PHE:CA	1.79	1.13
6:h:77:ILE:O	12:q:126:THR:OG1	1.67	1.12
7:r:120:GLU:OE1	8:t:79:PHE:CE2	2.02	1.12
9:j:60:ASP:CB	11:n:50:ARG:CB	2.25	1.13
12:q:9:ILE:HD11	14:u:90:LEU:HD22	1.14	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:17:ILE:HG21	12:q:171:VAL:CG2	1.77	1.12
12:q:89:GLN:HG2	12:q:90:PRO:CD	1.79	1.12
68:w:16:GLU:OE2	68:w:78:PHE:CB	1.98	1.12
3:d:169:PRO:HB3	55:PA:1795:PRO:HB2	1.31	1.12
9:j:59:HIS:O	11:n:50:ARG:CB	1.94	1.12
18:e:56:PHE:O	18:e:60:VAL:HG22	1.44	1.12
7:r:120:GLU:OE1	8:t:79:PHE:CZ	2.01	1.12
1:a:383:PRO:HA	69:x:92:LEU:HD21	1.21	1.12
2:m:14:ASN:C	5:g:39:LYS:NZ	2.07	1.12
3:d:117:ALA:HB2	5:g:163:MET:SD	1.89	1.12
3:d:128:ALA:HB3	14:u:108:VAL:HG23	1.31	1.12
36:DB:854:CYS:O	36:DB:858:ILE:HG13	1.47	1.12
5:g:93:LEU:HD22	9:j:106:LYS:HE3	1.25	1.12
7:r:62:GLY:CA	8:t:101:PHE:CE2	2.31	1.12
9:j:43:PHE:CE1	13:s:150:ALA:HB3	1.83	1.12
12:q:307:ILE:HG12	12:q:379:ILE:HG13	1.24	1.12
68:w:12:VAL:HG23	68:w:78:PHE:HE2	0.96	1.12
2:m:26:GLN:OE1	5:g:45:PHE:HD2	1.32	1.11
22:i:85:GLN:CG	22:i:86:ASP:H	1.60	1.11
68:w:9:PHE:HD2	68:w:66:PHE:CE2	1.67	1.11
11:n:158:ILE:HD13	12:q:11:ILE:HG21	1.12	1.11
21:o:715:LEU:CD2	69:x:25:ILE:HG13	1.78	1.11
4:f:180:LEU:CD1	11:n:299:PHE:HA	1.79	1.11
15:v:119:LEU:HD23	18:e:139:TRP:CE3	1.83	1.11
42:Di:73:LEU:HD22	44:Dl:105:HIS:NE2	1.63	1.11
69:x:485:PRO:HD2	69:x:486:ALA:H	1.08	1.11
1:a:467:MET:HE1	1:a:504:ILE:CD1	1.78	1.11
1:a:497:VAL:O	1:a:501:CYS:SG	2.09	1.11
9:j:43:PHE:HE1	13:s:150:ALA:HB3	1.05	1.11
12:q:9:ILE:HD11	14:u:90:LEU:CD2	1.80	1.11
15:v:119:LEU:HD23	18:e:139:TRP:CD2	1.81	1.11
9:j:43:PHE:HZ	13:s:151:GLY:N	1.45	1.11
10:k:24:ILE:HG22	12:q:164:ALA:CB	1.78	1.11
14:u:81:SER:HB2	14:u:85:LEU:HB2	1.23	1.10
5:g:93:LEU:HB3	9:j:106:LYS:HD3	1.23	1.10
2:m:30:ASN:CA	3:d:176:TYR:CB	2.29	1.10
9:j:53:LYS:HE2	11:n:57:PHE:C	1.76	1.10
44:Dl:76:LEU:CD1	44:Dl:84:LEU:HD11	1.81	1.10
49:DP:282:SER:HA	51:BA:206:VAL:HG21	1.33	1.10
9:j:19:ILE:HD13	9:j:45:VAL:HG22	1.32	1.10
36:DB:72:ILE:HG21	36:DB:148:ILE:CG2	1.82	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:74:GLN:NE2	12:q:129:PRO:HB3	1.67	1.10
9:j:75:ARG:CB	9:j:80:TYR:CD2	2.23	1.10
24:8:177:TRP:CZ2	55:PA:1677:SER:CB	2.35	1.10
2:m:30:ASN:HA	3:d:176:TYR:HB3	1.16	1.09
5:g:93:LEU:CB	9:j:106:LYS:NZ	2.14	1.09
9:j:75:ARG:CD	9:j:80:TYR:CZ	2.34	1.09
11:n:265:LEU:HD13	11:n:303:LEU:HD21	1.26	1.09
12:q:1:MET:HB2	16:z:541:PRO:HG3	1.11	1.09
17:c:204:MET:CE	17:c:208:PHE:N	2.14	1.09
2:m:116:GLN:HG2	16:z:595:PRO:HD2	1.21	1.09
21:o:761:LEU:O	68:w:74:LYS:CE	2.01	1.09
3:d:131:LYS:HB3	14:u:104:LEU:HD11	1.33	1.09
21:o:762:GLN:HA	68:w:74:LYS:CE	1.80	1.09
36:DB:563:PRO:HA	36:DB:580:GLN:HA	1.31	1.09
53:X:29:DG:N2	54:Y:-29:DC:O2	1.84	1.09
9:j:53:LYS:HG2	11:n:57:PHE:CA	1.83	1.09
69:x:955:LEU:HD22	69:x:967:VAL:HG22	1.15	1.09
1:a:360:ASN:CB	69:x:17:ARG:HH11	1.65	1.08
9:j:96:LYS:HD2	13:s:80:SER:HA	1.27	1.08
21:o:715:LEU:HD21	69:x:25:ILE:HG13	1.08	1.08
36:DB:689:GLN:O	36:DB:689:GLN:HG2	1.47	1.08
49:DP:300:ILE:HG21	49:DP:315:ALA:HB2	1.15	1.08
1:a:364:TYR:HB3	1:a:430:LEU:HD12	1.26	1.08
2:m:124:GLN:CG	16:z:581:SER:HB2	1.82	1.08
10:k:73:VAL:CG2	15:v:92:PRO:HD2	1.84	1.08
11:n:156:TYR:HE1	11:n:168:ARG:CG	1.66	1.08
11:n:247:LEU:CD2	11:n:278:VAL:HG23	1.82	1.08
68:w:12:VAL:HG23	68:w:78:PHE:CE2	1.87	1.08
1:a:321:LEU:CD2	1:a:407:ILE:HD12	1.83	1.08
9:j:56:GLN:HB3	11:n:53:THR:CB	1.84	1.08
9:j:77:PRO:O	9:j:81:THR:HB	0.92	1.08
14:u:105:GLU:HA	14:u:108:VAL:HG12	1.09	1.08
3:d:128:ALA:CB	14:u:108:VAL:HB	1.82	1.08
9:j:11:HIS:O	9:j:15:PHE:CD2	2.07	1.08
9:j:75:ARG:HD2	9:j:80:TYR:CE1	1.89	1.08
11:n:587:LEU:HD22	68:w:15:THR:HG22	1.27	1.08
14:u:105:GLU:HA	14:u:108:VAL:CG1	1.84	1.08
14:u:105:GLU:CA	14:u:108:VAL:HG12	1.83	1.08
53:X:-2:DC:H2"	53:X:-1:DT:C7	1.83	1.08
9:j:19:ILE:HG21	9:j:45:VAL:HG21	1.11	1.08
14:u:85:LEU:HD13	16:z:552:LEU:CD2	1.67	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:76:ASN:HB2	9:j:77:PRO:HD3	1.35	1.07
5:g:87:ILE:HG21	9:j:127:ILE:HD11	1.14	1.07
9:j:78:GLN:O	9:j:82:LYS:HG3	1.46	1.07
10:k:12:ARG:CB	10:k:66:GLN:NE2	1.97	1.07
3:d:44:LEU:HG	3:d:68:LEU:CD1	1.83	1.07
4:f:181:LEU:HD12	11:n:270:GLN:NE2	1.69	1.07
5:g:89:PHE:HE1	14:u:23:ILE:HD11	1.12	1.07
9:j:53:LYS:O	9:j:57:GLN:CG	2.03	1.07
11:n:545:LEU:HD11	11:n:653:PRO:HG3	1.12	1.07
12:q:138:LYS:HD2	12:q:140:ASN:OD1	1.54	1.07
53:X:-9:DG:N2	54:Y:9:DC:N3	2.03	1.07
6:h:40:LEU:CD1	6:h:45:VAL:HG11	1.84	1.07
2:m:31:PRO:HD2	3:d:176:TYR:CD2	1.90	1.07
5:g:93:LEU:CD2	9:j:106:LYS:CE	1.96	1.07
5:g:164:ILE:CD1	22:i:141:PHE:CD2	2.37	1.07
6:h:51:LEU:HB2	58:PD:140:PHE:HB3	1.37	1.07
11:n:245:TRP:CB	11:n:282:LEU:HD13	1.84	1.07
18:e:146:ILE:HG22	18:e:147:ASN:H	0.96	1.07
9:j:75:ARG:CB	9:j:80:TYR:HE2	1.42	1.06
11:n:172:CYS:SG	12:q:21:GLU:HA	1.94	1.06
11:n:686:LYS:HZ3	21:o:730:PRO:HG3	0.96	1.06
68:w:16:GLU:OE2	68:w:78:PHE:CG	2.08	1.06
10:k:29:GLY:O	10:k:33:LEU:HG	1.55	1.06
18:e:60:VAL:HB	19:b:179:LEU:CG	1.85	1.06
21:o:715:LEU:HD11	69:x:21:TYR:CB	1.85	1.06
36:DB:280:THR:HG23	36:DB:342:THR:HG21	1.30	1.06
2:m:120:ALA:HB1	16:z:592:ASN:HB3	1.38	1.06
6:h:72:ARG:NH1	12:q:134:ALA:H	1.53	1.06
9:j:73:GLN:O	9:j:80:TYR:OH	1.73	1.06
1:a:493:PHE:CD2	1:a:514:LYS:HD3	1.87	1.06
9:j:53:LYS:CE	11:n:57:PHE:O	2.04	1.06
11:n:156:TYR:CE1	11:n:168:ARG:CG	2.38	1.06
12:q:9:ILE:CG1	14:u:90:LEU:HD22	1.85	1.06
11:n:524:ASN:OD1	68:w:45:ARG:NH2	1.89	1.06
2:m:59:LYS:NZ	2:m:77:GLU:OE2	1.87	1.05
4:f:188:PHE:HB3	11:n:281:ARG:HD3	1.15	1.05
15:v:85:PHE:CE1	15:v:86:LEU:HD22	1.90	1.05
38:De:488:GLY:HA3	38:De:546:VAL:CG2	1.85	1.05
3:d:113:GLN:NE2	5:g:163:MET:HE2	1.70	1.05
3:d:121:LEU:HD21	5:g:160:VAL:HG11	1.19	1.05
44:Dl:102:LEU:HD13	44:Dl:118:LEU:CD2	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:124:GLN:NE2	16:z:581:SER:HB2	1.71	1.05
3:d:126:TYR:OH	12:q:36:MET:HE3	1.56	1.05
5:g:136:ARG:HA	14:u:86:GLN:NE2	1.70	1.05
9:j:77:PRO:HD2	9:j:78:GLN:H	1.20	1.05
10:k:12:ARG:CG	10:k:66:GLN:HE21	1.56	1.05
11:n:587:LEU:HD22	68:w:15:THR:HG21	1.36	1.05
54:Y:3:DG:H2"	54:Y:4:DA:OP2	1.49	1.05
9:j:102:MET:CA	14:u:26:LEU:HD21	1.86	1.05
11:n:156:TYR:CZ	11:n:168:ARG:HG2	1.91	1.05
11:n:254:VAL:HG13	11:n:304:GLN:HE21	1.13	1.05
11:n:861:LYS:HE3	17:c:30:ARG:HE	1.17	1.05
36:DB:72:ILE:HG21	36:DB:148:ILE:HG23	1.09	1.05
1:a:321:LEU:HD21	1:a:407:ILE:HG23	1.32	1.05
6:h:77:ILE:HG13	12:q:126:THR:CG2	1.85	1.05
11:n:130:VAL:CB	14:u:27:GLN:HG3	1.87	1.05
2:m:124:GLN:CD	16:z:590:ARG:HD3	1.81	1.04
10:k:104:LEU:HD21	15:v:123:ILE:HD11	1.39	1.04
12:q:647:SER:CB	18:e:93:CYS:SG	2.45	1.04
38:De:488:GLY:HA3	38:De:546:VAL:HG22	1.08	1.04
3:d:131:LYS:HD3	14:u:104:LEU:CG	1.87	1.04
9:j:102:MET:HB3	14:u:26:LEU:HD21	1.38	1.04
45:Dc:77:LEU:HD13	43:Dj:116:LEU:HD23	1.40	1.04
4:f:180:LEU:CD1	11:n:302:SER:OG	2.05	1.04
18:e:60:VAL:HB	19:b:179:LEU:CD1	1.88	1.04
44:DL:106:ARG:HD2	44:DL:114:LYS:NZ	1.71	1.04
44:DL:106:ARG:NE	44:DL:115:ASP:OD1	1.89	1.04
44:DL:106:ARG:HH22	44:DL:114:LYS:C	1.63	1.04
2:m:30:ASN:CA	3:d:176:TYR:HB2	1.85	1.04
9:j:53:LYS:HE2	11:n:57:PHE:O	1.55	1.04
14:u:117:LYS:NZ	22:i:140:MET:HG3	1.72	1.04
19:b:174:ILE:HG12	20:l:75:LEU:HD21	1.33	1.04
1:a:467:MET:HE2	1:a:504:ILE:HD11	1.30	1.04
12:q:7:VAL:HB	14:u:90:LEU:HD11	1.37	1.04
14:u:117:LYS:CE	22:i:140:MET:HG3	1.88	1.04
44:Dl:102:LEU:HD13	44:Dl:118:LEU:HD21	1.06	1.04
51:BA:125:ALA:HB1	51:BA:132:ARG:HB2	1.39	1.04
68:w:8:ILE:O	68:w:12:VAL:HG13	1.58	1.04
2:m:104:HIS:CD2	11:n:169:LEU:CA	2.40	1.03
6:h:29:PHE:CE2	12:q:102:LEU:HD11	1.92	1.03
10:k:114:MET:CE	18:e:129:VAL:HG21	1.87	1.03
17:c:110:ALA:HB1	19:b:168:ILE:CG2	1.63	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DD:890:GLY:O	44:DL:104:ARG:NH2	1.91	1.03
53:X:29:DG:H1	54:Y:-29:DC:N4	1.54	1.03
2:m:120:ALA:O	16:z:592:ASN:ND2	1.91	1.03
2:m:124:GLN:HE21	16:z:581:SER:HB2	1.18	1.03
3:d:148:ILE:HG12	11:n:161:LEU:HD12	1.37	1.03
9:j:92:ASN:HD22	13:s:83:LEU:CD2	1.51	1.03
17:c:204:MET:HE3	17:c:208:PHE:H	1.22	1.03
19:b:174:ILE:HD11	20:l:75:LEU:CD2	1.76	1.03
2:m:121:GLU:CA	16:z:592:ASN:ND2	2.21	1.03
12:q:92:LEU:CD1	12:q:99:ARG:CZ	2.29	1.03
22:i:85:GLN:HG3	22:i:86:ASP:OD1	1.56	1.03
36:DB:579:LEU:HD22	36:DB:588:HIS:HB3	1.41	1.03
2:m:116:GLN:CG	16:z:595:PRO:HD2	1.88	1.03
5:g:93:LEU:HD13	9:j:106:LYS:CD	1.87	1.03
10:k:78:PRO:O	10:k:79:HIS:ND1	1.91	1.03
17:c:110:ALA:HB2	19:b:168:ILE:CG2	1.81	1.03
1:a:417:TYR:HD1	1:a:469:VAL:HG23	1.24	1.02
1:a:439:GLN:CD	69:x:15:LYS:CD	2.30	1.02
5:g:136:ARG:HA	14:u:86:GLN:HE22	0.89	1.02
6:h:170:LYS:HE3	6:h:172:THR:HG22	1.07	1.02
9:j:59:HIS:C	11:n:50:ARG:CA	2.31	1.02
9:j:96:LYS:HD2	13:s:80:SER:CA	1.88	1.02
6:h:166:LEU:CD1	61:PG:125:PRO:HB2	1.85	1.02
11:n:225:ARG:HB2	11:n:231:GLU:OE1	1.56	1.02
19:b:174:ILE:HG12	20:l:75:LEU:CD1	1.89	1.02
4:f:177:VAL:HG22	11:n:266:VAL:CG2	1.90	1.02
5:g:93:LEU:CD1	9:j:106:LYS:HE2	1.89	1.02
6:h:19:VAL:CG1	12:q:113:TYR:HB2	1.87	1.02
10:k:114:MET:HE1	18:e:129:VAL:HG21	1.35	1.02
12:q:290:HIS:CE1	12:q:294:LYS:CE	2.43	1.02
36:DB:331:HIS:HE2	36:DB:342:THR:HB	1.23	1.02
45:Dc:77:LEU:CD1	43:Dj:116:LEU:HD23	1.90	1.02
2:m:124:GLN:HE21	16:z:581:SER:CA	1.72	1.02
5:g:93:LEU:HA	9:j:106:LYS:NZ	1.72	1.02
6:h:77:ILE:HG13	12:q:126:THR:OG1	1.55	1.02
9:j:19:ILE:CD1	9:j:45:VAL:HG22	1.88	1.02
14:u:85:LEU:CD1	16:z:552:LEU:HD21	1.69	1.02
18:e:49:GLU:HG2	20:l:89:PHE:CE1	1.94	1.02
23:0:194:VAL:CG2	23:0:198:LEU:CD2	2.30	1.02
12:q:451:LEU:CD1	12:q:529:MET:HE1	1.90	1.02
36:DB:280:THR:HG23	36:DB:342:THR:CG2	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:FB:126:ARG:HA	52:FB:129:ARG:HG2	1.37	1.02
53:X:-11:DG:C5'	54:Y:12:DG:N2	2.22	1.02
69:x:956:VAL:HB	69:x:968:LEU:HD21	1.04	1.02
9:j:78:GLN:O	9:j:82:LYS:CB	2.06	1.01
17:c:204:MET:HE3	17:c:206:SER:O	1.60	1.01
1:a:383:PRO:HA	69:x:92:LEU:CD2	1.89	1.01
6:h:77:ILE:C	12:q:126:THR:HG1	1.67	1.01
9:j:43:PHE:CZ	13:s:151:GLY:N	2.28	1.01
55:PA:686:THR:HG23	55:PA:765:ASN:ND2	1.75	1.01
2:m:56:LEU:HD21	2:m:80:GLN:NE2	1.75	1.01
4:f:177:VAL:CG2	11:n:266:VAL:CG2	2.39	1.01
4:f:180:LEU:CG	11:n:299:PHE:HD1	1.61	1.01
9:j:89:LEU:CD2	13:s:93:TYR:CZ	2.42	1.01
17:c:110:ALA:HB3	19:b:168:ILE:HG21	1.37	1.01
1:a:109:TYR:CZ	1:a:154:LEU:HD21	1.95	1.01
2:m:68:LYS:HD3	5:g:45:PHE:CZ	1.95	1.01
5:g:13:PRO:HA	55:PA:1660:THR:HA	1.42	1.01
6:h:42:TRP:HB2	6:h:43:PRO:HD3	1.40	1.01
7:r:62:GLY:CA	8:t:101:PHE:HE2	1.70	1.01
9:j:75:ARG:HD2	9:j:80:TYR:CE2	1.96	1.01
10:k:17:ILE:HG23	12:q:171:VAL:HG21	1.37	1.01
11:n:527:THR:CG2	68:w:42:GLY:CA	2.37	1.01
18:e:60:VAL:CA	19:b:179:LEU:HD12	1.90	1.01
3:d:126:TYR:OH	12:q:36:MET:HE1	1.21	1.00
9:j:19:ILE:CG2	9:j:45:VAL:HG21	1.91	1.00
9:j:78:GLN:O	9:j:82:LYS:HD2	1.56	1.00
14:u:83:ALA:O	14:u:87:ALA:N	1.92	1.00
3:d:121:LEU:HD21	5:g:160:VAL:CG1	1.91	1.00
9:j:53:LYS:NZ	11:n:60:HIS:CB	2.24	1.00
12:q:212:ALA:HA	12:q:387:LEU:CD1	1.90	1.00
42:Di:73:LEU:HD22	44:Dl:105:HIS:CD2	1.95	1.00
3:d:121:LEU:HD13	5:g:160:VAL:CG2	1.88	1.00
4:f:188:PHE:CB	11:n:281:ARG:HD3	1.89	1.00
8:t:98:LEU:HB2	8:t:102:PHE:HE2	1.22	1.00
11:n:266:VAL:CG2	11:n:303:LEU:HD11	1.90	1.00
4:f:16:VAL:HG12	4:f:103:GLY:O	1.60	1.00
11:n:659:LEU:HD13	68:w:14:LYS:HG2	1.40	1.00
2:m:26:GLN:OE1	5:g:45:PHE:CD2	2.15	1.00
21:o:762:GLN:HA	68:w:74:LYS:HE3	1.44	1.00
1:a:321:LEU:HD22	1:a:407:ILE:HD12	1.42	1.00
22:i:85:GLN:CG	22:i:86:ASP:OD1	2.09	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:X:29:DG:C2	54:Y:-29:DC:N3	2.29	1.00
69:x:956:VAL:HB	69:x:968:LEU:CD2	1.91	1.00
2:m:121:GLU:HA	16:z:592:ASN:HD21	1.16	0.99
53:X:-11:DG:H5"	54:Y:12:DG:N2	1.76	0.99
5:g:89:PHE:CE1	14:u:23:ILE:HD11	1.96	0.99
6:h:170:LYS:CE	6:h:172:THR:CG2	2.40	0.99
68:w:16:GLU:OE2	68:w:78:PHE:HB3	1.58	0.99
2:m:116:GLN:NE2	16:z:579:CYS:SG	2.36	0.99
53:X:2:DG:N2	54:Y:-1:DT:C2	2.29	0.99
4:f:132:GLU:OE2	4:f:132:GLU:C	2.05	0.99
11:n:247:LEU:HD23	11:n:278:VAL:HG23	1.40	0.99
11:n:545:LEU:HD11	11:n:653:PRO:CD	1.92	0.99
11:n:545:LEU:CD1	11:n:653:PRO:HG3	1.92	0.99
18:e:95:PHE:HB3	20:l:38:GLN:HG2	1.44	0.99
38:De:542:HIS:CD2	38:De:546:VAL:HG12	1.97	0.99
1:a:493:PHE:CD2	1:a:514:LYS:HG3	1.97	0.99
5:g:164:ILE:HD13	22:i:141:PHE:CE2	1.96	0.99
9:j:11:HIS:O	9:j:15:PHE:HD2	1.44	0.99
11:n:130:VAL:CB	14:u:27:GLN:CD	2.35	0.99
4:f:176:ARG:HH12	11:n:331:ALA:HB1	1.27	0.99
53:X:29:DG:N1	54:Y:-29:DC:N3	2.09	0.99
10:k:73:VAL:HG21	15:v:92:PRO:HD2	1.41	0.99
19:b:174:ILE:HG12	20:l:75:LEU:CD2	1.92	0.99
38:De:488:GLY:CA	38:De:546:VAL:HG22	1.93	0.99
5:g:87:ILE:HG23	9:j:127:ILE:HD13	1.43	0.99
10:k:17:ILE:HG21	12:q:171:VAL:HG22	1.40	0.99
54:Y:8:DA:H2'	54:Y:9:DC:C5	1.96	0.99
5:g:93:LEU:HB3	9:j:106:LYS:NZ	1.75	0.98
68:w:1:MET:N	68:w:1:MET:SD	2.32	0.98
11:n:686:LYS:NZ	21:o:730:PRO:HD3	1.78	0.98
2:m:30:ASN:ND2	3:d:176:TYR:CD1	2.31	0.98
3:d:169:PRO:HA	55:PA:1795:PRO:HG2	0.98	0.98
11:n:169:LEU:HB3	11:n:170:PRO:HD3	1.42	0.98
11:n:587:LEU:CD1	68:w:15:THR:CG2	2.42	0.98
3:d:128:ALA:HB1	14:u:108:VAL:HB	1.00	0.98
5:g:93:LEU:C	9:j:106:LYS:HZ3	1.70	0.98
19:b:181:CYS:SG	20:l:82:LEU:CD1	2.50	0.98
3:d:169:PRO:O	55:PA:1793:THR:HB	1.62	0.98
9:j:70:TYR:CD1	9:j:80:TYR:CB	2.46	0.98
10:k:28:ALA:HB2	12:q:161:LEU:HD23	1.43	0.98
9:j:19:ILE:HD13	9:j:45:VAL:CG2	1.94	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DB:72:ILE:CG2	36:DB:148:ILE:HG23	1.94	0.98
53:X:-16:DG:N2	54:Y:16:DC:N3	2.10	0.98
53:X:-11:DG:H5"	54:Y:12:DG:H21	1.28	0.98
69:x:955:LEU:CG	69:x:967:VAL:HG21	1.93	0.98
9:j:26:VAL:CB	9:j:38:ASN:HD21	1.76	0.97
14:u:77:PRO:CG	14:u:79:GLU:HG3	1.94	0.97
6:h:74:GLN:HA	12:q:129:PRO:HA	1.44	0.97
54:Y:8:DA:H2"	54:Y:9:DC:C6	1.98	0.97
1:a:493:PHE:CD2	1:a:514:LYS:CG	2.37	0.97
7:r:42:LEU:HD22	10:k:77:GLN:HB2	1.46	0.97
11:n:266:VAL:HG21	11:n:303:LEU:HD11	1.47	0.97
44:Dl:76:LEU:CD1	44:Dl:84:LEU:HD12	1.94	0.97
1:a:417:TYR:CE1	1:a:450:PHE:HD1	1.74	0.97
9:j:56:GLN:HB3	11:n:53:THR:CA	1.94	0.97
44:Dl:76:LEU:HD13	44:Dl:84:LEU:HD11	1.37	0.97
44:Dl:102:LEU:HD11	44:Dl:118:LEU:HD11	1.00	0.97
12:q:437:HIS:CE1	12:q:472:GLU:N	2.33	0.97
12:q:89:GLN:CB	12:q:90:PRO:HD2	1.94	0.97
19:b:174:ILE:HD13	20:l:75:LEU:HD21	1.44	0.97
44:Dl:76:LEU:HD13	44:Dl:84:LEU:HD12	1.44	0.97
3:d:113:GLN:HG2	5:g:166:ASN:HD21	1.26	0.97
8:t:110:ILE:HD12	8:t:197:PHE:HB3	1.47	0.97
53:X:-11:DG:H5'	54:Y:12:DG:H22	1.30	0.97
18:e:60:VAL:HB	19:b:179:LEU:HG	1.46	0.96
2:m:121:GLU:N	16:z:592:ASN:HD22	1.62	0.96
12:q:17:LYS:HE2	12:q:30:TYR:CE2	2.00	0.96
12:q:167:LEU:HD21	15:v:76:MET:HG3	1.48	0.96
13:s:92:ALA:O	13:s:96:PHE:HD2	1.36	0.96
12:q:578:TYR:CD1	12:q:646:LEU:CD1	2.49	0.96
14:u:85:LEU:HD13	16:z:552:LEU:HD21	0.97	0.96
44:Dl:118:LEU:HD12	44:Dl:119:HIS:N	1.81	0.96
12:q:288:SER:CB	12:q:289:PRO:CD	2.42	0.96
9:j:89:LEU:HD22	13:s:84:ILE:CG1	1.95	0.96
9:j:96:LYS:CE	13:s:80:SER:HA	1.95	0.96
15:v:119:LEU:HD21	18:e:139:TRP:CG	1.99	0.96
2:m:17:ARG:HH21	5:g:33:LYS:HD3	1.29	0.96
4:f:77:ILE:HG21	55:PA:1792:PRO:CG	1.96	0.96
7:r:68:PHE:HZ	8:t:98:LEU:HD22	1.29	0.96
9:j:70:TYR:HD1	9:j:80:TYR:CG	1.82	0.96
68:w:394:PRO:CA	70:p:171:PHE:CE1	2.48	0.96
5:g:136:ARG:CB	14:u:86:GLN:OE1	2.14	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:9:PHE:HB3	68:w:66:PHE:HE2	1.27	0.96
1:a:335:THR:O	1:a:391:THR:CG2	2.12	0.96
68:w:9:PHE:CD2	68:w:66:PHE:HD2	1.71	0.96
10:k:28:ALA:HB1	12:q:161:LEU:HD21	1.35	0.95
44:DL:106:ARG:CD	44:DL:114:LYS:HZ1	1.71	0.95
44:DL:87:ILE:O	44:DL:91:PHE:CD2	2.19	0.95
4:f:32:TYR:CD1	4:f:35:GLU:OE2	2.19	0.95
14:u:77:PRO:HG2	14:u:79:GLU:HG3	0.98	0.95
36:DB:72:ILE:CG2	36:DB:148:ILE:CG2	2.43	0.95
6:h:166:LEU:HD11	61:PG:125:PRO:HB3	1.45	0.95
42:Di:73:LEU:CD2	44:Dl:105:HIS:NE2	2.28	0.95
18:e:60:VAL:CB	19:b:179:LEU:HD12	1.97	0.95
18:e:146:ILE:HG22	18:e:147:ASN:N	1.78	0.95
21:o:715:LEU:HD11	69:x:21:TYR:HB2	0.98	0.95
6:h:147:CYS:SG	15:v:41:LYS:HB2	2.06	0.95
9:j:39:GLN:O	9:j:43:PHE:CD2	2.19	0.95
36:DB:290:PHE:CE2	36:DB:381:TRP:HB2	2.01	0.94
9:j:53:LYS:NZ	11:n:57:PHE:O	1.99	0.94
68:w:8:ILE:O	68:w:12:VAL:CG1	2.15	0.94
12:q:451:LEU:HD12	12:q:529:MET:HE1	1.49	0.94
44:Dl:57:VAL:HG21	44:Dl:92:ILE:CD1	1.97	0.94
9:j:26:VAL:CG1	9:j:38:ASN:ND2	1.94	0.94
10:k:12:ARG:HG2	10:k:66:GLN:HE21	0.80	0.94
42:DI:60:HIS:CE1	44:DL:106:ARG:CG	2.42	0.94
1:a:321:LEU:CD2	1:a:407:ILE:HG23	1.98	0.94
1:a:364:TYR:HB3	1:a:430:LEU:CG	1.96	0.94
2:m:66:TYR:CE2	5:g:38:ILE:HG23	2.01	0.94
2:m:71:GLN:OE1	3:d:175:PRO:HB2	1.67	0.94
11:n:545:LEU:CD1	11:n:653:PRO:CD	2.45	0.94
21:o:762:GLN:HA	68:w:74:LYS:HZ1	1.24	0.94
3:d:169:PRO:HB3	55:PA:1795:PRO:CB	1.98	0.94
24:8:177:TRP:CZ3	24:8:214:PRO:CA	2.50	0.94
51:BA:125:ALA:HB1	51:BA:132:ARG:CB	1.97	0.94
21:o:715:LEU:CD1	69:x:21:TYR:CB	2.42	0.94
44:Dl:87:ILE:O	44:Dl:91:PHE:HD2	1.43	0.94
2:m:104:HIS:CE1	11:n:168:ARG:CG	2.51	0.94
6:h:77:ILE:HG13	12:q:126:THR:HG21	1.49	0.94
11:n:254:VAL:CG1	11:n:304:GLN:NE2	2.31	0.94
36:DB:290:PHE:CD2	36:DB:381:TRP:HB2	2.02	0.94
3:d:44:LEU:HG	3:d:68:LEU:HD12	0.94	0.94
5:g:109:LEU:HD21	11:n:133:LEU:HG	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:527:THR:CG2	68:w:42:GLY:HA3	1.96	0.94
12:q:1:MET:CB	16:z:541:PRO:HG3	1.96	0.94
12:q:93:TRP:CE3	12:q:93:TRP:HA	2.02	0.94
36:DB:331:HIS:HE2	36:DB:342:THR:CB	1.81	0.94
42:DI:73:LEU:HD22	44:DL:105:HIS:CD2	2.01	0.94
2:m:70:PRO:HB2	11:n:166:TYR:HH	1.33	0.94
12:q:149:LYS:CE	15:v:40:ALA:HA	1.98	0.94
15:v:119:LEU:HD22	18:e:139:TRP:CD2	2.00	0.94
53:X:29:DG:N1	54:Y:-29:DC:N4	2.15	0.93
36:DB:67:SER:OG	36:DB:70:CYS:HB2	1.68	0.93
3:d:118:GLU:HA	3:d:121:LEU:HB2	1.47	0.93
2:m:112:ARG:HH22	16:z:598:CYS:C	1.50	0.93
36:DB:106:PHE:HB2	36:DB:954:TRP:CH2	2.03	0.93
44:DL:106:ARG:HD3	44:DL:114:LYS:HZ1	1.20	0.93
68:w:9:PHE:HB3	68:w:66:PHE:CE2	2.04	0.93
1:a:232:LEU:CD1	1:a:502:MET:HE1	1.99	0.93
44:DL:106:ARG:HH11	44:DL:114:LYS:HZ2	0.93	0.93
6:h:40:LEU:HD12	6:h:45:VAL:HG11	1.47	0.93
9:j:75:ARG:CD	9:j:80:TYR:CE2	2.48	0.93
17:c:111:TYR:CE1	19:b:136:HIS:CD2	2.57	0.93
21:o:696:SER:CB	69:x:111:HIS:HE1	1.80	0.93
10:k:28:ALA:HB1	12:q:161:LEU:HD23	0.97	0.93
68:w:9:PHE:CB	68:w:66:PHE:CE2	2.50	0.93
2:m:116:GLN:HE21	16:z:595:PRO:HD3	1.33	0.93
1:a:493:PHE:HD2	1:a:514:LYS:HD3	1.22	0.92
3:d:128:ALA:HB3	14:u:108:VAL:CG2	1.90	0.92
11:n:274:ILE:O	11:n:278:VAL:HG22	1.68	0.92
2:m:124:GLN:OE1	16:z:590:ARG:CG	2.17	0.92
5:g:93:LEU:CB	9:j:106:LYS:HE2	1.87	0.92
5:g:103:ILE:H	5:g:103:ILE:HD12	1.34	0.92
36:DB:806:VAL:HG22	36:DB:829:ILE:HD12	1.50	0.92
1:a:493:PHE:HD2	1:a:514:LYS:CD	1.74	0.92
10:k:73:VAL:CG2	15:v:92:PRO:CD	2.47	0.92
14:u:85:LEU:CD1	16:z:551:ASP:HB2	2.00	0.92
9:j:59:HIS:O	11:n:50:ARG:CA	2.17	0.92
11:n:586:LEU:HD22	68:w:11:GLU:HB3	1.48	0.92
58:PD:51:ALA:HB3	58:PD:54:GLU:CG	1.99	0.92
5:g:97:ILE:HG23	9:j:103:LYS:NZ	1.83	0.92
9:j:78:GLN:C	9:j:82:LYS:HG3	1.94	0.92
12:q:149:LYS:CD	15:v:40:ALA:HA	1.99	0.92
44:Dl:76:LEU:HD11	44:Dl:84:LEU:CD1	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:445:LEU:HD13	69:x:54:PRO:HB3	1.48	0.92
9:j:102:MET:HA	14:u:26:LEU:HD21	1.52	0.92
17:c:111:TYR:CD1	19:b:136:HIS:CD2	2.58	0.92
24:8:177:TRP:CZ2	55:PA:1677:SER:HB2	2.02	0.91
2:m:56:LEU:CD2	2:m:80:GLN:NE2	2.33	0.91
10:k:87:ARG:HH11	10:k:87:ARG:HG3	1.33	0.91
11:n:130:VAL:CB	14:u:27:GLN:CG	2.47	0.91
18:e:146:ILE:CG2	18:e:147:ASN:H	1.82	0.91
37:Dd:885:ILE:HG21	44:Dl:96:VAL:HG12	1.52	0.91
3:d:131:LYS:NZ	14:u:104:LEU:CD2	2.28	0.91
3:d:131:LYS:CB	14:u:104:LEU:HD11	2.00	0.91
8:t:98:LEU:HB2	8:t:102:PHE:CE2	2.05	0.91
9:j:53:LYS:CE	11:n:57:PHE:HA	2.01	0.91
15:v:122:GLU:HG3	18:e:139:TRP:HE1	1.35	0.91
18:e:60:VAL:HB	19:b:179:LEU:HD12	1.51	0.91
21:o:761:LEU:C	68:w:74:LYS:HE3	1.94	0.91
2:m:104:HIS:NE2	11:n:169:LEU:N	2.17	0.91
11:n:253:LEU:O	11:n:255:GLU:HG3	1.70	0.91
11:n:686:LYS:NZ	21:o:730:PRO:CD	2.26	0.91
11:n:870:GLN:HG2	21:o:655:THR:HG22	1.53	0.91
12:q:89:GLN:CG	12:q:90:PRO:CD	2.38	0.91
23:0:194:VAL:HG22	23:0:198:LEU:HD23	1.49	0.91
9:j:53:LYS:HZ1	11:n:60:HIS:C	1.78	0.91
12:q:1:MET:N	16:z:540:LEU:CD1	2.33	0.91
68:w:6:GLN:CA	68:w:62:TRP:HH2	1.83	0.91
2:m:104:HIS:HE1	11:n:168:ARG:HG3	1.05	0.91
6:h:170:LYS:HE2	6:h:172:THR:CG2	2.01	0.91
10:k:21:ILE:HG21	12:q:168:THR:OG1	1.68	0.91
18:e:49:GLU:CD	19:b:186:THR:HG21	1.96	0.91
42:Di:73:LEU:HD13	44:Dl:105:HIS:NE2	1.85	0.91
2:m:68:LYS:CE	5:g:50:GLN:HE22	1.83	0.91
54:Y:8:DA:C2'	54:Y:9:DC:C5	2.54	0.91
5:g:164:ILE:HG21	22:i:141:PHE:CZ	2.06	0.91
9:j:82:LYS:CG	13:s:96:PHE:CD1	2.08	0.91
10:k:31:VAL:HG23	12:q:157:ALA:HB2	1.51	0.91
10:k:114:MET:HE2	18:e:129:VAL:HG11	1.49	0.91
11:n:527:THR:HG21	68:w:42:GLY:HA2	1.52	0.91
68:w:12:VAL:CG2	68:w:78:PHE:HE2	1.81	0.91
9:j:59:HIS:O	11:n:50:ARG:HA	1.69	0.90
11:n:172:CYS:SG	12:q:21:GLU:CA	2.60	0.90
44:DL:106:ARG:NH1	44:DL:114:LYS:NZ	2.16	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Dl:115:ASP:O	44:Dl:118:LEU:HG	1.71	0.90
1:a:381:PRO:O	69:x:92:LEU:HD13	1.69	0.90
7:r:62:GLY:HA3	8:t:101:PHE:CD2	2.06	0.90
9:j:69:GLU:O	9:j:73:GLN:CG	2.19	0.90
11:n:265:LEU:HD13	11:n:303:LEU:CD2	2.01	0.90
9:j:85:LEU:HD12	13:s:96:PHE:CZ	2.05	0.90
15:v:82:LEU:HD13	15:v:86:LEU:CD2	2.01	0.90
36:DB:119:PRO:HB2	36:DB:195:SER:HB3	1.53	0.90
44:Dl:102:LEU:HD11	44:Dl:118:LEU:CD1	1.96	0.90
2:m:17:ARG:NH2	5:g:33:LYS:CD	2.35	0.90
2:m:27:CYS:HA	3:d:177:PRO:HG3	0.92	0.90
2:m:104:HIS:NE2	11:n:168:ARG:CD	2.34	0.90
3:d:106:ASP:OD2	5:g:174:ASP:CB	2.19	0.90
11:n:159:ASP:OD2	11:n:167:PRO:HD2	1.68	0.90
39:DF:35:THR:O	39:DF:39:LEU:HG	1.72	0.90
53:X:-5:DG:N2	54:Y:6:DG:N2	2.19	0.90
6:h:77:ILE:N	12:q:126:THR:OG1	2.04	0.90
10:k:28:ALA:HB3	12:q:161:LEU:CD2	2.00	0.90
2:m:124:GLN:HE21	16:z:581:SER:C	1.80	0.90
3:d:176:TYR:HB2	3:d:177:PRO:HD2	1.54	0.90
2:m:124:GLN:NE2	16:z:581:SER:C	2.29	0.90
3:d:131:LYS:CB	14:u:104:LEU:CD1	2.50	0.90
5:g:93:LEU:CB	9:j:106:LYS:HD3	2.01	0.90
15:v:75:LEU:HD23	15:v:78:LEU:HD12	1.51	0.90
19:b:62:MET:HE2	19:b:62:MET:HA	1.52	0.90
1:a:417:TYR:CB	1:a:469:VAL:HG21	2.02	0.90
10:k:99:TYR:OH	20:l:169:ASP:OD2	1.90	0.90
11:n:244:PRO:HB2	11:n:283:PHE:CD1	2.07	0.90
36:DB:579:LEU:HD22	36:DB:588:HIS:CB	2.01	0.90
7:r:45:ASN:ND2	10:k:82:SER:O	2.04	0.90
49:DP:300:ILE:CG2	49:DP:315:ALA:CB	2.50	0.90
58:PD:51:ALA:CB	58:PD:54:GLU:HG3	2.02	0.90
6:h:40:LEU:CG	6:h:45:VAL:HG11	2.01	0.89
11:n:278:VAL:CG1	11:n:281:ARG:HH22	1.83	0.89
24:8:177:TRP:CH2	55:PA:1677:SER:HA	2.07	0.89
10:k:79:HIS:CD2	12:q:195:LYS:CD	2.55	0.89
12:q:89:GLN:CD	12:q:90:PRO:HD2	1.97	0.89
12:q:149:LYS:HD2	15:v:40:ALA:HA	1.53	0.89
1:a:382:LEU:C	69:x:92:LEU:HD11	1.96	0.89
1:a:360:ASN:CB	69:x:17:ARG:NH1	2.29	0.89
2:m:27:CYS:C	3:d:177:PRO:HG3	1.97	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:526:SER:OG	68:w:45:ARG:NH1	2.05	0.89
24:8:177:TRP:CZ2	55:PA:1677:SER:HA	2.08	0.89
69:x:956:VAL:CB	69:x:968:LEU:HD21	1.99	0.89
69:x:485:PRO:HD2	69:x:486:ALA:N	1.86	0.89
10:k:37:LYS:H	10:k:37:LYS:HE3	1.34	0.89
12:q:89:GLN:HG2	12:q:90:PRO:HD3	1.55	0.89
2:m:30:ASN:CB	3:d:176:TYR:HB2	2.03	0.89
2:m:116:GLN:HB3	16:z:594:LEU:CD2	2.02	0.89
11:n:715:ARG:HH22	17:c:311:GLN:HE22	1.20	0.89
37:Dd:844:ASN:O	37:Dd:847:GLU:HG2	1.73	0.89
11:n:861:LYS:HE3	17:c:30:ARG:NE	1.87	0.89
4:f:77:ILE:CG2	55:PA:1792:PRO:HG2	2.02	0.89
11:n:266:VAL:HG21	11:n:303:LEU:CD1	2.02	0.89
11:n:278:VAL:HG12	11:n:281:ARG:HH21	0.78	0.89
12:q:120:ARG:HG2	12:q:120:ARG:HH11	1.38	0.89
12:q:437:HIS:HE1	12:q:472:GLU:C	1.81	0.89
2:m:30:ASN:ND2	3:d:176:TYR:CG	2.41	0.89
9:j:102:MET:CB	14:u:26:LEU:CD2	2.50	0.89
12:q:482:GLN:HB3	12:q:634:ASN:HD22	1.36	0.89
2:m:23:GLU:OE1	5:g:44:MET:O	1.90	0.88
2:m:68:LYS:HD2	5:g:50:GLN:HE22	1.38	0.88
9:j:43:PHE:HZ	13:s:150:ALA:C	1.80	0.88
9:j:89:LEU:HD22	13:s:84:ILE:HG12	1.54	0.88
12:q:482:GLN:HB3	12:q:634:ASN:ND2	1.88	0.88
3:d:113:GLN:HE22	5:g:163:MET:HE2	1.32	0.88
12:q:375:LEU:HD21	12:q:431:ILE:HG13	1.56	0.88
1:a:467:MET:HE1	1:a:504:ILE:HD11	0.89	0.88
9:j:101:THR:O	9:j:105:PHE:CD2	2.26	0.88
12:q:1:MET:H3	16:z:540:LEU:HD13	1.37	0.88
1:a:364:TYR:CB	1:a:430:LEU:HG	2.03	0.88
6:h:77:ILE:CG1	12:q:126:THR:CB	2.51	0.88
17:c:111:TYR:CD2	19:b:136:HIS:HD2	1.90	0.88
9:j:89:LEU:CD2	13:s:84:ILE:HG12	2.04	0.88
36:DB:119:PRO:HG3	36:DB:194:ASP:O	1.72	0.88
2:m:68:LYS:CD	5:g:50:GLN:HE22	1.87	0.88
7:r:88:LEU:HD12	7:r:88:LEU:H	1.37	0.88
9:j:53:LYS:HE2	11:n:57:PHE:CA	2.03	0.88
68:w:13:VAL:HG12	68:w:75:ARG:HG3	1.54	0.88
2:m:17:ARG:HH21	5:g:33:LYS:CD	1.86	0.88
2:m:116:GLN:CG	16:z:595:PRO:CD	2.50	0.88
2:m:121:GLU:N	16:z:592:ASN:ND2	2.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:29:PHE:CE2	12:q:102:LEU:CD1	2.56	0.88
9:j:79:LEU:HD11	13:s:111:ASP:CB	2.02	0.88
21:o:715:LEU:HD21	69:x:25:ILE:CG1	2.00	0.88
2:m:116:GLN:NE2	16:z:595:PRO:HD3	1.89	0.88
12:q:645:ALA:HB2	18:e:100:LEU:CD2	2.03	0.88
2:m:124:GLN:HG3	16:z:581:SER:HB2	1.54	0.88
10:k:28:ALA:HB3	12:q:161:LEU:HD21	1.55	0.88
1:a:509:ARG:HB2	1:a:509:ARG:NH1	1.89	0.87
2:m:62:GLU:HG3	5:g:38:ILE:HD11	1.56	0.87
11:n:245:TRP:HB2	11:n:282:LEU:HD13	0.89	0.87
11:n:545:LEU:HD12	11:n:653:PRO:HD3	1.55	0.87
33:EA:129:CYS:HB2	33:EA:154:CYS:SG	2.14	0.87
1:a:423:SER:CB	1:a:503:SER:HB2	2.04	0.87
2:m:39:GLN:HB3	55:PA:1654:SER:HB3	1.55	0.87
3:d:131:LYS:HZ3	14:u:104:LEU:CD2	1.84	0.87
9:j:101:THR:O	9:j:105:PHE:HD2	1.57	0.87
21:o:696:SER:OG	69:x:111:HIS:HE1	1.56	0.87
38:De:542:HIS:HD2	38:De:546:VAL:HG12	1.36	0.87
7:r:45:ASN:HB2	10:k:81:GLY:HA2	1.55	0.87
12:q:290:HIS:NE2	12:q:294:LYS:HE3	1.88	0.87
21:o:715:LEU:CD2	69:x:25:ILE:CG1	2.51	0.87
12:q:290:HIS:HE1	12:q:294:LYS:HE3	1.33	0.87
14:u:83:ALA:CA	14:u:86:GLN:HB3	2.05	0.87
5:g:89:PHE:HE1	14:u:23:ILE:CD1	1.88	0.87
6:h:29:PHE:HE2	12:q:102:LEU:HD11	1.36	0.87
9:j:39:GLN:O	9:j:43:PHE:HD2	1.55	0.87
1:a:232:LEU:HD12	1:a:502:MET:CE	2.04	0.87
9:j:78:GLN:O	9:j:82:LYS:HB2	1.73	0.87
10:k:111:CYS:SG	18:e:133:LEU:HG	2.15	0.87
1:a:467:MET:HE2	1:a:504:ILE:CD1	1.91	0.87
2:m:100:GLN:HB3	11:n:170:PRO:HG3	1.57	0.87
4:f:16:VAL:CG1	4:f:103:GLY:O	2.22	0.87
5:g:164:ILE:CG2	22:i:141:PHE:CE2	2.56	0.87
12:q:139:GLN:NE2	12:q:139:GLN:O	2.08	0.87
42:Di:73:LEU:CD2	44:Dl:105:HIS:CD2	2.58	0.87
11:n:659:LEU:CD1	68:w:14:LYS:CG	2.51	0.86
68:w:13:VAL:CG1	68:w:75:ARG:HG3	2.05	0.86
11:n:526:SER:HB2	68:w:45:ARG:NH2	1.89	0.86
36:DB:579:LEU:CD2	36:DB:588:HIS:HB3	2.04	0.86
44:DL:87:ILE:O	44:DL:91:PHE:HD2	1.58	0.86
44:DL:106:ARG:CZ	44:DL:114:LYS:HG3	2.02	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:70:TYR:HD1	9:j:80:TYR:CB	1.85	0.86
11:n:545:LEU:CD1	11:n:653:PRO:HD3	2.04	0.86
15:v:82:LEU:HD13	15:v:86:LEU:HD21	1.55	0.86
2:m:124:GLN:NE2	16:z:581:SER:CB	2.33	0.86
5:g:146:ARG:HH12	14:u:97:ASN:HB3	1.40	0.86
10:k:79:HIS:CD2	12:q:195:LYS:HD2	2.09	0.86
44:DL:76:LEU:HD11	44:DL:84:LEU:HD11	1.56	0.86
3:d:131:LYS:CG	14:u:104:LEU:HD13	2.05	0.86
15:v:82:LEU:CD1	15:v:86:LEU:HD21	2.06	0.86
1:a:417:TYR:CD1	1:a:469:VAL:HG23	2.03	0.86
9:j:77:PRO:HD2	9:j:78:GLN:N	1.90	0.86
17:c:204:MET:CE	17:c:208:PHE:O	2.23	0.86
36:DB:304:PHE:CE1	36:DB:353:GLN:OE1	2.28	0.86
10:k:45:LEU:O	10:k:45:LEU:HD22	1.76	0.86
1:a:367:LEU:HD13	1:a:509:ARG:CZ	2.05	0.86
2:m:116:GLN:NE2	16:z:595:PRO:CD	2.38	0.86
3:d:128:ALA:CB	14:u:108:VAL:HG23	1.93	0.86
7:r:68:PHE:CZ	8:t:98:LEU:HD22	2.09	0.86
11:n:172:CYS:SG	12:q:20:HIS:O	2.33	0.86
15:v:85:PHE:CD1	15:v:86:LEU:HD22	2.10	0.86
4:f:94:PRO:HB2	12:q:130:VAL:HG22	1.55	0.86
44:DL:106:ARG:HH11	44:DL:114:LYS:HG3	1.38	0.86
6:h:67:LYS:CE	23:0:141:THR:HG23	2.05	0.86
68:w:41:LEU:HD11	68:w:85:MET:HB3	1.55	0.86
2:m:101:GLN:HA	11:n:169:LEU:CD2	2.06	0.85
2:m:112:ARG:NH2	16:z:598:CYS:C	2.27	0.85
11:n:73:LEU:O	11:n:77:SER:N	2.09	0.85
11:n:154:ILE:HB	11:n:155:PRO:HD2	1.56	0.85
17:c:204:MET:HE1	17:c:208:PHE:C	2.00	0.85
18:e:60:VAL:HA	19:b:179:LEU:HD12	1.56	0.85
23:0:11:THR:N	23:0:34:CYS:SG	2.49	0.85
23:0:11:THR:H	23:0:34:CYS:HG	1.24	0.85
2:m:104:HIS:CG	11:n:169:LEU:CA	2.57	0.85
4:f:32:TYR:HD1	4:f:35:GLU:OE2	1.56	0.85
6:h:72:ARG:HH12	12:q:134:ALA:H	1.18	0.85
11:n:230:PHE:CE2	11:n:296:LEU:CB	2.59	0.85
19:b:78:ALA:HB3	21:o:621:LEU:HD21	1.58	0.85
68:w:16:GLU:OE2	68:w:78:PHE:CD2	2.29	0.85
2:m:104:HIS:CD2	11:n:169:LEU:N	2.45	0.85
4:f:181:LEU:CD1	11:n:270:GLN:NE2	2.39	0.85
11:n:247:LEU:CD2	11:n:278:VAL:CG2	2.53	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:204:MET:SD	17:c:208:PHE:O	2.35	0.85
7:r:117:PHE:CE1	8:t:79:PHE:HD2	1.94	0.85
11:n:226:VAL:HG12	11:n:230:PHE:O	1.76	0.85
11:n:244:PRO:HB2	11:n:283:PHE:CE1	2.11	0.85
11:n:141:ARG:HH21	14:u:20:CYS:HB3	1.41	0.85
1:a:417:TYR:CG	1:a:469:VAL:HG21	2.12	0.85
5:g:136:ARG:HB2	14:u:86:GLN:CD	2.00	0.85
8:t:173:PRO:HG3	8:t:192:GLN:HE21	1.42	0.85
17:c:110:ALA:HB1	19:b:168:ILE:HG23	0.85	0.85
4:f:116:ASN:HB3	15:v:52:THR:HG21	1.56	0.85
7:r:125:MET:C	7:r:125:MET:HE3	2.02	0.85
11:n:159:ASP:O	11:n:163:THR:O	1.95	0.85
2:m:104:HIS:CE1	11:n:169:LEU:H	1.94	0.85
6:h:18:GLN:HA	6:h:18:GLN:NE2	1.92	0.85
6:h:77:ILE:CA	12:q:126:THR:OG1	2.25	0.85
7:r:124:ARG:NH1	7:r:124:ARG:HB2	1.92	0.85
9:j:99:ILE:O	9:j:102:MET:HG2	1.77	0.85
2:m:124:GLN:CD	16:z:581:SER:HB2	2.01	0.84
4:f:181:LEU:HD12	11:n:270:GLN:HE22	1.34	0.84
12:q:578:TYR:CD1	12:q:646:LEU:HD13	2.11	0.84
37:Dd:873:LEU:HD13	44:Dl:92:ILE:HD11	1.59	0.84
2:m:104:HIS:CD2	11:n:169:LEU:H	1.95	0.84
15:v:85:PHE:CE1	15:v:86:LEU:CD2	2.59	0.84
9:j:92:ASN:CG	13:s:83:LEU:HD21	1.99	0.84
11:n:169:LEU:HB3	11:n:170:PRO:HD2	1.57	0.84
21:o:762:GLN:CA	68:w:74:LYS:NZ	2.40	0.84
42:Di:73:LEU:CD2	44:Dl:105:HIS:CE1	2.57	0.84
49:DP:300:ILE:HG22	49:DP:315:ALA:N	1.91	0.84
6:h:22:LEU:HD12	6:h:22:LEU:O	1.78	0.84
12:q:212:ALA:CA	12:q:387:LEU:HD11	2.04	0.84
44:Dl:76:LEU:HD11	44:Dl:84:LEU:HD11	1.59	0.84
5:g:131:ALA:HB2	11:n:152:PHE:CE2	2.12	0.84
7:r:62:GLY:HA3	8:t:101:PHE:HE2	1.05	0.84
9:j:59:HIS:CB	11:n:50:ARG:N	2.39	0.84
9:j:78:GLN:CA	9:j:82:LYS:HG3	2.08	0.84
12:q:1:MET:H1	16:z:540:LEU:HD13	1.41	0.84
1:a:423:SER:HB2	1:a:503:SER:HB2	1.56	0.84
3:d:131:LYS:NZ	14:u:104:LEU:CB	2.41	0.84
44:Dl:102:LEU:CD1	44:Dl:118:LEU:HD21	2.00	0.84
21:o:765:ASP:OD2	68:w:73:PRO:HD3	1.76	0.84
69:x:482:SER:O	69:x:485:PRO:CD	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:113:TRP:CH2	19:b:175:HIS:CB	2.56	0.84
68:w:5:LEU:HA	68:w:8:ILE:HD12	1.59	0.84
1:a:383:PRO:N	69:x:92:LEU:HD11	1.93	0.84
2:m:120:ALA:CB	16:z:592:ASN:HB3	2.07	0.84
9:j:53:LYS:HZ1	11:n:60:HIS:CB	1.87	0.84
5:g:97:ILE:CG2	9:j:103:LYS:CE	2.18	0.84
6:h:40:LEU:HG	6:h:45:VAL:HG11	1.60	0.84
55:PA:358:ARG:HA	56:PB:1085:ARG:HA	1.60	0.84
2:m:68:LYS:NZ	5:g:50:GLN:NE2	2.26	0.83
9:j:56:GLN:CB	11:n:53:THR:CB	2.47	0.83
11:n:706:LEU:HD22	12:q:615:TRP:CZ3	2.12	0.83
12:q:9:ILE:HG13	14:u:90:LEU:CD1	2.05	0.83
6:h:22:LEU:HA	6:h:56:LEU:HD13	1.57	0.83
6:h:23:LYS:NZ	6:h:23:LYS:HB3	1.92	0.83
11:n:172:CYS:SG	12:q:21:GLU:HB2	2.18	0.83
1:a:335:THR:O	1:a:391:THR:HG21	1.76	0.83
3:d:121:LEU:HD13	5:g:160:VAL:HG22	1.60	0.83
15:v:84:GLN:NE2	15:v:85:PHE:HB3	1.92	0.83
1:a:423:SER:OG	1:a:505:PRO:HD3	1.79	0.83
11:n:907:LEU:HD11	19:b:118:LEU:HB2	1.58	0.83
14:u:25:VAL:HG21	14:u:58:PHE:CE2	2.13	0.83
19:b:174:ILE:HD13	20:l:75:LEU:CD2	2.02	0.83
23:0:41:ARG:HA	33:EA:171:LYS:HD2	1.58	0.83
4:f:137:CYS:SG	6:h:42:TRP:HB3	2.18	0.83
9:j:85:LEU:CD1	13:s:96:PHE:CZ	2.62	0.83
11:n:254:VAL:HG11	11:n:304:GLN:HE21	1.42	0.83
53:X:-11:DG:C5'	54:Y:12:DG:H22	1.88	0.83
11:n:707:ASP:HB2	21:o:684:ARG:HH21	1.40	0.83
9:j:53:LYS:NZ	11:n:60:HIS:C	2.35	0.83
12:q:443:ARG:NE	12:q:443:ARG:HA	1.92	0.83
17:c:113:TRP:CZ2	19:b:175:HIS:CG	2.65	0.83
5:g:31:ALA:H	5:g:32:PRO:CD	1.92	0.82
15:v:20:LYS:HE3	58:PD:70:ARG:HG3	1.61	0.82
17:c:204:MET:HE1	17:c:208:PHE:CA	2.08	0.82
55:PA:381:PRO:HB3	55:PA:480:SER:HA	1.61	0.82
1:a:321:LEU:HD21	1:a:407:ILE:CG2	2.08	0.82
4:f:180:LEU:HD23	11:n:299:PHE:CZ	2.14	0.82
3:d:113:GLN:HG2	5:g:166:ASN:ND2	1.94	0.82
11:n:244:PRO:CB	11:n:283:PHE:CD1	2.61	0.82
12:q:462:ALA:O	15:v:131:GLU:HG2	1.80	0.82
17:c:111:TYR:CE2	19:b:136:HIS:HD2	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DB:304:PHE:HE1	36:DB:353:GLN:HE22	1.25	0.82
44:DL:106:ARG:NH1	44:DL:114:LYS:HZ2	1.75	0.82
11:n:225:ARG:CB	11:n:231:GLU:OE1	2.27	0.82
1:a:417:TYR:HB2	1:a:469:VAL:HG21	1.60	0.82
2:m:30:ASN:HB2	3:d:176:TYR:HB2	1.58	0.82
2:m:66:TYR:OH	5:g:38:ILE:CG2	2.27	0.82
6:h:77:ILE:CD1	12:q:126:THR:HG21	2.09	0.82
11:n:586:LEU:CD2	68:w:11:GLU:HB3	2.10	0.82
11:n:680:HIS:HE2	12:q:557:LEU:HD11	1.44	0.82
3:d:131:LYS:CD	14:u:104:LEU:HD22	2.08	0.82
11:n:73:LEU:O	11:n:77:SER:CA	2.28	0.82
12:q:339:LEU:HD22	12:q:439:PHE:CD2	2.14	0.82
3:d:159:ASN:HA	3:d:162:CYS:HB3	1.61	0.82
11:n:254:VAL:HG13	11:n:304:GLN:NE2	1.92	0.82
44:Dl:93:GLU:O	44:Dl:97:THR:HG23	1.79	0.82
12:q:451:LEU:CD1	12:q:529:MET:CE	2.57	0.82
24:8:177:TRP:CZ2	55:PA:1677:SER:CA	2.63	0.82
4:f:180:LEU:HD13	11:n:302:SER:HG	1.44	0.82
10:k:103:LYS:HB3	20:l:166:LEU:HD12	1.60	0.82
11:n:686:LYS:CE	21:o:730:PRO:HG3	2.09	0.82
12:q:437:HIS:HE1	12:q:472:GLU:N	1.77	0.82
12:q:441:ARG:NH1	20:l:168:TRP:CE2	2.48	0.82
9:j:102:MET:HB3	14:u:26:LEU:CD2	2.10	0.81
42:DI:60:HIS:HE1	44:DL:106:ARG:HG3	1.45	0.81
36:DB:280:THR:CG2	36:DB:342:THR:HG21	2.08	0.81
4:f:180:LEU:HD11	11:n:299:PHE:HA	0.90	0.81
8:t:144:TYR:HD2	8:t:147:CYS:HB2	1.46	0.81
9:j:56:GLN:HB3	11:n:53:THR:HA	1.60	0.81
11:n:130:VAL:CB	14:u:27:GLN:NE2	2.43	0.81
11:n:265:LEU:CD1	11:n:303:LEU:CD2	2.58	0.81
12:q:93:TRP:HA	12:q:93:TRP:HE3	1.41	0.81
19:b:174:ILE:CG1	20:l:75:LEU:CD2	2.39	0.81
25:9:183:ASN:HB3	25:9:186:ILE:HG23	1.60	0.81
44:DL:106:ARG:NE	44:DL:114:LYS:HZ3	1.78	0.81
3:d:121:LEU:CG	5:g:160:VAL:HG21	2.10	0.81
22:i:85:GLN:HG3	22:i:86:ASP:H	0.73	0.81
6:h:77:ILE:CG1	12:q:126:THR:OG1	2.28	0.81
14:u:83:ALA:HA	14:u:86:GLN:HB3	1.61	0.81
13:s:92:ALA:HB1	13:s:96:PHE:HE2	1.45	0.81
57:PC:78:ILE:HD11	57:PC:127:VAL:HG23	1.61	0.81
2:m:117:GLN:HA	16:z:594:LEU:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:278:VAL:HG13	11:n:281:ARG:NH2	1.95	0.81
44:Dl:57:VAL:HG21	44:Dl:92:ILE:HD12	1.62	0.81
6:h:77:ILE:CG1	12:q:126:THR:HG21	2.08	0.81
9:j:96:LYS:HD2	13:s:80:SER:O	1.79	0.81
12:q:437:HIS:HE1	12:q:472:GLU:CA	1.92	0.81
11:n:265:LEU:CD1	11:n:303:LEU:HD21	2.08	0.81
11:n:527:THR:HG21	68:w:42:GLY:N	1.96	0.81
15:v:126:ASP:HB3	18:e:132:HIS:CD2	2.15	0.81
1:a:514:LYS:NZ	1:a:514:LYS:HB3	1.96	0.81
3:d:170:GLY:N	55:PA:1793:THR:HG21	1.95	0.81
5:g:93:LEU:HD13	9:j:106:LYS:HG2	0.81	0.81
12:q:482:GLN:CB	12:q:634:ASN:ND2	2.43	0.81
17:c:111:TYR:CZ	19:b:136:HIS:CD2	2.69	0.81
53:X:-11:DG:H22	54:Y:11:DC:N4	1.78	0.81
1:a:364:TYR:CB	1:a:430:LEU:HD12	2.10	0.80
14:u:8:LEU:HD12	14:u:72:LEU:CD2	2.10	0.80
21:o:762:GLN:CA	68:w:74:LYS:HE3	2.11	0.80
23:0:46:CYS:HG	71:0:401:ZN:ZN	0.91	0.80
36:DB:689:GLN:O	36:DB:689:GLN:CG	2.29	0.80
1:a:383:PRO:C	69:x:92:LEU:HD21	2.05	0.80
1:a:417:TYR:HE1	1:a:450:PHE:HD1	1.06	0.80
1:a:441:GLU:HB3	69:x:14:TRP:HZ2	1.45	0.80
6:h:74:GLN:CD	12:q:129:PRO:HB3	2.05	0.80
12:q:138:LYS:CB	12:q:140:ASN:OD1	2.27	0.80
17:c:204:MET:CE	17:c:208:PHE:C	2.54	0.80
1:a:364:TYR:O	1:a:428:THR:OG1	1.98	0.80
3:d:170:GLY:HA2	55:PA:1793:THR:HG22	1.63	0.80
5:g:136:ARG:CA	14:u:86:GLN:NE2	2.35	0.80
11:n:265:LEU:HD11	11:n:307:VAL:HG21	1.64	0.80
19:b:174:ILE:HG12	20:l:75:LEU:CG	2.11	0.80
11:n:587:LEU:HD13	68:w:15:THR:HB	0.82	0.80
12:q:451:LEU:HD12	12:q:529:MET:CE	2.11	0.80
23:0:121:LYS:O	23:0:124:ILE:CG1	2.30	0.80
42:Di:73:LEU:CD1	44:Dl:105:HIS:NE2	2.44	0.80
55:PA:686:THR:HG23	55:PA:765:ASN:HD21	1.42	0.80
2:m:104:HIS:HB3	11:n:169:LEU:HD23	1.63	0.80
9:j:78:GLN:HA	9:j:82:LYS:HG3	1.62	0.80
11:n:230:PHE:CZ	11:n:296:LEU:CB	2.65	0.80
11:n:587:LEU:CD2	68:w:15:THR:HG21	2.03	0.80
23:0:196:LEU:HD13	23:0:200:GLN:OE1	1.81	0.80
36:DB:218:GLY:CA	36:DB:238:LEU:HD13	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DB:563:PRO:CA	36:DB:580:GLN:HA	2.09	0.80
2:m:104:HIS:ND1	11:n:169:LEU:HG	1.96	0.80
11:n:259:THR:OG1	11:n:311:GLN:NE2	2.13	0.80
44:DL:93:GLU:O	44:DL:97:THR:HG23	1.81	0.80
3:d:131:LYS:CD	14:u:104:LEU:CD1	2.00	0.80
3:d:131:LYS:HZ2	14:u:104:LEU:HB2	1.47	0.80
7:r:29:ASP:OD1	7:r:29:ASP:N	2.15	0.80
2:m:104:HIS:NE2	11:n:168:ARG:HD3	1.97	0.80
9:j:26:VAL:HG11	9:j:38:ASN:HD21	0.75	0.80
9:j:53:LYS:HZ3	11:n:61:ARG:H	0.82	0.80
19:b:178:LEU:HD23	20:l:82:LEU:HD11	1.64	0.80
44:Dl:102:LEU:CD1	44:Dl:118:LEU:CD1	2.59	0.80
2:m:116:GLN:NE2	16:z:595:PRO:CG	2.44	0.80
9:j:75:ARG:HB3	9:j:80:TYR:CD2	2.15	0.80
12:q:647:SER:HB2	18:e:97:GLN:NE2	1.97	0.80
36:DB:564:LEU:HB2	36:DB:581:ILE:HD11	1.64	0.80
48:DO:92:LYS:HE2	50:DQ:332:GLU:HB3	1.64	0.80
49:DP:300:ILE:HG21	49:DP:315:ALA:CB	2.06	0.80
11:n:278:VAL:HG13	11:n:281:ARG:HH22	1.46	0.79
40:DG:181:TRP:HZ2	40:DG:183:ILE:HD11	1.48	0.79
45:Dc:89:PRO:HB3	43:Dj:127:THR:H	1.46	0.79
8:t:8:GLN:HE22	8:t:200:ILE:HG23	1.48	0.79
9:j:89:LEU:HD21	13:s:93:TYR:OH	1.81	0.79
69:x:485:PRO:CD	69:x:486:ALA:H	1.93	0.79
2:m:116:GLN:CB	16:z:594:LEU:HG	2.12	0.79
15:v:82:LEU:CD1	15:v:86:LEU:CD2	2.60	0.79
18:e:95:PHE:HB3	20:l:38:GLN:CG	2.12	0.79
1:a:57:HIS:HA	1:a:148:ASP:OD2	1.81	0.79
1:a:493:PHE:HE2	1:a:514:LYS:HG3	1.00	0.79
2:m:121:GLU:CA	16:z:592:ASN:HD22	1.92	0.79
12:q:633:ARG:CZ	12:q:633:ARG:HB3	2.11	0.79
53:X:-15:DG:N2	54:Y:15:DC:O2	2.15	0.79
56:PB:567:ILE:HD11	56:PB:577:HIS:HB2	1.64	0.79
2:m:71:GLN:HA	11:n:166:TYR:HE2	1.47	0.79
9:j:26:VAL:HG13	9:j:33:SER:OG	1.83	0.79
9:j:53:LYS:CD	11:n:57:PHE:CA	2.59	0.79
12:q:644:SER:O	18:e:97:GLN:HG2	1.82	0.79
1:a:321:LEU:HD21	1:a:407:ILE:HD12	1.63	0.79
1:a:462:LEU:HD11	69:x:49:GLN:HG2	1.64	0.79
1:a:439:GLN:NE2	69:x:15:LYS:CD	2.44	0.79
2:m:68:LYS:HD2	5:g:50:GLN:NE2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:124:ARG:CZ	7:r:124:ARG:HA	2.13	0.79
9:j:34:GLN:OE1	9:j:37:LEU:HD11	1.82	0.79
12:q:644:SER:HA	12:q:647:SER:OG	1.82	0.79
42:Di:73:LEU:HD22	44:Dl:105:HIS:CG	2.17	0.79
6:h:32:LYS:NZ	6:h:40:LEU:HD11	1.97	0.79
36:DB:216:SER:HB3	36:DB:236:TYR:CG	2.18	0.79
3:d:155:ILE:HD11	3:d:161:VAL:HB	1.65	0.79
10:k:37:LYS:H	10:k:37:LYS:CE	1.96	0.79
3:d:169:PRO:O	55:PA:1793:THR:CB	2.30	0.79
12:q:290:HIS:HE1	12:q:294:LYS:CE	1.91	0.79
14:u:103:CYS:O	14:u:107:VAL:HG23	1.82	0.79
6:h:170:LYS:HE2	6:h:172:THR:HG22	1.58	0.78
12:q:9:ILE:CG1	14:u:90:LEU:HD13	2.08	0.78
7:r:42:LEU:CD2	10:k:77:GLN:HB2	2.11	0.78
9:j:70:TYR:HD1	9:j:80:TYR:CD1	2.00	0.78
10:k:12:ARG:HB3	10:k:66:GLN:HE22	0.63	0.78
23:0:194:VAL:HG21	23:0:198:LEU:HD22	1.65	0.78
2:m:30:ASN:HA	3:d:176:TYR:CG	2.17	0.78
3:d:99:GLU:OE2	3:d:103:ARG:CZ	2.32	0.78
19:b:178:LEU:HD11	20:l:78:LEU:HD13	1.64	0.78
22:i:118:LEU:HD23	22:i:118:LEU:C	2.08	0.78
5:g:83:MET:CG	9:j:120:ASP:OD1	2.31	0.78
9:j:92:ASN:HD21	13:s:83:LEU:HD21	0.95	0.78
4:f:32:TYR:O	4:f:35:GLU:HG3	1.84	0.78
7:r:125:MET:HE3	7:r:125:MET:O	1.83	0.78
56:PB:714:PRO:HD2	56:PB:1001:PRO:HB3	1.66	0.78
4:f:176:ARG:NH1	11:n:331:ALA:HB1	1.98	0.78
6:h:40:LEU:CD1	6:h:45:VAL:CG1	2.61	0.78
11:n:368:LYS:HE2	11:n:371:GLN:HB3	1.66	0.78
37:Dd:873:LEU:CD1	44:Dl:92:ILE:HD11	2.14	0.78
5:g:93:LEU:CD1	9:j:106:LYS:CD	2.61	0.78
15:v:119:LEU:HD22	18:e:139:TRP:CE2	2.17	0.78
23:0:9:CYS:SG	23:0:34:CYS:HB3	2.24	0.78
68:w:6:GLN:HB2	68:w:62:TRP:CH2	2.18	0.78
68:w:357:HIS:HE1	68:w:397:LYS:CE	1.90	0.78
5:g:25:ASN:HA	5:g:27:GLN:NE2	1.98	0.78
5:g:93:LEU:HD13	9:j:106:LYS:CE	2.14	0.78
5:g:97:ILE:CG2	9:j:103:LYS:NZ	2.42	0.78
6:h:19:VAL:HG11	12:q:113:TYR:HB2	1.65	0.78
24:8:177:TRP:CZ2	55:PA:1677:SER:HB3	2.18	0.78
42:DI:73:LEU:HD13	44:DL:105:HIS:NE2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DL:106:ARG:HD3	44:DL:114:LYS:HZ3	0.89	0.78
9:j:54:CYS:HA	9:j:57:GLN:CD	2.09	0.78
11:n:659:LEU:HD13	68:w:14:LYS:CG	2.10	0.78
69:x:481:GLU:HB3	69:x:485:PRO:HG2	1.65	0.78
4:f:78:LEU:HD11	6:h:81:LEU:HD23	1.65	0.77
5:g:37:PRO:HG2	5:g:39:LYS:HE3	1.64	0.77
11:n:73:LEU:C	11:n:77:SER:CB	2.57	0.77
1:a:504:ILE:HA	1:a:507:THR:HG23	1.67	0.77
6:h:67:LYS:HD2	23:0:141:THR:HG21	1.35	0.77
11:n:231:GLU:HB2	11:n:253:LEU:HD21	1.66	0.77
12:q:288:SER:CB	12:q:289:PRO:HD3	2.13	0.77
44:DL:106:ARG:HH22	44:DL:115:ASP:N	1.81	0.77
3:d:128:ALA:CB	14:u:108:VAL:HG21	2.14	0.77
5:g:83:MET:SD	9:j:120:ASP:CG	2.67	0.77
9:j:76:ASN:HB2	9:j:77:PRO:CD	2.14	0.77
10:k:21:ILE:CD1	12:q:168:THR:OG1	2.30	0.77
34:EB:224:THR:HG22	34:EB:227:SER:HB2	1.66	0.77
44:DL:76:LEU:CD1	44:DL:84:LEU:CD1	2.62	0.77
3:d:131:LYS:CD	14:u:104:LEU:CD2	2.63	0.77
9:j:43:PHE:CE1	13:s:150:ALA:CB	2.67	0.77
11:n:589:GLN:HE22	68:w:25:MET:HB2	1.48	0.77
12:q:92:LEU:HD11	12:q:99:ARG:NH1	2.00	0.77
55:PA:509:LEU:HD13	60:PF:71:LEU:HA	1.67	0.77
2:m:29:ALA:O	3:d:176:TYR:HB3	1.84	0.77
10:k:33:LEU:HA	10:k:36:SER:OG	1.85	0.77
14:u:82:THR:C	14:u:86:GLN:HB2	2.09	0.77
17:c:111:TYR:CG	19:b:136:HIS:CD2	2.73	0.77
23:0:26:CYS:HB2	23:0:53:LEU:HD11	1.66	0.77
36:DB:608:ASN:ND2	36:DB:657:ARG:HD2	1.99	0.77
11:n:587:LEU:CG	68:w:15:THR:CG2	2.62	0.77
11:n:706:LEU:O	21:o:684:ARG:NH2	2.16	0.77
1:a:382:LEU:O	69:x:92:LEU:CD2	2.33	0.77
2:m:68:LYS:NZ	5:g:50:GLN:HE22	1.82	0.77
6:h:29:PHE:HE2	12:q:102:LEU:CD1	1.93	0.77
7:r:117:PHE:HE1	8:t:79:PHE:HD2	1.33	0.77
10:k:21:ILE:CG2	12:q:168:THR:OG1	2.32	0.77
24:8:177:TRP:HZ3	24:8:214:PRO:HA	1.44	0.77
38:De:546:VAL:HG23	38:De:546:VAL:O	1.84	0.77
68:w:9:PHE:CG	68:w:66:PHE:CE2	2.73	0.77
6:h:29:PHE:CD2	12:q:102:LEU:HD11	2.19	0.77
9:j:116:VAL:HG13	14:u:67:LYS:CE	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:659:LEU:HD21	68:w:17:VAL:CB	2.15	0.77
54:Y:4:DA:H2"	54:Y:5:DC:OP2	1.83	0.77
1:a:509:ARG:HB2	1:a:509:ARG:CZ	2.15	0.77
2:m:117:GLN:N	16:z:594:LEU:HD21	1.99	0.77
6:h:166:LEU:HD13	61:PG:125:PRO:HB2	1.67	0.77
10:k:111:CYS:SG	18:e:129:VAL:CG1	2.73	0.77
11:n:119:SER:CB	13:s:83:LEU:HD22	2.15	0.77
21:o:787:ALA:HB3	69:x:21:TYR:OH	1.85	0.77
36:DB:304:PHE:HE1	36:DB:353:GLN:NE2	1.81	0.77
2:m:26:GLN:O	3:d:177:PRO:HB3	1.84	0.76
6:h:61:LYS:HB2	15:v:56:GLN:HE22	1.48	0.76
6:h:147:CYS:HB2	15:v:41:LYS:HB2	1.67	0.76
2:m:70:PRO:HD2	3:d:161:VAL:HG21	1.65	0.76
2:m:124:GLN:HE22	16:z:582:LEU:N	1.84	0.76
11:n:158:ILE:CD1	12:q:11:ILE:HG21	2.05	0.76
23:0:121:LYS:O	23:0:124:ILE:HG12	1.84	0.76
23:0:192:LEU:HD22	23:0:196:LEU:HA	1.66	0.76
69:x:955:LEU:CD2	69:x:967:VAL:HG22	1.85	0.76
11:n:686:LYS:HZ1	21:o:730:PRO:HD3	1.47	0.76
23:0:194:VAL:HG23	23:0:198:LEU:HD22	1.65	0.76
36:DB:119:PRO:CG	36:DB:194:ASP:O	2.34	0.76
53:X:-2:DC:C2'	53:X:-1:DT:H71	2.12	0.76
5:g:93:LEU:CB	9:j:106:LYS:CD	2.47	0.76
9:j:96:LYS:HD2	13:s:80:SER:C	2.09	0.76
11:n:159:ASP:OD1	11:n:163:THR:CG2	2.34	0.76
15:v:119:LEU:HD22	18:e:139:TRP:CG	2.15	0.76
36:DB:724:THR:HA	36:DB:728:CYS:HB2	1.67	0.76
36:DB:806:VAL:HG22	36:DB:829:ILE:CD1	2.14	0.76
49:DP:277:HIS:HB3	49:DP:280:PHE:HB2	1.66	0.76
1:a:109:TYR:OH	1:a:154:LEU:HD21	1.84	0.76
3:d:131:LYS:HZ3	14:u:104:LEU:HB3	1.50	0.76
6:h:40:LEU:HG	6:h:45:VAL:HG21	1.67	0.76
12:q:34:LEU:N	12:q:34:LEU:HD23	2.01	0.76
36:DB:72:ILE:HG23	36:DB:148:ILE:HG22	1.65	0.76
36:DB:873:LEU:O	36:DB:877:TYR:HD2	1.68	0.76
9:j:102:MET:HB3	14:u:26:LEU:HD11	1.66	0.76
10:k:104:LEU:CD2	15:v:123:ILE:HD11	2.16	0.76
11:n:686:LYS:NZ	21:o:730:PRO:CB	2.48	0.76
11:n:944:PHE:HE2	19:b:101:ARG:HH22	1.32	0.76
12:q:149:LYS:HE2	15:v:39:THR:O	1.86	0.76
23:0:9:CYS:SG	23:0:34:CYS:SG	2.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:X:-9:DG:H1	54:Y:9:DC:H42	1.30	0.76
3:d:117:ALA:CB	5:g:163:MET:SD	2.72	0.76
9:j:53:LYS:HE2	11:n:57:PHE:HA	1.65	0.76
10:k:28:ALA:HB2	12:q:161:LEU:CD2	2.05	0.76
10:k:88:LYS:HD2	10:k:88:LYS:O	1.86	0.76
5:g:84:SER:HB3	13:s:67:LEU:HD22	1.67	0.76
9:j:56:GLN:CB	11:n:53:THR:HA	2.15	0.76
44:DL:106:ARG:CZ	44:DL:115:ASP:CG	2.58	0.76
54:Y:8:DA:C2'	54:Y:9:DC:C6	2.68	0.76
68:w:14:LYS:HA	68:w:17:VAL:HG23	1.67	0.76
1:a:224:TYR:CE2	1:a:253:MET:HB3	2.21	0.76
2:m:17:ARG:NH2	5:g:33:LYS:CG	2.49	0.76
8:t:131:MET:HB2	8:t:136:ARG:HD2	1.67	0.76
68:w:6:GLN:HB2	68:w:62:TRP:CZ2	2.21	0.76
68:w:394:PRO:HA	70:p:171:PHE:HZ	0.98	0.76
1:a:337:ALA:HB1	1:a:338:PRO:CD	2.16	0.76
9:j:75:ARG:HA	9:j:79:LEU:HD12	1.66	0.76
9:j:92:ASN:HD22	13:s:83:LEU:HD21	0.94	0.76
12:q:190:LEU:HG	12:q:196:LEU:HD11	1.66	0.76
31:6:127:VAL:HG12	31:6:163:TYR:HA	1.66	0.76
7:r:149:PHE:HB3	7:r:160:THR:HB	1.68	0.75
10:k:101:ARG:HB3	10:k:101:ARG:CZ	2.16	0.75
12:q:120:ARG:HG2	12:q:120:ARG:NH1	1.98	0.75
53:X:-23:DG:OP1	53:X:-23:DG:H4'	1.86	0.75
53:X:-2:DC:H2"	53:X:-1:DT:C5	2.20	0.75
2:m:124:GLN:NE2	16:z:581:SER:CA	2.48	0.75
3:d:170:GLY:HA2	55:PA:1793:THR:HG21	0.77	0.75
6:h:61:LYS:CB	15:v:56:GLN:HE22	1.98	0.75
8:t:8:GLN:NE2	8:t:200:ILE:HG23	2.00	0.75
11:n:526:SER:CB	68:w:45:ARG:NH2	2.49	0.75
11:n:678:PHE:HB2	12:q:555:VAL:HG21	1.66	0.75
12:q:135:LEU:HD12	12:q:135:LEU:O	1.86	0.75
12:q:458:PRO:HG3	12:q:533:GLN:HE21	1.50	0.75
16:z:540:LEU:HB3	16:z:541:PRO:HD3	1.68	0.75
19:b:174:ILE:HD11	20:l:75:LEU:HD23	1.65	0.75
25:9:183:ASN:HB3	25:9:186:ILE:CG2	2.16	0.75
42:Di:73:LEU:HD22	44:Dl:105:HIS:ND1	2.01	0.75
1:a:417:TYR:CE1	1:a:450:PHE:HE1	2.01	0.75
2:m:17:ARG:HH22	5:g:33:LYS:HB2	1.50	0.75
4:f:132:GLU:OE2	4:f:132:GLU:O	2.04	0.75
12:q:9:ILE:HG12	14:u:90:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:o:707:ILE:HG23	21:o:720:PRO:HA	1.69	0.75
68:w:357:HIS:CE1	68:w:397:LYS:CE	2.65	0.75
6:h:40:LEU:HD12	6:h:45:VAL:CG1	2.16	0.75
6:h:42:TRP:O	6:h:45:VAL:HG22	1.87	0.75
9:j:53:LYS:HE3	11:n:60:HIS:CA	2.13	0.75
11:n:222:VAL:HG22	11:n:234:LEU:O	1.86	0.75
14:u:85:LEU:HD12	16:z:552:LEU:HD23	0.77	0.75
41:DH:92:ASP:O	41:DH:95:VAL:HG12	1.86	0.75
53:X:1:DA:C2	54:Y:0:DG:N1	2.53	0.75
6:h:67:LYS:HD3	23:0:141:THR:HG21	1.42	0.75
6:h:102:HIS:CD2	6:h:102:HIS:H	2.03	0.75
6:h:144:ASN:HA	15:v:41:LYS:HG3	1.69	0.75
11:n:127:ILE:C	14:u:27:GLN:NE2	2.44	0.75
2:m:116:GLN:CD	16:z:595:PRO:CD	2.59	0.75
6:h:41:THR:HB	6:h:44:SER:OG	1.86	0.75
11:n:278:VAL:HG12	11:n:295:CYS:SG	2.26	0.75
11:n:529:PRO:HG2	68:w:35:THR:HB	1.68	0.75
37:DD:890:GLY:C	44:DL:104:ARG:NH2	2.44	0.75
9:j:96:LYS:HE3	13:s:80:SER:HA	1.68	0.75
11:n:229:GLU:HG3	11:n:300:CYS:SG	2.25	0.75
6:h:33:LEU:HD23	6:h:40:LEU:CD2	2.16	0.75
6:h:72:ARG:NH1	12:q:134:ALA:N	2.33	0.75
10:k:21:ILE:HG21	12:q:168:THR:HG1	1.49	0.75
12:q:92:LEU:CD1	12:q:99:ARG:HH22	1.92	0.75
10:k:24:ILE:HG22	12:q:164:ALA:HB2	1.36	0.74
11:n:359:ILE:HA	11:n:372:ILE:HD12	1.68	0.74
12:q:152:SER:HB2	15:v:58:ASN:HA	1.68	0.74
2:m:30:ASN:CA	3:d:176:TYR:HB3	2.01	0.74
11:n:229:GLU:CG	11:n:300:CYS:SG	2.75	0.74
7:r:140:ILE:HD12	7:r:182:VAL:HG11	1.66	0.74
11:n:545:LEU:CD1	11:n:653:PRO:CG	2.51	0.74
12:q:633:ARG:HB3	12:q:633:ARG:NH2	2.02	0.74
21:o:762:GLN:CA	68:w:74:LYS:HZ1	1.97	0.74
1:a:77:MET:HE3	1:a:77:MET:HA	1.69	0.74
5:g:93:LEU:CD1	9:j:106:LYS:CE	2.59	0.74
12:q:596:PHE:CZ	20:l:117:TYR:OH	2.11	0.74
12:q:645:ALA:HB2	18:e:100:LEU:HD21	1.69	0.74
29:4:159:VAL:HG22	29:4:175:LEU:HD21	1.67	0.74
69:x:955:LEU:CD1	69:x:967:VAL:HG21	2.17	0.74
5:g:136:ARG:CB	14:u:86:GLN:HE22	2.01	0.74
7:r:84:HIS:NE2	12:q:398:ALA:HA	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:79:HIS:ND1	15:v:91:PHE:CE1	2.56	0.74
10:k:87:ARG:HG3	10:k:87:ARG:NH1	2.01	0.74
10:k:101:ARG:HB3	10:k:101:ARG:NH1	2.02	0.74
11:n:587:LEU:HB3	68:w:15:THR:HG21	1.69	0.74
14:u:105:GLU:C	14:u:108:VAL:HG12	2.13	0.74
15:v:133:GLU:OE2	18:e:125:LYS:CE	2.22	0.74
24:8:214:PRO:CG	55:PA:1674:THR:HG21	2.18	0.74
53:X:-2:DC:C2'	53:X:-1:DT:C7	2.65	0.74
2:m:66:TYR:CZ	5:g:38:ILE:HG23	2.21	0.74
3:d:131:LYS:HB3	14:u:104:LEU:CD1	2.12	0.74
23:0:78:VAL:HA	23:0:82:TYR:HB2	1.67	0.74
3:d:121:LEU:CD1	5:g:160:VAL:HG22	2.06	0.74
15:v:119:LEU:HD21	18:e:139:TRP:CB	2.16	0.74
17:c:111:TYR:CZ	19:b:136:HIS:CB	2.70	0.74
6:h:22:LEU:HD12	6:h:22:LEU:C	2.13	0.74
9:j:19:ILE:CG2	9:j:45:VAL:CG2	2.54	0.74
10:k:24:ILE:HG21	12:q:164:ALA:CA	2.16	0.74
12:q:437:HIS:CE1	12:q:472:GLU:CA	2.71	0.74
21:o:787:ALA:CB	69:x:21:TYR:OH	2.36	0.74
68:w:101:LEU:HD11	68:w:121:LEU:HD23	1.70	0.74
2:m:116:GLN:HG3	16:z:594:LEU:CG	2.11	0.74
3:d:117:ALA:HB2	5:g:163:MET:CG	2.17	0.74
11:n:170:PRO:HB3	12:q:22:VAL:HG23	1.70	0.74
11:n:937:ARG:NE	11:n:943:LEU:HD21	2.03	0.74
1:a:417:TYR:HE1	1:a:450:PHE:CE1	1.88	0.74
21:o:696:SER:CB	69:x:111:HIS:CE1	2.64	0.74
21:o:761:LEU:O	68:w:74:LYS:CD	2.35	0.74
3:d:131:LYS:HE2	14:u:104:LEU:HD22	0.74	0.73
5:g:95:ILE:HD13	13:s:72:PRO:HB3	1.68	0.73
17:c:111:TYR:CG	19:b:136:HIS:HD2	2.05	0.73
6:h:83:PRO:CG	55:PA:1790:TYR:CZ	2.69	0.73
15:v:126:ASP:CG	18:e:132:HIS:HD2	1.96	0.73
54:Y:-21:DC:H1'	54:Y:-20:DT:H5'	1.68	0.73
11:n:156:TYR:HE1	11:n:168:ARG:HG2	0.96	0.73
11:n:278:VAL:CG1	11:n:281:ARG:HH21	1.73	0.73
19:b:174:ILE:CG1	20:l:75:LEU:HD11	2.14	0.73
9:j:77:PRO:CD	9:j:78:GLN:H	1.99	0.73
11:n:659:LEU:HD12	68:w:14:LYS:HG2	1.66	0.73
21:o:696:SER:OG	69:x:111:HIS:ND1	2.20	0.73
37:Dd:1056:THR:HB	44:Dl:74:GLU:HA	1.69	0.73
5:g:96:LEU:CB	9:j:102:MET:HE1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:146:ARG:NH1	14:u:97:ASN:CG	2.46	0.73
8:t:129:VAL:HG21	8:t:200:ILE:HD12	1.69	0.73
11:n:587:LEU:CG	68:w:15:THR:HG21	2.18	0.73
13:s:84:ILE:HG22	13:s:90:GLU:HG2	1.68	0.73
15:v:50:ARG:O	15:v:51:ALA:C	2.31	0.73
36:DB:280:THR:CG2	36:DB:342:THR:CG2	2.66	0.73
1:a:229:SER:HB3	1:a:502:MET:HB2	1.69	0.73
3:d:155:ILE:HD12	3:d:158:SER:HB3	1.71	0.73
4:f:95:LEU:O	12:q:130:VAL:CG1	2.36	0.73
11:n:172:CYS:SG	12:q:21:GLU:CB	2.77	0.73
17:c:111:TYR:OH	19:b:136:HIS:HB2	1.88	0.73
32:7:8:LEU:HD11	32:7:61:ARG:HD3	1.71	0.73
5:g:75:LYS:HD2	14:u:77:PRO:HA	1.70	0.73
2:m:66:TYR:HE2	5:g:38:ILE:HG23	1.50	0.73
5:g:88:ASN:HD21	13:s:69:ARG:HD3	1.53	0.73
11:n:482:VAL:HG22	11:n:489:ILE:HG12	1.69	0.73
44:Dl:87:ILE:C	44:Dl:91:PHE:CD2	2.67	0.73
1:a:337:ALA:HB1	1:a:338:PRO:HD2	1.70	0.73
2:m:70:PRO:CB	11:n:166:TYR:OH	2.30	0.73
5:g:168:LEU:O	5:g:172:PRO:HD2	1.89	0.73
17:c:135:ARG:NH2	18:e:92:GLU:OE1	2.21	0.73
53:X:-13:DG:H1	54:Y:13:DC:H42	1.37	0.73
58:PD:51:ALA:CB	58:PD:54:GLU:CG	2.63	0.73
3:d:113:GLN:HG3	5:g:163:MET:SD	2.29	0.73
3:d:131:LYS:HE2	14:u:104:LEU:HD21	1.65	0.73
8:t:154:TRP:HB2	8:t:176:PHE:CD2	2.22	0.73
11:n:134:ASP:OD2	14:u:24:GLY:HA2	1.89	0.73
12:q:595:GLN:HG2	12:q:619:ARG:HB2	1.70	0.73
23:0:9:CYS:SG	23:0:34:CYS:CB	2.77	0.73
55:PA:886:VAL:HG21	59:PE:165:LEU:HD22	1.71	0.73
58:PD:32:LEU:HD12	58:PD:37:VAL:HG22	1.70	0.73
4:f:101:ILE:HD11	6:h:105:VAL:HG11	1.70	0.72
5:g:93:LEU:C	9:j:106:LYS:NZ	2.42	0.72
9:j:43:PHE:CZ	13:s:151:GLY:CA	2.71	0.72
9:j:52:ASP:OD1	9:j:53:LYS:N	2.22	0.72
11:n:686:LYS:HZ3	21:o:730:PRO:CB	1.98	0.72
11:n:707:ASP:HB2	21:o:684:ARG:NH2	2.04	0.72
55:PA:805:ARG:NH2	55:PA:808:PRO:HA	2.04	0.72
55:PA:1242:ASP:HA	55:PA:1262:MET:HB2	1.71	0.72
38:De:563:GLU:HA	38:De:587:PRO:HB3	1.71	0.72
53:X:-37:DG:H2'	53:X:-37:DG:OP2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:139:MET:HB3	14:u:93:LEU:HD13	1.69	0.72
44:DL:106:ARG:NH2	44:DL:115:ASP:HA	2.04	0.72
1:a:417:TYR:CZ	1:a:450:PHE:CD1	2.77	0.72
2:m:15:ARG:HA	5:g:39:LYS:HZ3	1.53	0.72
2:m:112:ARG:HH12	16:z:600:ASP:H	1.34	0.72
10:k:17:ILE:HG23	12:q:171:VAL:CG2	2.06	0.72
11:n:458:LEU:HD12	12:q:325:ILE:HG23	1.71	0.72
53:X:29:DG:C6	54:Y:-29:DC:N4	2.49	0.72
1:a:382:LEU:C	69:x:92:LEU:CD1	2.62	0.72
26:1:277:LEU:C	26:1:279:GLU:H	1.96	0.72
37:Dd:844:ASN:O	37:Dd:847:GLU:CG	2.37	0.72
55:PA:363:ALA:HB1	55:PA:384:ILE:HD13	1.72	0.72
68:w:9:PHE:CE2	68:w:66:PHE:CD2	2.72	0.72
4:f:134:MET:SD	4:f:134:MET:C	2.73	0.72
5:g:96:LEU:HB3	9:j:102:MET:HE1	1.71	0.72
5:g:131:ALA:HB2	11:n:152:PHE:HE2	1.54	0.72
9:j:92:ASN:HD22	13:s:83:LEU:CG	2.02	0.72
9:j:96:LYS:CG	13:s:80:SER:HA	2.18	0.72
11:n:587:LEU:CD1	68:w:15:THR:HG22	2.17	0.72
23:0:196:LEU:CD1	23:0:200:GLN:OE1	2.36	0.72
7:r:42:LEU:HD22	10:k:77:GLN:CB	2.18	0.72
8:t:6:VAL:HG22	8:t:141:GLU:HB2	1.71	0.72
12:q:109:MET:CA	12:q:109:MET:HE3	2.19	0.72
15:v:84:GLN:HE22	15:v:85:PHE:HB3	1.53	0.72
48:DO:28:ILE:HB	48:DO:32:LEU:HD23	1.71	0.72
10:k:24:ILE:CG2	12:q:164:ALA:HB1	2.11	0.72
26:1:286:VAL:O	26:1:287:PRO:C	2.33	0.72
36:DB:119:PRO:CB	36:DB:194:ASP:O	2.37	0.72
37:Dd:843:VAL:HG13	37:Dd:844:ASN:H	1.55	0.72
2:m:124:GLN:OE1	16:z:590:ARG:HB2	1.87	0.72
12:q:428:LEU:HD12	12:q:428:LEU:O	1.89	0.72
16:z:548:THR:HB	16:z:551:ASP:OD1	1.90	0.72
54:Y:8:DA:H2'	54:Y:9:DC:H5	1.51	0.72
1:a:439:GLN:NE2	69:x:15:LYS:HD2	2.05	0.72
6:h:19:VAL:HG21	12:q:112:LEU:CD2	2.20	0.72
7:r:62:GLY:C	8:t:101:PHE:HE2	1.98	0.72
16:z:543:LEU:C	16:z:545:ARG:N	2.45	0.72
44:DL:106:ARG:NH1	44:DL:115:ASP:CG	2.47	0.72
55:PA:201:GLU:HB2	55:PA:213:LYS:HG3	1.71	0.72
3:d:113:GLN:CD	5:g:163:MET:SD	2.72	0.71
4:f:95:LEU:C	12:q:130:VAL:HG11	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:83:MET:O	5:g:83:MET:HE3	1.89	0.71
6:h:29:PHE:CD2	12:q:102:LEU:CD1	2.72	0.71
6:h:72:ARG:HH12	12:q:134:ALA:N	1.86	0.71
11:n:159:ASP:CG	11:n:167:PRO:HD3	2.14	0.71
42:DI:53:ASP:OD1	44:DL:122:ARG:NH2	2.22	0.71
53:X:-33:DG:N2	54:Y:34:DG:C2	2.58	0.71
7:r:47:GLU:H	7:r:47:GLU:CD	1.98	0.71
12:q:106:LEU:HD23	12:q:106:LEU:C	2.15	0.71
14:u:117:LYS:HZ3	22:i:140:MET:HG3	1.55	0.71
17:c:111:TYR:CZ	19:b:136:HIS:HB2	2.25	0.71
36:DB:414:LEU:HD21	36:DB:452:LYS:HD3	1.71	0.71
54:Y:-17:DA:H1'	54:Y:-16:DG:H5'	1.71	0.71
1:a:160:LEU:CD1	1:a:214:ARG:HH21	2.03	0.71
2:m:18:PHE:HB2	5:g:36:PRO:HB2	1.71	0.71
10:k:84:TYR:OH	12:q:206:ASP:O	2.08	0.71
11:n:127:ILE:HA	14:u:27:GLN:HE21	1.55	0.71
11:n:278:VAL:CG1	11:n:295:CYS:SG	2.78	0.71
68:w:394:PRO:CA	70:p:171:PHE:HZ	1.81	0.71
1:a:388:LEU:HD21	1:a:447:GLU:HG3	1.72	0.71
2:m:30:ASN:ND2	3:d:176:TYR:CE1	2.59	0.71
4:f:32:TYR:CE1	4:f:35:GLU:OE2	2.43	0.71
7:r:150:ARG:HG3	7:r:161:GLU:HB2	1.71	0.71
16:z:567:GLN:O	16:z:567:GLN:NE2	2.22	0.71
53:X:7:DG:C2	54:Y:-6:DG:N2	2.58	0.71
55:PA:1790:TYR:CD2	55:PA:1791:SER:N	2.58	0.71
6:h:146:MET:HB2	10:k:39:LYS:HZ2	1.54	0.71
9:j:7:HIS:O	9:j:11:HIS:CD2	2.43	0.71
11:n:658:ARG:HH22	68:w:21:ALA:HA	1.54	0.71
15:v:120:ARG:HG2	15:v:120:ARG:HH11	1.55	0.71
15:v:120:ARG:HG2	15:v:120:ARG:NH1	2.05	0.71
68:w:510:PRO:HD3	68:w:922:MET:HE1	1.71	0.71
4:f:139:TYR:HB2	6:h:43:PRO:HG2	1.72	0.71
5:g:13:PRO:HA	55:PA:1660:THR:CA	2.18	0.71
5:g:146:ARG:NH1	14:u:97:ASN:CB	2.54	0.71
7:r:42:LEU:HD11	10:k:75:THR:HG21	1.71	0.71
23:0:11:THR:CB	23:0:34:CYS:SG	2.79	0.71
37:Dd:845:LEU:HD23	37:Dd:845:LEU:H	1.55	0.71
68:w:6:GLN:HA	68:w:62:TRP:HH2	1.55	0.71
5:g:93:LEU:CD2	9:j:106:LYS:NZ	2.54	0.71
7:r:70:LEU:HD12	7:r:123:PHE:CE2	2.26	0.71
8:t:175:VAL:HG21	8:t:188:ASP:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:109:TYR:CZ	1:a:154:LEU:CD2	2.73	0.71
2:m:116:GLN:HB3	16:z:594:LEU:HD23	1.72	0.71
3:d:131:LYS:CG	14:u:104:LEU:CD1	2.64	0.71
5:g:31:ALA:H	5:g:32:PRO:HD2	1.56	0.71
7:r:24:GLN:HG2	7:r:170:GLU:HG2	1.73	0.71
9:j:53:LYS:CE	11:n:60:HIS:CA	2.68	0.71
14:u:84:ALA:HB2	16:z:540:LEU:HG	1.72	0.71
15:v:119:LEU:HD21	18:e:139:TRP:HB3	1.70	0.71
38:De:225:ILE:HD12	38:De:236:LEU:HB3	1.72	0.71
2:m:124:GLN:NE2	16:z:582:LEU:N	2.37	0.71
6:h:42:TRP:HB2	6:h:43:PRO:CD	2.20	0.71
9:j:76:ASN:CB	9:j:77:PRO:HD3	2.16	0.71
23:0:64:GLU:OE1	23:0:64:GLU:HA	1.91	0.71
1:a:441:GLU:HB3	69:x:14:TRP:CZ2	2.25	0.71
5:g:34:PRO:HB2	5:g:35:PRO:HD2	1.73	0.71
6:h:32:LYS:HZ3	6:h:40:LEU:HD11	1.53	0.71
9:j:53:LYS:NZ	11:n:61:ARG:H	1.65	0.71
38:DE:647:ALA:HA	38:DE:671:PRO:HB3	1.72	0.71
65:PK:22:ASN:HB2	65:PK:32:LEU:HB3	1.72	0.71
1:a:214:ARG:CZ	1:a:214:ARG:HB2	2.21	0.70
7:r:23:LEU:HD21	7:r:99:HIS:O	1.91	0.70
5:g:146:ARG:NH1	14:u:97:ASN:HB3	2.05	0.70
9:j:65:LEU:HB3	9:j:67:VAL:HG23	1.73	0.70
9:j:89:LEU:HD21	13:s:93:TYR:CE1	2.17	0.70
11:n:686:LYS:HZ2	21:o:730:PRO:HB3	1.55	0.70
12:q:194:TRP:CZ2	12:q:295:LEU:HB3	2.27	0.70
12:q:630:MET:HE3	12:q:631:GLU:H	1.55	0.70
18:e:95:PHE:CE1	20:l:37:GLY:HA3	2.26	0.70
38:De:495:ARG:HB3	38:De:536:LEU:HD11	1.73	0.70
53:X:1:DA:C2	54:Y:0:DG:C2	2.78	0.70
55:PA:1143:LEU:HB2	55:PA:1148:ALA:HB2	1.73	0.70
4:f:188:PHE:CB	11:n:281:ARG:HD2	2.08	0.70
6:h:41:THR:O	6:h:45:VAL:HG22	1.89	0.70
11:n:158:ILE:HD13	12:q:11:ILE:CG2	2.07	0.70
12:q:288:SER:CB	12:q:289:PRO:HD2	2.20	0.70
36:DB:605:PRO:HA	36:DB:611:GLU:HB3	1.73	0.70
2:m:59:LYS:HZ3	2:m:77:GLU:CD	1.97	0.70
11:n:172:CYS:HG	12:q:20:HIS:C	1.96	0.70
21:o:715:LEU:HD12	69:x:21:TYR:HB2	1.67	0.70
36:DB:806:VAL:CG2	36:DB:829:ILE:CD1	2.69	0.70
1:a:462:LEU:HD12	69:x:52:ILE:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:40:LEU:O	6:h:41:THR:C	2.34	0.70
12:q:9:ILE:CG1	14:u:90:LEU:CD2	2.68	0.70
37:DD:1085:LYS:NZ	44:DL:83:MET:SD	2.55	0.70
54:Y:-16:DG:H2"	54:Y:-15:DT:H5"	1.71	0.70
3:d:113:GLN:CD	5:g:163:MET:CE	2.63	0.70
6:h:147:CYS:HB3	15:v:41:LYS:HB2	1.70	0.70
9:j:41:LEU:O	9:j:45:VAL:HG23	1.92	0.70
51:BA:125:ALA:CB	51:BA:132:ARG:HB2	2.21	0.70
68:w:397:LYS:CB	70:p:171:PHE:HE2	2.05	0.70
1:a:60:SER:CB	1:a:148:ASP:CB	2.70	0.70
5:g:97:ILE:CB	9:j:103:LYS:HE2	2.20	0.70
6:h:12:LEU:C	6:h:12:LEU:HD13	2.17	0.70
7:r:70:LEU:HD12	7:r:123:PHE:CZ	2.27	0.70
12:q:437:HIS:CE1	12:q:472:GLU:C	2.69	0.70
12:q:644:SER:HB3	18:e:96:LEU:HB3	1.73	0.70
44:Dl:101:GLN:O	44:Dl:105:HIS:CD2	2.45	0.70
2:m:120:ALA:C	16:z:592:ASN:HD22	1.84	0.70
9:j:34:GLN:HB2	9:j:37:LEU:HD12	1.74	0.70
11:n:359:ILE:HA	11:n:372:ILE:CD1	2.21	0.70
3:d:120:ILE:HG23	5:g:156:HIS:CE1	2.27	0.70
3:d:121:LEU:HD11	5:g:160:VAL:HG23	1.60	0.70
9:j:53:LYS:NZ	11:n:60:HIS:CA	2.54	0.70
12:q:212:ALA:O	12:q:383:HIS:HB3	1.91	0.70
1:a:60:SER:CB	1:a:148:ASP:HB2	2.22	0.69
2:m:71:GLN:OE1	3:d:175:PRO:CB	2.39	0.69
7:r:35:LEU:HD13	7:r:35:LEU:C	2.17	0.69
11:n:234:LEU:HD21	11:n:282:LEU:HD22	1.72	0.69
18:e:60:VAL:CB	19:b:179:LEU:CD1	2.62	0.69
36:DB:329:LEU:O	36:DB:331:HIS:CD2	2.45	0.69
68:w:164:ARG:HH21	68:w:204:LEU:HB2	1.57	0.69
1:a:145:LYS:HA	1:a:145:LYS:HE3	1.74	0.69
9:j:110:ILE:HG21	9:j:128:ARG:NH2	2.07	0.69
15:v:67:ASN:CG	58:PD:142:TYR:O	2.35	0.69
42:DI:73:LEU:CD2	44:DL:105:HIS:CD2	2.76	0.69
10:k:79:HIS:HD2	12:q:195:LYS:CD	2.01	0.69
9:j:116:VAL:HG13	14:u:67:LYS:NZ	2.06	0.69
11:n:815:THR:HG21	11:n:841:ASN:HB3	1.75	0.69
11:n:937:ARG:HE	11:n:943:LEU:HD21	1.57	0.69
44:DL:76:LEU:HD11	44:DL:84:LEU:CD1	2.19	0.69
10:k:16:ASP:OD2	15:v:79:VAL:HG22	1.93	0.69
12:q:109:MET:HE3	12:q:109:MET:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:633:ARG:HG2	12:q:637:TYR:HD2	1.57	0.69
29:4:152:ALA:HB1	29:4:286:LEU:HG	1.74	0.69
32:7:38:GLY:HA2	32:7:475:PRO:HB3	1.73	0.69
36:DB:72:ILE:CG2	36:DB:148:ILE:HG22	2.18	0.69
36:DB:608:ASN:ND2	36:DB:657:ARG:CD	2.56	0.69
55:PA:526:VAL:HA	55:PA:533:PRO:HA	1.75	0.69
1:a:229:SER:HB3	1:a:502:MET:CB	2.23	0.69
5:g:164:ILE:HD13	22:i:141:PHE:HD2	1.48	0.69
6:h:8:LEU:C	6:h:8:LEU:HD23	2.18	0.69
6:h:16:LEU:CD2	12:q:116:LEU:HB3	2.22	0.69
6:h:19:VAL:HG21	12:q:112:LEU:HD23	1.73	0.69
6:h:67:LYS:HE2	23:0:141:THR:HG23	1.72	0.69
14:u:117:LYS:HE2	22:i:140:MET:HG3	1.71	0.69
53:X:-11:DG:H1	54:Y:11:DC:H42	1.40	0.69
59:PE:26:TYR:HA	59:PE:64:HIS:HA	1.74	0.69
1:a:259:ILE:HD12	1:a:259:ILE:H	1.56	0.69
2:m:108:TYR:CZ	11:n:168:ARG:NH1	2.60	0.69
4:f:134:MET:SD	4:f:134:MET:O	2.50	0.69
4:f:177:VAL:HG12	11:n:270:GLN:HB3	1.73	0.69
9:j:102:MET:HA	14:u:26:LEU:CD2	2.23	0.69
10:k:114:MET:HE2	18:e:129:VAL:HG21	1.75	0.69
11:n:254:VAL:HG11	11:n:304:GLN:HG2	1.74	0.69
11:n:861:LYS:CE	17:c:30:ARG:HE	2.01	0.69
23:0:31:CYS:SG	23:0:34:CYS:SG	2.90	0.69
36:DB:224:VAL:HG22	36:DB:235:HIS:HE1	1.57	0.69
38:DE:653:LEU:HB2	38:DE:663:ARG:HB2	1.75	0.69
44:DL:106:ARG:CD	44:DL:115:ASP:OD1	2.40	0.69
53:X:19:DG:N2	54:Y:-18:DG:C2	2.60	0.69
57:PC:75:SER:HB3	57:PC:79:VAL:HG23	1.74	0.69
1:a:60:SER:HB2	1:a:148:ASP:HB2	1.75	0.69
6:h:77:ILE:C	12:q:126:THR:OG1	2.21	0.69
28:3:271:CYS:HB3	28:3:285:CYS:HB3	1.75	0.69
36:DB:290:PHE:CE2	36:DB:381:TRP:CB	2.74	0.69
44:DL:106:ARG:NH1	44:DL:114:LYS:CD	2.56	0.69
1:a:131:ASN:ND2	1:a:131:ASN:H	1.90	0.69
3:d:128:ALA:CB	14:u:108:VAL:CB	2.39	0.69
4:f:77:ILE:CG2	55:PA:1792:PRO:CG	2.66	0.69
12:q:35:SER:HB3	12:q:42:ARG:HH22	1.58	0.69
12:q:109:MET:HA	12:q:109:MET:CE	2.23	0.69
13:s:92:ALA:C	13:s:96:PHE:CD2	2.71	0.69
17:c:111:TYR:CE2	19:b:136:HIS:CD2	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:PA:853:LYS:HB2	55:PA:1104:LEU:HB2	1.73	0.69
2:m:66:TYR:OH	5:g:38:ILE:HG23	1.91	0.68
6:h:74:GLN:NE2	12:q:129:PRO:CB	2.54	0.68
8:t:10:PRO:HB2	8:t:12:ALA:HB2	1.75	0.68
9:j:9:GLU:CD	9:j:56:GLN:HG2	2.18	0.68
9:j:11:HIS:HB3	9:j:15:PHE:HE2	1.58	0.68
11:n:156:TYR:OH	11:n:168:ARG:CG	2.41	0.68
12:q:1:MET:HE3	16:z:541:PRO:CB	2.22	0.68
15:v:50:ARG:HD2	15:v:51:ALA:H	1.58	0.68
15:v:123:ILE:HG22	20:l:167:ILE:HD11	1.75	0.68
18:e:95:PHE:CB	20:l:38:GLN:HG2	2.22	0.68
33:EA:114:ILE:HG12	33:EA:181:ASN:HB3	1.74	0.68
48:DO:76:LEU:HB3	48:DO:79:VAL:HG21	1.74	0.68
1:a:364:TYR:CB	1:a:430:LEU:CG	2.65	0.68
1:a:367:LEU:HD13	1:a:509:ARG:NH1	2.08	0.68
1:a:514:LYS:HB3	1:a:514:LYS:HZ3	1.56	0.68
3:d:120:ILE:CG2	5:g:156:HIS:ND1	2.56	0.68
11:n:159:ASP:OD1	11:n:163:THR:HG23	1.93	0.68
1:a:223:LYS:HZ1	1:a:251:LEU:C	2.01	0.68
11:n:247:LEU:HD23	11:n:278:VAL:CG2	2.20	0.68
11:n:937:ARG:HE	11:n:943:LEU:CD2	2.07	0.68
15:v:130:LEU:N	15:v:130:LEU:HD23	2.08	0.68
35:DA:704:TYR:HB2	35:DA:739:LEU:HD12	1.74	0.68
68:w:9:PHE:CE2	68:w:66:PHE:HD2	2.11	0.68
6:h:33:LEU:HD21	12:q:95:TRP:HZ3	1.59	0.68
9:j:53:LYS:CE	11:n:57:PHE:CA	2.68	0.68
9:j:112:GLU:O	9:j:116:VAL:HG23	1.92	0.68
15:v:82:LEU:O	15:v:86:LEU:HD23	1.93	0.68
37:Dd:889:HIS:HB3	44:Dl:104:ARG:HD2	1.76	0.68
49:DP:300:ILE:HG23	49:DP:315:ALA:HB2	1.73	0.68
1:a:109:TYR:OH	1:a:154:LEU:CD2	2.40	0.68
1:a:364:TYR:HB3	1:a:430:LEU:HD11	1.71	0.68
6:h:146:MET:HB2	10:k:39:LYS:NZ	2.09	0.68
12:q:441:ARG:NH1	20:l:168:TRP:CZ3	2.59	0.68
12:q:633:ARG:HG2	12:q:637:TYR:CD2	2.28	0.68
17:c:111:TYR:OH	19:b:136:HIS:CB	2.41	0.68
36:DB:313:TYR:CE1	36:DB:964:ASP:OD1	2.46	0.68
37:Dd:878:LEU:HD13	44:Dl:57:VAL:HG11	1.75	0.68
53:X:-9:DG:N2	54:Y:9:DC:C2	2.57	0.68
54:Y:7:DA:H2"	54:Y:8:DA:C8	2.28	0.68
12:q:428:LEU:HD12	12:q:428:LEU:C	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DH:65:LEU:HD11	43:DJ:159:ALA:HB1	1.76	0.68
44:DL:106:ARG:NH2	44:DL:115:ASP:N	2.40	0.68
68:w:6:GLN:CA	68:w:62:TRP:CH2	2.73	0.68
68:w:397:LYS:HB3	70:p:171:PHE:HE2	1.57	0.68
4:f:95:LEU:C	12:q:130:VAL:CG1	2.67	0.68
9:j:53:LYS:HD3	11:n:57:PHE:HA	1.73	0.68
31:6:375:LYS:HD3	31:6:391:ARG:HD3	1.75	0.68
39:DF:110:LYS:HE3	43:DJ:217:PHE:HB2	1.74	0.68
46:Dk:191:VAL:HG21	44:Dl:129:PRO:HG2	1.75	0.68
51:BA:245:VAL:HB	51:BA:248:ARG:HG3	1.76	0.68
5:g:146:ARG:NH1	14:u:97:ASN:ND2	2.42	0.68
6:h:166:LEU:CD2	61:PG:125:PRO:O	2.42	0.68
8:t:8:GLN:HA	8:t:138:ILE:O	1.94	0.68
15:v:134:TYR:HB2	20:l:156:LEU:HD22	1.75	0.68
36:DB:218:GLY:HA2	36:DB:238:LEU:HD13	1.74	0.68
37:Dd:885:ILE:CG2	44:Dl:96:VAL:HG12	2.23	0.68
2:m:66:TYR:OH	5:g:40:ASP:OD1	2.11	0.68
10:k:78:PRO:O	10:k:79:HIS:CE1	2.47	0.68
12:q:482:GLN:CB	12:q:634:ASN:HD22	2.06	0.68
61:PG:30:LEU:HD21	61:PG:51:ILE:HG21	1.76	0.68
2:m:17:ARG:NH2	5:g:33:LYS:HB2	2.09	0.67
2:m:124:GLN:CD	16:z:590:ARG:HB3	2.17	0.67
4:f:174:ARG:HD3	11:n:267:HIS:HD2	1.58	0.67
7:r:117:PHE:CE1	8:t:79:PHE:CD2	2.80	0.67
8:t:130:THR:HA	8:t:135:ALA:HA	1.76	0.67
9:j:34:GLN:HB2	9:j:37:LEU:CD1	2.23	0.67
11:n:254:VAL:HG11	11:n:304:GLN:CG	2.25	0.67
3:d:131:LYS:HZ3	14:u:104:LEU:CB	2.06	0.67
4:f:180:LEU:CG	11:n:299:PHE:CE1	2.63	0.67
8:t:173:PRO:HD2	8:t:176:PHE:CD2	2.30	0.67
12:q:28:GLU:HA	12:q:28:GLU:OE2	1.94	0.67
12:q:31:LEU:N	12:q:32:PRO:HD2	2.10	0.67
15:v:131:GLU:OE2	20:l:164:ARG:NH2	2.26	0.67
19:b:65:PRO:HA	19:b:68:LYS:HE2	1.76	0.67
4:f:181:LEU:HD12	11:n:270:GLN:CD	2.18	0.67
26:1:216:THR:H	26:1:219:GLU:HB3	1.59	0.67
53:X:26:DG:H2"	53:X:27:DC:H5'	1.77	0.67
69:x:955:LEU:HD22	69:x:967:VAL:HG21	0.68	0.67
10:k:73:VAL:HG23	15:v:92:PRO:CD	2.23	0.67
12:q:578:TYR:CD1	12:q:646:LEU:HD12	2.29	0.67
17:c:113:TRP:HH2	19:b:175:HIS:HB2	1.48	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:183:PRO:HD2	17:c:189:MET:HE2	1.75	0.67
48:DO:22:LEU:HD11	50:DQ:42:LEU:HB2	1.75	0.67
9:j:9:GLU:HG3	9:j:56:GLN:CG	2.24	0.67
9:j:75:ARG:CG	9:j:80:TYR:CZ	2.73	0.67
21:o:765:ASP:OD1	21:o:766:LYS:N	2.27	0.67
24:8:214:PRO:CG	55:PA:1674:THR:CG2	2.73	0.67
36:DB:806:VAL:HG23	36:DB:829:ILE:HD13	1.77	0.67
55:PA:606:HIS:HB3	55:PA:609:HIS:HB2	1.76	0.67
55:PA:927:GLU:HG2	55:PA:927:GLU:O	1.95	0.67
1:a:211:LEU:HD13	1:a:222:LEU:HD23	1.75	0.67
6:h:164:GLY:O	61:PG:138:GLN:NE2	2.25	0.67
10:k:45:LEU:HD22	10:k:45:LEU:C	2.19	0.67
11:n:402:ILE:CD1	12:q:327:VAL:HA	2.24	0.67
12:q:307:ILE:HG12	12:q:379:ILE:CG1	2.15	0.67
26:1:277:LEU:O	26:1:279:GLU:N	2.28	0.67
28:3:99:GLY:HA2	29:4:129:TRP:HB2	1.76	0.67
33:EA:117:ASP:HB3	33:EA:177:LEU:HB3	1.75	0.67
36:DB:308:PHE:CG	36:DB:330:LEU:HD21	2.30	0.67
44:DL:106:ARG:NH2	44:DL:115:ASP:CA	2.57	0.67
2:m:67:LEU:HD13	2:m:73:LEU:HD11	1.77	0.67
7:r:45:ASN:CB	10:k:81:GLY:HA2	2.25	0.67
12:q:149:LYS:HG3	15:v:42:ILE:HG13	1.75	0.67
55:PA:1347:LEU:HD22	55:PA:1354:PRO:HA	1.77	0.67
10:k:17:ILE:HD13	12:q:171:VAL:HG22	1.75	0.67
18:e:49:GLU:CG	20:l:89:PHE:CE1	2.76	0.67
21:o:715:LEU:HD23	69:x:25:ILE:CG1	2.24	0.67
29:4:275:LYS:HB2	29:4:278:SER:HB3	1.76	0.67
41:DH:40:VAL:HG11	43:DJ:130:ILE:HG12	1.77	0.67
51:BA:169:ARG:HD3	51:BA:207:ASP:H	1.60	0.67
55:PA:1365:ILE:HG23	55:PA:1369:LEU:HD12	1.77	0.67
68:w:1291:MET:SD	68:w:1328:ARG:NH2	2.67	0.67
2:m:124:GLN:CG	16:z:581:SER:CB	2.67	0.67
4:f:177:VAL:HG11	11:n:270:GLN:CB	2.25	0.67
5:g:30:LEU:C	5:g:30:LEU:HD12	2.20	0.67
5:g:136:ARG:CB	14:u:86:GLN:NE2	2.58	0.67
8:t:94:LEU:O	8:t:98:LEU:HG	1.93	0.67
9:j:56:GLN:CB	11:n:53:THR:CA	2.70	0.67
9:j:77:PRO:CD	9:j:78:GLN:N	2.58	0.67
11:n:169:LEU:O	12:q:19:VAL:HG13	1.95	0.67
11:n:685:LEU:HD22	21:o:729:TYR:HE2	1.59	0.67
12:q:24:LEU:HD22	55:PA:1796:SER:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:u:85:LEU:HD23	16:z:539:ASP:HB3	1.77	0.67
24:8:214:PRO:HD2	24:8:224:ARG:HG2	1.77	0.67
4:f:177:VAL:CG1	11:n:270:GLN:CB	2.73	0.67
9:j:26:VAL:HG21	9:j:38:ASN:OD1	1.95	0.67
11:n:680:HIS:NE2	12:q:557:LEU:HD11	2.09	0.67
14:u:7:GLN:NE2	16:z:594:LEU:HD22	2.10	0.67
1:a:219:LEU:HD13	1:a:258:THR:HB	1.75	0.66
2:m:30:ASN:HB2	3:d:177:PRO:HD2	1.77	0.66
5:g:93:LEU:O	9:j:106:LYS:NZ	2.28	0.66
6:h:16:LEU:HD23	12:q:116:LEU:HB3	1.78	0.66
11:n:226:VAL:CG1	11:n:230:PHE:O	2.42	0.66
12:q:167:LEU:HD22	15:v:76:MET:HE2	1.75	0.66
12:q:644:SER:HB3	18:e:96:LEU:CB	2.25	0.66
33:EA:22:ILE:HA	33:EA:26:TYR:HD1	1.60	0.66
36:DB:215:VAL:HG11	36:DB:307:VAL:HG21	1.77	0.66
39:Df:55:LEU:HD13	42:Di:28:ILE:HG12	1.77	0.66
49:DP:235:ARG:HH12	50:DQ:311:GLU:HA	1.60	0.66
57:PC:262:GLN:HG3	65:PK:18:LYS:HD2	1.77	0.66
68:w:29:THR:HA	68:w:33:GLU:OE2	1.95	0.66
2:m:15:ARG:HA	5:g:39:LYS:NZ	2.10	0.66
9:j:53:LYS:HG2	11:n:57:PHE:N	2.10	0.66
12:q:457:ASP:HB2	12:q:458:PRO:HD3	1.77	0.66
24:8:177:TRP:CE3	24:8:214:PRO:CA	2.68	0.66
36:DB:948:ALA:O	36:DB:952:GLN:HG3	1.95	0.66
45:Dc:77:LEU:HD13	43:Dj:116:LEU:CD2	2.22	0.66
39:Df:381:ALA:HA	39:Df:388:ILE:HG22	1.77	0.66
56:PB:937:SER:HB3	56:PB:941:GLN:HB2	1.77	0.66
62:PH:4:ILE:HD11	62:PH:7:GLU:HB2	1.77	0.66
68:w:318:GLU:HG2	68:w:320:LYS:H	1.59	0.66
1:a:160:LEU:HD11	1:a:219:LEU:HD21	1.77	0.66
1:a:364:TYR:HB2	1:a:430:LEU:HG	1.77	0.66
6:h:166:LEU:HD23	61:PG:123:SER:HB2	1.77	0.66
7:r:116:ASP:OD1	7:r:116:ASP:N	2.29	0.66
3:d:168:VAL:H	3:d:171:ASP:HB2	1.61	0.66
4:f:44:THR:HG22	24:8:265:GLY:HA2	1.76	0.66
5:g:143:LYS:NZ	5:g:143:LYS:HB3	2.10	0.66
9:j:82:LYS:CB	13:s:96:PHE:HD1	2.01	0.66
12:q:15:CYS:SG	12:q:15:CYS:O	2.52	0.66
14:u:28:GLN:CD	16:z:483:ASN:ND2	2.54	0.66
21:o:762:GLN:CA	68:w:74:LYS:CE	2.66	0.66
38:De:542:HIS:HD2	38:De:546:VAL:CG1	2.06	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:244:PRO:CB	11:n:283:PHE:HD1	2.06	0.66
11:n:527:THR:CG2	68:w:42:GLY:HA2	2.15	0.66
11:n:686:LYS:NZ	21:o:730:PRO:HB3	2.10	0.66
36:DB:290:PHE:CZ	36:DB:381:TRP:N	2.63	0.66
10:k:21:ILE:HD12	12:q:168:THR:CA	2.26	0.66
11:n:659:LEU:HD22	68:w:17:VAL:HG21	1.65	0.66
12:q:375:LEU:CD2	12:q:431:ILE:HG13	2.24	0.66
37:Dd:845:LEU:HD23	37:Dd:845:LEU:N	2.10	0.66
42:Di:56:ILE:HG22	42:Di:60:HIS:NE2	2.10	0.66
56:PB:246:GLY:H	56:PB:249:LYS:HE2	1.60	0.66
59:PE:71:GLN:HB2	59:PE:99:ILE:HG21	1.77	0.66
69:x:485:PRO:CD	69:x:486:ALA:N	2.55	0.66
2:m:101:GLN:HA	11:n:169:LEU:HD22	1.78	0.66
7:r:137:ARG:O	7:r:137:ARG:HG3	1.93	0.66
11:n:634:MET:HE2	12:q:519:GLN:NE2	2.10	0.66
12:q:92:LEU:HD11	12:q:99:ARG:HH22	1.43	0.66
32:7:647:ARG:HB3	32:7:650:ASP:HB3	1.77	0.66
55:PA:76:GLY:HA2	55:PA:80:GLU:HG2	1.78	0.66
2:m:27:CYS:HA	3:d:177:PRO:CB	2.23	0.66
2:m:104:HIS:NE2	11:n:168:ARG:CG	2.57	0.66
5:g:31:ALA:N	5:g:32:PRO:CD	2.59	0.66
9:j:76:ASN:CB	9:j:77:PRO:CD	2.74	0.66
29:4:32:ASP:HB3	29:4:113:ILE:HD12	1.77	0.66
36:DB:313:TYR:HE1	36:DB:964:ASP:OD1	1.77	0.66
39:DF:370:TRP:HB3	39:DF:419:GLY:HA3	1.77	0.66
38:De:423:PRO:HG2	38:De:426:ARG:HB2	1.78	0.66
38:De:546:VAL:CG2	38:De:546:VAL:O	2.44	0.66
4:f:176:ARG:HG2	11:n:306:GLU:HB3	1.78	0.66
5:g:83:MET:HG3	9:j:120:ASP:OD1	1.96	0.66
7:r:153:VAL:HB	7:r:156:ASN:HB2	1.78	0.66
8:t:74:SER:HB3	12:q:409:GLY:O	1.95	0.66
8:t:78:LEU:HD12	8:t:84:CYS:HB3	1.77	0.66
11:n:593:GLU:OE2	68:w:24:GLY:HA2	1.95	0.66
55:PA:929:ALA:HA	62:PH:105:SER:HB2	1.77	0.66
3:d:131:LYS:NZ	14:u:104:LEU:HB3	2.08	0.66
4:f:137:CYS:HA	6:h:42:TRP:HB3	1.76	0.66
38:De:647:ALA:HA	38:De:671:PRO:HB3	1.78	0.66
56:PB:452:ASN:HB3	56:PB:462:ALA:HB1	1.76	0.66
1:a:336:TYR:CZ	1:a:391:THR:OG1	2.45	0.65
4:f:139:TYR:HB2	6:h:43:PRO:CG	2.25	0.65
5:g:93:LEU:HA	9:j:106:LYS:HZ1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:166:LEU:HD22	61:PG:125:PRO:O	1.96	0.65
12:q:467:ILE:HD11	17:c:203:VAL:HG11	1.78	0.65
13:s:92:ALA:C	13:s:96:PHE:HD2	2.04	0.65
15:v:126:ASP:CB	18:e:132:HIS:CD2	2.80	0.65
36:DB:920:PRO:HA	36:DB:923:ARG:HD2	1.77	0.65
38:De:557:TYR:H	38:De:571:SER:HA	1.60	0.65
53:X:-5:DG:H2"	53:X:-4:DT:H71	1.77	0.65
68:w:1183:TRP:CZ2	68:w:1185:GLY:HA3	2.32	0.65
69:x:912:LEU:HD22	69:x:958:VAL:HG21	1.77	0.65
1:a:232:LEU:C	1:a:232:LEU:HD13	2.22	0.65
2:m:68:LYS:HZ2	5:g:50:GLN:NE2	1.91	0.65
9:j:35:ALA:O	9:j:39:GLN:HG2	1.96	0.65
10:k:43:ARG:HB2	10:k:43:ARG:HH11	1.62	0.65
11:n:245:TRP:CB	11:n:282:LEU:CD1	2.57	0.65
37:DD:872:PHE:N	44:DL:92:ILE:HD12	2.11	0.65
51:BA:211:THR:HG22	51:BA:250:PRO:HB3	1.78	0.65
68:w:41:LEU:HD21	68:w:85:MET:HG3	1.76	0.65
1:a:109:TYR:CE2	1:a:154:LEU:CD2	2.80	0.65
1:a:329:LEU:O	1:a:329:LEU:HD23	1.96	0.65
12:q:644:SER:O	18:e:97:GLN:CG	2.44	0.65
29:4:430:VAL:HG11	29:4:447:GLY:HA3	1.79	0.65
29:4:434:GLU:HG2	29:4:436:SER:OG	1.97	0.65
1:a:439:GLN:NE2	69:x:15:LYS:HD3	2.09	0.65
8:t:196:LEU:O	8:t:200:ILE:HD13	1.96	0.65
11:n:937:ARG:HH21	11:n:943:LEU:HD23	1.62	0.65
12:q:162:LYS:O	12:q:166:ARG:HG2	1.96	0.65
19:b:103:ASP:OD1	19:b:103:ASP:N	2.23	0.65
29:4:55:TRP:HZ3	29:4:71:VAL:HG13	1.61	0.65
36:DB:873:LEU:O	36:DB:877:TYR:CD2	2.48	0.65
42:DI:73:LEU:HD22	44:DL:105:HIS:NE2	2.11	0.65
4:f:169:SER:O	11:n:267:HIS:NE2	2.30	0.65
6:h:74:GLN:HE21	12:q:129:PRO:HB3	1.61	0.65
18:e:60:VAL:CA	19:b:179:LEU:CD1	2.72	0.65
21:o:761:LEU:O	68:w:74:LYS:HD2	1.97	0.65
62:PH:88:PHE:HA	62:PH:146:LYS:HB3	1.78	0.65
5:g:33:LYS:HZ3	5:g:33:LYS:N	1.94	0.65
8:t:11:VAL:HA	8:t:20:THR:HG21	1.77	0.65
14:u:83:ALA:N	14:u:86:GLN:CB	2.60	0.65
15:v:131:GLU:O	15:v:135:TYR:HD2	1.79	0.65
24:8:177:TRP:CH2	55:PA:1677:SER:CA	2.80	0.65
10:k:79:HIS:HD2	12:q:195:LYS:HD3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:z:537:PRO:HB2	16:z:543:LEU:HB2	1.77	0.65
23:0:121:LYS:O	23:0:124:ILE:HG13	1.95	0.65
38:DE:634:ARG:HH21	38:DE:677:PHE:HB2	1.62	0.65
39:Df:263:ILE:HD13	39:Df:286:VAL:HG22	1.77	0.65
4:f:71:LEU:HD12	4:f:82:ARG:HE	1.61	0.65
11:n:669:GLN:NE2	21:o:681:GLU:HG3	2.11	0.65
12:q:149:LYS:HE2	15:v:40:ALA:HA	1.77	0.65
36:DB:290:PHE:CE2	36:DB:381:TRP:CA	2.79	0.65
68:w:13:VAL:HG11	68:w:75:ARG:CG	2.27	0.65
4:f:95:LEU:O	12:q:130:VAL:HG11	1.96	0.65
4:f:170:SER:HA	11:n:267:HIS:NE2	2.12	0.65
4:f:177:VAL:CG1	11:n:270:GLN:HB3	2.26	0.65
11:n:526:SER:OG	68:w:45:ARG:CZ	2.45	0.65
14:u:8:LEU:HD12	14:u:72:LEU:HD22	1.77	0.65
22:i:119:GLN:OE1	22:i:119:GLN:HA	1.95	0.65
36:DB:876:SER:O	36:DB:882:HIS:CD2	2.49	0.65
68:w:18:ILE:HA	68:w:21:ALA:HB2	1.79	0.65
2:m:105:TRP:CZ2	3:d:163:ALA:HA	2.32	0.65
5:g:94:ASP:HA	5:g:97:ILE:HG13	1.79	0.65
12:q:138:LYS:CD	12:q:140:ASN:OD1	2.40	0.65
12:q:489:LYS:O	12:q:507:ARG:NH2	2.30	0.65
34:EB:76:GLY:HA3	52:FB:188:PHE:HB3	1.79	0.65
39:DF:92:ILE:HG13	39:DF:93:PRO:HD3	1.79	0.65
44:DL:106:ARG:CZ	44:DL:114:LYS:HZ3	2.09	0.65
1:a:360:ASN:HB3	69:x:17:ARG:HH11	0.69	0.64
6:h:19:VAL:HG12	12:q:113:TYR:HB2	1.75	0.64
7:r:121:MET:HG3	7:r:121:MET:O	1.97	0.64
9:j:78:GLN:CG	9:j:82:LYS:HE3	2.24	0.64
11:n:586:LEU:HD21	68:w:11:GLU:C	2.22	0.64
36:DB:216:SER:HB3	36:DB:236:TYR:CD1	2.32	0.64
56:PB:453:TRP:HB2	56:PB:466:VAL:HG21	1.78	0.64
5:g:146:ARG:HH12	14:u:97:ASN:CB	2.09	0.64
9:j:34:GLN:HB2	9:j:37:LEU:HG	1.78	0.64
11:n:74:PRO:HA	11:n:82:LYS:CB	2.27	0.64
14:u:83:ALA:N	14:u:86:GLN:HB3	2.12	0.64
16:z:538:THR:H	16:z:542:GLY:HA3	1.62	0.64
36:DB:331:HIS:NE2	36:DB:342:THR:CB	2.58	0.64
36:DB:426:ASN:HB2	36:DB:435:ILE:HG13	1.78	0.64
36:DB:806:VAL:CG2	36:DB:829:ILE:HD13	2.26	0.64
40:DG:181:TRP:CZ2	40:DG:183:ILE:HD11	2.32	0.64
45:Dc:27:GLN:HG2	39:Df:111:GLU:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:x:482:SER:O	69:x:485:PRO:HD3	1.97	0.64
69:x:482:SER:O	69:x:485:PRO:HD2	1.95	0.64
10:k:44:LEU:HD22	10:k:47:ARG:HH22	1.62	0.64
44:DL:106:ARG:NH2	44:DL:114:LYS:C	2.48	0.64
9:j:92:ASN:ND2	13:s:83:LEU:CG	2.58	0.64
16:z:543:LEU:HG	16:z:545:ARG:HB3	1.79	0.64
23:0:258:PRO:HA	25:9:239:LYS:HZ3	1.60	0.64
27:2:69:ARG:H	27:2:69:ARG:HE	1.46	0.64
27:2:222:ILE:HG23	27:2:228:TYR:HB2	1.78	0.64
32:7:28:LEU:HD23	32:7:55:LEU:HD23	1.79	0.64
36:DB:327:THR:HB	41:DH:227:LEU:HD11	1.79	0.64
8:t:112:THR:HG22	8:t:129:VAL:HG22	1.77	0.64
10:k:111:CYS:HB3	18:e:133:LEU:HD21	1.80	0.64
11:n:156:TYR:OH	11:n:168:ARG:HG2	1.97	0.64
12:q:631:GLU:HA	12:q:631:GLU:OE2	1.97	0.64
4:f:70:LEU:HD21	4:f:73:ALA:HB2	1.79	0.64
9:j:34:GLN:OE1	9:j:37:LEU:CD1	2.44	0.64
10:k:37:LYS:HB3	12:q:150:LYS:HE3	1.79	0.64
10:k:78:PRO:O	10:k:79:HIS:CG	2.51	0.64
11:n:528:HIS:H	68:w:38:ILE:HG22	1.63	0.64
11:n:790:ILE:HG22	11:n:792:ALA:H	1.62	0.64
4:f:15:TRP:HE1	5:g:10:ALA:N	1.96	0.64
9:j:96:LYS:CE	13:s:80:SER:CA	2.73	0.64
10:k:21:ILE:HD12	12:q:168:THR:CB	2.26	0.64
18:e:45:VAL:HG13	20:l:92:LEU:HD11	1.79	0.64
40:DG:79:THR:HG23	40:DG:79:THR:O	1.98	0.64
37:Dd:845:LEU:H	37:Dd:845:LEU:CD2	2.10	0.64
55:PA:1161:LEU:HB3	55:PA:1307:VAL:HG21	1.79	0.64
1:a:220:MET:HB2	1:a:257:VAL:HG12	1.80	0.64
8:t:197:PHE:HA	8:t:200:ILE:HD11	1.80	0.64
21:o:723:LEU:HD11	21:o:734:PRO:HB2	1.78	0.64
25:9:161:HIS:HB3	25:9:209:PRO:HG3	1.80	0.64
39:DF:123:PRO:HD2	41:DH:32:ALA:HA	1.79	0.64
53:X:25:DA:N1	54:Y:-24:DC:O2	2.31	0.64
55:PA:791:GLN:HG2	55:PA:839:HIS:HA	1.79	0.64
67:FA:18:VAL:HG22	67:FA:137:ALA:HB3	1.79	0.64
1:a:424:CYS:HA	1:a:505:PRO:HG3	1.80	0.64
7:r:70:LEU:CD1	7:r:123:PHE:CE2	2.81	0.64
9:j:34:GLN:HB2	9:j:37:LEU:CG	2.27	0.64
14:u:117:LYS:NZ	22:i:140:MET:CG	2.56	0.64
21:o:765:ASP:CB	68:w:72:SER:OG	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Dk:120:ARG:HH11	47:Dm:44:GLY:HA2	1.61	0.64
55:PA:1655:PRO:O	55:PA:1656:SER:C	2.40	0.64
61:PG:147:ILE:HD11	61:PG:150:THR:HB	1.80	0.64
69:x:780:THR:HG22	69:x:816:CYS:HB3	1.80	0.64
1:a:321:LEU:HA	1:a:410:LEU:HD12	1.80	0.64
1:a:417:TYR:CD1	1:a:450:PHE:HE1	2.15	0.64
3:d:131:LYS:HD2	14:u:104:LEU:HD13	1.62	0.64
25:9:181:LEU:H	25:9:181:LEU:HD13	1.63	0.64
32:7:40:LEU:HD23	32:7:479:ALA:HB3	1.80	0.64
35:DA:480:TRP:HB2	39:Df:306:PRO:HG3	1.78	0.64
36:DB:309:ILE:HD11	36:DB:324:ILE:HG23	1.80	0.64
44:DL:76:LEU:CD1	44:DL:84:LEU:HD11	2.25	0.64
68:w:6:GLN:CB	68:w:62:TRP:HH2	2.10	0.64
1:a:382:LEU:O	69:x:92:LEU:HD22	1.97	0.63
1:a:462:LEU:CD1	69:x:49:GLN:HG2	2.26	0.63
3:d:169:PRO:CB	55:PA:1795:PRO:HG2	2.28	0.63
8:t:148:VAL:HG11	17:c:217:TYR:HB3	1.80	0.63
12:q:89:GLN:HB3	12:q:90:PRO:HD2	1.78	0.63
33:EA:127:PHE:HB3	33:EA:161:VAL:HB	1.79	0.63
42:Di:56:ILE:O	42:Di:60:HIS:CD2	2.51	0.63
55:PA:909:LEU:HD23	55:PA:966:LEU:HB3	1.79	0.63
56:PB:754:PRO:HB2	56:PB:773:PRO:HG2	1.80	0.63
69:x:143:ARG:HH22	69:x:205:ASN:HB2	1.62	0.63
1:a:364:TYR:HB2	1:a:428:THR:OG1	1.98	0.63
9:j:59:HIS:C	11:n:50:ARG:HA	2.16	0.63
10:k:17:ILE:CG2	12:q:171:VAL:HG22	2.10	0.63
11:n:679:SER:H	12:q:557:LEU:HD22	1.64	0.63
12:q:93:TRP:H	12:q:94:PRO:CD	2.12	0.63
32:7:60:GLN:HE22	32:7:70:LEU:HB2	1.63	0.63
68:w:361:ALA:HB1	70:p:250:SER:HB2	1.81	0.63
1:a:160:LEU:HD11	1:a:214:ARG:HH21	1.61	0.63
1:a:364:TYR:HB3	1:a:430:LEU:HG	1.67	0.63
5:g:83:MET:CE	9:j:120:ASP:OD1	2.46	0.63
10:k:24:ILE:HG23	12:q:164:ALA:HB2	1.59	0.63
10:k:39:LYS:HG3	10:k:39:LYS:O	1.97	0.63
12:q:34:LEU:HD23	12:q:34:LEU:H	1.64	0.63
14:u:85:LEU:HD11	16:z:551:ASP:CB	2.19	0.63
69:x:637:GLU:O	69:x:641:GLN:NE2	2.31	0.63
12:q:92:LEU:HD21	12:q:99:ARG:NE	2.14	0.63
17:c:166:ILE:HD13	17:c:190:LEU:HD21	1.80	0.63
31:6:448:ALA:HA	31:6:480:LEU:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DB:368:TRP:HB3	36:DB:449:PHE:HE1	1.62	0.63
44:Dl:102:LEU:HD13	44:Dl:118:LEU:CG	2.29	0.63
55:PA:119:VAL:HG21	55:PA:147:LEU:HB3	1.80	0.63
4:f:14:SER:O	55:PA:1660:THR:N	2.32	0.63
11:n:587:LEU:CB	68:w:15:THR:HG21	2.28	0.63
16:z:529:HIS:HA	16:z:568:ASP:HA	1.79	0.63
61:PG:18:PHE:HA	61:PG:22:LEU:HD13	1.80	0.63
3:d:169:PRO:CA	55:PA:1795:PRO:CG	2.50	0.63
5:g:10:ALA:N	55:PA:1662:PRO:HA	2.14	0.63
5:g:98:ARG:HB3	13:s:75:THR:HG23	1.80	0.63
6:h:97:VAL:HA	55:PA:1648:PRO:HA	1.79	0.63
10:k:111:CYS:SG	18:e:129:VAL:HG13	2.39	0.63
12:q:166:ARG:CZ	12:q:166:ARG:HB3	2.27	0.63
17:c:21:ILE:HD13	19:b:116:LEU:HB3	1.79	0.63
28:3:68:ARG:HD3	28:3:114:GLU:HG3	1.81	0.63
10:k:79:HIS:CD2	12:q:195:LYS:HD3	2.33	0.63
19:b:103:ASP:HB3	21:o:645:ALA:HB2	1.81	0.63
39:DF:243:LEU:HG	39:DF:288:ALA:HB2	1.80	0.63
39:Df:122:LEU:HD12	39:Df:123:PRO:HD2	1.79	0.63
42:Di:73:LEU:HD13	44:Dl:105:HIS:CE1	2.33	0.63
44:Dl:87:ILE:C	44:Dl:91:PHE:HD2	2.03	0.63
55:PA:265:VAL:HB	55:PA:271:ARG:HG2	1.79	0.63
55:PA:802:PHE:HD2	56:PB:671:GLU:HA	1.64	0.63
68:w:1184:VAL:O	68:w:1184:VAL:HG22	1.98	0.63
3:d:125:VAL:CB	14:u:112:ASP:OD1	2.34	0.63
11:n:753:LEU:HD12	17:c:283:ARG:HD2	1.80	0.63
23:0:258:PRO:HA	25:9:239:LYS:NZ	2.14	0.63
53:X:24:DG:H2"	53:X:25:DA:H5'	1.80	0.63
1:a:364:TYR:O	1:a:428:THR:HG21	1.98	0.63
2:m:116:GLN:CG	16:z:594:LEU:CG	2.66	0.63
4:f:188:PHE:HB3	11:n:281:ARG:NE	2.09	0.63
9:j:70:TYR:CD1	9:j:80:TYR:CD1	2.84	0.63
10:k:12:ARG:CD	10:k:66:GLN:NE2	2.61	0.63
11:n:154:ILE:HB	11:n:155:PRO:CD	2.29	0.63
11:n:354:VAL:HG12	11:n:355:HIS:H	1.64	0.63
14:u:77:PRO:O	14:u:79:GLU:OE1	2.17	0.63
14:u:82:THR:C	14:u:86:GLN:CB	2.71	0.63
20:l:108:PRO:HD2	20:l:109:ILE:HD12	1.81	0.63
27:2:65:VAL:HB	27:2:108:VAL:HG22	1.81	0.63
27:2:249:LEU:HD21	28:3:266:TYR:HB3	1.80	0.63
29:4:212:LEU:HD11	29:4:286:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:p:50:ASP:HA	70:p:59:THR:HG22	1.79	0.63
6:h:55:GLN:HA	58:PD:140:PHE:CE2	2.34	0.62
12:q:1:MET:HE3	16:z:541:PRO:HG2	1.81	0.62
42:DI:73:LEU:HD22	44:DL:105:HIS:CG	2.34	0.62
70:p:47:PHE:HE2	70:p:49:MET:HE2	1.64	0.62
12:q:647:SER:OG	18:e:93:CYS:SG	2.56	0.62
29:4:270:LEU:HD23	29:4:286:LEU:HB3	1.81	0.62
32:7:262:ASN:HD21	32:7:394:PHE:HA	1.64	0.62
38:DE:697:ASP:HB3	38:DE:700:HIS:HB2	1.81	0.62
1:a:382:LEU:O	69:x:92:LEU:HD21	1.97	0.62
3:d:136:GLU:OE1	5:g:146:ARG:HD3	1.98	0.62
9:j:76:ASN:H	9:j:79:LEU:HD12	1.64	0.62
10:k:13:ALA:HB2	15:v:83:LYS:HD2	1.81	0.62
12:q:93:TRP:H	12:q:94:PRO:HD2	1.63	0.62
36:DB:923:ARG:HB2	36:DB:967:LEU:HD21	1.81	0.62
53:X:20:DA:H2"	53:X:21:DG:H5'	1.81	0.62
57:PC:78:ILE:HG22	57:PC:81:LYS:HD2	1.81	0.62
4:f:15:TRP:CZ2	4:f:35:GLU:OE1	2.52	0.62
4:f:43:ARG:HB2	24:8:264:ALA:HB3	1.79	0.62
7:r:152:LEU:H	7:r:160:THR:HA	1.64	0.62
12:q:327:VAL:HG23	12:q:328:LYS:H	1.64	0.62
29:4:433:PHE:H	29:4:442:VAL:HG21	1.65	0.62
36:DB:331:HIS:CD2	36:DB:342:THR:OG1	2.52	0.62
53:X:-16:DG:OP2	53:X:-16:DG:H8	1.81	0.62
55:PA:1790:TYR:CG	55:PA:1791:SER:N	2.59	0.62
68:w:9:PHE:CB	68:w:66:PHE:HE2	1.93	0.62
4:f:188:PHE:CB	11:n:281:ARG:NE	2.61	0.62
11:n:226:VAL:CG1	11:n:230:PHE:H	2.11	0.62
12:q:93:TRP:N	12:q:94:PRO:CD	2.62	0.62
68:w:107:LEU:HD11	68:w:115:TRP:HA	1.81	0.62
1:a:62:LEU:HB3	3:d:69:LEU:HG	1.80	0.62
2:m:56:LEU:HG	2:m:80:GLN:HE22	1.65	0.62
3:d:117:ALA:HB2	5:g:163:MET:HG3	1.81	0.62
5:g:131:ALA:HB2	11:n:152:PHE:CD2	2.34	0.62
6:h:77:ILE:HG13	12:q:126:THR:HB	1.77	0.62
18:e:146:ILE:C	18:e:148:VAL:H	2.07	0.62
21:o:717:SER:HB3	69:x:66:TYR:OH	1.99	0.62
35:DA:950:VAL:HG21	35:DA:1065:GLU:HB3	1.80	0.62
44:Dl:129:PRO:HB2	47:Dm:56:ILE:HG23	1.80	0.62
54:Y:34:DG:H2"	54:Y:35:DC:H2'	1.80	0.62
55:PA:1654:SER:HB2	55:PA:1655:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:127:HIS:CE1	1:a:171:THR:HG22	2.34	0.62
4:f:180:LEU:CD2	11:n:299:PHE:CZ	2.77	0.62
6:h:144:ASN:HD21	15:v:42:ILE:HG22	1.64	0.62
9:j:43:PHE:CZ	13:s:150:ALA:C	2.70	0.62
14:u:25:VAL:HG21	14:u:58:PHE:HE2	1.62	0.62
39:Df:390:THR:HG23	39:Df:391:LEU:HD22	1.81	0.62
49:DP:169:VAL:HG21	53:X:-26:DA:C2	2.35	0.62
56:PB:502:HIS:HB3	56:PB:505:LEU:HD23	1.81	0.62
68:w:19:GLU:HA	68:w:25:MET:HG2	1.81	0.62
4:f:15:TRP:HH2	4:f:35:GLU:CD	2.06	0.62
4:f:139:TYR:CB	6:h:43:PRO:HG2	2.30	0.62
10:k:105:SER:HA	18:e:140:GLN:NE2	2.15	0.62
11:n:158:ILE:CD1	12:q:11:ILE:HD13	2.30	0.62
11:n:169:LEU:CB	11:n:170:PRO:CD	2.59	0.62
11:n:944:PHE:CE2	19:b:101:ARG:NH2	2.67	0.62
12:q:142:GLN:H	12:q:142:GLN:CD	2.08	0.62
12:q:213:GLY:HA3	12:q:386:THR:OG1	1.99	0.62
15:v:122:GLU:CG	18:e:139:TRP:HE1	2.10	0.62
55:PA:752:THR:HB	55:PA:786:ALA:HB1	1.82	0.62
16:z:543:LEU:O	16:z:544:THR:C	2.43	0.62
38:DE:423:PRO:HG2	38:DE:426:ARG:HB2	1.82	0.62
55:PA:58:MET:HG2	55:PA:258:LEU:HD11	1.80	0.62
68:w:6:GLN:N	68:w:62:TRP:CH2	2.68	0.62
1:a:109:TYR:CE2	1:a:154:LEU:HD21	2.34	0.62
9:j:43:PHE:CE1	13:s:147:THR:O	2.53	0.62
9:j:78:GLN:CA	9:j:82:LYS:HE3	2.26	0.62
9:j:99:ILE:HA	9:j:102:MET:HG2	1.82	0.62
11:n:634:MET:N	11:n:634:MET:SD	2.73	0.62
14:u:4:ARG:NE	16:z:596:TYR:N	2.47	0.62
68:w:19:GLU:HA	68:w:25:MET:CG	2.30	0.62
68:w:33:GLU:HB3	68:w:36:LYS:HB3	1.82	0.62
70:p:148:GLU:HB3	70:p:370:VAL:HG21	1.82	0.62
6:h:42:TRP:CB	6:h:43:PRO:HD3	2.25	0.61
10:k:109:ARG:HH11	10:k:109:ARG:HG3	1.65	0.61
11:n:229:GLU:HG2	11:n:300:CYS:SG	2.40	0.61
12:q:89:GLN:CB	12:q:90:PRO:CD	2.68	0.61
12:q:109:MET:HE3	12:q:109:MET:O	2.00	0.61
15:v:119:LEU:O	15:v:120:ARG:C	2.43	0.61
17:c:214:VAL:H	17:c:243:THR:HG22	1.65	0.61
68:w:40:CYS:HB3	68:w:82:CYS:SG	2.40	0.61
68:w:101:LEU:HD22	68:w:118:THR:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:33:LYS:HD2	5:g:33:LYS:C	2.25	0.61
14:u:57:LEU:HD13	16:z:492:ARG:CG	2.30	0.61
31:6:503:ALA:HB2	31:6:646:ALA:HA	1.82	0.61
34:EB:129:LYS:HB3	34:EB:143:TYR:OH	2.01	0.61
38:De:561:SER:HB2	38:De:588:VAL:HB	1.82	0.61
68:w:281:ASP:OD1	68:w:281:ASP:N	2.31	0.61
69:x:650:LEU:HB2	69:x:659:TYR:HE2	1.64	0.61
4:f:87:GLN:HE21	23:0:239:HIS:CB	2.13	0.61
9:j:19:ILE:HD12	9:j:45:VAL:HG22	1.82	0.61
36:DB:280:THR:HG23	36:DB:342:THR:HG22	1.79	0.61
37:DD:935:GLU:HB2	42:DI:130:LYS:HG2	1.80	0.61
48:DO:97:ALA:HB1	50:DQ:339:TYR:HB3	1.81	0.61
62:PH:64:LEU:HD11	62:PH:91:VAL:HG11	1.82	0.61
68:w:1181:THR:O	68:w:1184:VAL:HB	2.00	0.61
4:f:58:GLU:HB2	4:f:61:ASN:HD21	1.65	0.61
9:j:70:TYR:CD1	9:j:80:TYR:CG	2.74	0.61
11:n:229:GLU:HB2	11:n:254:VAL:HG22	1.82	0.61
11:n:237:MET:HE1	12:q:45:GLN:HG2	1.81	0.61
11:n:417:LYS:HG3	11:n:421:ARG:HE	1.64	0.61
14:u:57:LEU:CD1	16:z:492:ARG:NE	2.63	0.61
14:u:110:ARG:HH22	22:i:141:PHE:CB	2.14	0.61
28:3:241:LEU:HD21	29:4:55:TRP:HE1	1.64	0.61
53:X:-26:DA:H3'	53:X:-26:DA:OP2	2.01	0.61
53:X:28:DA:C2	54:Y:-27:DG:N2	2.69	0.61
68:w:6:GLN:CB	68:w:62:TRP:CH2	2.83	0.61
1:a:383:PRO:HA	69:x:92:LEU:CG	2.30	0.61
2:m:100:GLN:HE22	11:n:172:CYS:HB2	1.65	0.61
6:h:72:ARG:HH11	12:q:134:ALA:H	1.48	0.61
6:h:99:VAL:O	6:h:99:VAL:HG23	2.01	0.61
9:j:53:LYS:HZ1	11:n:61:ARG:N	1.84	0.61
14:u:28:GLN:OE1	16:z:483:ASN:ND2	2.34	0.61
24:8:214:PRO:HG3	55:PA:1674:THR:HB	1.82	0.61
54:Y:3:DG:C2'	54:Y:4:DA:OP2	2.35	0.61
55:PA:686:THR:CG2	55:PA:765:ASN:HD21	2.14	0.61
63:PI:27:LYS:HG2	63:PI:38:ALA:HB2	1.82	0.61
8:t:204:GLN:O	8:t:205:GLN:C	2.42	0.61
12:q:24:LEU:HD22	55:PA:1796:SER:CB	2.29	0.61
18:e:71:GLU:OE1	18:e:74:ARG:NH2	2.33	0.61
36:DB:368:TRP:HB3	36:DB:449:PHE:CE1	2.35	0.61
42:DI:60:HIS:CE1	44:DL:106:ARG:HG3	2.26	0.61
38:De:488:GLY:CA	38:De:546:VAL:CG2	2.67	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:X:7:DG:N2	54:Y:-6:DG:N2	2.47	0.61
55:PA:983:LEU:HD11	55:PA:1045:LEU:HD12	1.83	0.61
7:r:124:ARG:HA	7:r:124:ARG:NE	2.15	0.61
9:j:102:MET:HB3	14:u:26:LEU:CD1	2.30	0.61
39:DF:12:THR:HB	42:DI:22:ILE:HG12	1.82	0.61
63:PI:80:ARG:HG2	63:PI:95:VAL:HG12	1.83	0.61
69:x:251:GLU:HG3	69:x:263:LEU:HD13	1.82	0.61
70:p:225:ASN:ND2	70:p:245:CYS:SG	2.74	0.61
8:t:151:SER:HA	8:t:154:TRP:HB3	1.81	0.61
9:j:9:GLU:HG3	9:j:56:GLN:HG3	1.82	0.61
9:j:53:LYS:HZ1	11:n:60:HIS:CA	2.12	0.61
11:n:526:SER:OG	68:w:45:ARG:NH2	2.33	0.61
31:6:568:LEU:HB2	31:6:606:PHE:HB3	1.82	0.61
35:DA:638:PRO:HB3	40:DG:39:LEU:HD23	1.82	0.61
36:DB:656:GLU:HB3	36:DB:662:GLN:HG3	1.83	0.61
4:f:87:GLN:HB2	23:0:239:HIS:CB	2.31	0.61
5:g:153:PHE:CZ	14:u:107:VAL:HG12	2.36	0.61
9:j:12:LEU:HD13	9:j:52:ASP:HB3	1.83	0.61
10:k:42:GLU:HA	10:k:42:GLU:OE2	2.00	0.61
11:n:226:VAL:HG13	11:n:230:PHE:H	1.64	0.61
11:n:526:SER:CB	68:w:45:ARG:CZ	2.79	0.61
12:q:543:VAL:HG11	17:c:135:ARG:HE	1.66	0.61
37:Dd:843:VAL:HG13	37:Dd:844:ASN:N	2.16	0.61
55:PA:25:VAL:HG22	55:PA:243:ALA:HA	1.82	0.61
1:a:224:TYR:CZ	1:a:253:MET:HB3	2.36	0.61
1:a:232:LEU:CG	1:a:502:MET:HE1	2.30	0.61
2:m:56:LEU:CD2	2:m:80:GLN:HE22	2.12	0.61
8:t:136:ARG:HG3	8:t:136:ARG:O	2.00	0.61
37:DD:1060:LEU:HA	44:DL:80:VAL:HG22	1.81	0.61
56:PB:1123:GLY:HA3	56:PB:1170:ARG:HA	1.82	0.61
1:a:509:ARG:CZ	1:a:509:ARG:CB	2.79	0.60
3:d:153:HIS:HB2	5:g:56:ILE:HG23	1.83	0.60
4:f:181:LEU:CD1	11:n:270:GLN:CD	2.74	0.60
9:j:19:ILE:HG21	9:j:45:VAL:HG23	1.72	0.60
9:j:89:LEU:HD21	13:s:84:ILE:HG12	1.82	0.60
12:q:255:ALA:HB3	12:q:301:VAL:HG22	1.81	0.60
24:8:177:TRP:CE2	55:PA:1677:SER:HB2	2.35	0.60
53:X:2:DG:N2	54:Y:-1:DT:N3	2.49	0.60
69:x:414:GLU:OE2	69:x:460:LYS:NZ	2.34	0.60
1:a:60:SER:HB3	1:a:148:ASP:CB	2.31	0.60
1:a:329:LEU:HD21	1:a:393:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:23:LYS:HB3	6:h:23:LYS:HZ3	1.64	0.60
10:k:78:PRO:C	10:k:79:HIS:ND1	2.58	0.60
11:n:377:PRO:HG2	11:n:408:ARG:HH21	1.66	0.60
12:q:263:LYS:HE2	12:q:439:PHE:CE2	2.36	0.60
15:v:16:GLN:HE21	15:v:20:LYS:HE3	1.66	0.60
15:v:127:LEU:HD12	15:v:127:LEU:O	2.01	0.60
44:DL:76:LEU:HD13	44:DL:84:LEU:HD12	1.81	0.60
44:DL:106:ARG:HH11	44:DL:114:LYS:CE	2.14	0.60
49:DP:300:ILE:CG2	49:DP:315:ALA:CA	2.79	0.60
53:X:-37:DG:H2'	53:X:-37:DG:P	2.41	0.60
57:PC:37:VAL:HG13	57:PC:41:GLU:HB2	1.83	0.60
68:w:25:MET:SD	68:w:28:ASP:HB3	2.40	0.60
3:d:164:PRO:HD2	3:d:167:TRP:HB2	1.82	0.60
4:f:133:ALA:O	4:f:137:CYS:SG	2.59	0.60
11:n:141:ARG:NH2	14:u:20:CYS:HB3	2.15	0.60
11:n:315:LEU:HD22	11:n:319:ARG:HD2	1.83	0.60
12:q:1:MET:HE3	16:z:541:PRO:CG	2.31	0.60
22:i:118:LEU:HD23	22:i:118:LEU:O	2.00	0.60
26:1:198:ARG:NH2	26:1:317:ALA:O	2.31	0.60
31:6:272:VAL:HG13	31:6:276:MET:HE3	1.84	0.60
36:DB:304:PHE:HE1	36:DB:353:GLN:CD	2.08	0.60
43:DJ:146:ALA:HB1	43:DJ:152:ILE:HD11	1.82	0.60
56:PB:94:SER:HB3	56:PB:123:PRO:HG2	1.83	0.60
1:a:60:SER:CB	1:a:148:ASP:HB3	2.31	0.60
9:j:99:ILE:C	9:j:102:MET:HG2	2.25	0.60
10:k:73:VAL:HG23	15:v:92:PRO:CG	2.31	0.60
15:v:85:PHE:HE1	15:v:86:LEU:CD2	2.14	0.60
56:PB:125:TYR:HB3	56:PB:146:LYS:HA	1.83	0.60
9:j:34:GLN:OE1	9:j:37:LEU:CG	2.50	0.60
24:8:214:PRO:HG2	55:PA:1674:THR:CG2	2.31	0.60
36:DB:571:LEU:HB3	36:DB:597:ARG:HB2	1.82	0.60
53:X:-16:DG:H1	54:Y:16:DC:H42	1.46	0.60
2:m:124:GLN:CD	16:z:590:ARG:CD	2.58	0.60
10:k:115:LEU:HD11	18:e:133:LEU:HD12	1.84	0.60
11:n:651:ASN:OD1	11:n:680:HIS:NE2	2.34	0.60
12:q:19:VAL:O	12:q:19:VAL:HG22	2.01	0.60
28:3:227:LEU:HA	28:3:231:PHE:HD2	1.66	0.60
31:6:104:ALA:HB2	31:6:118:LEU:HD23	1.82	0.60
53:X:27:DC:H2'	53:X:27:DC:OP2	2.00	0.60
55:PA:805:ARG:CZ	55:PA:808:PRO:HA	2.32	0.60
56:PB:834:ARG:HA	56:PB:840:MET:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:394:PRO:HG3	70:p:171:PHE:CE1	2.37	0.60
6:h:19:VAL:HG11	12:q:113:TYR:CB	2.30	0.60
9:j:59:HIS:H	11:n:50:ARG:HA	1.66	0.60
10:k:21:ILE:CD1	12:q:168:THR:CA	2.80	0.60
12:q:597:PRO:HA	12:q:619:ARG:HA	1.84	0.60
19:b:59:ARG:HH21	19:b:63:LEU:HD11	1.66	0.60
19:b:78:ALA:CB	21:o:621:LEU:HD21	2.31	0.60
24:8:65:LEU:HD22	24:8:133:ILE:HD13	1.84	0.60
32:7:458:SER:HB2	32:7:461:LEU:HG	1.83	0.60
36:DB:529:VAL:HG11	36:DB:560:TYR:HB2	1.82	0.60
38:DE:610:ARG:HH11	38:DE:619:PRO:HG2	1.66	0.60
37:Dd:909:ARG:HG2	44:Dl:91:PHE:CE1	2.37	0.60
37:Dd:1078:LEU:HD21	44:Dl:90:ASP:OD2	2.02	0.60
55:PA:1301:ILE:HB	55:PA:1304:ILE:HG12	1.83	0.60
55:PA:1473:LEU:HB2	61:PG:59:ILE:HB	1.83	0.60
68:w:113:GLN:HE22	68:w:159:GLN:HE22	1.49	0.60
7:r:108:ILE:HD13	8:t:91:PHE:HA	1.84	0.60
9:j:82:LYS:CB	13:s:96:PHE:CD1	2.82	0.60
10:k:101:ARG:HH11	10:k:101:ARG:CG	2.14	0.60
15:v:120:ARG:HH11	15:v:120:ARG:CG	2.13	0.60
17:c:111:TYR:CZ	19:b:136:HIS:CG	2.90	0.60
46:Dk:156:GLY:HA3	47:Dm:103:LEU:HD11	1.84	0.60
56:PB:116:ARG:HB2	56:PB:118:LEU:HG	1.82	0.60
56:PB:1112:ASP:HB2	56:PB:1153:TYR:HB3	1.84	0.60
4:f:143:LYS:HD2	12:q:226:LYS:HD2	1.83	0.60
6:h:175:PRO:HA	6:h:178:THR:HG23	1.84	0.60
9:j:102:MET:HB3	14:u:26:LEU:CG	2.31	0.60
28:3:133:LEU:HD22	28:3:165:LYS:HD2	1.82	0.60
2:m:54:TYR:OH	5:g:35:PRO:HA	2.02	0.60
2:m:68:LYS:HD2	5:g:50:GLN:CD	2.27	0.60
3:d:111:GLN:HA	3:d:114:LEU:CD2	2.32	0.60
6:h:19:VAL:HG12	12:q:113:TYR:HD2	1.67	0.60
7:r:23:LEU:HD12	7:r:171:LEU:HD23	1.82	0.60
7:r:108:ILE:CD1	8:t:91:PHE:HA	2.31	0.60
9:j:42:ASN:O	9:j:46:THR:HG23	2.01	0.60
11:n:252:ILE:HD11	11:n:271:ILE:HG12	1.83	0.60
22:i:86:ASP:N	22:i:86:ASP:OD1	2.25	0.60
27:2:116:LYS:HE2	27:2:119:GLU:HA	1.83	0.60
31:6:663:VAL:HG13	31:6:669:GLU:HB3	1.82	0.60
36:DB:713:TRP:HD1	36:DB:715:GLY:H	1.49	0.60
56:PB:633:LEU:HG	56:PB:683:GLN:HE22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:316:ALA:HB2	1:a:447:GLU:HG2	1.82	0.59
3:d:120:ILE:HG23	5:g:156:HIS:ND1	2.16	0.59
5:g:87:ILE:CD1	9:j:123:LYS:HB2	2.32	0.59
6:h:39:ARG:HD2	6:h:39:ARG:O	2.01	0.59
6:h:67:LYS:HD3	23:0:141:THR:CB	2.32	0.59
9:j:53:LYS:CG	11:n:57:PHE:CA	2.53	0.59
9:j:82:LYS:HA	13:s:96:PHE:CD1	2.37	0.59
9:j:96:LYS:HE3	13:s:80:SER:CB	2.31	0.59
11:n:158:ILE:HD11	12:q:11:ILE:HD13	1.84	0.59
15:v:126:ASP:OD2	18:e:132:HIS:HD2	1.85	0.59
44:DL:106:ARG:HD2	44:DL:114:LYS:HZ2	1.63	0.59
68:w:895:ASP:O	68:w:899:ARG:NH1	2.34	0.59
2:m:15:ARG:N	5:g:39:LYS:NZ	2.49	0.59
4:f:37:SER:HB3	5:g:10:ALA:HA	1.83	0.59
9:j:61:ILE:HG22	9:j:61:ILE:O	2.01	0.59
12:q:167:LEU:CD2	15:v:76:MET:HE2	2.32	0.59
17:c:113:TRP:CZ2	19:b:175:HIS:HB2	2.34	0.59
18:e:60:VAL:C	19:b:179:LEU:CD1	2.75	0.59
21:o:765:ASP:HB3	68:w:72:SER:OG	2.02	0.59
32:7:444:ILE:HD11	32:7:471:LEU:HD22	1.83	0.59
39:Df:292:ASN:HD22	39:Df:295:LEU:HD23	1.67	0.59
58:PD:79:THR:HG21	58:PD:141:GLN:HE21	1.67	0.59
2:m:116:GLN:CG	16:z:595:PRO:HD3	2.31	0.59
29:4:163:MET:HG2	29:4:196:ILE:HG23	1.84	0.59
29:4:431:LEU:HD12	29:4:442:VAL:HG23	1.84	0.59
4:f:101:ILE:CD1	6:h:105:VAL:CG1	2.80	0.59
8:t:3:VAL:HG21	8:t:153:CYS:HB2	1.82	0.59
9:j:97:GLY:O	9:j:101:THR:HG23	2.02	0.59
12:q:162:LYS:O	12:q:166:ARG:CG	2.50	0.59
15:v:119:LEU:HD22	18:e:139:TRP:CD1	2.37	0.59
18:e:91:THR:OG1	20:l:41:VAL:HG21	2.00	0.59
29:4:334:MET:HA	29:4:344:ALA:HA	1.85	0.59
29:4:401:LEU:HD21	30:5:53:LEU:HD23	1.84	0.59
35:DA:690:LEU:HD22	35:DA:747:LEU:HD22	1.83	0.59
38:DE:543:SER:HB3	41:DH:77:LYS:HE2	1.84	0.59
38:DE:724:GLU:HA	38:DE:741:ILE:HG12	1.84	0.59
41:DH:186:VAL:HG21	39:Df:220:GLN:HG2	1.84	0.59
38:De:490:ALA:HA	38:De:545:PRO:HB3	1.84	0.59
38:De:689:THR:HA	38:De:713:THR:HG23	1.83	0.59
56:PB:564:ALA:HB3	56:PB:576:ILE:HD12	1.83	0.59
1:a:232:LEU:HB3	1:a:502:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:336:TYR:CE1	1:a:391:THR:OG1	2.52	0.59
4:f:106:TYR:CE2	6:h:106:PRO:HG3	2.38	0.59
6:h:33:LEU:CD2	6:h:40:LEU:CD2	2.81	0.59
11:n:169:LEU:CB	11:n:170:PRO:HD3	2.26	0.59
11:n:715:ARG:NH2	17:c:311:GLN:HE22	1.96	0.59
12:q:451:LEU:HD11	12:q:529:MET:CE	2.32	0.59
31:6:537:ASN:HB3	31:6:540:LYS:HB3	1.85	0.59
36:DB:290:PHE:CZ	36:DB:381:TRP:HA	2.37	0.59
36:DB:608:ASN:OD1	36:DB:610:GLU:O	2.20	0.59
1:a:160:LEU:CD1	1:a:219:LEU:HD21	2.33	0.59
2:m:15:ARG:CA	5:g:39:LYS:HZ3	2.14	0.59
6:h:8:LEU:HD23	6:h:8:LEU:O	2.03	0.59
10:k:114:MET:HE2	18:e:129:VAL:CG1	2.27	0.59
12:q:591:LYS:NZ	12:q:593:MET:SD	2.75	0.59
22:i:85:GLN:HG2	22:i:86:ASP:OD1	1.98	0.59
31:6:514:MET:HE3	31:6:518:PHE:HB3	1.83	0.59
32:7:269:THR:HA	32:7:272:ARG:HE	1.67	0.59
37:Dd:856:ASN:HD21	46:Dk:126:ARG:HB3	1.68	0.59
51:BA:125:ALA:HB1	51:BA:132:ARG:HB3	1.85	0.59
68:w:9:PHE:HZ	68:w:63:ILE:HG12	1.68	0.59
5:g:164:ILE:HG21	22:i:141:PHE:HE2	1.55	0.59
10:k:73:VAL:HG21	15:v:90:ASP:OD1	2.03	0.59
10:k:79:HIS:ND1	15:v:91:PHE:HE1	1.99	0.59
11:n:402:ILE:HD13	12:q:327:VAL:HG12	1.85	0.59
15:v:82:LEU:O	15:v:86:LEU:CD2	2.51	0.59
21:o:715:LEU:HD23	69:x:25:ILE:HG12	1.85	0.59
24:8:177:TRP:CE2	55:PA:1677:SER:CB	2.85	0.59
35:DA:409:HIS:CE1	35:DA:411:GLU:HB2	2.38	0.59
44:Dl:58:LEU:HD23	44:Dl:85:LEU:HD23	1.85	0.59
56:PB:422:PHE:HD2	56:PB:429:PHE:HA	1.67	0.59
1:a:367:LEU:HD22	1:a:509:ARG:HH11	1.67	0.59
2:m:26:GLN:O	3:d:177:PRO:CB	2.49	0.59
3:d:131:LYS:CE	14:u:104:LEU:CG	2.77	0.59
4:f:132:GLU:CD	12:q:98:VAL:HG22	2.26	0.59
4:f:180:LEU:HD21	11:n:299:PHE:CD2	2.32	0.59
5:g:56:ILE:HD12	5:g:56:ILE:N	2.18	0.59
10:k:101:ARG:HH11	10:k:101:ARG:HG2	1.67	0.59
53:X:7:DG:N2	54:Y:-6:DG:C2	2.71	0.59
55:PA:193:ARG:HA	55:PA:198:LEU:HA	1.84	0.59
68:w:13:VAL:HG11	68:w:75:ARG:HG3	1.84	0.59
5:g:27:GLN:CD	5:g:32:PRO:HG3	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:77:ILE:CG1	12:q:126:THR:HB	2.33	0.59
8:t:6:VAL:HA	8:t:140:VAL:O	2.03	0.59
9:j:89:LEU:HD21	13:s:93:TYR:CE2	2.30	0.59
9:j:96:LYS:HE3	13:s:80:SER:CA	2.32	0.59
9:j:99:ILE:O	9:j:102:MET:CG	2.47	0.59
10:k:29:GLY:O	10:k:33:LEU:CG	2.42	0.59
10:k:88:LYS:HD2	10:k:88:LYS:C	2.27	0.59
11:n:375:ASP:HB3	11:n:376:PRO:HD3	1.85	0.59
14:u:110:ARG:NH2	22:i:141:PHE:HB2	2.18	0.59
69:x:482:SER:C	69:x:485:PRO:HD3	2.27	0.59
3:d:145:SER:HA	5:g:135:LEU:HD13	1.85	0.59
3:d:169:PRO:CB	55:PA:1795:PRO:CB	2.76	0.59
5:g:48:GLN:OE1	5:g:48:GLN:N	2.22	0.59
6:h:26:LEU:HD22	12:q:102:LEU:HD22	1.84	0.59
12:q:290:HIS:HE1	12:q:294:LYS:NZ	2.01	0.59
16:z:543:LEU:O	16:z:545:ARG:N	2.36	0.59
34:EB:81:ILE:HG23	34:EB:102:ILE:HG21	1.83	0.59
36:DB:290:PHE:CZ	36:DB:381:TRP:CA	2.86	0.59
68:w:13:VAL:CG1	68:w:75:ARG:CG	2.79	0.59
68:w:425:MET:N	68:w:425:MET:SD	2.72	0.59
1:a:232:LEU:HD13	1:a:232:LEU:O	2.02	0.58
7:r:83:TRP:CE3	7:r:114:LEU:HD22	2.38	0.58
8:t:78:LEU:HD22	8:t:78:LEU:N	2.18	0.58
8:t:131:MET:O	8:t:131:MET:HE3	2.02	0.58
10:k:32:ILE:HG13	12:q:157:ALA:HB1	1.85	0.58
29:4:433:PHE:HB2	30:5:9:LEU:HD22	1.84	0.58
56:PB:931:ILE:HA	56:PB:945:CYS:HB3	1.85	0.58
57:PC:53:ASP:HA	66:PL:52:LEU:HD22	1.84	0.58
57:PC:106:ARG:HD3	57:PC:158:GLU:HB3	1.85	0.58
63:PI:24:LEU:HB3	63:PI:37:TYR:HB3	1.85	0.58
2:m:31:PRO:HD2	3:d:176:TYR:HD2	1.61	0.58
7:r:41:GLY:O	10:k:79:HIS:HB2	2.03	0.58
11:n:131:ASP:N	14:u:27:GLN:OE1	2.36	0.58
11:n:175:ASP:OD2	12:q:20:HIS:CE1	2.56	0.58
11:n:685:LEU:CD2	21:o:729:TYR:HE2	2.16	0.58
12:q:534:VAL:HG11	12:q:567:SER:HB3	1.83	0.58
21:o:696:SER:HB3	69:x:111:HIS:HE1	1.66	0.58
31:6:340:LEU:HD12	31:6:466:LEU:HD22	1.84	0.58
32:7:493:MET:HA	32:7:705:ASN:HB3	1.85	0.58
38:DE:495:ARG:HB3	38:DE:536:LEU:HD11	1.84	0.58
54:Y:-8:DT:H2"	54:Y:-7:DC:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:PI:68:ILE:HG13	63:PI:122:ARG:HD2	1.83	0.58
10:k:109:ARG:HH11	10:k:109:ARG:CG	2.14	0.58
11:n:821:SER:O	11:n:833:ILE:HA	2.02	0.58
36:DB:329:LEU:O	36:DB:331:HIS:HD2	1.84	0.58
39:DF:35:THR:HG23	42:DI:71:VAL:HG21	1.85	0.58
46:Dk:139:GLN:HG2	46:Dk:145:SER:HA	1.84	0.58
53:X:-9:DG:H5'	53:X:-9:DG:C8	2.38	0.58
53:X:-5:DG:N2	54:Y:6:DG:N1	2.51	0.58
53:X:2:DG:N2	54:Y:-1:DT:O2	2.35	0.58
56:PB:801:VAL:HG13	56:PB:929:PRO:HD2	1.85	0.58
68:w:765:ARG:HA	68:w:768:LYS:HE2	1.84	0.58
70:p:61:MET:HE2	70:p:75:SER:HB3	1.85	0.58
1:a:329:LEU:HD23	1:a:329:LEU:C	2.27	0.58
1:a:364:TYR:O	1:a:428:THR:CG2	2.51	0.58
4:f:101:ILE:CD1	6:h:105:VAL:HG11	2.33	0.58
6:h:43:PRO:HA	6:h:46:LEU:HD23	1.85	0.58
6:h:77:ILE:CG1	12:q:126:THR:CG2	2.69	0.58
9:j:30:GLN:HG2	9:j:31:PRO:HD2	1.84	0.58
10:k:21:ILE:HD12	12:q:168:THR:HA	1.84	0.58
21:o:691:VAL:HA	21:o:708:CYS:HA	1.84	0.58
55:PA:922:PHE:H	55:PA:1052:ARG:HH11	1.52	0.58
5:g:136:ARG:CB	14:u:86:GLN:CD	2.67	0.58
10:k:21:ILE:HD12	12:q:168:THR:HG1	1.61	0.58
11:n:234:LEU:HD21	11:n:282:LEU:CD2	2.33	0.58
11:n:292:MET:HA	11:n:295:CYS:SG	2.42	0.58
12:q:36:MET:HE2	12:q:40:LEU:HD23	1.83	0.58
12:q:645:ALA:HB2	18:e:100:LEU:HD22	1.85	0.58
21:o:718:VAL:HG11	21:o:743:TYR:CE1	2.38	0.58
24:8:16:ASP:HB3	24:8:28:LYS:HB3	1.85	0.58
36:DB:215:VAL:HG11	36:DB:307:VAL:CG2	2.33	0.58
42:Di:73:LEU:HB2	44:Dl:105:HIS:CE1	2.38	0.58
55:PA:367:ILE:HG22	55:PA:482:PHE:HB2	1.86	0.58
70:p:166:PRO:HG2	70:p:169:THR:HG22	1.84	0.58
2:m:29:ALA:HB3	3:d:177:PRO:HD3	1.85	0.58
3:d:136:GLU:CD	5:g:146:ARG:HD3	2.28	0.58
5:g:130:GLN:O	5:g:134:THR:HG23	2.03	0.58
7:r:17:ASN:OD1	7:r:17:ASN:N	2.35	0.58
12:q:130:VAL:O	12:q:130:VAL:HG12	2.02	0.58
31:6:505:VAL:HG11	31:6:640:LEU:HD11	1.85	0.58
36:DB:802:LEU:HB3	36:DB:829:ILE:HG23	1.86	0.58
53:X:-5:DG:C2'	53:X:-4:DT:H71	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:PA:381:PRO:HG2	55:PA:384:ILE:HB	1.86	0.58
56:PB:748:ALA:HB3	56:PB:811:TYR:HB2	1.85	0.58
1:a:131:ASN:H	1:a:131:ASN:HD22	1.49	0.58
3:d:136:GLU:HB3	14:u:101:ALA:CB	2.34	0.58
4:f:178:ASP:HA	11:n:270:GLN:HE22	1.67	0.58
6:h:21:ASP:HB3	6:h:56:LEU:HD22	1.86	0.58
11:n:231:GLU:CB	11:n:253:LEU:HD21	2.34	0.58
17:c:111:TYR:CE1	19:b:136:HIS:CG	2.91	0.58
38:DE:578:LEU:HD13	42:DI:115:LEU:HD11	1.85	0.58
39:DF:106:PHE:HA	43:DJ:217:PHE:HB3	1.86	0.58
52:FB:126:ARG:HA	52:FB:129:ARG:CG	2.22	0.58
68:w:764:TYR:OH	68:w:799:GLU:OE2	2.22	0.58
11:n:234:LEU:HD22	11:n:245:TRP:HB3	1.86	0.58
11:n:937:ARG:NE	11:n:943:LEU:CD2	2.65	0.58
14:u:57:LEU:HD11	16:z:492:ARG:CZ	2.33	0.58
36:DB:294:ILE:HG13	36:DB:295:LEU:HG	1.85	0.58
60:PF:110:LEU:HD12	60:PF:114:SER:HB2	1.86	0.58
2:m:68:LYS:HD2	5:g:50:GLN:OE1	2.03	0.58
3:d:155:ILE:CD1	3:d:161:VAL:HB	2.34	0.58
9:j:92:ASN:HD21	13:s:83:LEU:CD2	1.75	0.58
13:s:84:ILE:HG22	13:s:90:GLU:HA	1.86	0.58
14:u:4:ARG:HD2	16:z:596:TYR:HB2	1.84	0.58
19:b:178:LEU:CD2	20:l:82:LEU:HD11	2.33	0.58
33:EA:114:ILE:HA	33:EA:181:ASN:HD22	1.69	0.58
49:DP:264:VAL:HG23	49:DP:266:PHE:H	1.69	0.58
49:DP:295:MET:HB3	49:DP:298:PRO:HD2	1.86	0.58
55:PA:93:PRO:HD2	55:PA:219:GLU:HG3	1.86	0.58
1:a:374:TYR:HA	1:a:440:PHE:O	2.04	0.58
2:m:15:ARG:HA	5:g:39:LYS:CE	2.34	0.58
3:d:99:GLU:CD	3:d:103:ARG:NH2	2.59	0.58
4:f:45:CYS:HB2	4:f:66:ILE:HB	1.85	0.58
10:k:24:ILE:HG21	12:q:164:ALA:HB2	0.58	0.58
12:q:153:LEU:HD11	15:v:40:ALA:HB1	1.85	0.58
15:v:134:TYR:HB2	20:l:156:LEU:CD2	2.34	0.58
17:c:162:VAL:HG13	17:c:207:LEU:HD13	1.86	0.58
36:DB:368:TRP:HH2	36:DB:519:ILE:HD12	1.69	0.58
69:x:439:LEU:HB3	69:x:495:ILE:HG21	1.86	0.58
1:a:94:LEU:HD23	1:a:94:LEU:H	1.68	0.57
7:r:117:PHE:HE1	8:t:79:PHE:CD2	2.15	0.57
7:r:192:GLN:CB	10:k:77:GLN:HE21	2.17	0.57
11:n:820:ILE:HD11	11:n:833:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DA:957:THR:HG23	40:DG:147:ARG:HA	1.85	0.57
36:DB:638:ARG:O	36:DB:638:ARG:HD3	2.03	0.57
43:DJ:198:GLU:H	43:DJ:198:GLU:CD	2.12	0.57
38:De:548:GLY:HA3	38:De:590:ASP:HA	1.87	0.57
3:d:111:GLN:O	3:d:114:LEU:HG	2.04	0.57
3:d:113:GLN:CG	5:g:163:MET:SD	2.92	0.57
6:h:143:LEU:HA	10:k:39:LYS:NZ	2.18	0.57
8:t:3:VAL:HG13	8:t:176:PHE:CZ	2.39	0.57
2:m:26:GLN:O	3:d:177:PRO:CG	2.52	0.57
5:g:45:PHE:CD1	5:g:45:PHE:C	2.83	0.57
6:h:41:THR:O	6:h:42:TRP:C	2.44	0.57
8:t:103:GLN:NE2	8:t:103:GLN:HA	2.19	0.57
12:q:93:TRP:N	12:q:94:PRO:HD2	2.20	0.57
18:e:132:HIS:CE1	20:l:163:LEU:HD11	2.39	0.57
22:i:118:LEU:C	22:i:118:LEU:CD2	2.77	0.57
36:DB:595:LYS:HD3	36:DB:598:ARG:HH22	1.68	0.57
39:DF:211:ARG:HH12	41:DH:168:PRO:HD3	1.68	0.57
55:PA:199:TYR:HB2	55:PA:213:LYS:HG2	1.85	0.57
55:PA:828:LEU:HA	56:PB:978:ILE:HG21	1.86	0.57
1:a:504:ILE:N	1:a:505:PRO:CD	2.67	0.57
4:f:177:VAL:HG21	11:n:266:VAL:CG2	2.10	0.57
6:h:143:LEU:HD22	10:k:39:LYS:HE2	1.86	0.57
8:t:16:SER:O	8:t:17:VAL:C	2.46	0.57
9:j:43:PHE:CE2	13:s:151:GLY:HA2	2.39	0.57
9:j:75:ARG:HB2	9:j:80:TYR:HE2	0.74	0.57
12:q:38:GLN:HB2	12:q:42:ARG:HH21	1.70	0.57
12:q:647:SER:CB	18:e:93:CYS:HG	2.18	0.57
26:1:382:TYR:OH	28:3:271:CYS:HB2	2.04	0.57
31:6:168:LEU:HD11	31:6:175:TYR:HB3	1.86	0.57
32:7:657:MET:HG3	32:7:692:LYS:HB2	1.85	0.57
44:DL:58:LEU:HA	44:DL:62:LYS:HD2	1.86	0.57
48:DO:31:GLN:O	48:DO:31:GLN:HG3	2.02	0.57
68:w:726:ASN:ND2	68:w:726:ASN:H	2.01	0.57
1:a:316:ALA:CB	1:a:447:GLU:HG2	2.34	0.57
3:d:160:ALA:HB1	3:d:175:PRO:HA	1.87	0.57
6:h:102:HIS:CE1	55:PA:1792:PRO:O	2.57	0.57
11:n:265:LEU:O	11:n:265:LEU:HD22	2.02	0.57
11:n:685:LEU:HD22	21:o:729:TYR:CE2	2.40	0.57
15:v:134:TYR:CD2	20:l:160:MET:HE1	2.40	0.57
27:2:221:VAL:HG11	32:7:725:ALA:HB1	1.85	0.57
39:DF:256:LEU:HD22	39:DF:295:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Dl:118:LEU:HD12	44:Dl:118:LEU:C	2.30	0.57
55:PA:552:ASP:HB2	62:PH:24:ARG:HB2	1.86	0.57
68:w:855:TRP:O	68:w:858:ASN:ND2	2.37	0.57
2:m:124:GLN:HG3	16:z:581:SER:CB	2.31	0.57
4:f:137:CYS:SG	6:h:46:LEU:HD22	2.45	0.57
11:n:266:VAL:HG23	11:n:303:LEU:HD11	1.84	0.57
16:z:543:LEU:C	16:z:545:ARG:H	2.13	0.57
21:o:756:MET:O	21:o:760:LEU:HG	2.05	0.57
25:9:93:ASN:HD22	25:9:153:GLN:HG3	1.69	0.57
26:1:199:THR:HA	26:1:317:ALA:HB2	1.85	0.57
36:DB:331:HIS:NE2	36:DB:342:THR:HB	2.07	0.57
69:x:404:GLN:NE2	69:x:408:GLN:OE1	2.37	0.57
1:a:267:LYS:H	1:a:267:LYS:HD2	1.70	0.57
6:h:166:LEU:HD12	61:PG:125:PRO:HG2	1.61	0.57
11:n:159:ASP:CG	11:n:167:PRO:CD	2.75	0.57
11:n:870:GLN:CG	21:o:655:THR:HG22	2.32	0.57
12:q:315:ALA:HB2	12:q:428:LEU:HD23	1.87	0.57
32:7:84:ILE:HG13	32:7:108:ALA:HB2	1.86	0.57
55:PA:1790:TYR:CE2	55:PA:1791:SER:O	2.58	0.57
59:PE:80:PRO:HA	59:PE:107:GLN:HB3	1.87	0.57
11:n:589:GLN:NE2	68:w:25:MET:HB2	2.19	0.57
12:q:562:SER:HB2	12:q:587:GLU:HB2	1.87	0.57
14:u:57:LEU:HD11	16:z:492:ARG:NE	2.20	0.57
38:DE:377:LEU:HG	38:DE:422:PRO:HG2	1.87	0.57
38:DE:709:GLY:HA3	38:DE:738:TRP:HH2	1.69	0.57
52:FB:8:ASP:HB3	52:FB:105:SER:HA	1.86	0.57
55:PA:577:PRO:HG2	55:PA:580:LEU:HG	1.85	0.57
56:PB:794:VAL:HG12	56:PB:967:ILE:HG22	1.87	0.57
62:PH:42:ASP:HB2	62:PH:121:LEU:HB3	1.86	0.57
68:w:122:VAL:O	68:w:126:ILE:HB	2.03	0.57
68:w:433:ASN:ND2	68:w:445:ILE:O	2.35	0.57
4:f:93:ILE:HG23	23:0:237:PRO:CB	2.34	0.57
4:f:178:ASP:HA	11:n:270:GLN:NE2	2.19	0.57
5:g:60:GLU:HG3	5:g:60:GLU:O	2.03	0.57
5:g:111:ASP:OD2	13:s:69:ARG:HG2	2.04	0.57
14:u:110:ARG:HH22	22:i:141:PHE:HB2	1.70	0.57
17:c:110:ALA:HB2	19:b:168:ILE:HG21	1.56	0.57
37:DD:944:LEU:HD11	42:DI:123:THR:HG21	1.85	0.57
37:Dd:1058:VAL:O	44:Dl:77:ASP:CG	2.47	0.57
56:PB:1116:VAL:HG11	56:PB:1151:MET:HE2	1.86	0.57
61:PG:34:VAL:HG11	61:PG:48:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:160:LEU:CD1	1:a:214:ARG:NH2	2.67	0.57
1:a:401:PRO:O	1:a:405:PRO:HD3	2.04	0.57
7:r:108:ILE:HD13	8:t:91:PHE:CA	2.34	0.57
10:k:111:CYS:SG	18:e:129:VAL:HG12	2.44	0.57
14:u:88:ALA:CB	16:z:552:LEU:HD11	2.35	0.57
24:8:304:GLY:HA2	24:8:307:LEU:HB2	1.87	0.57
39:DF:75:LEU:HD13	39:DF:82:PRO:HA	1.87	0.57
44:DL:76:LEU:CD1	44:DL:84:LEU:HD12	2.34	0.57
37:Dd:885:ILE:HB	44:Dl:96:VAL:HG11	1.87	0.57
59:PE:18:MET:HE3	59:PE:28:VAL:HG13	1.87	0.57
69:x:376:ALA:O	69:x:380:ASN:ND2	2.38	0.57
4:f:93:ILE:HG12	23:0:237:PRO:HA	1.86	0.56
7:r:59:LEU:O	7:r:59:LEU:HD23	2.04	0.56
7:r:64:GLN:HB2	8:t:101:PHE:HZ	1.69	0.56
8:t:94:LEU:HG	8:t:98:LEU:HD11	1.86	0.56
8:t:152:ASP:HA	17:c:278:GLN:HE21	1.69	0.56
9:j:53:LYS:CE	11:n:57:PHE:C	2.58	0.56
11:n:229:GLU:HG3	11:n:300:CYS:HB2	1.85	0.56
12:q:314:GLU:OE1	12:q:427:LEU:N	2.38	0.56
14:u:4:ARG:HD2	16:z:596:TYR:CA	2.34	0.56
31:6:364:LEU:HD22	31:6:410:TYR:H	1.70	0.56
56:PB:984:CYS:HB3	56:PB:1044:GLY:HA3	1.86	0.56
68:w:169:TYR:CZ	68:w:177:LEU:HD11	2.40	0.56
68:w:369:ARG:NH1	68:w:402:LEU:O	2.37	0.56
69:x:581:ILE:HD11	69:x:616:LEU:HD22	1.87	0.56
7:r:108:ILE:HD13	8:t:91:PHE:N	2.20	0.56
11:n:156:TYR:OH	11:n:168:ARG:NH1	2.34	0.56
11:n:706:LEU:HD22	12:q:615:TRP:CH2	2.40	0.56
31:6:168:LEU:HB2	31:6:291:LEU:HD22	1.87	0.56
34:EB:78:LEU:HD22	34:EB:123:ALA:HB1	1.86	0.56
44:DL:106:ARG:CZ	44:DL:114:LYS:NZ	2.67	0.56
39:Df:104:LEU:HD21	44:Dl:154:LEU:HD23	1.87	0.56
39:Df:334:ALA:HB1	39:Df:379:GLY:HA2	1.86	0.56
53:X:25:DA:C2	54:Y:-24:DC:O2	2.58	0.56
2:m:121:GLU:CA	16:z:592:ASN:HD21	1.95	0.56
5:g:75:LYS:HD2	14:u:77:PRO:CA	2.35	0.56
6:h:22:LEU:HG	12:q:109:MET:HG3	1.86	0.56
9:j:75:ARG:HA	9:j:79:LEU:CD1	2.34	0.56
9:j:119:GLU:O	9:j:123:LYS:HG3	2.05	0.56
11:n:141:ARG:HH22	14:u:16:ALA:C	2.12	0.56
11:n:369:PRO:O	11:n:370:LEU:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:589:GLN:HE21	11:n:591:PHE:HE1	1.52	0.56
13:s:92:ALA:HB1	13:s:96:PHE:CE2	2.34	0.56
18:e:45:VAL:HG13	20:l:92:LEU:CD1	2.35	0.56
33:EA:113:ARG:NH2	34:EB:217:GLN:HB3	2.19	0.56
36:DB:656:GLU:HG2	36:DB:661:ALA:HB3	1.87	0.56
38:DE:292:LYS:HA	38:DE:298:LEU:HD11	1.86	0.56
37:Dd:844:ASN:C	37:Dd:847:GLU:HG2	2.30	0.56
38:De:653:LEU:HB3	38:De:662:VAL:HG23	1.87	0.56
55:PA:64:VAL:HG22	55:PA:71:CYS:HB2	1.86	0.56
56:PB:198:GLU:HB2	56:PB:488:PRO:HD3	1.87	0.56
57:PC:101:PHE:HB3	57:PC:120:LEU:HD12	1.87	0.56
69:x:483:THR:C	69:x:485:PRO:HD3	2.30	0.56
1:a:430:LEU:N	1:a:430:LEU:HD23	2.21	0.56
2:m:104:HIS:CB	11:n:169:LEU:HA	2.32	0.56
6:h:19:VAL:CG2	12:q:112:LEU:CD2	2.84	0.56
6:h:23:LYS:HD3	12:q:110:CYS:SG	2.45	0.56
6:h:144:ASN:ND2	15:v:41:LYS:O	2.38	0.56
7:r:57:VAL:O	7:r:126:ASP:N	2.31	0.56
10:k:13:ALA:CB	15:v:83:LYS:HD2	2.35	0.56
12:q:1:MET:H2	16:z:540:LEU:CD1	2.17	0.56
12:q:477:VAL:HB	12:q:493:LEU:HB2	1.88	0.56
16:z:551:ASP:OD1	16:z:551:ASP:N	2.37	0.56
55:PA:64:VAL:HG21	55:PA:78:MET:H	1.70	0.56
55:PA:805:ARG:HG2	55:PA:812:LYS:HA	1.88	0.56
58:PD:79:THR:HG23	58:PD:137:LYS:HG3	1.87	0.56
2:m:30:ASN:CG	3:d:176:TYR:CD1	2.83	0.56
4:f:41:TYR:HE1	4:f:47:ASN:HD22	1.52	0.56
5:g:30:LEU:O	5:g:30:LEU:HG	2.05	0.56
7:r:88:LEU:HD12	7:r:88:LEU:N	2.11	0.56
9:j:106:LYS:O	9:j:110:ILE:HG13	2.05	0.56
11:n:319:ARG:HG3	11:n:320:TRP:HD1	1.71	0.56
11:n:587:LEU:HD21	68:w:15:THR:HG22	1.76	0.56
14:u:4:ARG:HD2	16:z:596:TYR:CB	2.35	0.56
18:e:60:VAL:C	19:b:179:LEU:HD11	2.29	0.56
26:1:198:ARG:HH21	26:1:320:ARG:HD3	1.70	0.56
33:EA:149:THR:HG21	33:EA:153:ARG:HG2	1.87	0.56
36:DB:164:PRO:HD2	36:DB:173:ARG:HD2	1.87	0.56
41:DH:109:ALA:HA	41:DH:112:LYS:HE2	1.88	0.56
53:X:-14:DG:C2	54:Y:15:DC:O2	2.58	0.56
54:Y:13:DC:H2"	54:Y:14:DC:C6	2.41	0.56
55:PA:465:HIS:HD2	55:PA:467:MET:HB2	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:PA:637:MET:HB3	62:PH:122:LEU:HD21	1.87	0.56
1:a:127:HIS:HE1	1:a:171:THR:CG2	2.19	0.56
2:m:68:LYS:HD3	5:g:45:PHE:CE1	2.40	0.56
5:g:93:LEU:CD1	9:j:106:LYS:CG	2.39	0.56
6:h:55:GLN:HB2	58:PD:137:LYS:NZ	2.20	0.56
7:r:124:ARG:HB2	7:r:124:ARG:HH11	1.69	0.56
9:j:105:PHE:CZ	14:u:52:GLU:HA	2.40	0.56
10:k:16:ASP:OD1	15:v:79:VAL:HG21	2.06	0.56
11:n:586:LEU:HD11	68:w:12:VAL:HG12	1.88	0.56
44:DL:106:ARG:HH12	44:DL:115:ASP:N	2.02	0.56
38:De:781:VAL:HG13	39:Df:62:LYS:HD3	1.86	0.56
58:PD:60:VAL:HG13	61:PG:103:PRO:HB3	1.87	0.56
2:m:116:GLN:HB3	16:z:594:LEU:HG	1.88	0.56
5:g:33:LYS:HZ3	5:g:33:LYS:H	1.53	0.56
9:j:85:LEU:HD12	13:s:96:PHE:CE1	2.41	0.56
10:k:92:MET:HE3	12:q:376:HIS:CB	2.36	0.56
15:v:122:GLU:OE1	15:v:122:GLU:HA	2.05	0.56
17:c:176:MET:HE1	17:c:267:MET:HB3	1.86	0.56
29:4:162:PHE:HB3	29:4:185:MET:SD	2.44	0.56
29:4:308:VAL:HG23	29:4:316:TYR:O	2.06	0.56
36:DB:532:TYR:HB2	36:DB:549:LYS:HG3	1.87	0.56
2:m:104:HIS:CE1	11:n:169:LEU:N	2.68	0.56
2:m:116:GLN:HB3	16:z:594:LEU:CG	2.35	0.56
4:f:29:VAL:HG21	4:f:79:PHE:CG	2.40	0.56
6:h:12:LEU:HD13	6:h:12:LEU:O	2.05	0.56
11:n:693:ILE:HD11	11:n:775:ARG:HG2	1.87	0.56
13:s:84:ILE:O	13:s:90:GLU:HG3	2.05	0.56
29:4:408:LEU:HD11	29:4:440:LEU:HD13	1.86	0.56
30:5:35:ILE:HB	30:5:44:PHE:HB3	1.88	0.56
36:DB:656:GLU:HG3	36:DB:658:ASP:H	1.69	0.56
38:DE:453:LEU:O	38:DE:457:CYS:HB3	2.05	0.56
38:DE:557:TYR:H	38:DE:571:SER:HA	1.71	0.56
53:X:29:DG:N1	54:Y:-29:DC:C4	2.47	0.56
1:a:107:MET:O	1:a:107:MET:HE2	2.06	0.56
1:a:417:TYR:CD1	1:a:450:PHE:CE1	2.89	0.56
8:t:13:GLU:HB3	8:t:15:LYS:H	1.71	0.56
9:j:82:LYS:HG2	13:s:96:PHE:CG	2.15	0.56
10:k:21:ILE:CD1	12:q:168:THR:HA	2.35	0.56
11:n:156:TYR:HE1	11:n:168:ARG:CB	2.19	0.56
15:v:126:ASP:CB	18:e:132:HIS:HD2	2.19	0.56
21:o:765:ASP:OD2	68:w:73:PRO:CD	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:187:LEU:HD21	23:0:200:GLN:HG2	1.86	0.56
33:EA:33:ALA:HA	33:EA:52:LEU:HD21	1.87	0.56
36:DB:287:VAL:HG11	36:DB:347:ALA:HA	1.88	0.56
38:DE:306:VAL:HG21	38:DE:363:ALA:HA	1.87	0.56
46:Dk:194:LEU:HB3	46:Dk:200:ILE:HG13	1.88	0.56
55:PA:997:ASN:HD22	55:PA:1000:LEU:HG	1.71	0.56
55:PA:1005:HIS:HD2	55:PA:1007:ILE:HG12	1.71	0.56
70:p:243:LYS:NZ	70:p:245:CYS:SG	2.79	0.56
6:h:3:ARG:HG2	6:h:6:LYS:HB2	1.88	0.56
7:r:192:GLN:HB2	10:k:77:GLN:HE21	1.71	0.56
12:q:633:ARG:CG	12:q:637:TYR:HD2	2.19	0.56
16:z:540:LEU:C	16:z:540:LEU:CD2	2.78	0.56
33:EA:129:CYS:SG	33:EA:131:VAL:HG21	2.37	0.56
55:PA:1087:VAL:HG12	55:PA:1400:LEU:HD22	1.88	0.56
57:PC:45:ILE:HD12	57:PC:82:LEU:HD22	1.88	0.56
3:d:106:ASP:CG	5:g:174:ASP:HB2	2.28	0.55
5:g:153:PHE:HD1	5:g:153:PHE:O	1.88	0.55
7:r:96:LYS:HG3	33:EA:148:MET:HE2	1.87	0.55
8:t:9:MET:H	8:t:138:ILE:HG22	1.71	0.55
10:k:43:ARG:HH11	10:k:43:ARG:CB	2.19	0.55
12:q:9:ILE:HG12	14:u:90:LEU:HB2	1.88	0.55
12:q:633:ARG:CG	12:q:637:TYR:CD2	2.88	0.55
14:u:105:GLU:O	14:u:108:VAL:HG12	2.04	0.55
36:DB:218:GLY:HA2	36:DB:238:LEU:CD1	2.36	0.55
47:Dm:100:VAL:HA	47:Dm:103:LEU:HD12	1.88	0.55
57:PC:103:LEU:HD13	57:PC:120:LEU:HD22	1.89	0.55
68:w:16:GLU:OE1	68:w:75:ARG:HA	2.06	0.55
2:m:30:ASN:N	3:d:177:PRO:HD2	2.20	0.55
6:h:81:LEU:HD12	6:h:101:SER:O	2.06	0.55
7:r:118:LEU:N	7:r:118:LEU:HD23	2.20	0.55
8:t:173:PRO:O	8:t:176:PHE:HB2	2.06	0.55
10:k:13:ALA:HB2	15:v:83:LYS:CE	2.37	0.55
11:n:643:HIS:CE1	12:q:560:ILE:HG13	2.41	0.55
26:1:244:ALA:HB1	26:1:306:ARG:HD3	1.88	0.55
36:DB:727:PHE:O	36:DB:736:VAL:HG23	2.06	0.55
46:Dk:120:ARG:NH1	47:Dm:44:GLY:HA2	2.21	0.55
55:PA:63:GLY:HA3	55:PA:258:LEU:HB3	1.89	0.55
61:PG:30:LEU:HD22	61:PG:70:VAL:HG21	1.88	0.55
4:f:137:CYS:HA	6:h:42:TRP:CB	2.37	0.55
7:r:27:VAL:HG22	7:r:197:VAL:HG21	1.88	0.55
7:r:108:ILE:HG12	8:t:90:ASN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:706:LEU:HB2	11:n:725:VAL:HG23	1.87	0.55
31:6:360:ARG:HD2	31:6:405:VAL:HG23	1.88	0.55
55:PA:46:THR:HB	55:PA:58:MET:HB2	1.87	0.55
67:FA:49:ARG:HB2	67:FA:54:LYS:NZ	2.21	0.55
1:a:439:GLN:CD	69:x:15:LYS:HD2	2.26	0.55
2:m:17:ARG:NH2	5:g:33:LYS:CB	2.69	0.55
7:r:151:ILE:HD11	7:r:157:THR:HA	1.88	0.55
8:t:21:VAL:O	8:t:25:THR:HG23	2.05	0.55
8:t:156:LEU:HD13	17:c:286:LYS:NZ	2.21	0.55
11:n:247:LEU:HB2	11:n:282:LEU:HD21	1.87	0.55
12:q:578:TYR:CE1	12:q:646:LEU:HD13	2.41	0.55
12:q:596:PHE:CZ	20:l:117:TYR:CZ	2.95	0.55
14:u:11:ALA:O	14:u:69:ILE:HD11	2.07	0.55
23:0:250:PRO:HG3	24:8:291:LYS:HE2	1.87	0.55
32:7:105:LEU:HG	32:7:202:ALA:HA	1.87	0.55
34:EB:214:GLU:HB3	34:EB:217:GLN:HB2	1.87	0.55
53:X:24:DG:C8	54:Y:-23:DG:N2	2.75	0.55
1:a:259:ILE:HD12	1:a:259:ILE:N	2.20	0.55
2:m:15:ARG:N	5:g:39:LYS:HZ1	1.99	0.55
6:h:51:LEU:HD12	58:PD:137:LYS:HZ1	1.72	0.55
11:n:870:GLN:HG2	21:o:655:THR:CG2	2.31	0.55
14:u:8:LEU:HD12	14:u:72:LEU:HD23	1.85	0.55
19:b:160:TYR:O	19:b:164:ILE:HG12	2.07	0.55
35:DA:466:SER:HB2	39:DF:261:THR:HG21	1.88	0.55
38:De:651:VAL:HG13	38:De:665:PHE:HB2	1.89	0.55
55:PA:529:GLN:HE21	55:PA:1393:VAL:HG22	1.71	0.55
57:PC:73:LEU:HB3	57:PC:127:VAL:HG13	1.88	0.55
67:FA:100:LEU:HB3	67:FA:110:PHE:HB2	1.88	0.55
68:w:726:ASN:O	68:w:873:SER:OG	2.21	0.55
1:a:441:GLU:O	1:a:452:VAL:HA	2.07	0.55
3:d:148:ILE:HG12	11:n:161:LEU:CD1	2.25	0.55
4:f:177:VAL:HG11	11:n:270:GLN:HB2	1.87	0.55
7:r:117:PHE:HD2	8:t:85:LEU:HD12	1.70	0.55
8:t:131:MET:C	8:t:131:MET:SD	2.89	0.55
12:q:437:HIS:ND1	12:q:472:GLU:N	2.53	0.55
12:q:451:LEU:HD12	12:q:460:ILE:HD12	1.89	0.55
14:u:81:SER:CB	14:u:85:LEU:HB2	2.16	0.55
15:v:64:ARG:HH12	58:PD:140:PHE:HE1	1.54	0.55
17:c:110:ALA:HB2	19:b:168:ILE:HG22	1.84	0.55
36:DB:119:PRO:HB3	36:DB:194:ASP:O	2.07	0.55
55:PA:362:SER:HB2	56:PB:1084:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:199:PRO:HG2	1:a:244:GLU:O	2.06	0.55
1:a:321:LEU:HD21	1:a:407:ILE:CD1	2.35	0.55
1:a:383:PRO:HD3	1:a:445:LEU:O	2.06	0.55
2:m:15:ARG:CA	5:g:39:LYS:NZ	2.69	0.55
4:f:49:VAL:HA	4:f:52:MET:HE3	1.87	0.55
6:h:15:LEU:HD21	6:h:64:LYS:HD3	1.88	0.55
7:r:68:PHE:CE2	8:t:98:LEU:HD13	2.41	0.55
21:o:765:ASP:HB2	68:w:72:SER:OG	2.07	0.55
39:DF:65:LYS:O	39:DF:66:LEU:HB2	2.06	0.55
39:DF:114:LEU:HG	41:DH:45:LEU:HD12	1.88	0.55
38:De:458:LEU:HD12	39:Df:140:GLY:HA2	1.87	0.55
42:Di:73:LEU:HD21	44:Dl:105:HIS:CD2	2.40	0.55
54:Y:35:DC:H2'	54:Y:35:DC:OP2	2.07	0.55
68:w:1034:LEU:HD22	68:w:1038:ARG:HD2	1.86	0.55
68:w:1185:GLY:O	68:w:1186:TYR:C	2.50	0.55
11:n:196:ASN:HD21	11:n:219:ASN:HA	1.70	0.55
12:q:259:VAL:HG22	12:q:343:ILE:HG23	1.88	0.55
14:u:88:ALA:HB1	16:z:552:LEU:HD11	1.89	0.55
21:o:697:HIS:C	69:x:957:LYS:HD3	2.31	0.55
21:o:722:GLU:HG3	21:o:737:ILE:HB	1.89	0.55
25:9:190:THR:HB	25:9:223:ARG:HH21	1.71	0.55
26:1:278:ASP:HA	32:7:126:PHE:HA	1.87	0.55
28:3:61:ALA:HB2	28:3:70:LEU:HD11	1.88	0.55
34:EB:155:LEU:HD13	34:EB:189:ILE:HG23	1.88	0.55
37:Dd:843:VAL:N	37:Dd:845:LEU:CD2	2.70	0.55
55:PA:382:ARG:NH1	65:PK:1:MET:N	2.55	0.55
55:PA:1311:LEU:HD23	55:PA:1311:LEU:H	1.72	0.55
3:d:164:PRO:HG2	3:d:173:ARG:HD2	1.88	0.55
7:r:54:HIS:C	7:r:54:HIS:CD2	2.85	0.55
7:r:124:ARG:CZ	7:r:124:ARG:CB	2.85	0.55
12:q:437:HIS:HD2	12:q:437:HIS:O	1.89	0.55
21:o:767:HIS:CD2	21:o:772:LEU:HD21	2.42	0.55
36:DB:27:LYS:HG2	36:DB:489:GLN:HB3	1.88	0.55
56:PB:584:MET:HE3	56:PB:605:ARG:HB2	1.89	0.55
69:x:172:THR:HB	69:x:965:LYS:HE2	1.88	0.55
3:d:110:LEU:HD11	5:g:170:SER:HB3	1.89	0.55
3:d:135:ILE:HB	12:q:12:GLU:OE2	2.06	0.55
7:r:120:GLU:CD	8:t:79:PHE:CD1	2.82	0.55
8:t:103:GLN:HA	8:t:103:GLN:HE21	1.70	0.55
12:q:92:LEU:HD13	12:q:99:ARG:NH2	2.09	0.55
20:l:30:THR:OG1	20:l:102:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:107:ASP:N	20:l:108:PRO:HD3	2.22	0.55
31:6:123:LEU:O	31:6:127:VAL:HG23	2.07	0.55
42:DI:73:LEU:HA	42:DI:76:GLN:HE21	1.72	0.55
55:PA:885:GLN:HA	59:PE:169:GLN:HA	1.89	0.55
68:w:18:ILE:O	68:w:18:ILE:HD13	2.06	0.55
70:p:232:ASP:OD1	70:p:232:ASP:N	2.31	0.55
1:a:471:ASP:HB2	1:a:474:HIS:HB2	1.89	0.54
4:f:174:ARG:HD3	11:n:267:HIS:CD2	2.41	0.54
7:r:121:MET:O	7:r:121:MET:HE3	2.07	0.54
8:t:4:THR:HG22	8:t:143:GLU:HB2	1.87	0.54
11:n:247:LEU:HD21	11:n:278:VAL:CG2	2.34	0.54
21:o:757:THR:O	21:o:761:LEU:HG	2.06	0.54
24:8:261:PHE:HZ	24:8:272:ILE:HG21	1.71	0.54
28:3:64:ILE:HA	28:3:131:THR:HA	1.87	0.54
36:DB:308:PHE:CD2	36:DB:330:LEU:HD21	2.42	0.54
44:DL:101:GLN:O	44:DL:105:HIS:CD2	2.60	0.54
68:w:68:HIS:NE2	68:w:114:LEU:HD11	2.21	0.54
1:a:59:VAL:O	1:a:63:GLU:HG3	2.07	0.54
1:a:420:LEU:CD1	1:a:475:VAL:HG21	2.37	0.54
4:f:82:ARG:HD2	4:f:84:GLN:HE21	1.71	0.54
5:g:24:GLU:O	5:g:27:GLN:NE2	2.41	0.54
9:j:58:LEU:O	9:j:59:HIS:CG	2.61	0.54
12:q:109:MET:HE3	12:q:109:MET:C	2.32	0.54
12:q:196:LEU:H	12:q:196:LEU:HD12	1.72	0.54
36:DB:917:ASP:HB3	36:DB:923:ARG:HG2	1.90	0.54
39:Df:317:LEU:HB2	39:Df:330:ARG:HH21	1.72	0.54
49:DP:200:VAL:HB	49:DP:213:ILE:HB	1.89	0.54
53:X:-39:DA:H61	54:Y:39:DT:H3	1.54	0.54
53:X:-11:DG:H22	54:Y:11:DC:H42	1.54	0.54
56:PB:795:ILE:HB	56:PB:966:ILE:HB	1.89	0.54
68:w:397:LYS:CB	70:p:171:PHE:CE2	2.88	0.54
1:a:160:LEU:CG	1:a:219:LEU:HD21	2.38	0.54
1:a:348:LEU:HD13	1:a:425:VAL:HG12	1.89	0.54
1:a:440:PHE:CE2	1:a:508:MET:HB3	2.43	0.54
12:q:437:HIS:C	12:q:437:HIS:CD2	2.86	0.54
27:2:117:LEU:HG	27:2:130:SER:HB2	1.89	0.54
35:DA:567:LEU:HD22	36:DB:745:GLN:HG3	1.88	0.54
36:DB:579:LEU:HD22	36:DB:588:HIS:HB2	1.87	0.54
3:d:122:ALA:HA	3:d:125:VAL:HG22	1.90	0.54
5:g:23:ASP:O	5:g:26:ILE:HG22	2.08	0.54
12:q:482:GLN:H	12:q:634:ASN:ND2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:v:126:ASP:OD2	18:e:132:HIS:CD2	2.61	0.54
17:c:127:LEU:HB2	18:e:81:ILE:HD13	1.89	0.54
36:DB:75:VAL:HG23	36:DB:84:PHE:CE1	2.43	0.54
36:DB:320:ALA:O	36:DB:321:SER:HB3	2.06	0.54
37:DD:1085:LYS:HZ3	44:DL:83:MET:CE	2.20	0.54
40:DG:31:ALA:HB1	40:DG:39:LEU:HB2	1.89	0.54
53:X:-16:DG:N2	54:Y:16:DC:C2	2.74	0.54
68:w:41:LEU:CD1	68:w:85:MET:HB3	2.33	0.54
69:x:955:LEU:HD13	69:x:967:VAL:HG21	1.89	0.54
10:k:109:ARG:CB	10:k:109:ARG:CZ	2.85	0.54
11:n:230:PHE:CD2	11:n:296:LEU:CB	2.89	0.54
24:8:214:PRO:HG3	55:PA:1674:THR:CG2	2.37	0.54
31:6:350:GLY:HA3	31:6:374:TRP:HZ3	1.73	0.54
31:6:437:LEU:HB3	31:6:462:CYS:HB2	1.90	0.54
35:DA:396:LEU:HD11	39:Df:394:PRO:HG2	1.89	0.54
36:DB:884:VAL:HA	36:DB:887:ARG:HD3	1.90	0.54
53:X:1:DA:H2	54:Y:0:DG:C2	2.25	0.54
62:PH:57:ARG:HB2	62:PH:148:LEU:HD11	1.88	0.54
1:a:128:HIS:CG	1:a:128:HIS:O	2.60	0.54
4:f:130:PHE:HE2	15:v:62:HIS:HB3	1.72	0.54
5:g:109:LEU:HD11	11:n:133:LEU:HD12	1.90	0.54
6:h:40:LEU:HG	6:h:45:VAL:CG1	2.36	0.54
9:j:78:GLN:C	9:j:82:LYS:CD	2.77	0.54
11:n:359:ILE:HG12	11:n:372:ILE:HD11	1.89	0.54
15:v:82:LEU:CD1	15:v:86:LEU:HD23	2.35	0.54
21:o:776:TRP:O	21:o:780:VAL:HG23	2.08	0.54
28:3:229:TRP:HH2	29:4:74:TRP:HB3	1.72	0.54
38:DE:599:TYR:HB3	38:DE:611:LEU:HD11	1.90	0.54
39:Df:94:PHE:HB3	39:Df:105:TYR:HD2	1.72	0.54
68:w:10:GLU:OE1	68:w:66:PHE:HZ	1.91	0.54
1:a:270:ILE:O	1:a:270:ILE:HG22	2.08	0.54
5:g:28:GLU:OE1	5:g:28:GLU:HA	1.99	0.54
9:j:60:ASP:C	11:n:50:ARG:CB	2.80	0.54
23:0:258:PRO:CA	25:9:239:LYS:HZ3	2.21	0.54
23:0:268:ARG:HG3	25:9:176:THR:HG21	1.89	0.54
44:DL:106:ARG:HD2	44:DL:115:ASP:OD1	2.08	0.54
37:Dd:1084:LEU:HD22	42:Di:99:ARG:HH21	1.73	0.54
55:PA:927:GLU:O	55:PA:927:GLU:CG	2.55	0.54
59:PE:3:ASP:HB2	59:PE:47:LYS:HB2	1.90	0.54
59:PE:61:LEU:HD13	59:PE:73:PHE:HD2	1.73	0.54
68:w:231:VAL:O	68:w:1099:ASN:ND2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:1072:ILE:HD11	68:w:1126:LEU:HD22	1.89	0.54
1:a:109:TYR:HE1	1:a:150:PHE:HZ	1.56	0.54
1:a:417:TYR:HB2	1:a:469:VAL:CG2	2.36	0.54
2:m:56:LEU:CG	2:m:80:GLN:HE22	2.19	0.54
3:d:121:LEU:CD1	5:g:160:VAL:HG23	2.22	0.54
14:u:83:ALA:N	14:u:86:GLN:HB2	2.23	0.54
24:8:214:PRO:HG3	55:PA:1674:THR:CB	2.38	0.54
36:DB:304:PHE:HE1	36:DB:353:GLN:OE1	1.88	0.54
55:PA:375:ILE:HG22	55:PA:485:ASN:HD22	1.72	0.54
59:PE:162:ARG:NH1	60:PF:52:ILE:HG21	2.23	0.54
68:w:169:TYR:CE2	68:w:177:LEU:HD11	2.43	0.54
68:w:627:LEU:HD22	68:w:645:VAL:HG23	1.89	0.54
68:w:681:GLU:OE2	68:w:685:ARG:NH1	2.41	0.54
69:x:976:PRO:HA	69:x:979:ARG:HE	1.73	0.54
4:f:82:ARG:HH11	4:f:94:PRO:HB3	1.72	0.54
6:h:40:LEU:O	6:h:42:TRP:N	2.41	0.54
11:n:333:LYS:O	11:n:360:LYS:HA	2.07	0.54
31:6:628:SER:HB3	31:6:672:TYR:CD2	2.43	0.54
36:DB:841:LYS:HG3	41:DH:214:ILE:HB	1.89	0.54
40:DG:24:TYR:HD2	40:DG:58:VAL:CG1	2.20	0.54
55:PA:66:GLU:HG2	55:PA:69:GLY:H	1.72	0.54
56:PB:896:LEU:HD13	56:PB:900:GLU:HB3	1.88	0.54
68:w:339:ILE:O	68:w:343:LEU:HB2	2.08	0.54
3:d:131:LYS:NZ	14:u:104:LEU:HB2	2.12	0.54
3:d:156:SER:HB2	11:n:150:PRO:HD2	1.90	0.54
7:r:96:LYS:HG2	33:EA:146:ASP:OD1	2.08	0.54
8:t:1:MET:HE2	8:t:183:VAL:HB	1.90	0.54
11:n:435:LEU:HG	12:q:325:ILE:HD11	1.90	0.54
11:n:777:TYR:HA	11:n:780:VAL:HG22	1.89	0.54
12:q:326:VAL:HG12	12:q:331:ILE:HG12	1.90	0.54
15:v:111:GLU:HA	15:v:114:ARG:HE	1.72	0.54
18:e:60:VAL:HG23	18:e:60:VAL:O	2.08	0.54
21:o:759:ARG:HE	21:o:762:GLN:HG2	1.73	0.54
36:DB:873:LEU:CD1	36:DB:877:TYR:HE2	2.21	0.54
44:DL:106:ARG:NH1	44:DL:114:LYS:HZ3	2.01	0.54
55:PA:1054:MET:HA	55:PA:1058:PHE:HD2	1.72	0.54
67:FA:49:ARG:HB2	67:FA:54:LYS:HZ1	1.71	0.54
68:w:397:LYS:HB3	70:p:171:PHE:CE2	2.39	0.54
1:a:336:TYR:CD1	1:a:391:THR:HG23	2.43	0.53
2:m:112:ARG:NH1	16:z:600:ASP:H	2.04	0.53
11:n:549:TYR:HB2	11:n:571:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:437:HIS:CE1	12:q:472:GLU:H	2.21	0.53
16:z:480:LEU:HD23	16:z:480:LEU:O	2.08	0.53
16:z:548:THR:O	16:z:549:GLN:C	2.48	0.53
22:i:85:GLN:HG3	22:i:86:ASP:CG	2.31	0.53
23:0:245:LEU:HA	24:8:296:SER:HB2	1.90	0.53
24:8:118:MET:HG3	24:8:203:LEU:HD13	1.90	0.53
24:8:132:TRP:HA	24:8:132:TRP:CE3	2.43	0.53
40:DG:140:LEU:HA	40:DG:146:ARG:HH22	1.73	0.53
38:De:364:LYS:HB2	38:De:368:ASN:HD22	1.73	0.53
4:f:180:LEU:HG	11:n:299:PHE:CE1	2.33	0.53
5:g:33:LYS:H	5:g:33:LYS:NZ	2.05	0.53
6:h:110:ARG:C	6:h:110:ARG:HD3	2.33	0.53
11:n:589:GLN:OE1	68:w:25:MET:HG2	2.07	0.53
12:q:166:ARG:CG	12:q:166:ARG:HH11	2.21	0.53
18:e:49:GLU:CD	19:b:186:THR:CG2	2.77	0.53
21:o:762:GLN:C	68:w:74:LYS:HZ2	2.15	0.53
23:0:74:ILE:HA	23:0:77:LYS:HE3	1.89	0.53
25:9:3:HIS:HD2	25:9:6:SER:HA	1.72	0.53
45:Dc:33:LEU:HD13	43:Dj:197:MET:HE1	1.89	0.53
45:Dc:77:LEU:CD1	43:Dj:116:LEU:CD2	2.76	0.53
38:De:450:ARG:HB2	38:De:788:ARG:HA	1.90	0.53
53:X:-26:DA:H3'	53:X:-26:DA:P	2.48	0.53
55:PA:245:PRO:HA	55:PA:248:MET:HE2	1.91	0.53
55:PA:1180:ASN:HB3	55:PA:1182:GLN:HG3	1.89	0.53
1:a:106:ASP:N	1:a:106:ASP:OD1	2.41	0.53
1:a:226:VAL:HG12	1:a:226:VAL:O	2.08	0.53
9:j:105:PHE:CE1	14:u:52:GLU:HA	2.43	0.53
11:n:707:ASP:CB	21:o:684:ARG:NH2	2.72	0.53
11:n:715:ARG:HH22	17:c:311:GLN:NE2	1.97	0.53
11:n:864:ASN:ND2	11:n:867:GLN:OE1	2.41	0.53
17:c:204:MET:CE	17:c:206:SER:O	2.47	0.53
39:DF:233:GLY:HA2	39:DF:239:ARG:HE	1.73	0.53
40:DG:17:ILE:HG12	40:DG:91:ILE:HG21	1.90	0.53
51:BA:297:PRO:HB3	51:BA:310:VAL:HG21	1.90	0.53
54:Y:14:DC:H2"	54:Y:15:DC:C6	2.43	0.53
66:PL:33:PRO:HB2	66:PL:35:ARG:HH12	1.73	0.53
68:w:1:MET:HE3	68:w:1:MET:H1	1.72	0.53
68:w:781:SER:O	68:w:783:GLN:NE2	2.41	0.53
1:a:423:SER:HB2	1:a:503:SER:CB	2.32	0.53
4:f:49:VAL:HB	24:8:109:LEU:HD22	1.90	0.53
9:j:59:HIS:CA	11:n:50:ARG:CA	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:633:ARG:CG	12:q:633:ARG:HH21	2.20	0.53
12:q:647:SER:HB2	18:e:97:GLN:HE21	1.73	0.53
28:3:59:VAL:HG12	28:3:70:LEU:HD12	1.90	0.53
40:DG:79:THR:OG1	40:DG:84:THR:O	2.20	0.53
39:Df:230:ALA:HB1	39:Df:239:ARG:HA	1.90	0.53
52:FB:50:GLY:HA3	52:FB:51:ARG:NH2	2.24	0.53
55:PA:575:PRO:HG3	55:PA:594:LEU:HD11	1.90	0.53
55:PA:621:ILE:HG13	62:PH:40:ILE:HD12	1.90	0.53
56:PB:29:VAL:HG11	56:PB:635:LEU:HD21	1.89	0.53
69:x:628:VAL:HG13	69:x:636:ARG:HG2	1.91	0.53
5:g:143:LYS:HB3	5:g:143:LYS:HZ2	1.73	0.53
7:r:32:LEU:HD11	7:r:167:TYR:CE2	2.43	0.53
8:t:129:VAL:HG21	8:t:200:ILE:CD1	2.37	0.53
11:n:149:LEU:HG	14:u:9:GLN:HE22	1.73	0.53
11:n:247:LEU:HD21	11:n:278:VAL:HG21	1.91	0.53
12:q:577:ASP:HB2	12:q:597:PRO:HG3	1.91	0.53
16:z:560:TRP:CD1	16:z:561:PRO:HD2	2.44	0.53
17:c:200:VAL:HG13	17:c:214:VAL:HG12	1.91	0.53
26:1:205:MET:O	26:1:209:GLU:HG3	2.08	0.53
36:DB:652:GLN:O	36:DB:656:GLU:HB2	2.08	0.53
68:w:522:PRO:HG3	68:w:565:GLU:HG2	1.90	0.53
69:x:54:PRO:HA	69:x:90:ARG:HH11	1.74	0.53
69:x:358:ASP:OD1	69:x:389:ARG:NE	2.41	0.53
1:a:321:LEU:C	1:a:321:LEU:HD13	2.34	0.53
3:d:131:LYS:HZ2	14:u:104:LEU:CB	2.05	0.53
3:d:155:ILE:HG21	11:n:153:ALA:HB2	1.90	0.53
5:g:153:PHE:CE1	14:u:107:VAL:HG12	2.43	0.53
6:h:147:CYS:CB	15:v:41:LYS:CB	2.70	0.53
13:s:83:LEU:N	13:s:83:LEU:HD23	2.24	0.53
15:v:48:VAL:HG22	15:v:53:GLN:HB2	1.91	0.53
17:c:204:MET:HE3	17:c:208:PHE:O	2.05	0.53
26:1:161:LYS:C	26:1:314:VAL:HG11	2.34	0.53
26:1:411:MET:HG2	28:3:119:MET:HB2	1.90	0.53
40:DG:21:PRO:O	40:DG:25:ALA:N	2.33	0.53
51:BA:125:ALA:HB2	51:BA:135:VAL:HG21	1.90	0.53
55:PA:1134:PRO:HD2	55:PA:1137:PRO:HB3	1.89	0.53
68:w:261:ASP:OD1	68:w:261:ASP:N	2.38	0.53
3:d:131:LYS:CD	14:u:104:LEU:CG	2.64	0.53
3:d:136:GLU:CD	14:u:101:ALA:HB2	2.34	0.53
5:g:25:ASN:HA	5:g:27:GLN:HE22	1.71	0.53
5:g:96:LEU:HB2	9:j:102:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:143:LEU:HA	10:k:39:LYS:HZ1	1.74	0.53
8:t:98:LEU:HD12	8:t:102:PHE:CZ	2.43	0.53
11:n:229:GLU:HG3	11:n:300:CYS:CB	2.38	0.53
11:n:254:VAL:HG11	11:n:304:GLN:NE2	2.11	0.53
11:n:659:LEU:HD11	68:w:14:LYS:HG2	1.81	0.53
11:n:923:CYS:SG	11:n:924:ILE:N	2.82	0.53
14:u:57:LEU:HD13	16:z:492:ARG:NE	2.24	0.53
27:2:186:ILE:HG12	27:2:211:LEU:HD13	1.91	0.53
32:7:626:VAL:HB	32:7:629:GLN:HB2	1.91	0.53
33:EA:106:LYS:HB3	34:EB:218:LYS:HE3	1.90	0.53
36:DB:62:ARG:HD3	36:DB:129:LYS:HA	1.91	0.53
38:DE:304:LYS:HB3	38:DE:338:TYR:H	1.73	0.53
37:Dd:843:VAL:N	37:Dd:845:LEU:HD21	2.24	0.53
55:PA:530:SER:HB2	55:PA:532:ARG:HG2	1.89	0.53
68:w:1:MET:H2	68:w:4:GLN:HG3	1.73	0.53
68:w:999:ASP:N	68:w:999:ASP:OD1	2.41	0.53
1:a:248:SER:HB3	1:a:251:LEU:HB2	1.90	0.53
7:r:70:LEU:CD1	7:r:123:PHE:CZ	2.92	0.53
12:q:140:ASN:N	12:q:141:PRO:HD2	2.24	0.53
12:q:437:HIS:ND1	12:q:471:TYR:C	2.67	0.53
14:u:71:VAL:HG21	16:z:582:LEU:HD11	1.90	0.53
17:c:204:MET:SD	17:c:208:PHE:C	2.92	0.53
21:o:748:PHE:O	21:o:752:VAL:HG13	2.09	0.53
23:0:192:LEU:CD2	23:0:196:LEU:HD22	2.39	0.53
31:6:644:LEU:HD23	31:6:657:ALA:HB1	1.91	0.53
38:DE:450:ARG:HB2	38:DE:788:ARG:HA	1.91	0.53
40:DG:23:GLU:O	40:DG:27:THR:HG23	2.08	0.53
38:De:473:LEU:HD23	38:De:796:ALA:HB2	1.91	0.53
39:Df:286:VAL:HG12	39:Df:290:MET:HE3	1.91	0.53
51:BA:111:ASP:HB3	51:BA:114:MET:HB2	1.90	0.53
69:x:472:ASN:ND2	69:x:496:SER:OG	2.42	0.53
5:g:98:ARG:HG2	13:s:74:SER:HA	1.90	0.53
5:g:109:LEU:HD21	11:n:133:LEU:CG	2.32	0.53
6:h:19:VAL:HG12	12:q:113:TYR:CD2	2.44	0.53
7:r:124:ARG:CZ	7:r:124:ARG:CA	2.86	0.53
7:r:171:LEU:HD11	7:r:186:MET:HG2	1.91	0.53
9:j:34:GLN:CB	9:j:37:LEU:HG	2.39	0.53
13:s:152:PHE:C	13:s:154:LEU:H	2.17	0.53
17:c:167:SER:OG	17:c:171:ARG:NH1	2.41	0.53
21:o:707:ILE:HG23	21:o:720:PRO:CA	2.37	0.53
32:7:471:LEU:HB2	32:7:473:PHE:HD1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DE:605:HIS:HA	38:DE:629:ASP:HB3	1.91	0.53
39:Df:72:ASP:HA	39:Df:75:LEU:HD12	1.91	0.53
68:w:1302:LYS:NZ	68:w:1308:ASP:OD1	2.41	0.53
69:x:175:ARG:HH21	69:x:221:LEU:HD22	1.73	0.53
2:m:30:ASN:CB	3:d:177:PRO:HD2	2.39	0.53
5:g:24:GLU:C	5:g:27:GLN:HE21	2.17	0.53
9:j:26:VAL:HG11	9:j:38:ASN:CG	2.18	0.53
12:q:123:LYS:HG2	12:q:124:PHE:CE2	2.43	0.53
13:s:84:ILE:CG2	13:s:90:GLU:HA	2.39	0.53
19:b:67:LEU:HD22	19:b:116:LEU:HD12	1.91	0.53
23:0:250:PRO:HD2	23:0:251:LEU:HD22	1.91	0.53
26:1:279:GLU:O	26:1:281:TYR:N	2.38	0.53
35:DA:747:LEU:HG	35:DA:883:GLU:HG3	1.90	0.53
36:DB:904:TYR:CE1	36:DB:908:GLN:CG	2.91	0.53
44:DL:106:ARG:NH1	44:DL:115:ASP:N	2.57	0.53
52:FB:147:LYS:HG3	52:FB:148:VAL:H	1.74	0.53
55:PA:1654:SER:CB	55:PA:1655:PRO:HD3	2.39	0.53
68:w:625:SER:HB2	68:w:674:THR:HG22	1.89	0.53
69:x:483:THR:C	69:x:485:PRO:CD	2.82	0.53
1:a:367:LEU:HD22	1:a:509:ARG:NH1	2.23	0.52
2:m:17:ARG:HH22	5:g:33:LYS:CB	2.22	0.52
4:f:177:VAL:HG12	11:n:270:GLN:CB	2.37	0.52
9:j:102:MET:CE	9:j:106:LYS:NZ	2.73	0.52
11:n:203:LEU:HD11	11:n:222:VAL:HG12	1.90	0.52
11:n:208:LEU:HD12	11:n:208:LEU:O	2.08	0.52
11:n:589:GLN:OE1	68:w:25:MET:CG	2.57	0.52
15:v:16:GLN:O	15:v:20:LYS:HG2	2.08	0.52
18:e:45:VAL:CG1	20:l:92:LEU:HD11	2.40	0.52
34:EB:88:ARG:HD3	34:EB:97:LEU:HD21	1.90	0.52
37:DD:886:GLY:HA3	37:DD:891:ILE:HG12	1.90	0.52
38:De:695:LEU:HD12	38:De:705:GLY:HA3	1.90	0.52
56:PB:815:LYS:HB3	56:PB:920:LYS:HG2	1.91	0.52
68:w:115:TRP:HE1	68:w:163:ALA:HB2	1.74	0.52
1:a:127:HIS:CE1	1:a:171:THR:CG2	2.91	0.52
1:a:229:SER:N	1:a:502:MET:HB2	2.23	0.52
1:a:439:GLN:HE22	69:x:15:LYS:NZ	2.07	0.52
4:f:37:SER:HB3	5:g:10:ALA:CA	2.39	0.52
5:g:99:SER:HB2	13:s:75:THR:HG21	1.89	0.52
6:h:41:THR:HG22	6:h:44:SER:H	1.73	0.52
7:r:192:GLN:OE1	15:v:8:PRO:HA	2.09	0.52
11:n:861:LYS:HE3	17:c:30:ARG:CD	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:s:92:ALA:O	13:s:96:PHE:CE2	2.58	0.52
14:u:73:ILE:C	14:u:75:SER:H	2.17	0.52
16:z:540:LEU:C	16:z:540:LEU:HD22	2.34	0.52
36:DB:920:PRO:HA	36:DB:923:ARG:CD	2.39	0.52
61:PG:143:ILE:HA	61:PG:169:GLY:HA2	1.91	0.52
69:x:567:MET:H	69:x:612:LYS:NZ	2.07	0.52
1:a:466:VAL:O	1:a:466:VAL:HG13	2.08	0.52
4:f:130:PHE:CE2	15:v:62:HIS:HB3	2.44	0.52
6:h:19:VAL:HG11	12:q:113:TYR:CA	2.39	0.52
11:n:449:SER:OG	11:n:450:GLU:N	2.41	0.52
12:q:7:VAL:HG21	14:u:87:ALA:HB1	1.91	0.52
12:q:9:ILE:CD1	14:u:90:LEU:CD2	2.55	0.52
12:q:166:ARG:CZ	12:q:166:ARG:CB	2.86	0.52
21:o:690:LEU:O	21:o:692:ASN:ND2	2.42	0.52
24:8:214:PRO:HG3	55:PA:1674:THR:HG21	1.91	0.52
32:7:2:LYS:HD3	32:7:9:LEU:HD13	1.91	0.52
34:EB:119:LEU:HA	34:EB:123:ALA:HB3	1.91	0.52
49:DP:163:PRO:HA	49:DP:262:CYS:HB3	1.90	0.52
59:PE:75:PHE:HE1	59:PE:93:ARG:HD3	1.75	0.52
62:PH:22:PHE:HB2	62:PH:25:VAL:HB	1.92	0.52
63:PI:88:LYS:HE3	63:PI:121:HIS:HB2	1.92	0.52
68:w:378:GLN:HE22	68:w:532:THR:HA	1.75	0.52
1:a:504:ILE:H	1:a:505:PRO:HD3	1.75	0.52
2:m:30:ASN:N	3:d:176:TYR:HB2	2.24	0.52
3:d:131:LYS:CB	14:u:104:LEU:HD13	2.29	0.52
8:t:1:MET:HB3	8:t:185:GLY:H	1.75	0.52
11:n:879:LEU:HA	11:n:882:ILE:HG22	1.90	0.52
56:PB:1025:ASN:HA	56:PB:1042:PHE:HA	1.91	0.52
1:a:364:TYR:CD1	1:a:430:LEU:HB2	2.45	0.52
3:d:154:ARG:CZ	3:d:155:ILE:HB	2.40	0.52
6:h:67:LYS:HD3	23:0:141:THR:OG1	2.10	0.52
9:j:70:TYR:CE1	9:j:80:TYR:HB3	2.39	0.52
10:k:101:ARG:NH1	10:k:101:ARG:CB	2.73	0.52
11:n:231:GLU:HB2	11:n:253:LEU:CD2	2.37	0.52
11:n:526:SER:HB2	68:w:45:ARG:CZ	2.39	0.52
11:n:836:GLY:O	11:n:846:ASN:ND2	2.38	0.52
29:4:152:ALA:HB2	29:4:284:THR:HG22	1.92	0.52
38:De:556:ASN:HD21	38:De:573:GLN:HG3	1.74	0.52
49:DP:314:GLY:HA3	53:X:-27:DA:H4'	1.92	0.52
53:X:-11:DG:N2	54:Y:11:DC:N4	2.54	0.52
55:PA:1231:ILE:HG12	55:PA:1298:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:PH:27:ARG:HD2	62:PH:40:ILE:HG23	1.91	0.52
1:a:107:MET:HE2	1:a:107:MET:C	2.35	0.52
5:g:97:ILE:HG23	9:j:103:LYS:HE2	0.54	0.52
7:r:53:ASP:OD2	12:q:396:ALA:HB2	2.08	0.52
12:q:482:GLN:HB2	12:q:634:ASN:ND2	2.22	0.52
14:u:18:GLN:HB3	14:u:62:ILE:HG13	1.92	0.52
15:v:130:LEU:N	15:v:130:LEU:CD2	2.73	0.52
31:6:401:ILE:HG23	31:6:433:GLN:NE2	2.25	0.52
34:EB:155:LEU:HD22	34:EB:189:ILE:HG12	1.90	0.52
35:DA:968:ILE:HG13	35:DA:969:PRO:HD2	1.91	0.52
38:De:463:PHE:HB2	39:Df:136:LEU:HB2	1.92	0.52
38:De:466:PHE:HB2	38:De:796:ALA:HA	1.91	0.52
59:PE:21:CYS:HB2	59:PE:26:TYR:HB2	1.91	0.52
70:p:304:SER:OG	70:p:349:ASP:O	2.28	0.52
1:a:423:SER:CB	1:a:503:SER:CB	2.85	0.52
4:f:181:LEU:HD23	4:f:184:LEU:HD21	1.91	0.52
7:r:51:PHE:O	7:r:51:PHE:CD1	2.63	0.52
9:j:12:LEU:O	9:j:16:VAL:HG23	2.10	0.52
11:n:156:TYR:CZ	11:n:168:ARG:CG	2.76	0.52
18:e:55:CYS:HG	20:l:52:PHE:HZ	1.57	0.52
20:l:51:ILE:O	20:l:55:LEU:HG	2.09	0.52
21:o:718:VAL:HG13	21:o:742:GLN:OE1	2.10	0.52
23:0:264:GLU:HB2	23:0:269:LEU:HB2	1.92	0.52
34:EB:136:LYS:N	34:EB:136:LYS:HD2	2.24	0.52
36:DB:212:MET:HA	36:DB:253:PRO:HA	1.91	0.52
38:DE:561:SER:HB2	38:DE:588:VAL:HB	1.91	0.52
61:PG:60:GLN:HE21	61:PG:63:ARG:HD3	1.75	0.52
68:w:8:ILE:O	68:w:12:VAL:HG12	2.04	0.52
3:d:149:ILE:O	3:d:152:ALA:HB3	2.10	0.52
6:h:97:VAL:HG23	6:h:104:VAL:HG21	1.92	0.52
10:k:38:GLU:HG3	10:k:38:GLU:O	2.10	0.52
11:n:780:VAL:HG12	11:n:808:LEU:HD11	1.90	0.52
11:n:904:PHE:HD1	11:n:916:LEU:HD11	1.74	0.52
14:u:20:CYS:SG	14:u:21:ASN:N	2.83	0.52
15:v:133:GLU:OE1	15:v:133:GLU:HA	2.10	0.52
20:l:44:ILE:O	20:l:48:THR:HG23	2.09	0.52
29:4:156:TRP:HB2	29:4:286:LEU:HD11	1.91	0.52
39:Df:62:LYS:H	39:Df:62:LYS:HD2	1.75	0.52
46:Dk:147:SER:HB3	46:Dk:150:VAL:HG23	1.92	0.52
49:DP:171:THR:HG22	49:DP:220:VAL:HG22	1.90	0.52
55:PA:790:GLN:HA	55:PA:822:PHE:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:PC:58:VAL:HG11	64:PJ:59:LEU:HB3	1.91	0.52
1:a:329:LEU:C	1:a:329:LEU:CD2	2.82	0.52
5:g:48:GLN:H	5:g:48:GLN:CD	2.13	0.52
5:g:83:MET:HE2	9:j:120:ASP:OD1	2.09	0.52
6:h:19:VAL:CG1	12:q:113:TYR:CB	2.75	0.52
8:t:129:VAL:HG11	8:t:200:ILE:CD1	2.40	0.52
11:n:845:SER:OG	11:n:846:ASN:N	2.43	0.52
12:q:561:GLU:OE2	12:q:588:SER:OG	2.28	0.52
12:q:576:GLY:O	12:q:619:ARG:NH2	2.43	0.52
14:u:7:GLN:HE22	16:z:594:LEU:HD22	1.75	0.52
29:4:75:VAL:HG11	29:4:83:GLN:HB2	1.90	0.52
39:DF:296:TYR:HD2	39:DF:299:LYS:HB2	1.74	0.52
37:Dd:885:ILE:HG13	44:Dl:96:VAL:HG11	1.91	0.52
37:Dd:894:LEU:HA	44:Dl:111:LEU:HB3	1.92	0.52
39:Df:96:PHE:HE1	39:Df:103:GLU:HA	1.75	0.52
51:BA:149:LYS:HA	51:BA:152:LYS:HB2	1.91	0.52
69:x:566:GLU:C	69:x:568:LYS:H	2.18	0.52
3:d:44:LEU:CD2	3:d:68:LEU:HD12	2.38	0.52
8:t:24:LEU:HG	8:t:126:VAL:HG11	1.92	0.52
9:j:74:GLY:O	9:j:75:ARG:HG3	2.10	0.52
9:j:89:LEU:CD2	13:s:93:TYR:OH	2.51	0.52
10:k:115:LEU:CD1	18:e:133:LEU:HD12	2.39	0.52
12:q:149:LYS:HE2	15:v:40:ALA:CA	2.40	0.52
19:b:181:CYS:SG	20:l:82:LEU:HD22	2.50	0.52
33:EA:110:MET:HB2	34:EB:218:LYS:HG3	1.91	0.52
42:DI:61:ALA:HB3	42:DI:63:LYS:HE2	1.92	0.52
38:De:271:GLN:HB2	38:De:279:LEU:HD11	1.92	0.52
54:Y:-15:DT:H1'	54:Y:-14:DG:H5'	1.92	0.52
55:PA:390:PHE:HA	55:PA:507:GLN:HE22	1.75	0.52
69:x:86:ASP:O	69:x:88:PHE:N	2.43	0.52
7:r:124:ARG:HB2	7:r:124:ARG:CZ	2.40	0.51
9:j:37:LEU:O	9:j:41:LEU:HG	2.10	0.51
10:k:41:ASN:O	10:k:45:LEU:HB2	2.10	0.51
11:n:156:TYR:OH	11:n:168:ARG:CD	2.58	0.51
11:n:643:HIS:CD2	12:q:560:ILE:HA	2.45	0.51
33:EA:129:CYS:CB	33:EA:154:CYS:SG	2.96	0.51
38:DE:294:ASN:HD22	38:DE:297:MET:HG2	1.76	0.51
53:X:-14:DG:H2'	53:X:-13:DG:C8	2.45	0.51
68:w:1:MET:N	68:w:1:MET:CE	2.73	0.51
5:g:74:HIS:H	5:g:74:HIS:CD2	2.27	0.51
5:g:93:LEU:HD22	9:j:106:LYS:NZ	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:32:LEU:HD11	7:r:167:TYR:CZ	2.46	0.51
7:r:32:LEU:CD1	7:r:167:TYR:CZ	2.93	0.51
9:j:26:VAL:HG12	9:j:38:ASN:ND2	2.15	0.51
9:j:76:ASN:OD1	9:j:78:GLN:N	2.42	0.51
9:j:78:GLN:HB3	9:j:82:LYS:NZ	2.18	0.51
10:k:73:VAL:HG23	15:v:92:PRO:HG2	1.91	0.51
20:l:36:ILE:O	20:l:39:GLU:HG2	2.10	0.51
25:9:11:TRP:HH2	25:9:154:LEU:HA	1.75	0.51
29:4:156:TRP:HZ2	29:4:211:GLN:HB3	1.75	0.51
39:DF:335:ARG:HE	39:DF:382:GLU:HB2	1.76	0.51
53:X:-26:DA:OP2	53:X:-26:DA:C3'	2.58	0.51
68:w:31:GLU:O	68:w:32:ASP:HB2	2.10	0.51
2:m:74:HIS:HB2	11:n:166:TYR:HB2	1.92	0.51
8:t:131:MET:SD	8:t:132:GLY:N	2.83	0.51
9:j:85:LEU:CD1	13:s:96:PHE:CE2	2.92	0.51
10:k:43:ARG:CB	10:k:43:ARG:NH1	2.73	0.51
11:n:292:MET:O	11:n:295:CYS:SG	2.62	0.51
21:o:725:VAL:HA	21:o:734:PRO:HB3	1.92	0.51
21:o:775:THR:HA	21:o:778:GLN:HG2	1.91	0.51
24:8:143:LEU:HD11	24:8:151:LEU:HG	1.93	0.51
32:7:506:SER:HB3	32:7:623:VAL:H	1.76	0.51
35:DA:484:ILE:HG23	39:Df:310:THR:HA	1.92	0.51
37:DD:936:GLN:HA	42:DI:127:TYR:HA	1.93	0.51
63:PI:73:SER:HA	63:PI:95:VAL:HG21	1.92	0.51
65:PK:81:TYR:HE2	65:PK:86:ALA:HB2	1.75	0.51
70:p:91:GLN:NE2	70:p:137:LEU:O	2.43	0.51
1:a:127:HIS:HE1	1:a:171:THR:HG22	1.73	0.51
3:d:131:LYS:NZ	14:u:104:LEU:CG	2.73	0.51
5:g:63:GLY:C	5:g:64:ILE:HG12	2.34	0.51
9:j:22:LEU:O	9:j:26:VAL:HG23	2.10	0.51
10:k:41:ASN:O	10:k:45:LEU:CB	2.59	0.51
11:n:545:LEU:CD1	11:n:653:PRO:N	2.73	0.51
13:s:78:THR:OG1	13:s:80:SER:OG	2.21	0.51
17:c:240:GLN:O	17:c:243:THR:OG1	2.26	0.51
56:PB:310:VAL:HG22	67:FA:164:TRP:HZ2	1.75	0.51
68:w:958:ASN:N	68:w:958:ASN:OD1	2.40	0.51
69:x:618:VAL:HG13	69:x:673:MET:HE1	1.92	0.51
2:m:64:ALA:HA	2:m:67:LEU:HD12	1.92	0.51
3:d:169:PRO:C	55:PA:1793:THR:HG21	2.35	0.51
3:d:169:PRO:C	55:PA:1795:PRO:HG2	2.33	0.51
4:f:169:SER:O	11:n:267:HIS:CE1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:19:VAL:HG11	12:q:113:TYR:HA	1.93	0.51
7:r:60:LEU:HB2	7:r:123:PHE:CE1	2.44	0.51
8:t:78:LEU:HD22	8:t:78:LEU:H	1.74	0.51
11:n:545:LEU:HD11	11:n:653:PRO:N	2.25	0.51
12:q:9:ILE:HD11	14:u:90:LEU:HD21	1.84	0.51
26:1:358:ILE:HG22	26:1:359:GLU:HG3	1.91	0.51
38:DE:586:TYR:HB3	38:DE:605:HIS:HB3	1.93	0.51
42:DI:73:LEU:HD22	44:DL:105:HIS:CE1	2.46	0.51
37:Dd:878:LEU:CD1	44:Dl:57:VAL:HG11	2.40	0.51
38:De:245:VAL:HG12	38:De:282:LEU:HD11	1.90	0.51
49:DP:174:LEU:HD12	49:DP:178:LEU:HD11	1.93	0.51
52:FB:160:GLN:HB3	56:PB:428:ASP:HB3	1.93	0.51
68:w:633:VAL:O	68:w:817:ARG:NH2	2.43	0.51
1:a:223:LYS:NZ	1:a:251:LEU:C	2.68	0.51
4:f:101:ILE:HD13	6:h:105:VAL:HB	1.92	0.51
7:r:21:TYR:O	7:r:172:SER:HA	2.10	0.51
9:j:59:HIS:CA	11:n:50:ARG:N	2.74	0.51
9:j:63:VAL:N	9:j:64:PRO:HD2	2.26	0.51
9:j:89:LEU:HD22	13:s:84:ILE:HG13	1.87	0.51
10:k:109:ARG:CB	10:k:109:ARG:NH1	2.74	0.51
11:n:306:GLU:HA	11:n:309:HIS:HB3	1.91	0.51
12:q:17:LYS:HE2	12:q:30:TYR:CD2	2.43	0.51
12:q:149:LYS:HD2	15:v:40:ALA:CA	2.34	0.51
16:z:572:ASN:N	16:z:572:ASN:OD1	2.42	0.51
33:EA:145:PHE:HA	33:EA:152:PHE:HA	1.92	0.51
39:DF:246:ILE:HA	39:DF:252:LEU:HD13	1.93	0.51
46:Dk:188:ARG:NH1	44:Dl:128:ILE:HG22	2.26	0.51
55:PA:1454:VAL:HA	55:PA:1465:PRO:HD2	1.92	0.51
56:PB:556:ILE:HG23	56:PB:560:ALA:HB3	1.91	0.51
1:a:94:LEU:O	1:a:94:LEU:HG	2.10	0.51
8:t:153:CYS:SG	8:t:156:LEU:HD23	2.50	0.51
11:n:259:THR:CG2	11:n:311:GLN:HE21	2.24	0.51
11:n:544:ARG:HD3	11:n:716:ASN:O	2.10	0.51
12:q:117:SER:O	12:q:120:ARG:HB3	2.11	0.51
15:v:85:PHE:HB2	15:v:89:ASN:HD22	1.76	0.51
18:e:77:VAL:HA	18:e:80:CYS:SG	2.51	0.51
22:i:118:LEU:HD22	22:i:119:GLN:NE2	2.26	0.51
29:4:385:PRO:HB2	29:4:387:ILE:HG22	1.93	0.51
32:7:415:THR:HB	32:7:438:MET:HE3	1.93	0.51
38:De:586:TYR:HB3	38:De:605:HIS:HB3	1.92	0.51
55:PA:460:ARG:HE	55:PA:494:ALA:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:1036:ASP:OD1	68:w:1036:ASP:N	2.39	0.51
3:d:136:GLU:HG3	14:u:104:LEU:HD21	1.93	0.51
5:g:69:PRO:HD2	5:g:77:GLU:OE2	2.11	0.51
8:t:47:HIS:HB3	8:t:103:GLN:HB3	1.93	0.51
8:t:96:VAL:O	8:t:99:LYS:HB3	2.11	0.51
8:t:154:TRP:HA	8:t:176:PHE:CE2	2.46	0.51
9:j:34:GLN:OE1	9:j:37:LEU:HG	2.11	0.51
10:k:14:LEU:N	10:k:14:LEU:HD23	2.24	0.51
11:n:446:CYS:SG	11:n:447:GLY:N	2.83	0.51
11:n:589:GLN:OE1	68:w:25:MET:SD	2.69	0.51
12:q:633:ARG:CZ	12:q:633:ARG:CB	2.86	0.51
24:8:261:PHE:CZ	24:8:272:ILE:HG21	2.46	0.51
26:1:285:SER:O	26:1:286:VAL:C	2.54	0.51
27:2:118:THR:HG22	27:2:126:LYS:HE3	1.92	0.51
36:DB:597:ARG:NH2	36:DB:603:LYS:O	2.44	0.51
39:Df:290:MET:HE1	39:Df:336:LEU:HG	1.93	0.51
55:PA:883:ILE:HD13	55:PA:1423:ASP:HB2	1.92	0.51
68:w:1241:THR:OG1	68:w:1242:GLU:N	2.44	0.51
6:h:61:LYS:HB2	15:v:56:GLN:NE2	2.22	0.51
6:h:147:CYS:SG	15:v:41:LYS:CB	2.92	0.51
7:r:152:LEU:N	7:r:160:THR:HA	2.26	0.51
9:j:102:MET:HB2	14:u:26:LEU:CD2	2.37	0.51
10:k:109:ARG:CZ	10:k:109:ARG:HB3	2.41	0.51
12:q:645:ALA:O	20:l:111:VAL:CG2	2.59	0.51
14:u:4:ARG:HD2	16:z:596:TYR:HA	1.93	0.51
18:e:49:GLU:OE1	19:b:186:THR:HG21	2.11	0.51
21:o:688:LYS:HG2	21:o:712:ASP:HB3	1.93	0.51
24:8:302:THR:HG22	24:8:304:GLY:H	1.75	0.51
26:1:377:LYS:HB2	28:3:286:GLU:HB2	1.93	0.51
28:3:219:GLN:HG2	28:3:221:PRO:HD2	1.92	0.51
49:DP:239:ARG:CZ	49:DP:239:ARG:HB3	2.40	0.51
56:PB:1137:CYS:HB3	56:PB:1142:ASN:HD21	1.76	0.51
67:FA:118:VAL:HG21	67:FA:142:ASN:HA	1.93	0.51
68:w:19:GLU:HG2	68:w:25:MET:HE3	1.93	0.51
70:p:437:SER:OG	70:p:438:TRP:N	2.43	0.51
3:d:169:PRO:CB	55:PA:1795:PRO:CG	2.89	0.51
5:g:109:LEU:HD11	11:n:133:LEU:CG	2.41	0.51
8:t:128:THR:O	8:t:128:THR:OG1	2.27	0.51
9:j:39:GLN:HB3	9:j:43:PHE:HE2	1.75	0.51
9:j:43:PHE:CE2	13:s:151:GLY:CA	2.93	0.51
9:j:89:LEU:HD22	13:s:84:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:327:GLU:HG3	11:n:356:LYS:HG2	1.91	0.51
11:n:915:ARG:NE	11:n:923:CYS:SG	2.84	0.51
12:q:166:ARG:CB	12:q:166:ARG:NH1	2.73	0.51
12:q:523:ASP:HB3	12:q:563:ILE:HD12	1.92	0.51
26:1:161:LYS:O	26:1:314:VAL:HG11	2.10	0.51
37:Dd:844:ASN:HA	37:Dd:847:GLU:CD	2.35	0.51
57:PC:206:SER:HB3	57:PC:209:SER:HB3	1.93	0.51
70:p:398:SER:OG	70:p:400:GLN:NE2	2.43	0.51
2:m:18:PHE:HA	5:g:36:PRO:HG3	1.93	0.50
4:f:177:VAL:CG1	11:n:270:GLN:HG3	2.41	0.50
11:n:907:LEU:HD21	19:b:118:LEU:HA	1.93	0.50
12:q:149:LYS:CE	15:v:40:ALA:CA	2.83	0.50
12:q:188:LEU:HD23	12:q:189:ARG:HG3	1.92	0.50
17:c:178:ILE:HG23	17:c:192:VAL:HG22	1.92	0.50
43:DJ:128:PRO:HB2	43:DJ:160:GLN:HE22	1.75	0.50
52:FB:127:LEU:HA	52:FB:130:LEU:HB2	1.92	0.50
55:PA:1028:PRO:O	55:PA:1029:LEU:HB3	2.11	0.50
55:PA:1668:SER:HB2	55:PA:1669:PRO:HD2	1.92	0.50
68:w:872:ARG:HB3	68:w:874:HIS:HD2	1.76	0.50
4:f:180:LEU:CD1	11:n:299:PHE:CD1	2.93	0.50
9:j:79:LEU:CD1	13:s:111:ASP:CB	2.83	0.50
11:n:256:ASP:HB2	11:n:395:LEU:HB2	1.92	0.50
23:0:300:ALA:HA	25:9:166:PRO:HB3	1.93	0.50
24:8:172:GLN:H	24:8:183:LEU:HD12	1.75	0.50
38:De:464:TYR:HB3	39:Df:131:LEU:HD11	1.92	0.50
52:FB:104:LEU:HD13	67:FA:47:LEU:HB3	1.93	0.50
55:PA:382:ARG:HH11	65:PK:1:MET:N	2.08	0.50
62:PH:65:TYR:HA	62:PH:84:ARG:HB3	1.92	0.50
68:w:366:ILE:HG23	68:w:369:ARG:HD3	1.94	0.50
1:a:429:ILE:O	1:a:429:ILE:HG13	2.11	0.50
2:m:107:HIS:O	2:m:111:LYS:HB3	2.12	0.50
3:d:176:TYR:HB2	3:d:177:PRO:CD	2.34	0.50
9:j:43:PHE:HZ	13:s:151:GLY:CA	2.11	0.50
11:n:127:ILE:HA	14:u:27:GLN:NE2	2.24	0.50
16:z:560:TRP:HD1	16:z:561:PRO:HD2	1.75	0.50
18:e:49:GLU:HG2	20:l:89:PHE:CD1	2.42	0.50
36:DB:741:PHE:CD1	36:DB:747:TYR:HB2	2.46	0.50
38:DE:718:ARG:HD2	38:DE:784:HIS:HA	1.94	0.50
38:De:332:ILE:HA	38:De:336:HIS:HD2	1.76	0.50
53:X:-21:DG:N2	53:X:-20:DG:C2	2.79	0.50
55:PA:1163:HIS:HA	55:PA:1300:GLY:HA3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:418:GLN:HA	68:w:421:HIS:HD2	1.75	0.50
68:w:1193:PHE:C	68:w:1195:ALA:H	2.19	0.50
3:d:128:ALA:C	14:u:108:VAL:HG21	2.36	0.50
3:d:128:ALA:O	3:d:131:LYS:HB2	2.11	0.50
3:d:136:GLU:OE2	14:u:101:ALA:HB2	2.12	0.50
5:g:158:GLU:OE2	5:g:158:GLU:HA	2.09	0.50
7:r:206:ARG:HE	7:r:206:ARG:C	2.19	0.50
12:q:186:GLU:HB3	12:q:243:LEU:CD2	2.42	0.50
12:q:633:ARG:NH2	12:q:633:ARG:CB	2.74	0.50
17:c:200:VAL:HA	17:c:214:VAL:HA	1.92	0.50
18:e:49:GLU:OE1	19:b:186:THR:CG2	2.60	0.50
24:8:271:LEU:HD13	24:8:292:MET:HG3	1.93	0.50
36:DB:722:LEU:HG	36:DB:726:MET:HE2	1.93	0.50
37:DD:1058:VAL:HB	44:DL:76:LEU:HD23	1.94	0.50
53:X:-24:DA:C5'	53:X:-24:DA:H8	2.25	0.50
53:X:-24:DA:H8	53:X:-24:DA:H5"	1.76	0.50
53:X:-15:DG:N2	54:Y:16:DC:C2	2.79	0.50
55:PA:948:ILE:HG23	55:PA:1007:ILE:HG23	1.93	0.50
68:w:363:ARG:HB3	68:w:365:LEU:HG	1.93	0.50
68:w:767:TRP:HE1	68:w:804:ASN:HD21	1.58	0.50
68:w:1200:TYR:CD2	68:w:1200:TYR:O	2.64	0.50
1:a:340:TYR:O	1:a:344:THR:HG23	2.11	0.50
5:g:83:MET:HG3	9:j:123:LYS:HE3	1.93	0.50
5:g:124:ASN:O	5:g:128:PRO:HD2	2.12	0.50
5:g:153:PHE:CD1	5:g:153:PHE:C	2.89	0.50
11:n:171:THR:OG1	12:q:20:HIS:HA	2.11	0.50
11:n:197:GLN:HA	11:n:200:ARG:HD2	1.93	0.50
11:n:207:ASP:N	11:n:207:ASP:OD1	2.44	0.50
12:q:95:TRP:N	12:q:95:TRP:CD1	2.79	0.50
12:q:523:ASP:CB	12:q:563:ILE:HD12	2.41	0.50
15:v:41:LYS:O	15:v:42:ILE:HB	2.10	0.50
15:v:119:LEU:CD1	15:v:123:ILE:HG13	2.42	0.50
18:e:49:GLU:CG	19:b:186:THR:HG21	2.41	0.50
22:i:79:ASP:HB2	22:i:85:GLN:HB3	1.92	0.50
27:2:344:PHE:HA	27:2:351:GLU:HA	1.94	0.50
29:4:407:VAL:HG11	29:4:448:HIS:HB2	1.93	0.50
32:7:634:LYS:HA	32:7:637:LEU:HD12	1.93	0.50
35:DA:1177:LYS:HE2	35:DA:1179:TYR:HB2	1.94	0.50
36:DB:33:VAL:HA	36:DB:49:VAL:HG22	1.94	0.50
36:DB:394:TRP:O	36:DB:398:GLU:HG2	2.12	0.50
44:DL:102:LEU:HD13	44:DL:118:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:De:570:TRP:HB3	38:De:577:CYS:HA	1.93	0.50
51:BA:137:ARG:HB2	56:PB:823:PHE:HE1	1.76	0.50
68:w:150:ASN:O	68:w:199:TRP:CE2	2.64	0.50
68:w:726:ASN:ND2	68:w:726:ASN:N	2.60	0.50
1:a:274:ILE:HG22	1:a:274:ILE:O	2.11	0.50
1:a:445:LEU:HD11	1:a:449:ARG:HH21	1.76	0.50
2:m:124:GLN:OE1	16:z:590:ARG:HD2	2.00	0.50
3:d:111:GLN:HA	3:d:114:LEU:HD23	1.94	0.50
3:d:121:LEU:CD2	5:g:160:VAL:CG1	2.78	0.50
4:f:78:LEU:HD11	6:h:81:LEU:CD2	2.39	0.50
5:g:33:LYS:HD2	5:g:33:LYS:O	2.12	0.50
5:g:157:LEU:HD23	5:g:157:LEU:C	2.36	0.50
6:h:170:LYS:HE2	6:h:172:THR:HG23	1.90	0.50
10:k:37:LYS:HE3	10:k:37:LYS:N	2.16	0.50
11:n:359:ILE:HG23	11:n:372:ILE:CD1	2.41	0.50
12:q:183:PHE:HA	12:q:242:PRO:HB2	1.94	0.50
19:b:132:ASP:C	19:b:132:ASP:OD1	2.54	0.50
21:o:759:ARG:HD3	68:w:26:PHE:HD2	1.77	0.50
22:i:85:GLN:CG	22:i:86:ASP:N	2.32	0.50
28:3:196:LEU:HD21	28:3:223:LEU:HD22	1.93	0.50
31:6:418:LYS:HG3	54:Y:-9:DA:H62	1.76	0.50
38:DE:633:THR:HG22	38:DE:644:THR:HG22	1.94	0.50
37:Dd:844:ASN:HA	37:Dd:847:GLU:OE1	2.11	0.50
37:Dd:885:ILE:CB	44:Dl:96:VAL:HG11	2.42	0.50
49:DP:168:ILE:HG21	49:DP:227:GLU:HA	1.93	0.50
49:DP:281:SER:HB3	49:DP:293:TYR:CD2	2.47	0.50
1:a:417:TYR:HB2	1:a:469:VAL:HG11	1.93	0.50
3:d:118:GLU:OE2	14:u:118:ILE:HD12	2.11	0.50
8:t:138:ILE:O	8:t:138:ILE:HG22	2.10	0.50
9:j:75:ARG:CA	9:j:79:LEU:HD12	2.37	0.50
11:n:707:ASP:HA	21:o:684:ARG:NH2	2.27	0.50
15:v:123:ILE:CD1	20:l:166:LEU:HD22	2.41	0.50
25:9:171:LEU:HG	25:9:188:ARG:HB2	1.93	0.50
27:2:378:SER:HB3	28:3:183:ALA:HA	1.94	0.50
33:EA:53:LYS:HB3	34:EB:201:LEU:HD11	1.92	0.50
37:Dd:1084:LEU:HD12	42:Di:98:GLN:HE21	1.76	0.50
56:PB:1091:ARG:HG3	56:PB:1103:LEU:HD11	1.94	0.50
68:w:113:GLN:HE22	68:w:159:GLN:NE2	2.08	0.50
68:w:394:PRO:CG	70:p:171:PHE:CE1	2.95	0.50
1:a:76:ALA:C	1:a:78:THR:H	2.19	0.50
6:h:77:ILE:O	12:q:126:THR:CB	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:99:ILE:CA	9:j:102:MET:HG2	2.41	0.50
12:q:482:GLN:H	12:q:634:ASN:HD22	1.60	0.50
12:q:644:SER:CA	12:q:647:SER:OG	2.58	0.50
23:0:192:LEU:HD21	23:0:196:LEU:CD2	2.42	0.50
32:7:244:ILE:HG23	32:7:437:CYS:HB2	1.93	0.50
38:DE:651:VAL:HG21	38:DE:686:THR:HG21	1.93	0.50
39:DF:122:LEU:HD13	41:DH:122:PRO:HA	1.94	0.50
53:X:-28:DT:H2'	53:X:-28:DT:O5'	2.12	0.50
55:PA:420:ILE:HB	55:PA:445:LYS:HB3	1.94	0.50
68:w:571:LEU:HB2	68:w:612:MET:HE1	1.93	0.50
1:a:420:LEU:HB3	1:a:504:ILE:HD12	1.94	0.50
2:m:27:CYS:SG	3:d:182:MET:HG2	2.52	0.50
3:d:89:ILE:HA	3:d:93:MET:HB2	1.94	0.50
3:d:122:ALA:O	3:d:125:VAL:HG22	2.12	0.50
4:f:169:SER:OG	4:f:170:SER:N	2.44	0.50
6:h:60:ASN:O	6:h:64:LYS:HG2	2.12	0.50
9:j:56:GLN:HB2	11:n:53:THR:HA	1.93	0.50
15:v:64:ARG:HH22	58:PD:140:PHE:HD1	1.56	0.50
25:9:231:TYR:O	25:9:234:GLU:HG3	2.12	0.50
38:De:722:ASP:HB2	38:De:724:GLU:HG2	1.94	0.50
53:X:-5:DG:C2	54:Y:6:DG:N2	2.79	0.50
59:PE:12:LYS:HE3	59:PE:136:LEU:HD22	1.94	0.50
69:x:555:GLU:HA	69:x:558:VAL:HG12	1.94	0.50
7:r:124:ARG:NE	7:r:124:ARG:CA	2.73	0.49
9:j:19:ILE:HD13	9:j:45:VAL:HG23	1.89	0.49
10:k:44:LEU:HD22	10:k:47:ARG:HH12	1.76	0.49
11:n:776:LEU:O	11:n:780:VAL:HG13	2.12	0.49
24:8:265:GLY:HA3	24:8:268:LEU:HB3	1.93	0.49
27:2:91:PHE:HB2	27:2:232:LEU:HB3	1.94	0.49
29:4:240:LEU:HB3	29:4:287:ALA:HB1	1.93	0.49
36:DB:392:ARG:HH21	36:DB:634:MET:HE2	1.77	0.49
41:DH:116:ARG:HD3	43:DJ:126:TYR:CE1	2.46	0.49
49:DP:300:ILE:CG2	49:DP:315:ALA:N	2.70	0.49
56:PB:817:GLN:HE21	56:PB:916:TYR:HB2	1.77	0.49
56:PB:827:GLU:HG2	56:PB:871:VAL:HG13	1.93	0.49
57:PC:37:VAL:HG12	57:PC:248:ALA:HB1	1.94	0.49
70:p:51:LEU:HB2	70:p:58:LEU:HB3	1.94	0.49
1:a:60:SER:HB3	1:a:148:ASP:HB2	1.93	0.49
1:a:197:ALA:HB1	1:a:201:ASP:HB2	1.94	0.49
6:h:8:LEU:C	6:h:8:LEU:CD2	2.85	0.49
6:h:41:THR:O	6:h:42:TRP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:83:PRO:CG	55:PA:1790:TYR:CE1	2.72	0.49
11:n:368:LYS:HB2	11:n:369:PRO:HD2	1.93	0.49
21:o:762:GLN:C	68:w:74:LYS:NZ	2.69	0.49
43:DJ:139:LEU:HB3	43:DJ:144:PHE:HD2	1.75	0.49
37:Dd:844:ASN:O	37:Dd:848:GLU:HG2	2.12	0.49
37:Dd:885:ILE:HG21	44:Dl:96:VAL:CG1	2.32	0.49
56:PB:1138:ARG:HG3	56:PB:1141:ARG:HH12	1.76	0.49
70:p:168:LEU:HD11	70:p:248:VAL:HG23	1.94	0.49
1:a:229:SER:N	1:a:502:MET:CB	2.75	0.49
5:g:91:ASP:OD1	9:j:127:ILE:HG21	2.12	0.49
6:h:36:GLU:O	6:h:38:GLY:N	2.45	0.49
8:t:130:THR:O	8:t:130:THR:OG1	2.25	0.49
12:q:441:ARG:CZ	20:l:168:TRP:CE3	2.90	0.49
21:o:682:VAL:HG22	21:o:691:VAL:HG11	1.93	0.49
35:DA:593:ILE:HG12	35:DA:663:PHE:HE2	1.78	0.49
41:DH:190:LEU:HD21	39:Df:222:LEU:HD23	1.93	0.49
39:Df:62:LYS:HD2	39:Df:62:LYS:N	2.27	0.49
53:X:-15:DG:N2	54:Y:16:DC:N3	2.60	0.49
55:PA:1214:VAL:HB	55:PA:1257:LEU:HB2	1.94	0.49
68:w:23:PRO:HA	68:w:26:PHE:CD1	2.48	0.49
68:w:1195:ALA:C	68:w:1197:HIS:N	2.69	0.49
70:p:38:ALA:HA	70:p:435:GLN:HE21	1.78	0.49
4:f:93:ILE:HG12	23:0:237:PRO:CB	2.42	0.49
5:g:87:ILE:HD11	9:j:123:LYS:HB2	1.94	0.49
5:g:109:LEU:HD11	11:n:133:LEU:HG	1.94	0.49
8:t:176:PHE:HE1	8:t:184:TYR:CE1	2.30	0.49
10:k:107:VAL:HG12	18:e:136:LEU:CD1	2.42	0.49
11:n:870:GLN:CG	21:o:655:THR:CG2	2.90	0.49
12:q:484:TYR:CD1	12:q:636:VAL:HG11	2.48	0.49
14:u:105:GLU:O	14:u:108:VAL:CG1	2.61	0.49
15:v:111:GLU:O	15:v:115:LYS:HG2	2.12	0.49
17:c:46:GLU:H	17:c:46:GLU:CD	2.17	0.49
24:8:137:ASP:HB3	24:8:158:LEU:HD13	1.94	0.49
33:EA:183:GLN:O	33:EA:186:PRO:HD2	2.12	0.49
35:DA:410:TRP:HH2	39:DF:351:ILE:HA	1.78	0.49
36:DB:304:PHE:CE1	36:DB:353:GLN:CD	2.85	0.49
36:DB:455:LEU:HD13	36:DB:637:LEU:HD11	1.94	0.49
37:DD:963:ARG:HH12	37:DD:981:GLN:HA	1.76	0.49
55:PA:1023:VAL:H	55:PA:1034:GLN:HB2	1.78	0.49
56:PB:59:VAL:HG11	56:PB:91:ILE:HD11	1.94	0.49
5:g:73:ASP:O	5:g:74:HIS:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:102:HIS:H	6:h:102:HIS:HD2	1.58	0.49
12:q:330:GLN:HG3	12:q:344:SER:HB3	1.93	0.49
23:0:87:GLU:O	23:0:90:PRO:HD2	2.12	0.49
24:8:176:ARG:H	24:8:176:ARG:HD2	1.77	0.49
27:2:174:LEU:HD13	32:7:532:PRO:HA	1.93	0.49
27:2:358:TYR:HB2	27:2:367:PHE:HB2	1.94	0.49
35:DA:592:SER:HA	35:DA:663:PHE:HZ	1.77	0.49
36:DB:833:ILE:HD11	36:DB:861:LEU:HD12	1.94	0.49
38:DE:548:GLY:HA3	38:DE:590:ASP:HA	1.94	0.49
39:Df:83:LEU:HD11	42:Di:42:PHE:HB2	1.95	0.49
60:PF:100:ARG:HB3	60:PF:121:ASP:HA	1.94	0.49
68:w:397:LYS:HB2	70:p:171:PHE:CE2	2.47	0.49
1:a:223:LYS:NZ	1:a:251:LEU:O	2.46	0.49
2:m:116:GLN:CD	16:z:595:PRO:CG	2.86	0.49
3:d:159:ASN:HA	3:d:162:CYS:CB	2.39	0.49
3:d:169:PRO:HA	55:PA:1795:PRO:HG3	1.82	0.49
5:g:38:ILE:HG22	5:g:38:ILE:O	2.12	0.49
5:g:103:ILE:H	5:g:103:ILE:CD1	2.12	0.49
6:h:55:GLN:HA	58:PD:140:PHE:HE2	1.75	0.49
6:h:106:PRO:HA	55:PA:1657:TYR:OH	2.11	0.49
8:t:184:TYR:CZ	8:t:188:ASP:HB2	2.47	0.49
11:n:116:ALA:HA	13:s:83:LEU:HD13	1.95	0.49
11:n:545:LEU:HD11	11:n:653:PRO:CA	2.42	0.49
24:8:177:TRP:HZ3	24:8:214:PRO:CA	2.11	0.49
36:DB:67:SER:HG	36:DB:70:CYS:HB2	1.71	0.49
36:DB:287:VAL:HG12	36:DB:291:TYR:CE2	2.47	0.49
43:Dj:208:GLY:HA2	46:Dk:207:LYS:O	2.11	0.49
56:PB:718:GLN:HG2	56:PB:720:PRO:HD2	1.93	0.49
68:w:1187:PRO:HA	68:w:1190:LEU:HB3	1.94	0.49
68:w:1195:ALA:C	68:w:1197:HIS:H	2.21	0.49
1:a:246:ASN:N	1:a:246:ASN:OD1	2.44	0.49
4:f:16:VAL:HG13	4:f:104:VAL:HA	1.94	0.49
5:g:12:PRO:O	55:PA:1661:SER:N	2.46	0.49
6:h:50:ALA:HB1	15:v:63:VAL:HG22	1.95	0.49
8:t:3:VAL:HG12	8:t:157:LEU:HD23	1.95	0.49
10:k:21:ILE:CD1	12:q:168:THR:N	2.76	0.49
12:q:9:ILE:HG12	14:u:90:LEU:CB	2.42	0.49
23:0:254:GLU:H	24:8:130:GLN:HE22	1.60	0.49
29:4:38:PRO:HA	29:4:117:ASN:HB3	1.95	0.49
35:DA:1193:ALA:HB3	40:DG:166:VAL:HG21	1.94	0.49
36:DB:67:SER:OG	36:DB:70:CYS:CB	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DD:878:LEU:O	37:DD:882:ILE:HG13	2.12	0.49
38:De:610:ARG:HD3	38:De:619:PRO:HG3	1.95	0.49
61:PG:15:PRO:HA	61:PG:18:PHE:CD2	2.47	0.49
68:w:337:GLN:HE21	68:w:341:PHE:HE2	1.59	0.49
68:w:1118:SER:OG	68:w:1119:GLY:N	2.43	0.49
1:a:71:VAL:HA	22:i:74:LYS:HE2	1.95	0.49
2:m:29:ALA:C	3:d:176:TYR:HB3	2.37	0.49
5:g:123:ILE:HD13	14:u:9:GLN:HG2	1.94	0.49
6:h:20:ALA:HB2	12:q:113:TYR:HE2	1.77	0.49
7:r:18:MET:O	7:r:105:CYS:N	2.42	0.49
7:r:120:GLU:CD	8:t:79:PHE:CE1	2.86	0.49
11:n:149:LEU:HG	14:u:9:GLN:NE2	2.27	0.49
11:n:808:LEU:HB2	11:n:822:ILE:HB	1.94	0.49
12:q:1:MET:HB2	16:z:541:PRO:HG2	1.84	0.49
12:q:106:LEU:C	12:q:106:LEU:CD2	2.85	0.49
12:q:183:PHE:CG	12:q:184:ASN:N	2.80	0.49
19:b:162:ALA:HA	19:b:165:LYS:HD3	1.94	0.49
21:o:715:LEU:HD11	69:x:21:TYR:CA	2.41	0.49
33:EA:22:ILE:HA	33:EA:26:TYR:CD1	2.44	0.49
33:EA:102:VAL:HA	33:EA:105:TYR:HB3	1.94	0.49
36:DB:71:ARG:C	36:DB:72:ILE:HD13	2.37	0.49
36:DB:290:PHE:CZ	36:DB:380:LEU:C	2.90	0.49
55:PA:896:LEU:HD23	55:PA:1080:ILE:HA	1.94	0.49
68:w:671:ASP:OD1	68:w:671:ASP:N	2.44	0.49
68:w:777:ILE:HA	68:w:810:VAL:HG22	1.95	0.49
5:g:159:ARG:HA	5:g:162:GLU:HB2	1.95	0.49
6:h:67:LYS:HD2	23:0:141:THR:HG23	1.44	0.49
6:h:110:ARG:C	6:h:110:ARG:CD	2.85	0.49
10:k:114:MET:CE	18:e:129:VAL:CG2	2.77	0.49
12:q:255:ALA:CB	12:q:301:VAL:HG22	2.41	0.49
15:v:131:GLU:HG3	15:v:135:TYR:HE2	1.78	0.49
17:c:124:ALA:HA	18:e:81:ILE:HD11	1.94	0.49
25:9:102:ARG:HD3	25:9:103:ILE:HG12	1.94	0.49
36:DB:290:PHE:CE2	36:DB:381:TRP:N	2.80	0.49
51:BA:33:ILE:HG12	51:BA:40:VAL:HG12	1.94	0.49
1:a:467:MET:HE1	1:a:504:ILE:CG1	2.40	0.49
3:d:117:ALA:CB	5:g:163:MET:HG3	2.41	0.49
3:d:188:GLY:HA3	5:g:15:MET:HB2	1.94	0.49
4:f:97:ASP:HB2	6:h:75:VAL:HG11	1.94	0.49
11:n:266:VAL:HG21	11:n:303:LEU:HD12	1.89	0.49
12:q:1:MET:HG2	12:q:2:SER:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:62:MET:HA	19:b:62:MET:CE	2.34	0.49
51:BA:149:LYS:HG2	51:BA:152:LYS:HD2	1.94	0.49
68:w:980:VAL:O	68:w:983:SER:OG	2.31	0.49
1:a:337:ALA:CB	1:a:338:PRO:CD	2.89	0.48
4:f:35:GLU:O	4:f:36:ARG:HB2	2.12	0.48
5:g:109:LEU:CD2	11:n:133:LEU:HG	2.32	0.48
6:h:157:GLU:HG2	10:k:53:THR:HG21	1.95	0.48
7:r:64:GLN:HB2	8:t:101:PHE:CZ	2.48	0.48
8:t:5:CYS:O	8:t:141:GLU:HA	2.13	0.48
9:j:26:VAL:CB	9:j:38:ASN:ND2	2.57	0.48
9:j:116:VAL:HG13	14:u:67:LYS:HE3	1.92	0.48
10:k:37:LYS:CE	10:k:37:LYS:N	2.73	0.48
12:q:456:GLU:HG2	15:v:140:SER:HA	1.95	0.48
18:e:146:ILE:CG2	18:e:147:ASN:N	2.52	0.48
19:b:178:LEU:HD13	20:l:55:LEU:CD2	2.44	0.48
21:o:644:PRO:O	21:o:648:ALA:N	2.44	0.48
22:i:71:ASN:HA	22:i:74:LYS:HD2	1.93	0.48
29:4:163:MET:HG3	29:4:185:MET:SD	2.53	0.48
38:DE:561:SER:HB3	38:DE:591:THR:HB	1.95	0.48
38:DE:634:ARG:HG3	38:DE:675:LEU:HB3	1.95	0.48
39:DF:20:LYS:HA	39:DF:31:ILE:HD11	1.94	0.48
44:DL:106:ARG:NH1	44:DL:114:LYS:CE	2.75	0.48
55:PA:459:ASN:HB3	55:PA:469:MET:HG3	1.95	0.48
56:PB:640:ILE:HG22	56:PB:644:LYS:HE3	1.95	0.48
2:m:57:TYR:CZ	5:g:36:PRO:HD2	2.48	0.48
3:d:34:LEU:O	3:d:38:GLU:HG3	2.14	0.48
4:f:16:VAL:O	55:PA:1662:PRO:HD3	2.13	0.48
7:r:117:PHE:CD2	8:t:85:LEU:HD12	2.47	0.48
7:r:127:HIS:ND1	7:r:127:HIS:N	2.60	0.48
8:t:203:GLN:O	8:t:204:GLN:C	2.56	0.48
12:q:19:VAL:CG2	12:q:22:VAL:HG22	2.43	0.48
12:q:106:LEU:HD23	12:q:106:LEU:O	2.12	0.48
12:q:109:MET:HE1	12:q:112:LEU:HD22	1.95	0.48
14:u:28:GLN:HG3	16:z:483:ASN:CG	2.38	0.48
15:v:49:SER:HB3	15:v:50:ARG:CZ	2.42	0.48
15:v:93:SER:O	15:v:96:GLU:HG3	2.13	0.48
15:v:126:ASP:CG	18:e:132:HIS:CD2	2.86	0.48
33:EA:146:ASP:HB3	33:EA:149:THR:HG22	1.95	0.48
36:DB:488:PHE:HB3	36:DB:491:HIS:HB2	1.95	0.48
37:DD:928:TYR:HB2	42:DI:127:TYR:CD1	2.49	0.48
38:De:633:THR:HG22	38:De:644:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Di:73:LEU:CG	44:Dl:105:HIS:CE1	2.96	0.48
53:X:-11:DG:N2	54:Y:11:DC:H42	2.10	0.48
53:X:-5:DG:H2"	53:X:-4:DT:C7	2.42	0.48
54:Y:7:DA:H2"	54:Y:8:DA:H8	1.73	0.48
67:FA:45:ALA:HB1	67:FA:100:LEU:HD11	1.94	0.48
68:w:10:GLU:HB3	68:w:14:LYS:HE3	1.94	0.48
68:w:726:ASN:N	68:w:726:ASN:HD22	2.10	0.48
1:a:160:LEU:HD12	1:a:214:ARG:NH2	2.26	0.48
1:a:335:THR:O	1:a:391:THR:HG22	2.07	0.48
2:m:29:ALA:O	3:d:176:TYR:CB	2.59	0.48
7:r:20:GLU:HB2	7:r:174:VAL:HG22	1.95	0.48
8:t:184:TYR:CE1	8:t:188:ASP:HB2	2.47	0.48
10:k:101:ARG:NH1	10:k:101:ARG:CG	2.73	0.48
11:n:136:LEU:HD23	11:n:139:LEU:HD21	1.95	0.48
11:n:188:LYS:HB3	11:n:188:LYS:HE3	1.74	0.48
18:e:75:THR:O	18:e:79:GLN:HG2	2.14	0.48
29:4:265:LEU:HB3	29:4:271:VAL:HB	1.95	0.48
4:f:170:SER:HA	11:n:267:HIS:CE1	2.48	0.48
5:g:162:GLU:O	5:g:165:GLN:HG2	2.12	0.48
8:t:125:LYS:HB2	8:t:125:LYS:HE2	1.52	0.48
10:k:64:SER:HB2	10:k:68:ARG:CZ	2.44	0.48
10:k:70:LEU:HB2	15:v:85:PHE:CE1	2.49	0.48
10:k:73:VAL:HG21	15:v:92:PRO:CD	2.21	0.48
11:n:365:ASP:HB3	11:n:368:LYS:O	2.13	0.48
11:n:659:LEU:CD2	68:w:17:VAL:CG2	2.23	0.48
11:n:678:PHE:HA	12:q:557:LEU:HB2	1.95	0.48
11:n:937:ARG:NH2	11:n:943:LEU:HD23	2.27	0.48
12:q:263:LYS:HE2	12:q:439:PHE:CZ	2.49	0.48
17:c:176:MET:HG2	17:c:194:LEU:HG	1.95	0.48
26:1:380:ASP:O	26:1:384:HIS:HD2	1.95	0.48
29:4:314:ARG:HD3	29:4:314:ARG:HA	1.77	0.48
36:DB:257:LEU:HB3	36:DB:267:HIS:HB2	1.94	0.48
36:DB:535:PHE:HD2	36:DB:544:LEU:HD11	1.78	0.48
36:DB:608:ASN:OD1	36:DB:608:ASN:C	2.55	0.48
37:Dd:1057:ARG:HG2	44:Dl:77:ASP:OD1	2.13	0.48
53:X:-5:DG:H2"	53:X:-4:DT:C6	2.47	0.48
53:X:15:DA:H1'	53:X:16:DC:H5'	1.95	0.48
55:PA:1308:TYR:HB2	55:PA:1337:GLU:HG2	1.95	0.48
59:PE:45:GLY:HA3	59:PE:53:PRO:HD3	1.95	0.48
68:w:101:LEU:HD11	68:w:121:LEU:CD2	2.41	0.48
2:m:116:GLN:CD	16:z:595:PRO:HD2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:113:GLN:HE21	5:g:163:MET:CG	2.25	0.48
10:k:73:VAL:CG2	15:v:92:PRO:CG	2.88	0.48
11:n:593:GLU:OE1	68:w:27:MET:HG3	2.13	0.48
12:q:17:LYS:CE	12:q:30:TYR:CD2	2.97	0.48
14:u:80:GLU:CB	16:z:539:ASP:H	2.26	0.48
29:4:76:LYS:HB3	29:4:79:PHE:HD2	1.78	0.48
32:7:508:PHE:HD1	32:7:510:THR:H	1.62	0.48
35:DA:469:PRO:C	35:DA:470:ILE:HG13	2.38	0.48
35:DA:925:ASP:O	35:DA:929:THR:HG23	2.12	0.48
56:PB:779:ILE:HA	56:PB:1045:PRO:HA	1.94	0.48
70:p:367:ASP:HA	70:p:370:VAL:HG22	1.96	0.48
1:a:108:PHE:O	1:a:108:PHE:CD1	2.66	0.48
1:a:420:LEU:HD22	1:a:504:ILE:HG13	1.95	0.48
3:d:184:SER:HB3	55:PA:1664:TYR:CZ	2.49	0.48
10:k:24:ILE:HG22	12:q:164:ALA:HB1	1.80	0.48
11:n:156:TYR:OH	11:n:168:ARG:HD2	2.13	0.48
11:n:711:ARG:HH12	11:n:723:GLU:CD	2.21	0.48
12:q:484:TYR:O	12:q:488:CYS:HB2	2.14	0.48
12:q:645:ALA:O	20:l:111:VAL:HG21	2.14	0.48
14:u:26:LEU:CD1	14:u:26:LEU:C	2.86	0.48
14:u:80:GLU:HB2	16:z:539:ASP:H	1.79	0.48
21:o:714:ASP:O	69:x:25:ILE:HG12	2.14	0.48
31:6:628:SER:HB3	31:6:672:TYR:HD2	1.77	0.48
56:PB:473:LEU:HD23	56:PB:731:GLN:HA	1.95	0.48
61:PG:27:LYS:HA	61:PG:30:LEU:HD23	1.94	0.48
68:w:108:GLU:HG3	68:w:111:ARG:H	1.77	0.48
69:x:481:GLU:CB	69:x:485:PRO:HG2	2.37	0.48
1:a:489:CYS:HA	1:a:514:LYS:NZ	2.29	0.48
2:m:117:GLN:HG3	16:z:594:LEU:CD2	2.44	0.48
3:d:169:PRO:HB3	55:PA:1795:PRO:CG	2.44	0.48
5:g:97:ILE:HB	5:g:98:ARG:HD2	1.95	0.48
6:h:50:ALA:HB1	15:v:63:VAL:HG13	1.94	0.48
6:h:102:HIS:CD2	6:h:102:HIS:N	2.73	0.48
6:h:102:HIS:HE1	55:PA:1792:PRO:O	1.96	0.48
9:j:11:HIS:C	9:j:15:PHE:HD2	2.19	0.48
12:q:379:ILE:HD11	12:q:427:LEU:HD22	1.94	0.48
14:u:81:SER:OG	14:u:82:THR:N	2.45	0.48
23:0:192:LEU:HD22	23:0:196:LEU:HD22	1.96	0.48
25:9:212:ILE:HG12	25:9:255:MET:HE1	1.94	0.48
28:3:67:SER:HB2	28:3:139:LYS:HD2	1.94	0.48
36:DB:119:PRO:HB2	36:DB:195:SER:CB	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DE:781:VAL:HG13	39:DF:62:LYS:HD3	1.95	0.48
39:DF:287:LYS:HA	39:DF:290:MET:HE2	1.96	0.48
46:Dk:168:GLU:HB3	46:Dk:190:ALA:HB1	1.95	0.48
68:w:164:ARG:NE	68:w:204:LEU:HD22	2.29	0.48
68:w:1193:PHE:C	68:w:1195:ALA:N	2.70	0.48
69:x:843:TYR:HD1	69:x:847:PHE:HE2	1.62	0.48
1:a:364:TYR:CD1	1:a:430:LEU:HD12	2.49	0.48
1:a:504:ILE:H	1:a:505:PRO:CD	2.27	0.48
5:g:88:ASN:ND2	13:s:69:ARG:HD3	2.26	0.48
10:k:35:LEU:HD12	10:k:35:LEU:O	2.14	0.48
11:n:587:LEU:CG	68:w:15:THR:HG22	2.33	0.48
11:n:796:ILE:O	11:n:816:LYS:NZ	2.34	0.48
11:n:851:ILE:HD11	11:n:911:SER:HA	1.96	0.48
12:q:633:ARG:HG2	12:q:633:ARG:HH21	1.78	0.48
16:z:582:LEU:HG	16:z:584:PRO:HD3	1.95	0.48
18:e:146:ILE:O	18:e:148:VAL:N	2.46	0.48
23:0:31:CYS:SG	23:0:34:CYS:HB2	2.54	0.48
24:8:177:TRP:CH2	55:PA:1677:SER:CB	2.93	0.48
26:1:278:ASP:O	26:1:280:GLY:N	2.43	0.48
32:7:462:SER:HB3	32:7:463:PRO:HD2	1.96	0.48
45:Dc:89:PRO:HB3	43:Dj:127:THR:N	2.23	0.48
52:FB:187:LEU:HD21	52:FB:213:LEU:HD11	1.95	0.48
56:PB:119:THR:HG23	56:PB:187:ILE:HA	1.95	0.48
56:PB:1115:GLN:HG2	56:PB:1150:ARG:HG2	1.95	0.48
1:a:321:LEU:HA	1:a:410:LEU:CD1	2.43	0.48
2:m:20:LEU:HB2	5:g:21:TYR:HE2	1.79	0.48
2:m:30:ASN:ND2	3:d:176:TYR:CD2	2.73	0.48
3:d:180:LEU:HD13	4:f:18:SER:HB2	1.94	0.48
7:r:192:GLN:O	10:k:75:THR:HG22	2.14	0.48
9:j:76:ASN:OD1	9:j:79:LEU:N	2.44	0.48
12:q:149:LYS:HE2	15:v:39:THR:C	2.37	0.48
26:1:134:SER:O	26:1:135:GLN:CB	2.62	0.48
29:4:209:PRO:HG3	29:4:295:SER:HB3	1.95	0.48
32:7:154:HIS:HD2	32:7:159:GLU:HG3	1.79	0.48
36:DB:45:VAL:HG22	36:DB:155:PRO:HG3	1.95	0.48
36:DB:204:LEU:HB2	36:DB:236:TYR:HB2	1.96	0.48
39:Df:356:THR:HG22	39:Df:383:LEU:HD13	1.96	0.48
44:Dl:87:ILE:O	44:Dl:91:PHE:CE2	2.61	0.48
57:PC:103:LEU:HB2	57:PC:120:LEU:HD13	1.96	0.48
69:x:621:VAL:HG11	69:x:670:LEU:HD22	1.96	0.48
5:g:83:MET:SD	9:j:120:ASP:OD2	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:125:MET:HE2	7:r:125:MET:HB3	1.76	0.48
9:j:43:PHE:CZ	13:s:151:GLY:HA2	2.48	0.48
17:c:111:TYR:OH	19:b:136:HIS:HB3	2.13	0.48
18:e:56:PHE:HE1	20:l:52:PHE:CE1	2.32	0.48
26:1:291:ASN:O	26:1:292:SER:CB	2.61	0.48
31:6:127:VAL:HG22	31:6:160:THR:HG23	1.96	0.48
36:DB:605:PRO:HA	36:DB:611:GLU:CB	2.41	0.48
38:DE:474:THR:HG22	39:DF:61:GLY:HA2	1.96	0.48
49:DP:268:ILE:HD13	49:DP:332:LEU:HD22	1.96	0.48
60:PF:75:MET:HE3	61:PG:64:GLY:HA3	1.94	0.48
70:p:24:TRP:HD1	70:p:51:LEU:HD12	1.79	0.48
1:a:259:ILE:HD12	1:a:259:ILE:O	2.14	0.47
1:a:440:PHE:CD1	1:a:454:PHE:HB3	2.49	0.47
3:d:113:GLN:CG	5:g:166:ASN:HD21	2.12	0.47
11:n:226:VAL:HG12	11:n:230:PHE:C	2.39	0.47
26:1:264:ASN:O	26:1:265:PRO:C	2.57	0.47
42:Di:73:LEU:CG	44:Dl:105:HIS:NE2	2.76	0.47
53:X:8:DA:H3'	53:X:9:DT:H73	1.96	0.47
69:x:374:SER:O	69:x:377:SER:OG	2.29	0.47
70:p:207:CYS:HB3	70:p:242:TYR:HE2	1.79	0.47
1:a:432:GLU:OE1	1:a:432:GLU:HA	2.14	0.47
2:m:107:HIS:O	2:m:111:LYS:CB	2.62	0.47
3:d:128:ALA:HB1	14:u:108:VAL:HG21	1.76	0.47
4:f:191:LYS:HE3	11:n:284:ALA:HB1	1.96	0.47
5:g:158:GLU:O	5:g:162:GLU:N	2.44	0.47
7:r:206:ARG:C	7:r:206:ARG:NE	2.72	0.47
8:t:128:THR:O	8:t:130:THR:N	2.46	0.47
12:q:214:SER:HB3	12:q:383:HIS:CE1	2.48	0.47
12:q:339:LEU:CD2	12:q:439:PHE:CD2	2.93	0.47
12:q:378:LEU:HG	20:l:176:MET:HE2	1.96	0.47
12:q:644:SER:HB3	18:e:96:LEU:HB2	1.96	0.47
16:z:528:LEU:HA	16:z:582:LEU:HD12	1.95	0.47
24:8:18:LEU:HG	24:8:28:LYS:HB2	1.96	0.47
33:EA:23:ARG:HB3	34:EB:209:GLN:HB3	1.96	0.47
36:DB:308:PHE:CD2	36:DB:330:LEU:CD2	2.97	0.47
39:DF:256:LEU:N	39:DF:257:PRO:HD2	2.30	0.47
52:FB:12:ALA:HB1	67:FA:39:PHE:HB3	1.96	0.47
55:PA:1002:SER:HB3	55:PA:1059:ARG:HA	1.95	0.47
68:w:270:LEU:HD23	68:w:303:GLN:HG3	1.96	0.47
68:w:863:ASP:OD1	68:w:863:ASP:N	2.45	0.47
70:p:88:GLU:OE2	70:p:288:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:232:LEU:HB3	1:a:502:MET:CE	2.44	0.47
1:a:467:MET:HE2	1:a:504:ILE:HD13	1.88	0.47
3:d:117:ALA:CB	5:g:163:MET:CG	2.89	0.47
3:d:131:LYS:CG	14:u:104:LEU:HD11	2.41	0.47
3:d:152:ALA:HB1	11:n:152:PHE:CG	2.49	0.47
4:f:116:ASN:HB3	15:v:52:THR:CG2	2.37	0.47
5:g:27:GLN:NE2	5:g:32:PRO:HA	2.29	0.47
6:h:40:LEU:HG	6:h:45:VAL:CG2	2.41	0.47
7:r:147:LYS:HB3	7:r:149:PHE:HE1	1.79	0.47
8:t:28:LEU:HD13	8:t:31:LEU:HD12	1.96	0.47
11:n:156:TYR:CZ	11:n:168:ARG:NH1	2.82	0.47
11:n:247:LEU:H	11:n:279:GLN:CD	2.22	0.47
12:q:335:PRO:HB3	12:q:436:LYS:HG3	1.95	0.47
19:b:71:LEU:O	19:b:75:MET:HG2	2.15	0.47
21:o:762:GLN:HB2	68:w:29:THR:HG21	1.97	0.47
32:7:256:LEU:HD11	32:7:340:VAL:HG12	1.96	0.47
35:DA:504:PRO:HG2	39:DF:208:LEU:HD23	1.96	0.47
36:DB:833:ILE:HD11	36:DB:861:LEU:CD1	2.44	0.47
38:DE:450:ARG:HG3	38:DE:789:ASN:HB2	1.95	0.47
42:DI:118:ASP:HA	42:DI:121:CYS:HB2	1.96	0.47
44:DL:58:LEU:O	44:DL:85:LEU:HD22	2.15	0.47
45:Dc:80:LEU:HB3	43:Dj:119:PHE:CZ	2.49	0.47
38:De:254:ASN:H	38:De:288:LYS:HD2	1.79	0.47
55:PA:807:LEU:HB2	55:PA:810:PHE:CD2	2.49	0.47
56:PB:285:LEU:HD22	56:PB:285:LEU:HA	1.75	0.47
57:PC:184:PHE:HE1	57:PC:229:PHE:HB3	1.78	0.47
68:w:164:ARG:NH2	68:w:204:LEU:HB2	2.26	0.47
68:w:394:PRO:C	70:p:171:PHE:HZ	2.21	0.47
68:w:1229:LYS:O	68:w:1233:GLU:HB2	2.15	0.47
3:d:186:LEU:HD11	5:g:44:MET:HB2	1.96	0.47
4:f:78:LEU:CD1	6:h:81:LEU:HD23	2.42	0.47
5:g:84:SER:CB	13:s:67:LEU:HB3	2.44	0.47
6:h:48:SER:HA	6:h:51:LEU:CD2	2.44	0.47
9:j:53:LYS:CE	11:n:60:HIS:N	2.77	0.47
14:u:68:ASP:OD1	16:z:585:HIS:CE1	2.66	0.47
17:c:134:LYS:HD3	20:l:46:TYR:HB2	1.97	0.47
23:0:49:CYS:SG	23:0:49:CYS:O	2.73	0.47
26:1:198:ARG:NH2	26:1:320:ARG:HD3	2.28	0.47
27:2:321:SER:HA	27:2:324:HIS:HD2	1.80	0.47
35:DA:472:ASN:O	35:DA:476:VAL:HG23	2.15	0.47
36:DB:382:MET:HG3	36:DB:386:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Dc:33:LEU:HD11	43:Dj:211:VAL:HG11	1.96	0.47
44:Dl:71:ASP:HB3	44:Dl:74:GLU:HB3	1.96	0.47
44:Dl:118:LEU:CD1	44:Dl:119:HIS:N	2.66	0.47
49:DP:299:ARG:O	49:DP:300:ILE:HG23	2.15	0.47
55:PA:1212:LEU:HB3	55:PA:1259:ILE:HB	1.97	0.47
56:PB:230:ARG:HB3	56:PB:231:PRO:HD3	1.94	0.47
58:PD:103:LEU:HG	58:PD:115:ILE:HD11	1.95	0.47
68:w:615:ILE:O	68:w:620:ARG:NH2	2.48	0.47
68:w:1172:ILE:O	68:w:1244:GLN:NE2	2.41	0.47
69:x:20:ASP:OD1	69:x:20:ASP:N	2.44	0.47
70:p:100:ASP:OD1	70:p:100:ASP:N	2.47	0.47
1:a:393:VAL:HG13	1:a:393:VAL:O	2.13	0.47
4:f:100:ILE:HG12	4:f:105:ILE:HG12	1.96	0.47
7:r:18:MET:O	7:r:105:CYS:HB3	2.14	0.47
9:j:53:LYS:HD3	11:n:57:PHE:CA	2.38	0.47
10:k:17:ILE:HG21	12:q:171:VAL:CG1	2.43	0.47
11:n:127:ILE:CA	14:u:27:GLN:NE2	2.76	0.47
31:6:493:TRP:HA	31:6:496:LEU:HD12	1.97	0.47
36:DB:325:PHE:HB3	36:DB:329:LEU:HD12	1.97	0.47
36:DB:402:ILE:HD12	36:DB:455:LEU:HD12	1.97	0.47
38:De:651:VAL:HG11	38:De:686:THR:HG21	1.96	0.47
39:Df:263:ILE:HA	39:Df:282:LEU:HD22	1.96	0.47
67:FA:16:VAL:HG22	67:FA:135:PHE:HB2	1.96	0.47
2:m:66:TYR:OH	5:g:38:ILE:HG22	2.13	0.47
2:m:68:LYS:CD	5:g:50:GLN:NE2	2.64	0.47
5:g:103:ILE:HD12	5:g:103:ILE:N	2.16	0.47
6:h:23:LYS:CD	12:q:110:CYS:SG	3.03	0.47
6:h:29:PHE:HD2	12:q:102:LEU:CD1	2.26	0.47
9:j:82:LYS:CA	13:s:96:PHE:CD1	2.97	0.47
11:n:229:GLU:HB3	11:n:254:VAL:HG13	1.96	0.47
11:n:229:GLU:HB3	11:n:304:GLN:NE2	2.29	0.47
11:n:362:ASP:N	11:n:370:LEU:HD22	2.30	0.47
31:6:171:LYS:HA	31:6:299:ASN:HB3	1.97	0.47
33:EA:129:CYS:HG	33:EA:131:VAL:CG2	2.22	0.47
38:DE:331:ASN:HA	38:DE:334:GLN:HE21	1.79	0.47
39:DF:213:ILE:HG22	41:DH:165:TYR:HA	1.96	0.47
39:DF:379:GLY:O	39:DF:383:LEU:HG	2.15	0.47
38:De:308:ARG:HH21	38:De:342:PHE:HB3	1.79	0.47
42:Di:56:ILE:HG22	42:Di:60:HIS:CD2	2.49	0.47
49:DP:300:ILE:HG22	49:DP:315:ALA:CA	2.45	0.47
51:BA:131:PRO:HG3	56:PB:101:ARG:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:FB:3:GLU:HB3	52:FB:6:GLU:HB3	1.96	0.47
55:PA:760:LEU:HD11	55:PA:781:ILE:HG21	1.97	0.47
56:PB:132:VAL:HG13	56:PB:140:LEU:HB3	1.95	0.47
56:PB:627:ILE:HD11	56:PB:663:GLU:HB2	1.96	0.47
1:a:58:LEU:O	1:a:62:LEU:HG	2.15	0.47
1:a:157:LEU:HD23	1:a:217:GLY:HA2	1.96	0.47
1:a:421:ILE:HD11	1:a:450:PHE:CD1	2.50	0.47
1:a:431:LYS:HD3	1:a:431:LYS:HA	1.70	0.47
2:m:120:ALA:O	16:z:592:ASN:CG	2.56	0.47
4:f:43:ARG:CB	24:8:264:ALA:HB3	2.45	0.47
4:f:72:HIS:CE1	6:h:79:LEU:O	2.68	0.47
4:f:82:ARG:NH1	4:f:94:PRO:HB3	2.30	0.47
6:h:62:VAL:HA	6:h:65:HIS:CE1	2.50	0.47
7:r:36:ILE:HD11	7:r:134:HIS:CD2	2.50	0.47
8:t:6:VAL:HG22	8:t:141:GLU:CB	2.41	0.47
10:k:58:HIS:C	10:k:58:HIS:ND1	2.73	0.47
10:k:78:PRO:C	10:k:79:HIS:HD1	2.23	0.47
11:n:156:TYR:O	11:n:160:VAL:HG23	2.15	0.47
11:n:387:GLU:HG3	11:n:391:LYS:HE3	1.97	0.47
12:q:166:ARG:HH11	12:q:166:ARG:HG3	1.80	0.47
12:q:431:ILE:HD13	12:q:431:ILE:HA	1.75	0.47
13:s:84:ILE:HG23	13:s:93:TYR:CD2	2.49	0.47
13:s:87:TYR:HB2	13:s:89:LEU:HG	1.96	0.47
15:v:122:GLU:HG3	18:e:139:TRP:NE1	2.16	0.47
15:v:123:ILE:HD12	20:l:166:LEU:CD2	2.44	0.47
23:0:192:LEU:CD2	23:0:196:LEU:CD2	2.93	0.47
24:8:177:TRP:CZ3	24:8:214:PRO:CB	2.97	0.47
31:6:420:SER:O	31:6:421:TRP:C	2.58	0.47
32:7:609:ASP:HA	32:7:666:ARG:HD3	1.97	0.47
36:DB:709:MET:HE3	36:DB:709:MET:HB2	1.82	0.47
37:DD:874:LEU:HD23	37:DD:874:LEU:H	1.79	0.47
38:DE:572:LEU:HD22	38:DE:572:LEU:HA	1.76	0.47
37:Dd:848:GLU:HA	37:Dd:848:GLU:OE2	2.14	0.47
37:Dd:878:LEU:HD13	44:Dl:57:VAL:CG1	2.43	0.47
37:Dd:878:LEU:O	37:Dd:882:ILE:HG13	2.14	0.47
44:Dl:102:LEU:CD1	44:Dl:118:LEU:CG	2.93	0.47
55:PA:566:PHE:CE1	65:PK:62:LYS:HB2	2.50	0.47
55:PA:1216:LEU:HD11	55:PA:1257:LEU:HG	1.95	0.47
56:PB:1115:GLN:HE21	56:PB:1150:ARG:HH11	1.62	0.47
57:PC:172:GLU:HG2	65:PK:10:PHE:HE2	1.79	0.47
62:PH:96:VAL:HG22	62:PH:116:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:151:ILE:HA	7:r:160:THR:HG22	1.97	0.47
12:q:263:LYS:HE2	12:q:439:PHE:HE2	1.78	0.47
14:u:110:ARG:NH2	22:i:141:PHE:CB	2.76	0.47
15:v:84:GLN:HE22	15:v:85:PHE:CB	2.26	0.47
16:z:488:SER:HB2	16:z:492:ARG:NH2	2.29	0.47
24:8:177:TRP:CE2	55:PA:1677:SER:HB3	2.48	0.47
32:7:552:TRP:HB3	32:7:558:LEU:HB2	1.97	0.47
34:EB:129:LYS:HB2	34:EB:140:LYS:HG3	1.96	0.47
38:DE:464:TYR:HB3	39:DF:131:LEU:HD11	1.96	0.47
43:Dj:195:LEU:HD11	43:Dj:200:LEU:HD13	1.96	0.47
55:PA:1020:LEU:HD21	55:PA:1073:GLU:HA	1.96	0.47
56:PB:37:LYS:O	56:PB:41:ARG:HB2	2.13	0.47
56:PB:566:LYS:HA	56:PB:576:ILE:HG22	1.96	0.47
56:PB:776:ILE:HD12	56:PB:806:PHE:H	1.80	0.47
57:PC:260:GLN:HB2	65:PK:91:ILE:HG21	1.96	0.47
65:PK:18:LYS:O	65:PK:35:ILE:HA	2.14	0.47
1:a:364:TYR:CB	1:a:430:LEU:CD1	2.54	0.47
2:m:30:ASN:N	3:d:176:TYR:CB	2.77	0.47
2:m:68:LYS:HD3	5:g:45:PHE:CE2	2.47	0.47
4:f:137:CYS:CB	6:h:42:TRP:HB3	2.45	0.47
6:h:48:SER:HA	6:h:51:LEU:HD23	1.96	0.47
7:r:47:GLU:OE2	7:r:47:GLU:N	2.35	0.47
10:k:44:LEU:CD1	10:k:44:LEU:C	2.87	0.47
11:n:202:ARG:HH22	11:n:243:VAL:HG12	1.80	0.47
11:n:929:ARG:HB2	11:n:933:VAL:HG13	1.97	0.47
14:u:88:ALA:HB1	16:z:552:LEU:CD1	2.45	0.47
21:o:762:GLN:N	68:w:74:LYS:HE3	2.30	0.47
22:i:70:HIS:O	22:i:74:LYS:HG3	2.15	0.47
24:8:103:LYS:HD3	24:8:103:LYS:HA	1.73	0.47
24:8:136:ARG:H	24:8:159:ALA:HA	1.79	0.47
27:2:156:LEU:HB3	27:2:165:ARG:HE	1.80	0.47
36:DB:290:PHE:CD2	36:DB:381:TRP:CB	2.90	0.47
38:DE:585:ASN:HD22	38:DE:585:ASN:HA	1.57	0.47
38:DE:691:GLY:HA2	38:DE:714:VAL:HG23	1.97	0.47
55:PA:496:PHE:HD2	56:PB:791:GLU:HB3	1.79	0.47
59:PE:108:GLN:HB3	59:PE:109:GLY:H	1.57	0.47
59:PE:164:LYS:HB2	60:PF:111:PRO:HG2	1.97	0.47
60:PF:81:VAL:HG22	60:PF:101:LYS:HD2	1.96	0.47
68:w:9:PHE:HB2	68:w:66:PHE:CE2	2.46	0.47
68:w:113:GLN:NE2	68:w:159:GLN:HE22	2.10	0.47
68:w:787:PRO:HB3	68:w:822:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:x:255:ASN:OD1	69:x:255:ASN:N	2.47	0.47
69:x:544:HIS:HD2	69:x:546:CYS:H	1.62	0.47
69:x:708:LYS:HB2	70:p:128:GLY:HA3	1.97	0.47
2:m:18:PHE:HB3	5:g:39:LYS:HD3	1.96	0.47
2:m:39:GLN:HB3	55:PA:1654:SER:CB	2.37	0.47
5:g:92:LEU:HD11	11:n:133:LEU:HD11	1.96	0.47
9:j:75:ARG:HB3	9:j:79:LEU:HB2	1.97	0.47
11:n:802:VAL:HG22	11:n:809:ILE:HB	1.97	0.47
12:q:9:ILE:HG12	14:u:90:LEU:CD2	2.42	0.47
14:u:18:GLN:HE22	14:u:65:THR:HG21	1.79	0.47
24:8:185:PHE:HB3	24:8:243:LEU:HD23	1.97	0.47
31:6:530:ARG:HA	31:6:533:LEU:HD12	1.97	0.47
31:6:546:PHE:HD2	31:6:693:LEU:HD13	1.79	0.47
33:EA:18:ALA:O	33:EA:22:ILE:HG23	2.15	0.47
36:DB:210:ALA:HA	36:DB:232:LYS:HD2	1.96	0.47
38:DE:474:THR:HB	38:DE:547:TYR:HA	1.97	0.47
39:DF:276:LEU:HD13	39:DF:323:VAL:HG21	1.97	0.47
45:Dc:99:PHE:HB3	45:Dc:100:PRO:HD3	1.96	0.47
37:Dd:960:GLU:HG2	37:Dd:963:ARG:HH21	1.79	0.47
48:DO:82:ARG:HH21	48:DO:87:LEU:HB2	1.80	0.47
53:X:-9:DG:H2'	53:X:-8:DT:H71	1.96	0.47
68:w:234:SER:HB2	68:w:660:GLU:HG3	1.96	0.47
3:d:113:GLN:CG	5:g:166:ASN:ND2	2.71	0.46
6:h:130:ARG:HG3	6:h:131:ILE:H	1.79	0.46
9:j:49:GLN:HA	9:j:52:ASP:OD2	2.14	0.46
12:q:484:TYR:CD1	12:q:636:VAL:CG1	2.98	0.46
19:b:174:ILE:HD13	20:l:58:MET:HE2	1.97	0.46
26:1:286:VAL:O	26:1:289:ALA:N	2.47	0.46
26:1:387:THR:HG23	26:1:388:PRO:HD2	1.97	0.46
33:EA:169:PRO:HB2	33:EA:172:ASP:HB2	1.97	0.46
35:DA:1061:ARG:HA	35:DA:1061:ARG:HD3	1.74	0.46
36:DB:817:ARG:HE	36:DB:865:GLY:HA2	1.79	0.46
37:DD:914:VAL:O	37:DD:917:ILE:HG12	2.15	0.46
38:DE:636:HIS:HD2	38:DE:637:PRO:HD2	1.79	0.46
40:DG:129:LYS:HA	40:DG:129:LYS:HD2	1.45	0.46
44:DL:76:LEU:HD13	44:DL:84:LEU:CD1	2.39	0.46
38:De:636:HIS:CD2	38:De:637:PRO:HD2	2.50	0.46
56:PB:725:GLN:HG3	56:PB:938:ARG:O	2.14	0.46
60:PF:72:GLN:HB3	60:PF:77:ALA:HB2	1.96	0.46
70:p:266:ARG:HH11	70:p:341:ILE:HD13	1.80	0.46
4:f:32:TYR:O	4:f:35:GLU:CG	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:51:LYS:HE2	4:f:51:LYS:HB3	1.50	0.46
10:k:109:ARG:CG	10:k:109:ARG:NH1	2.73	0.46
11:n:170:PRO:HG2	11:n:173:ILE:HD11	1.97	0.46
11:n:753:LEU:HG	17:c:305:PHE:CE1	2.50	0.46
12:q:103:ARG:HH11	12:q:103:ARG:HB2	1.81	0.46
12:q:428:LEU:C	12:q:428:LEU:CD1	2.85	0.46
12:q:609:VAL:HG23	21:o:674:ILE:HD13	1.96	0.46
15:v:53:GLN:HE21	15:v:53:GLN:HB3	1.48	0.46
16:z:529:HIS:CE1	16:z:582:LEU:HD13	2.51	0.46
18:e:45:VAL:CG1	20:l:92:LEU:CD1	2.92	0.46
19:b:129:GLN:NE2	19:b:129:GLN:HA	2.31	0.46
29:4:55:TRP:HE3	29:4:96:TRP:HH2	1.62	0.46
31:6:340:LEU:HD13	31:6:349:VAL:HG21	1.98	0.46
36:DB:954:TRP:HA	36:DB:957:MET:HE2	1.97	0.46
45:Dc:55:LEU:HD21	37:Dd:920:THR:HG23	1.97	0.46
39:Df:69:SER:HA	39:Df:87:HIS:HE1	1.80	0.46
51:BA:182:ALA:HB2	52:FB:155:PRO:HD2	1.97	0.46
59:PE:84:ILE:H	59:PE:84:ILE:HG13	1.56	0.46
60:PF:107:ARG:HG3	60:PF:115:TYR:HB2	1.98	0.46
68:w:11:GLU:HA	68:w:14:LYS:HD2	1.98	0.46
69:x:847:PHE:HB2	69:x:899:ARG:HG2	1.97	0.46
1:a:160:LEU:HG	1:a:219:LEU:HD21	1.96	0.46
1:a:437:LEU:HD13	1:a:439:GLN:HE21	1.81	0.46
7:r:35:LEU:C	7:r:35:LEU:CD1	2.85	0.46
8:t:154:TRP:CD1	8:t:179:ARG:HH22	2.32	0.46
8:t:156:LEU:HD13	17:c:286:LYS:HZ3	1.79	0.46
11:n:587:LEU:CD1	68:w:15:THR:CB	2.40	0.46
11:n:658:ARG:NH2	68:w:21:ALA:HA	2.25	0.46
12:q:17:LYS:CE	12:q:30:TYR:CE2	2.87	0.46
12:q:120:ARG:HH11	12:q:120:ARG:CG	2.14	0.46
12:q:548:VAL:HA	12:q:571:VAL:HG12	1.96	0.46
26:1:277:LEU:C	26:1:279:GLU:N	2.62	0.46
31:6:623:LEU:HD13	31:6:643:VAL:HG11	1.97	0.46
35:DA:496:GLU:HG3	35:DA:497:PRO:HD2	1.95	0.46
38:De:684:LEU:HB2	38:De:698:ILE:HD11	1.97	0.46
56:PB:194:LEU:HA	56:PB:467:SER:HA	1.98	0.46
56:PB:862:GLY:HA3	56:PB:899:SER:H	1.80	0.46
57:PC:193:ARG:HD3	57:PC:220:TYR:HB2	1.97	0.46
68:w:41:LEU:HD11	68:w:85:MET:C	2.40	0.46
68:w:370:ASP:OD1	68:w:370:ASP:N	2.48	0.46
1:a:145:LYS:HA	1:a:145:LYS:CE	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:187:MET:HE1	1:a:401:PRO:HB2	1.96	0.46
1:a:417:TYR:CZ	1:a:450:PHE:HD1	2.21	0.46
7:r:42:LEU:HD13	10:k:77:GLN:HG3	1.96	0.46
9:j:101:THR:HB	9:j:105:PHE:HE2	1.79	0.46
10:k:73:VAL:CG2	15:v:92:PRO:HG2	2.46	0.46
10:k:80:GLU:N	10:k:80:GLU:OE1	2.48	0.46
15:v:133:GLU:O	15:v:136:SER:N	2.46	0.46
15:v:139:SER:HA	20:l:149:LEU:CD1	2.45	0.46
19:b:107:GLU:HB3	21:o:649:ILE:HD11	1.96	0.46
19:b:178:LEU:HD13	20:l:55:LEU:HD21	1.98	0.46
21:o:678:LEU:HD11	21:o:725:VAL:HG11	1.96	0.46
25:9:250:ASP:HA	25:9:253:LYS:HE2	1.98	0.46
28:3:152:LYS:HB2	28:3:155:GLN:HG2	1.96	0.46
36:DB:608:ASN:CG	36:DB:657:ARG:HG3	2.41	0.46
51:BA:235:ILE:HG23	51:BA:299:LEU:HB3	1.97	0.46
53:X:-23:DG:H2"	53:X:-22:DG:H5"	1.97	0.46
53:X:-19:DG:H2"	53:X:-18:DT:H71	1.97	0.46
55:PA:1121:VAL:N	55:PA:1122:PRO:HD2	2.30	0.46
68:w:6:GLN:HA	68:w:62:TRP:CH2	2.44	0.46
68:w:394:PRO:CB	70:p:171:PHE:CE1	2.99	0.46
68:w:1090:CYS:SG	68:w:1091:ASP:N	2.87	0.46
1:a:232:LEU:CB	1:a:502:MET:HE1	2.44	0.46
2:m:21:GLU:O	2:m:25:VAL:HG23	2.16	0.46
2:m:93:CYS:O	2:m:97:ILE:HG22	2.16	0.46
2:m:99:GLU:OE2	55:PA:1794:SER:O	2.33	0.46
4:f:64:VAL:HB	4:f:86:ARG:O	2.15	0.46
4:f:118:ARG:HH21	12:q:111:VAL:HG12	1.80	0.46
5:g:109:LEU:HD11	11:n:133:LEU:CD1	2.46	0.46
9:j:78:GLN:HB3	9:j:82:LYS:HE3	0.56	0.46
10:k:13:ALA:HB2	15:v:83:LYS:CD	2.44	0.46
10:k:37:LYS:H	10:k:37:LYS:CD	2.26	0.46
11:n:529:PRO:CG	68:w:35:THR:HB	2.41	0.46
12:q:506:HIS:CD2	12:q:508:ASP:H	2.34	0.46
17:c:281:CYS:SG	17:c:306:HIS:N	2.84	0.46
19:b:116:LEU:HD23	19:b:116:LEU:HA	1.80	0.46
21:o:715:LEU:HD12	21:o:748:PHE:CZ	2.50	0.46
25:9:248:LEU:O	25:9:252:MET:HG2	2.16	0.46
32:7:283:ASP:HA	32:7:286:ARG:HD2	1.97	0.46
35:DA:1165:LEU:HB2	35:DA:1191:ILE:HG12	1.97	0.46
36:DB:671:LYS:HB2	36:DB:671:LYS:HE2	1.53	0.46
39:DF:109:GLU:O	39:DF:110:LYS:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Dc:15:ALA:HA	39:Df:114:LEU:HD22	1.97	0.46
45:Dc:51:ARG:HB3	37:Dd:1065:PHE:HE1	1.79	0.46
44:Dl:60:LYS:HE2	44:Dl:85:LEU:HD11	1.97	0.46
53:X:-9:DG:C2'	53:X:-8:DT:H71	2.46	0.46
55:PA:1016:LEU:HD23	55:PA:1045:LEU:HD11	1.97	0.46
57:PC:189:ASP:HB3	57:PC:218:ALA:HB2	1.98	0.46
1:a:99:THR:HG22	1:a:112:VAL:HG13	1.96	0.46
1:a:224:TYR:HE1	1:a:254:ASN:C	2.23	0.46
4:f:74:GLN:HB3	4:f:78:LEU:HB2	1.97	0.46
5:g:130:GLN:HB2	16:z:596:TYR:OH	2.15	0.46
7:r:83:TRP:CE3	7:r:114:LEU:CD2	2.99	0.46
10:k:88:LYS:HG3	12:q:380:ARG:HH11	1.80	0.46
11:n:855:LEU:HD11	11:n:868:LEU:HD22	1.98	0.46
12:q:466:ASN:ND2	17:c:205:ARG:HG3	2.30	0.46
14:u:73:ILE:C	14:u:75:SER:N	2.74	0.46
15:v:75:LEU:HD23	15:v:78:LEU:CD1	2.35	0.46
15:v:128:TYR:HD2	17:c:205:ARG:NH2	2.14	0.46
36:DB:568:VAL:HG22	36:DB:628:ILE:HG23	1.96	0.46
38:DE:243:LEU:HD11	38:DE:333:VAL:HG22	1.98	0.46
41:DH:193:PHE:HE2	39:Df:226:GLU:HB3	1.81	0.46
44:DL:58:LEU:O	44:DL:85:LEU:CD2	2.63	0.46
39:Df:409:GLY:HA3	39:Df:417:ARG:HH22	1.80	0.46
48:DO:56:VAL:HG11	48:DO:83:GLU:HA	1.97	0.46
55:PA:201:GLU:HG2	55:PA:212:LYS:HG3	1.96	0.46
56:PB:203:ASN:O	56:PB:571:GLY:HA3	2.16	0.46
56:PB:355:ASP:O	56:PB:358:GLU:HG2	2.16	0.46
68:w:332:GLN:O	68:w:335:SER:OG	2.27	0.46
1:a:329:LEU:HD22	1:a:330:PHE:CD2	2.51	0.46
4:f:14:SER:HB2	55:PA:1659:PRO:HB3	1.97	0.46
6:h:32:LYS:HZ2	6:h:40:LEU:HD11	1.78	0.46
7:r:32:LEU:HD12	7:r:167:TYR:CE1	2.51	0.46
11:n:230:PHE:CE1	11:n:296:LEU:CB	2.99	0.46
12:q:494:GLN:HB2	17:c:251:LEU:HD11	1.96	0.46
15:v:139:SER:HA	20:l:149:LEU:HD11	1.97	0.46
17:c:209:ILE:HB	17:c:250:LEU:HD13	1.96	0.46
22:i:100:LEU:C	22:i:100:LEU:HD13	2.41	0.46
27:2:379:LEU:HA	28:3:183:ALA:HB2	1.96	0.46
32:7:320:PRO:O	32:7:323:ILE:HG12	2.16	0.46
36:DB:435:ILE:HG23	36:DB:441:LEU:HD21	1.98	0.46
36:DB:769:LYS:HD3	36:DB:825:ASP:OD2	2.15	0.46
38:DE:559:LEU:HD11	38:DE:600:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DF:366:GLU:HA	39:DF:402:ARG:HH22	1.81	0.46
42:Di:57:TYR:HE2	42:Di:74:ALA:HA	1.80	0.46
47:Dm:30:ARG:HH11	47:Dm:58:GLU:HB3	1.80	0.46
49:DP:269:ARG:HG3	49:DP:337:LYS:HG2	1.98	0.46
51:BA:194:CYS:O	51:BA:198:ILE:HG13	2.15	0.46
61:PG:79:PRO:HG3	61:PG:157:ILE:HG21	1.97	0.46
1:a:167:ASN:O	1:a:171:THR:HG23	2.14	0.46
4:f:60:LEU:O	4:f:86:ARG:HD2	2.15	0.46
8:t:48:THR:HA	8:t:61:LYS:O	2.16	0.46
9:j:53:LYS:CE	11:n:60:HIS:H	2.29	0.46
10:k:88:LYS:CG	12:q:380:ARG:HH11	2.28	0.46
10:k:114:MET:HE2	18:e:129:VAL:CG2	2.45	0.46
11:n:512:LEU:HD21	12:q:565:ASN:HD22	1.80	0.46
21:o:752:VAL:HA	21:o:755:CYS:SG	2.56	0.46
24:8:264:ALA:HA	24:8:269:LEU:HD23	1.98	0.46
33:EA:105:TYR:CE1	34:EB:222:SER:HB2	2.51	0.46
38:DE:515:LEU:HD12	38:DE:516:ILE:HG23	1.98	0.46
43:Dj:135:THR:O	43:Dj:139:LEU:HG	2.16	0.46
49:DP:172:VAL:HB	49:DP:253:PHE:HD1	1.80	0.46
49:DP:281:SER:HB3	49:DP:293:TYR:HD2	1.81	0.46
56:PB:283:ASP:O	56:PB:286:GLU:HG3	2.16	0.46
56:PB:591:ARG:HD3	56:PB:603:MET:HE1	1.98	0.46
56:PB:674:MET:HG3	56:PB:693:TYR:HD1	1.79	0.46
68:w:758:LYS:HA	68:w:758:LYS:HD3	1.81	0.46
1:a:297:VAL:HG12	1:a:299:LEU:HG	1.98	0.46
2:m:26:GLN:O	3:d:177:PRO:HG3	2.16	0.46
2:m:29:ALA:C	3:d:176:TYR:CB	2.89	0.46
2:m:56:LEU:CD2	2:m:80:GLN:HE21	2.23	0.46
5:g:75:LYS:HD2	14:u:76:LEU:O	2.15	0.46
7:r:194:LYS:HE2	7:r:198:HIS:CE1	2.50	0.46
9:j:96:LYS:CD	13:s:80:SER:CA	2.51	0.46
9:j:96:LYS:HG3	13:s:80:SER:HA	1.94	0.46
11:n:281:ARG:HH21	11:n:295:CYS:CB	2.27	0.46
15:v:85:PHE:CE1	15:v:86:LEU:HD21	2.49	0.46
19:b:178:LEU:HD21	20:l:78:LEU:HB3	1.98	0.46
21:o:720:PRO:O	21:o:721:LEU:C	2.58	0.46
24:8:214:PRO:HG2	55:PA:1674:THR:HG22	1.97	0.46
31:6:350:GLY:HA3	31:6:374:TRP:CZ3	2.51	0.46
35:DA:1168:TYR:HB2	40:DG:180:ARG:HB3	1.97	0.46
39:DF:148:ASN:HB3	39:DF:150:PRO:HD2	1.97	0.46
39:Df:229:GLU:O	39:Df:232:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Dl:106:ARG:HH12	44:Dl:114:LYS:HB2	1.79	0.46
44:Dl:118:LEU:HD12	44:Dl:119:HIS:CA	2.45	0.46
55:PA:1037:ALA:HA	59:PE:200:ALA:HB1	1.98	0.46
1:a:60:SER:HB2	1:a:148:ASP:CB	2.42	0.46
4:f:141:PRO:HB3	12:q:167:LEU:HD23	1.98	0.46
5:g:83:MET:HE3	5:g:83:MET:CA	2.45	0.46
11:n:281:ARG:NH2	11:n:295:CYS:HB2	2.31	0.46
11:n:367:SER:HB2	11:n:368:LYS:HD3	1.97	0.46
14:u:81:SER:N	16:z:539:ASP:HB2	2.31	0.46
21:o:710:LEU:HG	21:o:776:TRP:CH2	2.50	0.46
21:o:733:SER:HB3	21:o:766:LYS:HA	1.98	0.46
26:1:430:THR:HG21	28:3:225:GLN:HB3	1.97	0.46
28:3:34:LEU:HD21	28:3:119:MET:HG3	1.98	0.46
31:6:311:LYS:H	31:6:381:TRP:HB2	1.81	0.46
36:DB:213:VAL:O	36:DB:213:VAL:HG13	2.17	0.46
38:DE:563:GLU:HA	38:DE:587:PRO:HB3	1.98	0.46
44:DL:106:ARG:NH1	44:DL:115:ASP:OD1	2.37	0.46
38:De:556:ASN:HD22	38:De:556:ASN:HA	1.61	0.46
1:a:445:LEU:HD11	1:a:449:ARG:NH2	2.30	0.45
2:m:17:ARG:NH2	5:g:33:LYS:HD2	2.23	0.45
2:m:105:TRP:CZ2	3:d:164:PRO:HD3	2.51	0.45
3:d:40:LEU:O	3:d:43:GLU:HG3	2.15	0.45
3:d:144:SER:CB	12:q:9:ILE:HB	2.47	0.45
4:f:94:PRO:C	12:q:130:VAL:HG13	2.41	0.45
6:h:23:LYS:NZ	6:h:23:LYS:CB	2.73	0.45
9:j:11:HIS:C	9:j:15:PHE:CD2	2.91	0.45
9:j:43:PHE:CZ	13:s:150:ALA:HB3	2.46	0.45
11:n:238:GLY:N	11:n:243:VAL:HG21	2.31	0.45
11:n:507:GLN:NE2	11:n:636:ALA:O	2.49	0.45
12:q:89:GLN:OE1	12:q:90:PRO:HD2	2.16	0.45
12:q:543:VAL:CG1	17:c:135:ARG:HE	2.29	0.45
21:o:681:GLU:OE1	21:o:768:SER:OG	2.35	0.45
30:5:24:ASP:HA	30:5:33:PHE:HB3	1.98	0.45
38:DE:359:LEU:HD11	38:DE:648:ASP:HB2	1.97	0.45
41:DH:193:PHE:CE2	39:Df:226:GLU:HB3	2.51	0.45
44:DL:102:LEU:HB2	44:DL:115:ASP:HB3	1.98	0.45
44:Dl:120:LEU:HG	44:Dl:126:MET:HB2	1.98	0.45
52:FB:160:GLN:H	52:FB:160:GLN:HG3	1.61	0.45
56:PB:796:MET:HB3	56:PB:948:GLN:HG2	1.98	0.45
64:PJ:48:MET:HE2	64:PJ:48:MET:HA	1.98	0.45
68:w:10:GLU:OE1	68:w:66:PHE:CZ	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:111:ARG:HB3	68:w:114:LEU:HB3	1.97	0.45
70:p:191:SER:HA	70:p:200:LEU:O	2.15	0.45
2:m:104:HIS:NE2	11:n:168:ARG:HD2	2.25	0.45
6:h:12:LEU:C	6:h:12:LEU:CD1	2.85	0.45
8:t:98:LEU:O	8:t:100:GLY:N	2.44	0.45
9:j:9:GLU:CG	9:j:56:GLN:CG	2.93	0.45
11:n:478:MET:HE3	11:n:492:TRP:HB3	1.98	0.45
11:n:509:ILE:HG21	11:n:540:ILE:HD13	1.97	0.45
12:q:17:LYS:HB3	12:q:30:TYR:HE2	1.81	0.45
23:0:295:ARG:NH2	24:8:132:TRP:HB3	2.32	0.45
28:3:177:PHE:O	28:3:180:VAL:HG22	2.16	0.45
33:EA:128:LYS:HB2	33:EA:135:THR:HA	1.97	0.45
36:DB:431:LEU:HD11	36:DB:435:ILE:HG12	1.97	0.45
37:Dd:904:HIS:O	37:Dd:908:GLN:HG2	2.16	0.45
54:Y:-6:DG:H4'	54:Y:-5:DC:OP1	2.16	0.45
55:PA:686:THR:CG2	55:PA:765:ASN:ND2	2.62	0.45
55:PA:1170:THR:HA	55:PA:1216:LEU:HA	1.98	0.45
59:PE:104:ILE:HG23	59:PE:127:LEU:HD22	1.97	0.45
68:w:37:LEU:HD23	68:w:85:MET:HE3	1.98	0.45
1:a:200:LEU:C	1:a:200:LEU:HD13	2.42	0.45
4:f:106:TYR:CZ	6:h:106:PRO:HG3	2.50	0.45
6:h:19:VAL:CG2	12:q:112:LEU:HD23	2.45	0.45
6:h:33:LEU:HD23	6:h:40:LEU:HD21	1.97	0.45
12:q:118:ILE:CG2	12:q:125:MET:HG2	2.46	0.45
14:u:57:LEU:HD11	16:z:492:ARG:NH2	2.30	0.45
25:9:139:ALA:O	25:9:143:ILE:HG12	2.16	0.45
29:4:55:TRP:CZ3	29:4:71:VAL:HG13	2.48	0.45
31:6:621:ASN:O	31:6:622:VAL:HB	2.16	0.45
36:DB:923:ARG:HD3	36:DB:967:LEU:HD11	1.97	0.45
41:DH:47:GLU:H	41:DH:47:GLU:HG3	1.60	0.45
51:BA:125:ALA:HA	51:BA:135:VAL:HG11	1.99	0.45
51:BA:134:ILE:HG23	51:BA:171:GLU:HG3	1.98	0.45
52:FB:142:SER:HB3	56:PB:93:LEU:HD12	1.97	0.45
55:PA:465:HIS:CD2	55:PA:467:MET:HB2	2.50	0.45
55:PA:894:ASP:HB3	55:PA:1396:ARG:HH12	1.80	0.45
55:PA:1654:SER:HB2	55:PA:1655:PRO:CD	2.46	0.45
56:PB:735:VAL:HB	56:PB:750:VAL:HG13	1.99	0.45
68:w:1:MET:N	68:w:1:MET:HE3	2.31	0.45
68:w:1135:PRO:O	68:w:1136:LEU:HB2	2.17	0.45
1:a:259:ILE:O	1:a:259:ILE:CD1	2.64	0.45
1:a:364:TYR:O	1:a:428:THR:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:17:ARG:NH2	5:g:33:LYS:HG2	2.31	0.45
4:f:177:VAL:HG22	11:n:266:VAL:HG23	1.92	0.45
5:g:68:HIS:HB2	5:g:77:GLU:OE1	2.17	0.45
8:t:129:VAL:HG11	8:t:200:ILE:HG13	1.98	0.45
9:j:9:GLU:CD	9:j:56:GLN:CG	2.89	0.45
9:j:110:ILE:HG21	9:j:128:ARG:HH21	1.81	0.45
11:n:184:THR:O	11:n:188:LYS:HG3	2.16	0.45
11:n:385:LEU:HD23	11:n:407:ALA:HA	1.99	0.45
11:n:637:PHE:HD2	11:n:639:LYS:HG2	1.82	0.45
12:q:640:GLU:CD	18:e:96:LEU:HD21	2.42	0.45
12:q:644:SER:CB	18:e:96:LEU:HB3	2.44	0.45
13:s:67:LEU:HA	13:s:69:ARG:NH1	2.32	0.45
17:c:41:ASN:HD22	17:c:41:ASN:C	2.24	0.45
21:o:634:PHE:O	21:o:637:SER:OG	2.25	0.45
31:6:339:VAL:HB	31:6:490:GLU:HA	1.98	0.45
36:DB:516:GLN:N	36:DB:517:PRO:HD2	2.31	0.45
36:DB:723:PHE:HD2	36:DB:753:MET:HB3	1.81	0.45
38:De:461:ILE:HG23	38:De:791:VAL:HB	1.97	0.45
59:PE:80:PRO:HB3	59:PE:108:GLN:HE21	1.81	0.45
68:w:10:GLU:HB3	68:w:14:LYS:NZ	2.31	0.45
1:a:518:ILE:HG22	1:a:518:ILE:O	2.17	0.45
2:m:68:LYS:HZ1	5:g:50:GLN:NE2	2.13	0.45
3:d:81:LYS:HD3	3:d:81:LYS:HA	1.65	0.45
3:d:117:ALA:HB2	5:g:163:MET:CE	2.46	0.45
4:f:52:MET:HE1	24:8:263:ALA:HB2	1.98	0.45
6:h:18:GLN:HG2	6:h:63:LEU:HD12	1.98	0.45
6:h:139:GLN:HG3	10:k:37:LYS:O	2.17	0.45
6:h:146:MET:CB	10:k:39:LYS:HZ2	2.26	0.45
11:n:274:ILE:HG22	11:n:278:VAL:HG13	1.98	0.45
11:n:801:ARG:NE	11:n:811:CYS:HB3	2.31	0.45
12:q:113:TYR:CD1	12:q:113:TYR:C	2.93	0.45
15:v:127:LEU:HD23	20:l:167:ILE:HD12	1.98	0.45
17:c:111:TYR:CD2	19:b:136:HIS:CD2	2.82	0.45
25:9:252:MET:O	25:9:256:ARG:HG2	2.17	0.45
29:4:17:ARG:HD3	29:4:21:GLU:HB2	1.97	0.45
31:6:378:PHE:HA	31:6:381:TRP:NE1	2.31	0.45
32:7:325:THR:HB	32:7:328:HIS:CD2	2.51	0.45
35:DA:414:ILE:HG21	39:DF:310:THR:HB	1.99	0.45
37:DD:1064:ILE:HG23	37:DD:1079:LEU:HD11	1.97	0.45
37:Dd:901:TYR:CZ	44:Dl:117:GLN:HG2	2.52	0.45
44:Dl:101:GLN:C	44:Dl:105:HIS:CD2	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:PA:45:GLU:H	55:PA:45:GLU:HG3	1.47	0.45
69:x:669:ILE:HG22	69:x:673:MET:HE2	1.99	0.45
70:p:15:LEU:HD11	70:p:453:SER:HB2	1.99	0.45
2:m:105:TRP:CH2	3:d:164:PRO:HD3	2.52	0.45
5:g:83:MET:HE3	5:g:83:MET:C	2.41	0.45
6:h:90:MET:HG2	6:h:95:GLY:HA2	1.99	0.45
9:j:73:GLN:HB3	9:j:80:TYR:OH	2.17	0.45
12:q:437:HIS:HE1	12:q:472:GLU:O	1.99	0.45
12:q:449:ASP:OD2	20:l:157:LYS:HD3	2.16	0.45
12:q:484:TYR:CE1	12:q:636:VAL:CG1	2.99	0.45
16:z:552:LEU:HD23	16:z:552:LEU:N	2.31	0.45
23:0:92:LEU:HB2	23:0:127:LYS:NZ	2.32	0.45
24:8:177:TRP:CH2	55:PA:1677:SER:HB3	2.50	0.45
25:9:7:GLN:HE21	25:9:7:GLN:HB2	1.47	0.45
26:1:264:ASN:C	26:1:266:LEU:N	2.74	0.45
33:EA:157:CYS:HB2	33:EA:158:HIS:H	1.63	0.45
35:DA:1165:LEU:HD22	35:DA:1165:LEU:HA	1.85	0.45
38:DE:285:LEU:H	38:DE:285:LEU:HG	1.64	0.45
44:DL:106:ARG:CZ	44:DL:115:ASP:N	2.79	0.45
55:PA:104:MET:HE2	55:PA:104:MET:HB2	1.90	0.45
56:PB:862:GLY:HA3	56:PB:899:SER:N	2.31	0.45
68:w:339:ILE:HD11	68:w:378:GLN:HB3	1.99	0.45
68:w:512:THR:OG1	68:w:513:ASN:ND2	2.50	0.45
69:x:676:ASP:OD1	69:x:676:ASP:N	2.50	0.45
1:a:145:LYS:HD2	1:a:145:LYS:N	2.32	0.45
1:a:160:LEU:HG	1:a:219:LEU:HD11	1.98	0.45
5:g:98:ARG:CG	13:s:74:SER:HA	2.46	0.45
5:g:136:ARG:CG	14:u:86:GLN:OE1	2.65	0.45
5:g:153:PHE:HD1	5:g:153:PHE:C	2.25	0.45
11:n:647:MET:HG2	11:n:651:ASN:ND2	2.32	0.45
13:s:82:ASN:HB2	13:s:84:ILE:HG13	1.98	0.45
16:z:582:LEU:HD22	16:z:593:ILE:HD11	1.99	0.45
23:0:121:LYS:C	23:0:124:ILE:HG12	2.41	0.45
27:2:58:MET:HE2	27:2:58:MET:HB3	1.89	0.45
29:4:188:THR:O	29:4:193:PRO:HD2	2.16	0.45
36:DB:313:TYR:HD1	36:DB:920:PRO:HB2	1.82	0.45
38:DE:509:GLN:O	38:DE:513:LEU:HG	2.17	0.45
38:DE:573:GLN:H	38:DE:573:GLN:HG3	1.57	0.45
39:DF:246:ILE:HG23	39:DF:252:LEU:HD22	1.99	0.45
53:X:-5:DG:H21	54:Y:6:DG:N2	2.09	0.45
54:Y:30:DA:H2'	54:Y:31:DG:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:PA:1261:ILE:HD12	55:PA:1261:ILE:HA	1.87	0.45
58:PD:103:LEU:HD22	58:PD:103:LEU:HA	1.74	0.45
68:w:1139:ARG:O	68:w:1140:GLU:HG3	2.17	0.45
1:a:428:THR:HB	1:a:430:LEU:CD2	2.46	0.45
3:d:121:LEU:CD2	5:g:160:VAL:HG21	2.46	0.45
8:t:28:LEU:HG	8:t:117:TYR:CD2	2.51	0.45
8:t:76:PHE:CD2	8:t:86:ILE:HG23	2.52	0.45
10:k:68:ARG:O	10:k:69:TYR:C	2.59	0.45
11:n:368:LYS:O	11:n:369:PRO:C	2.58	0.45
11:n:443:LEU:HD12	11:n:500:LEU:HD22	1.98	0.45
11:n:444:GLU:HB3	11:n:445:PRO:HD3	1.98	0.45
11:n:544:ARG:NE	11:n:716:ASN:HA	2.32	0.45
24:8:113:HIS:CD2	24:8:308:PRO:HD3	2.51	0.45
26:1:434:LEU:HD12	29:4:58:ARG:HH22	1.82	0.45
27:2:334:ILE:HG13	27:2:357:VAL:HB	1.97	0.45
29:4:172:SER:C	29:4:174:ASP:H	2.25	0.45
31:6:444:HIS:NE2	31:6:638:GLN:HG3	2.32	0.45
32:7:494:ILE:HB	32:7:706:LEU:HA	1.98	0.45
36:DB:69:GLN:HE22	36:DB:963:HIS:HB3	1.82	0.45
41:DH:87:GLN:H	42:DI:126:ASN:HD21	1.63	0.45
44:DL:102:LEU:O	44:DL:106:ARG:HG3	2.17	0.45
47:Dm:37:ARG:HG2	47:Dm:54:VAL:HG21	1.98	0.45
53:X:-37:DG:H2'	53:X:-37:DG:O5'	2.16	0.45
68:w:1195:ALA:O	68:w:1197:HIS:N	2.50	0.45
1:a:109:TYR:CE1	1:a:150:PHE:CZ	3.05	0.45
1:a:259:ILE:H	1:a:259:ILE:CD1	2.22	0.45
3:d:28:GLU:H	3:d:28:GLU:HG3	1.42	0.45
3:d:172:PRO:O	3:d:174:ARG:HG2	2.17	0.45
6:h:61:LYS:HB3	6:h:61:LYS:HE2	1.66	0.45
6:h:191:LEU:HD21	7:r:129:PHE:HB3	1.97	0.45
7:r:30:HIS:O	7:r:33:GLU:OE2	2.35	0.45
7:r:150:ARG:N	7:r:161:GLU:O	2.46	0.45
10:k:31:VAL:CG2	12:q:157:ALA:HB2	2.35	0.45
10:k:113:GLN:HA	10:k:116:GLU:OE1	2.17	0.45
14:u:117:LYS:HZ1	22:i:140:MET:HG3	1.75	0.45
15:v:119:LEU:HD11	15:v:123:ILE:HG13	1.99	0.45
15:v:133:GLU:C	15:v:133:GLU:CD	2.85	0.45
27:2:69:ARG:HG3	27:2:141:GLY:H	1.82	0.45
31:6:404:SER:HA	31:6:433:GLN:HB3	1.98	0.45
32:7:653:THR:HG22	32:7:692:LYS:HG3	1.99	0.45
33:EA:154:CYS:SG	33:EA:161:VAL:HG13	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DE:366:GLU:HA	38:DE:369:LYS:HG2	1.97	0.45
39:DF:332:PHE:O	39:DF:335:ARG:HG2	2.17	0.45
38:De:321:LEU:HD22	38:De:329:ILE:HG23	1.98	0.45
38:De:424:GLN:HE21	38:De:424:GLN:HB2	1.61	0.45
38:De:477:ASP:HB3	38:De:551:PHE:HB2	1.98	0.45
38:De:721:ARG:HG2	38:De:787:ARG:HA	1.99	0.45
46:Dk:183:GLN:HB2	46:Dk:186:HIS:HD2	1.82	0.45
44:Dl:57:VAL:HG21	44:Dl:92:ILE:HD11	1.93	0.45
53:X:13:DA:H2"	53:X:14:DC:C6	2.51	0.45
57:PC:172:GLU:HG2	65:PK:10:PHE:CE2	2.52	0.45
58:PD:51:ALA:CB	58:PD:54:GLU:HG2	2.44	0.45
58:PD:137:LYS:HD2	58:PD:137:LYS:HA	1.61	0.45
64:PJ:3:ILE:HD12	64:PJ:4:PRO:HD2	1.99	0.45
67:FA:102:VAL:HB	67:FA:108:ARG:HB3	1.98	0.45
1:a:177:LEU:HB2	1:a:259:ILE:HG13	1.99	0.45
1:a:330:PHE:HZ	1:a:393:VAL:HA	1.82	0.45
2:m:54:TYR:HE1	5:g:35:PRO:N	2.15	0.45
6:h:5:GLU:C	6:h:5:GLU:CD	2.85	0.45
8:t:8:GLN:HE21	8:t:196:LEU:HD13	1.80	0.45
11:n:148:ARG:HD3	14:u:9:GLN:HB3	1.98	0.45
11:n:707:ASP:CG	21:o:684:ARG:HD3	2.42	0.45
11:n:959:LEU:HD12	11:n:963:LEU:HD23	1.98	0.45
12:q:484:TYR:CE1	12:q:636:VAL:HG12	2.52	0.45
18:e:74:ARG:HD2	18:e:78:ASP:OD2	2.16	0.45
32:7:77:VAL:N	32:7:78:PRO:HD2	2.31	0.45
32:7:445:LYS:N	32:7:446:PRO:HD2	2.32	0.45
33:EA:144:LEU:HD13	33:EA:161:VAL:HG21	1.97	0.45
36:DB:788:LYS:HB2	36:DB:788:LYS:HE3	1.40	0.45
41:DH:105:ASP:O	41:DH:108:PRO:HD2	2.17	0.45
38:De:251:LEU:O	38:De:256:HIS:HB2	2.17	0.45
39:Df:282:LEU:O	39:Df:286:VAL:HG23	2.17	0.45
49:DP:300:ILE:HD11	49:DP:324:ALA:HB2	1.99	0.45
56:PB:587:LEU:HB3	56:PB:603:MET:HE3	1.98	0.45
70:p:41:CYS:SG	70:p:42:ARG:N	2.90	0.45
1:a:340:TYR:HB2	1:a:378:LYS:HB3	1.99	0.44
3:d:31:LEU:HD21	22:i:100:LEU:HD23	1.99	0.44
6:h:33:LEU:HD21	12:q:95:TRP:CZ3	2.48	0.44
7:r:38:ARG:HD2	10:k:75:THR:HG21	1.99	0.44
9:j:29:PHE:CD2	9:j:30:GLN:HB2	2.52	0.44
11:n:464:GLN:CD	12:q:323:PRO:HG3	2.42	0.44
12:q:167:LEU:CD2	15:v:76:MET:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:v:48:VAL:CG2	15:v:53:GLN:HB2	2.47	0.44
25:9:198:ILE:HG22	25:9:204:TYR:HD1	1.82	0.44
26:1:165:GLY:HA2	26:1:196:ILE:HG12	1.98	0.44
28:3:59:VAL:H	28:3:71:TYR:HB2	1.82	0.44
31:6:109:ARG:HB2	31:6:682:ASP:HA	1.98	0.44
32:7:606:GLU:HA	32:7:666:ARG:HH22	1.81	0.44
32:7:683:ARG:HB3	32:7:689:LYS:HD3	2.00	0.44
36:DB:627:TRP:HE1	36:DB:629:ARG:HD2	1.81	0.44
36:DB:774:PHE:O	36:DB:778:LEU:HG	2.16	0.44
37:DD:872:PHE:HD2	44:DL:56:GLN:HA	1.81	0.44
38:DE:441:ILE:HG22	38:DE:445:LYS:HE3	1.99	0.44
38:DE:718:ARG:HB2	38:DE:783:LEU:HB3	1.99	0.44
39:Df:297:LEU:HB2	39:Df:344:PHE:CZ	2.52	0.44
55:PA:698:THR:HG21	55:PA:759:SER:HB3	1.99	0.44
55:PA:1217:ASP:O	55:PA:1221:MET:HG2	2.17	0.44
57:PC:25:ASN:H	57:PC:227:GLU:HG2	1.81	0.44
69:x:495:ILE:HG22	69:x:499:MET:HE2	1.99	0.44
69:x:543:ASP:OD1	69:x:543:ASP:N	2.48	0.44
1:a:109:TYR:CE2	1:a:154:LEU:HD23	2.52	0.44
3:d:131:LYS:HB2	14:u:104:LEU:CD1	2.42	0.44
3:d:169:PRO:C	55:PA:1793:THR:CB	2.88	0.44
6:h:55:GLN:HB2	58:PD:137:LYS:HZ3	1.80	0.44
6:h:132:GLY:HA2	6:h:136:ALA:HB2	1.98	0.44
8:t:9:MET:HG3	8:t:165:LEU:HD11	2.00	0.44
10:k:88:LYS:HZ3	12:q:303:LEU:HD22	1.83	0.44
11:n:781:LEU:HD23	11:n:781:LEU:HA	1.88	0.44
12:q:89:GLN:CD	12:q:90:PRO:CD	2.82	0.44
12:q:166:ARG:CG	12:q:166:ARG:NH1	2.79	0.44
12:q:223:GLU:HB2	12:q:246:GLN:HB3	1.98	0.44
12:q:549:LEU:HD11	12:q:572:ALA:HB2	1.99	0.44
12:q:633:ARG:NH1	18:e:114:ASP:OD1	2.49	0.44
19:b:156:PRO:HD2	19:b:159:GLN:HG2	1.99	0.44
21:o:712:ASP:N	21:o:712:ASP:OD1	2.48	0.44
23:0:272:LEU:HD22	23:0:272:LEU:HA	1.76	0.44
29:4:52:ALA:HB2	29:4:86:SER:HB2	1.99	0.44
32:7:637:LEU:HD13	32:7:648:GLU:HG3	1.99	0.44
40:DG:79:THR:O	40:DG:79:THR:CG2	2.65	0.44
53:X:-39:DA:OP1	53:X:-39:DA:C8	2.71	0.44
53:X:7:DG:N3	54:Y:-6:DG:N2	2.65	0.44
56:PB:1115:GLN:HB3	56:PB:1148:LEU:HD11	2.00	0.44
62:PH:58:LEU:HD11	62:PH:143:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:1183:TRP:CH2	68:w:1185:GLY:HA3	2.52	0.44
69:x:53:GLY:O	69:x:54:PRO:C	2.60	0.44
70:p:40:SER:HB3	70:p:89:TRP:CD2	2.52	0.44
2:m:101:GLN:HA	11:n:169:LEU:HD23	1.97	0.44
6:h:20:ALA:HB2	12:q:113:TYR:CE2	2.51	0.44
8:t:78:LEU:CD1	8:t:84:CYS:HB3	2.46	0.44
12:q:213:GLY:O	12:q:383:HIS:HA	2.17	0.44
12:q:491:ILE:HG23	12:q:506:HIS:HE1	1.82	0.44
14:u:71:VAL:HG23	16:z:528:LEU:HD21	1.98	0.44
19:b:85:ASN:ND2	21:o:641:THR:HB	2.32	0.44
23:0:92:LEU:HB2	23:0:127:LYS:HZ1	1.82	0.44
27:2:145:LEU:HD11	27:2:169:ILE:HD13	1.97	0.44
28:3:177:PHE:O	28:3:181:ILE:HG13	2.18	0.44
29:4:212:LEU:HD22	29:4:270:LEU:HD21	1.98	0.44
32:7:606:GLU:HA	32:7:666:ARG:NH2	2.33	0.44
36:DB:399:LEU:O	36:DB:403:VAL:HG22	2.16	0.44
36:DB:428:ALA:HB1	36:DB:430:HIS:CE1	2.52	0.44
36:DB:899:LYS:HA	36:DB:935:PRO:HA	1.99	0.44
38:De:243:LEU:HD13	38:De:243:LEU:HA	1.76	0.44
39:Df:402:ARG:CZ	39:Df:424:GLN:HB2	2.48	0.44
49:DP:193:ASN:HD22	49:DP:194:PRO:HD2	1.82	0.44
52:FB:19:TRP:HD1	52:FB:112:GLN:HB3	1.82	0.44
52:FB:126:ARG:CA	52:FB:129:ARG:HG2	2.27	0.44
55:PA:488:VAL:O	55:PA:491:PRO:HD2	2.18	0.44
55:PA:1669:PRO:HB2	55:PA:1670:SER:H	1.61	0.44
57:PC:47:ILE:HA	57:PC:165:ALA:HA	1.99	0.44
61:PG:51:ILE:HG22	61:PG:72:TYR:HB3	1.98	0.44
68:w:273:VAL:HG21	68:w:286:MET:HE1	1.99	0.44
69:x:269:MET:HB2	69:x:269:MET:HE2	1.76	0.44
11:n:173:ILE:H	11:n:173:ILE:HG13	1.63	0.44
11:n:274:ILE:H	11:n:274:ILE:HG13	1.61	0.44
11:n:865:VAL:O	11:n:869:LEU:HG	2.17	0.44
12:q:160:LEU:HA	12:q:160:LEU:HD23	1.81	0.44
12:q:186:GLU:HB3	12:q:243:LEU:HD22	1.99	0.44
12:q:194:TRP:HB3	12:q:222:PHE:HZ	1.82	0.44
14:u:102:THR:O	14:u:105:GLU:HG2	2.17	0.44
22:i:72:ILE:HG23	22:i:88:ASN:OD1	2.16	0.44
31:6:437:LEU:H	31:6:437:LEU:HG	1.57	0.44
36:DB:30:HIS:HE1	36:DB:32:VAL:HG22	1.82	0.44
36:DB:75:VAL:HG23	36:DB:84:PHE:CD1	2.52	0.44
36:DB:913:MET:O	36:DB:917:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DE:780:VAL:HG13	38:DE:793:ALA:HB1	1.99	0.44
55:PA:36:VAL:HA	56:PB:1138:ARG:HH12	1.82	0.44
55:PA:457:ILE:O	55:PA:503:LEU:HA	2.18	0.44
55:PA:1147:SER:HA	55:PA:1153:ARG:HB3	1.98	0.44
55:PA:1481:LYS:HD3	61:PG:20:PRO:HA	2.00	0.44
55:PA:1655:PRO:C	55:PA:1657:TYR:N	2.75	0.44
56:PB:1156:LYS:HE3	56:PB:1156:LYS:HB3	1.86	0.44
58:PD:135:GLN:HE21	58:PD:135:GLN:HB3	1.55	0.44
65:PK:36:ASN:HA	65:PK:70:LYS:HG3	2.00	0.44
69:x:431:SER:O	69:x:431:SER:OG	2.31	0.44
1:a:428:THR:HB	1:a:430:LEU:HD21	1.99	0.44
1:a:465:VAL:HG22	1:a:479:LEU:HG	1.99	0.44
7:r:135:LEU:HD11	7:r:142:LYS:HE3	2.00	0.44
8:t:76:PHE:CG	8:t:190:MET:HG3	2.53	0.44
9:j:49:GLN:HB3	11:n:60:HIS:CB	2.48	0.44
9:j:59:HIS:N	11:n:50:ARG:HA	2.31	0.44
9:j:85:LEU:HD12	13:s:96:PHE:CE2	2.50	0.44
11:n:509:ILE:HD11	11:n:516:SER:HB2	2.00	0.44
12:q:7:VAL:HG23	14:u:90:LEU:HD21	1.99	0.44
12:q:290:HIS:CE1	12:q:294:LYS:NZ	2.82	0.44
12:q:443:ARG:NE	12:q:443:ARG:CA	2.73	0.44
18:e:146:ILE:C	18:e:148:VAL:N	2.71	0.44
20:l:91:LYS:O	20:l:94:LEU:HG	2.18	0.44
21:o:706:LEU:HG	21:o:723:LEU:HB3	1.99	0.44
32:7:72:TYR:O	32:7:206:VAL:HA	2.17	0.44
36:DB:661:ALA:O	36:DB:664:GLU:HG2	2.17	0.44
49:DP:223:GLY:HA3	54:Y:26:DT:H4'	1.99	0.44
55:PA:567:LEU:HD21	55:PA:595:ILE:HG12	2.00	0.44
68:w:236:ALA:HB2	68:w:663:PRO:HG3	2.00	0.44
68:w:381:SER:O	68:w:534:HIS:ND1	2.48	0.44
68:w:383:SER:O	68:w:383:SER:OG	2.32	0.44
68:w:547:VAL:HG13	68:w:559:LEU:HD11	2.00	0.44
70:p:131:ILE:HD13	70:p:183:THR:HG22	1.99	0.44
1:a:382:LEU:C	69:x:92:LEU:HD21	2.41	0.44
4:f:50:VAL:HG12	4:f:56:THR:HG21	2.00	0.44
7:r:69:VAL:O	7:r:69:VAL:HG12	2.17	0.44
8:t:173:PRO:HD2	8:t:176:PHE:CG	2.53	0.44
11:n:231:GLU:CB	11:n:253:LEU:CD2	2.96	0.44
12:q:247:ILE:HD11	12:q:294:LYS:HD3	2.00	0.44
15:v:123:ILE:HD12	20:l:166:LEU:HD22	2.00	0.44
31:6:153:MET:O	31:6:157:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:EB:127:ASN:HB2	34:EB:130:ILE:HB	2.00	0.44
34:EB:204:ASN:HD22	34:EB:204:ASN:HA	1.61	0.44
36:DB:806:VAL:CG2	36:DB:829:ILE:HD12	2.30	0.44
37:DD:961:GLN:O	37:DD:964:GLU:HG3	2.18	0.44
38:DE:601:VAL:HG21	38:DE:642:VAL:HG11	2.00	0.44
44:DL:106:ARG:HH12	44:DL:114:LYS:HG3	0.62	0.44
38:De:427:ILE:HD11	38:De:657:LEU:HB2	1.99	0.44
38:De:585:ASN:HD22	38:De:585:ASN:HA	1.64	0.44
39:Df:389:LYS:HA	39:Df:393:LEU:HD23	1.99	0.44
53:X:1:DA:N1	54:Y:0:DG:C6	2.86	0.44
55:PA:689:ILE:H	55:PA:689:ILE:HG13	1.48	0.44
55:PA:959:MET:HE3	55:PA:959:MET:HB2	1.85	0.44
56:PB:389:GLY:HA3	56:PB:668:LEU:HG	1.99	0.44
56:PB:626:LEU:H	56:PB:626:LEU:HG	1.64	0.44
56:PB:707:CYS:O	56:PB:710:ILE:HG12	2.17	0.44
68:w:326:THR:HA	68:w:329:LEU:HD13	1.99	0.44
68:w:485:SER:OG	68:w:486:GLU:N	2.49	0.44
68:w:786:PRO:HA	68:w:787:PRO:HD3	1.82	0.44
69:x:529:MET:HE3	69:x:529:MET:HB3	1.78	0.44
69:x:561:LEU:O	69:x:608:ASN:ND2	2.51	0.44
69:x:577:ALA:O	69:x:581:ILE:HG13	2.18	0.44
70:p:145:LEU:HD22	70:p:359:LEU:HD21	2.00	0.44
1:a:321:LEU:HD21	1:a:407:ILE:CG1	2.47	0.44
1:a:378:LYS:O	1:a:379:ASP:HB2	2.18	0.44
2:m:30:ASN:CB	3:d:176:TYR:CB	2.78	0.44
8:t:36:GLN:HG3	8:t:118:GLN:HB2	1.98	0.44
9:j:75:ARG:CB	9:j:80:TYR:HD2	2.17	0.44
11:n:306:GLU:HG3	11:n:306:GLU:O	2.18	0.44
11:n:591:PHE:HE1	68:w:22:PHE:HE1	1.64	0.44
11:n:591:PHE:CE1	68:w:22:PHE:HE1	2.36	0.44
11:n:909:GLN:OE1	19:b:114:ASP:OD1	2.36	0.44
12:q:469:ASP:HB2	17:c:231:TRP:CD2	2.52	0.44
15:v:67:ASN:ND2	58:PD:142:TYR:O	2.50	0.44
31:6:562:ALA:HB3	31:6:568:LEU:HD23	1.99	0.44
32:7:35:LYS:HE2	32:7:35:LYS:HB3	1.89	0.44
33:EA:30:HIS:O	33:EA:34:LEU:HG	2.16	0.44
38:DE:665:PHE:HE1	38:DE:701:GLY:HA2	1.83	0.44
45:Dc:110:PRO:HD3	45:Dc:122:GLU:HA	1.99	0.44
46:Dk:134:ILE:O	46:Dk:138:ILE:HG13	2.18	0.44
47:Dm:82:GLN:H	47:Dm:82:GLN:HG3	1.55	0.44
56:PB:1015:LEU:HD12	56:PB:1015:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:PB:1143:LYS:O	56:PB:1146:ILE:HG22	2.18	0.44
69:x:832:GLN:NE2	69:x:835:ARG:HH21	2.15	0.44
69:x:959:SER:O	69:x:965:LYS:N	2.51	0.44
70:p:398:SER:O	70:p:400:GLN:N	2.51	0.44
1:a:62:LEU:O	1:a:65:LEU:HB2	2.17	0.44
1:a:167:ASN:HD22	1:a:167:ASN:HA	1.65	0.44
1:a:348:LEU:HD12	1:a:348:LEU:HA	1.74	0.44
2:m:59:LYS:NZ	2:m:77:GLU:CD	2.66	0.44
2:m:59:LYS:CE	2:m:77:GLU:OE2	2.65	0.44
4:f:137:CYS:CA	6:h:42:TRP:HB3	2.47	0.44
5:g:97:ILE:HG22	9:j:103:LYS:NZ	2.30	0.44
8:t:146:PRO:HB3	17:c:239:PHE:CE2	2.52	0.44
11:n:307:VAL:O	11:n:311:GLN:HG3	2.18	0.44
11:n:529:PRO:O	11:n:533:LEU:HG	2.18	0.44
11:n:936:ILE:N	11:n:1197:GLY:O	2.49	0.44
12:q:32:PRO:HB2	12:q:34:LEU:HD21	1.99	0.44
12:q:119:VAL:CG1	12:q:127:LEU:HD13	2.48	0.44
12:q:127:LEU:HG	12:q:127:LEU:O	2.16	0.44
14:u:96:GLU:O	14:u:99:GLU:HG3	2.17	0.44
15:v:84:GLN:NE2	15:v:85:PHE:CB	2.73	0.44
21:o:764:PRO:HD3	68:w:20:GLU:HG3	1.99	0.44
21:o:765:ASP:OD2	68:w:72:SER:HA	2.17	0.44
41:DH:60:THR:HG21	43:DJ:211:VAL:HG23	2.00	0.44
38:De:225:ILE:HG13	38:De:240:PHE:CZ	2.52	0.44
49:DP:232:LEU:HG	49:DP:236:LYS:HE3	1.99	0.44
50:DQ:319:ASP:O	50:DQ:320:VAL:HG22	2.17	0.44
55:PA:1374:VAL:HG11	55:PA:1411:LEU:HD11	2.00	0.44
68:w:726:ASN:H	68:w:726:ASN:HD22	1.63	0.44
69:x:484:LYS:N	69:x:485:PRO:HD3	2.32	0.44
69:x:765:VAL:HG13	69:x:812:LEU:HB2	1.99	0.44
1:a:400:HIS:HE1	1:a:403:ARG:HG2	1.83	0.44
3:d:136:GLU:OE2	5:g:146:ARG:NH1	2.50	0.44
5:g:92:LEU:HD23	5:g:92:LEU:HA	1.73	0.44
8:t:11:VAL:HG12	8:t:138:ILE:HD12	2.00	0.44
9:j:82:LYS:HE2	13:s:96:PHE:HA	1.99	0.44
11:n:197:GLN:O	11:n:200:ARG:HB2	2.17	0.44
11:n:482:VAL:HG13	11:n:489:ILE:HD11	2.00	0.44
11:n:659:LEU:HD11	68:w:14:LYS:CG	2.42	0.44
12:q:437:HIS:O	12:q:437:HIS:CD2	2.71	0.44
12:q:457:ASP:O	12:q:634:ASN:OD1	2.36	0.44
14:u:28:GLN:CD	14:u:28:GLN:C	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:v:127:LEU:CD2	20:l:167:ILE:HD12	2.47	0.44
16:z:489:TYR:HA	16:z:492:ARG:HD2	1.99	0.44
21:o:694:ASP:HB2	21:o:705:HIS:HB2	2.00	0.44
27:2:182:ILE:O	27:2:186:ILE:HG13	2.18	0.44
29:4:383:LEU:HD12	29:4:383:LEU:HA	1.90	0.44
31:6:170:LEU:HD22	31:6:461:HIS:HB3	1.99	0.44
32:7:121:VAL:HG13	32:7:133:LYS:HB3	1.99	0.44
35:DA:791:VAL:HA	35:DA:887:ALA:HB1	2.00	0.44
35:DA:929:THR:HG22	35:DA:954:ALA:HA	1.99	0.44
36:DB:339:THR:HB	36:DB:340:PRO:HD3	2.00	0.44
38:De:376:LEU:HA	38:De:638:ASN:HD21	1.83	0.44
38:De:747:LEU:H	38:De:747:LEU:HG	1.60	0.44
39:Df:280:ILE:HG12	39:Df:329:LEU:HD13	1.99	0.44
53:X:-5:DG:H2"	53:X:-4:DT:C5	2.53	0.44
56:PB:206:TYR:HB2	56:PB:208:PHE:CZ	2.53	0.44
56:PB:304:SER:O	56:PB:307:GLU:HG2	2.17	0.44
61:PG:89:VAL:HA	61:PG:99:THR:HA	2.00	0.44
68:w:150:ASN:O	68:w:199:TRP:NE1	2.51	0.44
1:a:324:CYS:HB3	1:a:403:ARG:HD2	1.99	0.43
10:k:83:SER:HB3	15:v:102:ASN:OD1	2.17	0.43
14:u:4:ARG:NE	16:z:594:LEU:O	2.45	0.43
17:c:296:TRP:NE1	17:c:311:GLN:HG3	2.33	0.43
24:8:177:TRP:CZ3	24:8:214:PRO:HB3	2.53	0.43
24:8:177:TRP:CE3	24:8:215:GLY:N	2.86	0.43
31:6:105:GLU:HG3	31:6:122:SER:HB3	2.00	0.43
36:DB:94:CYS:SG	36:DB:954:TRP:HZ2	2.40	0.43
36:DB:961:THR:HG22	36:DB:967:LEU:HB3	1.99	0.43
44:DL:89:ASP:O	44:DL:93:GLU:HG3	2.18	0.43
39:Df:105:TYR:HB2	43:Dj:217:PHE:HB2	1.99	0.43
44:Dl:57:VAL:HG11	44:Dl:92:ILE:HD13	2.00	0.43
50:DQ:10:VAL:HG13	50:DQ:366:ILE:HD11	2.00	0.43
56:PB:634:LEU:HD23	56:PB:634:LEU:HA	1.81	0.43
56:PB:763:SER:HA	56:PB:766:TYR:HD2	1.82	0.43
67:FA:47:LEU:HG	67:FA:98:TRP:CE3	2.53	0.43
68:w:673:LYS:HE2	68:w:678:ALA:HB2	1.99	0.43
1:a:373:CYS:HB3	1:a:439:GLN:HG2	2.00	0.43
1:a:417:TYR:OH	1:a:450:PHE:CD1	2.70	0.43
3:d:73:ASP:HA	3:d:76:PHE:CE1	2.53	0.43
6:h:147:CYS:SG	15:v:41:LYS:HA	2.57	0.43
7:r:32:LEU:HD12	7:r:167:TYR:CZ	2.53	0.43
7:r:126:ASP:HB3	7:r:127:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:1:MET:HE3	16:z:541:PRO:HB2	1.96	0.43
12:q:311:LEU:HG	12:q:427:LEU:HD23	2.00	0.43
12:q:577:ASP:OD1	12:q:577:ASP:N	2.51	0.43
14:u:4:ARG:CD	16:z:596:TYR:CA	2.96	0.43
16:z:548:THR:C	16:z:550:ASP:N	2.75	0.43
17:c:307:ASP:N	17:c:307:ASP:OD1	2.52	0.43
20:l:92:LEU:HA	20:l:95:VAL:HG22	2.00	0.43
25:9:194:PHE:O	25:9:198:ILE:HG12	2.18	0.43
27:2:156:LEU:HD22	27:2:165:ARG:HB3	2.01	0.43
31:6:640:LEU:HD12	31:6:644:LEU:HD13	1.99	0.43
44:DL:87:ILE:C	44:DL:91:PHE:CD2	2.95	0.43
38:De:761:LEU:HD23	38:De:762:PRO:HD2	1.99	0.43
58:PD:90:LYS:HD3	58:PD:130:ILE:HG12	2.00	0.43
63:PI:78:LEU:HD22	63:PI:97:PHE:HB3	1.99	0.43
2:m:17:ARG:HA	5:g:21:TYR:OH	2.18	0.43
2:m:104:HIS:CG	11:n:169:LEU:HG	2.52	0.43
3:d:150:LYS:HE2	3:d:150:LYS:HA	2.00	0.43
4:f:122:ALA:HB2	12:q:108:GLU:HG2	2.00	0.43
4:f:122:ALA:O	4:f:126:ILE:HG13	2.18	0.43
7:r:38:ARG:NH1	10:k:75:THR:HG23	2.33	0.43
9:j:78:GLN:C	9:j:82:LYS:HD2	2.35	0.43
9:j:119:GLU:H	9:j:119:GLU:HG3	1.61	0.43
10:k:36:SER:HB3	10:k:37:LYS:HZ2	1.83	0.43
11:n:160:VAL:HG22	11:n:166:TYR:HE1	1.83	0.43
12:q:375:LEU:CD2	12:q:431:ILE:CG1	2.95	0.43
12:q:440:LEU:CD2	12:q:502:ILE:HD11	2.46	0.43
14:u:77:PRO:CG	14:u:79:GLU:CG	2.67	0.43
26:1:519:THR:O	26:1:520:ASN:C	2.61	0.43
29:4:19:LEU:HB3	29:4:47:GLU:HG3	2.00	0.43
29:4:337:ARG:O	29:4:338:PHE:CD1	2.72	0.43
32:7:233:PHE:HB3	32:7:236:ALA:HB2	2.01	0.43
35:DA:403:LEU:HD12	35:DA:403:LEU:HA	1.77	0.43
37:DD:1085:LYS:NZ	44:DL:83:MET:HE1	2.33	0.43
39:DF:274:ASN:HD22	39:DF:274:ASN:HA	1.51	0.43
41:DH:156:PRO:O	41:DH:160:ILE:HB	2.18	0.43
39:Df:104:LEU:HB3	43:Dj:216:TYR:HB2	1.99	0.43
39:Df:290:MET:HE2	39:Df:340:ILE:HB	1.99	0.43
53:X:15:DA:C6	54:Y:-14:DG:N2	2.66	0.43
56:PB:34:PHE:HZ	56:PB:528:LEU:HB3	1.83	0.43
56:PB:50:PHE:HA	56:PB:54:SER:HB3	2.00	0.43
56:PB:588:ARG:O	56:PB:592:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:PB:757:PRO:HG2	56:PB:764:MET:HE1	2.00	0.43
57:PC:42:VAL:HG21	57:PC:244:ILE:HG23	2.00	0.43
2:m:116:GLN:CD	16:z:595:PRO:HD3	2.37	0.43
6:h:89:LEU:HD22	6:h:89:LEU:HA	1.75	0.43
10:k:103:LYS:HA	10:k:103:LYS:HD3	1.70	0.43
11:n:948:LYS:HD2	11:n:948:LYS:HA	1.70	0.43
12:q:203:ILE:O	12:q:203:ILE:HG13	2.18	0.43
14:u:57:LEU:HD13	16:z:492:ARG:HG3	2.00	0.43
15:v:45:GLU:H	15:v:45:GLU:HG3	1.63	0.43
15:v:131:GLU:O	15:v:135:TYR:CD2	2.66	0.43
23:0:192:LEU:HD11	23:0:196:LEU:HD23	2.01	0.43
23:0:281:GLN:NE2	24:8:244:PRO:HD3	2.34	0.43
25:9:58:LYS:HA	25:9:58:LYS:HD3	1.79	0.43
29:4:188:THR:O	29:4:189:GLU:HB2	2.17	0.43
32:7:255:THR:HA	32:7:258:ARG:HD2	2.00	0.43
39:DF:320:ARG:HG2	39:DF:415:ILE:HG13	2.00	0.43
37:Dd:885:ILE:HB	44:Dl:96:VAL:CG1	2.48	0.43
51:BA:138:THR:HG23	51:BA:163:CYS:HB3	2.01	0.43
55:PA:276:LEU:HD23	55:PA:276:LEU:H	1.82	0.43
55:PA:1471:PHE:CZ	60:PF:61:GLU:HA	2.54	0.43
61:PG:117:MET:H	61:PG:117:MET:HG3	1.65	0.43
62:PH:94:GLY:HA3	62:PH:118:TYR:HA	2.01	0.43
68:w:316:GLU:OE2	68:w:366:ILE:N	2.49	0.43
69:x:821:TYR:HE2	69:x:946:PHE:HE2	1.67	0.43
1:a:107:MET:O	1:a:107:MET:SD	2.77	0.43
5:g:13:PRO:O	5:g:15:MET:N	2.44	0.43
10:k:79:HIS:NE2	12:q:195:LYS:HD2	2.32	0.43
11:n:909:GLN:HB2	11:n:913:HIS:O	2.18	0.43
12:q:475:VAL:HG22	12:q:495:LEU:HB2	2.01	0.43
12:q:633:ARG:NH2	12:q:633:ARG:CG	2.78	0.43
15:v:77:LYS:O	15:v:80:SER:OG	2.27	0.43
17:c:42:LYS:HB2	17:c:48:ARG:HB3	1.99	0.43
22:i:121:LEU:HD22	22:i:121:LEU:HA	1.80	0.43
25:9:85:MET:HE3	25:9:85:MET:HB3	1.92	0.43
36:DB:359:ILE:HG23	36:DB:496:MET:O	2.18	0.43
38:De:547:TYR:CD1	39:Df:60:MET:HB3	2.54	0.43
46:Dk:170:LEU:HD21	47:Dm:45:ASP:HA	1.99	0.43
44:Dl:115:ASP:HA	44:Dl:118:LEU:HD23	2.00	0.43
47:Dm:30:ARG:HB2	47:Dm:33:SER:HB2	2.01	0.43
51:BA:296:ALA:N	51:BA:297:PRO:HD2	2.33	0.43
53:X:1:DA:H2"	53:X:2:DG:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:PA:192:ARG:HB3	55:PA:213:LYS:HZ1	1.83	0.43
55:PA:546:ARG:HH22	55:PA:550:LYS:HE2	1.83	0.43
56:PB:911:LEU:HD12	66:PL:42:ARG:HD3	2.00	0.43
68:w:770:MET:HB3	68:w:776:ILE:HD11	1.99	0.43
69:x:187:SER:O	69:x:190:THR:OG1	2.35	0.43
69:x:420:ILE:HA	69:x:423:THR:HG22	1.99	0.43
2:m:116:GLN:NE2	16:z:595:PRO:HG2	2.31	0.43
2:m:116:GLN:CD	16:z:595:PRO:HG2	2.43	0.43
3:d:135:ILE:O	3:d:136:GLU:HB2	2.17	0.43
5:g:31:ALA:N	5:g:32:PRO:HD3	2.33	0.43
6:h:55:GLN:CD	58:PD:137:LYS:HD3	2.44	0.43
7:r:85:LEU:HG	7:r:114:LEU:HD11	2.00	0.43
8:t:81:ASN:N	8:t:81:ASN:OD1	2.50	0.43
11:n:276:GLN:H	11:n:276:GLN:HG3	1.64	0.43
11:n:808:LEU:O	11:n:821:SER:HA	2.18	0.43
11:n:857:GLU:O	11:n:861:LYS:HG2	2.19	0.43
22:i:88:ASN:OD1	22:i:88:ASN:C	2.61	0.43
24:8:131:HIS:O	24:8:132:TRP:HB2	2.18	0.43
31:6:65:MET:HE2	31:6:65:MET:HB2	1.92	0.43
32:7:623:VAL:HG21	32:7:689:LYS:HE2	2.01	0.43
36:DB:608:ASN:HB3	36:DB:657:ARG:HG3	2.01	0.43
39:DF:359:PHE:HB3	39:DF:380:LEU:HG	2.01	0.43
43:DJ:204:LEU:HB3	43:DJ:209:ILE:O	2.19	0.43
53:X:-14:DG:N2	54:Y:15:DC:O2	2.52	0.43
55:PA:577:PRO:HD3	62:PH:75:TYR:HB2	2.01	0.43
55:PA:952:LEU:HD21	55:PA:1006:PRO:HB2	2.00	0.43
56:PB:109:MET:HB2	56:PB:112:GLU:HB2	2.01	0.43
56:PB:896:LEU:HD23	56:PB:896:LEU:HA	1.80	0.43
63:PI:65:LEU:HD23	63:PI:68:ILE:HD11	2.01	0.43
1:a:489:CYS:HA	1:a:514:LYS:HZ1	1.83	0.43
1:a:514:LYS:HB3	1:a:514:LYS:HZ2	1.82	0.43
3:d:121:LEU:HA	3:d:121:LEU:HD12	1.76	0.43
9:j:90:ALA:O	9:j:94:GLN:HG3	2.19	0.43
10:k:16:ASP:OD2	15:v:79:VAL:CG2	2.64	0.43
10:k:88:LYS:C	10:k:88:LYS:CD	2.89	0.43
11:n:244:PRO:HB3	11:n:283:PHE:CD1	2.47	0.43
11:n:376:PRO:HD2	11:n:377:PRO:HD3	2.00	0.43
11:n:436:PRO:HG3	11:n:458:LEU:HD21	1.99	0.43
11:n:541:LYS:HG3	11:n:549:TYR:CZ	2.54	0.43
12:q:146:LEU:HD22	12:q:150:LYS:HG3	1.99	0.43
12:q:161:LEU:HD22	12:q:161:LEU:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:348:SER:OG	12:q:350:ASN:OD1	2.37	0.43
18:e:45:VAL:O	18:e:48:LEU:HG	2.18	0.43
18:e:95:PHE:CZ	20:l:37:GLY:HA3	2.54	0.43
24:8:106:SER:HB3	24:8:209:ARG:CZ	2.49	0.43
31:6:427:MET:HE2	31:6:427:MET:HB3	1.92	0.43
32:7:35:LYS:HD3	32:7:452:GLN:HG2	1.99	0.43
34:EB:140:LYS:N	34:EB:141:PRO:HD2	2.33	0.43
35:DA:405:VAL:HG23	35:DA:410:TRP:HZ2	1.84	0.43
36:DB:49:VAL:HG21	36:DB:190:PHE:CD2	2.53	0.43
36:DB:105:TYR:CD1	36:DB:105:TYR:C	2.97	0.43
36:DB:319:TYR:HE2	36:DB:324:ILE:HB	1.84	0.43
38:DE:376:LEU:HD22	38:DE:637:PRO:HB2	2.00	0.43
38:DE:503:LYS:HB2	38:DE:533:ALA:HB1	2.01	0.43
38:DE:605:HIS:HA	38:DE:629:ASP:CB	2.48	0.43
38:DE:609:ALA:HB3	38:DE:623:PHE:HD2	1.83	0.43
38:DE:636:HIS:CD2	38:DE:637:PRO:HD2	2.53	0.43
38:De:550:SER:HB3	38:De:559:LEU:HB2	2.00	0.43
49:DP:301:VAL:HG11	53:X:-28:DT:H4'	2.01	0.43
52:FB:56:PHE:HE2	52:FB:58:LEU:HD23	1.83	0.43
55:PA:57:LEU:HD23	55:PA:57:LEU:HA	1.72	0.43
55:PA:339:LEU:HD23	56:PB:1165:MET:HG2	2.00	0.43
55:PA:461:GLN:HB2	55:PA:462:PRO:HD3	2.00	0.43
55:PA:1253:GLU:H	55:PA:1253:GLU:HG3	1.65	0.43
56:PB:505:LEU:HD12	56:PB:509:VAL:HB	2.01	0.43
56:PB:737:ILE:HD12	56:PB:737:ILE:HA	1.84	0.43
67:FA:37:VAL:HB	67:FA:42:TRP:HZ2	1.83	0.43
68:w:68:HIS:CD2	68:w:114:LEU:HD11	2.54	0.43
68:w:315:SER:OG	68:w:319:GLU:OE1	2.31	0.43
68:w:782:MET:O	68:w:785:SER:OG	2.33	0.43
1:a:231:LEU:O	1:a:241:ILE:HB	2.19	0.43
2:m:117:GLN:CA	16:z:594:LEU:HD11	2.41	0.43
3:d:132:LEU:HD21	14:u:105:GLU:HB2	2.00	0.43
5:g:33:LYS:HZ2	5:g:33:LYS:HG3	1.59	0.43
5:g:120:HIS:HA	5:g:123:ILE:HD12	2.01	0.43
6:h:29:PHE:CZ	6:h:49:PHE:HB2	2.54	0.43
7:r:191:GLU:O	7:r:194:LYS:HB2	2.19	0.43
8:t:85:LEU:HA	8:t:85:LEU:HD23	1.76	0.43
8:t:154:TRP:HB2	8:t:176:PHE:HD2	1.80	0.43
11:n:259:THR:HG21	11:n:311:GLN:HE21	1.84	0.43
11:n:907:LEU:HD11	19:b:118:LEU:CB	2.40	0.43
12:q:7:VAL:HG21	14:u:87:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:188:LEU:HD12	12:q:191:ARG:HH22	1.84	0.43
12:q:640:GLU:HG2	18:e:96:LEU:HD22	2.01	0.43
12:q:646:LEU:HD21	20:l:115:ILE:CD1	2.49	0.43
16:z:485:ILE:H	16:z:485:ILE:HG13	1.67	0.43
24:8:66:LEU:HD12	24:8:66:LEU:HA	1.71	0.43
25:9:54:MET:HE3	25:9:54:MET:HB3	1.88	0.43
31:6:78:VAL:HG11	31:6:148:VAL:HG13	2.00	0.43
31:6:401:ILE:H	31:6:401:ILE:HG13	1.55	0.43
32:7:708:LEU:HD13	32:7:713:GLY:HA2	2.00	0.43
38:De:479:THR:HG21	38:De:555:ARG:HG2	2.01	0.43
42:Di:32:GLU:HB2	42:Di:35:VAL:HG23	2.01	0.43
53:X:-16:DG:OP2	53:X:-16:DG:C8	2.67	0.43
55:PA:676:ILE:HD13	55:PA:676:ILE:HA	1.79	0.43
55:PA:1132:LYS:H	55:PA:1132:LYS:HG3	1.69	0.43
55:PA:1427:LEU:HD23	55:PA:1427:LEU:HA	1.86	0.43
68:w:1064:ASP:OD1	68:w:1064:ASP:N	2.37	0.43
2:m:24:PHE:CE1	5:g:18:ILE:HD11	2.54	0.43
2:m:31:PRO:HD2	3:d:176:TYR:CG	2.49	0.43
2:m:120:ALA:HB1	16:z:592:ASN:CB	2.28	0.43
4:f:27:GLY:HA2	4:f:30:LEU:HD23	2.00	0.43
4:f:60:LEU:HB2	4:f:86:ARG:CZ	2.49	0.43
5:g:94:ASP:HB3	13:s:72:PRO:HG2	2.01	0.43
5:g:95:ILE:HD13	5:g:95:ILE:HA	1.84	0.43
5:g:122:LEU:HD12	5:g:122:LEU:HA	1.86	0.43
5:g:153:PHE:HE2	14:u:108:VAL:HA	1.84	0.43
11:n:526:SER:CB	68:w:45:ARG:HH22	2.26	0.43
11:n:793:HIS:CD2	11:n:794:LEU:HG	2.54	0.43
12:q:36:MET:SD	12:q:37:SER:N	2.92	0.43
12:q:544:MET:HE2	12:q:544:MET:HB3	1.84	0.43
18:e:79:GLN:O	18:e:82:GLN:HG2	2.18	0.43
23:0:192:LEU:CD1	23:0:196:LEU:HD23	2.48	0.43
23:0:303:GLY:O	23:0:304:LEU:HB2	2.18	0.43
25:9:247:GLN:O	25:9:251:ILE:HG13	2.18	0.43
28:3:50:PHE:HE2	29:4:118:LEU:HD22	1.83	0.43
29:4:286:LEU:HD23	29:4:286:LEU:HA	1.81	0.43
30:5:17:LYS:HD3	30:5:40:ASP:HA	1.99	0.43
32:7:113:LYS:HB2	32:7:113:LYS:HE2	1.78	0.43
34:EB:127:ASN:HB3	34:EB:140:LYS:HD2	2.01	0.43
36:DB:72:ILE:HD13	36:DB:72:ILE:N	2.34	0.43
36:DB:136:LYS:HZ2	36:DB:136:LYS:HG2	1.77	0.43
39:DF:26:MET:HB3	39:DF:28:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Dk:183:GLN:HB2	46:Dk:186:HIS:CD2	2.54	0.43
44:Dl:56:GLN:HG3	44:Dl:56:GLN:O	2.18	0.43
52:FB:15:ASN:HA	52:FB:109:ILE:HD13	2.01	0.43
53:X:-19:DG:C8	53:X:-18:DT:H73	2.54	0.43
53:X:20:DA:C2'	53:X:21:DG:H5'	2.47	0.43
55:PA:563:LEU:HD22	55:PA:675:VAL:HG13	2.01	0.43
55:PA:1206:ARG:HA	55:PA:1206:ARG:HD3	1.80	0.43
56:PB:56:GLN:HE22	56:PB:90:GLN:HA	1.83	0.43
56:PB:216:ALA:HB2	56:PB:241:ALA:HA	2.01	0.43
56:PB:302:LYS:N	56:PB:303:PRO:HD2	2.34	0.43
59:PE:138:ASN:O	59:PE:141:GLU:HG2	2.19	0.43
69:x:101:MET:HE1	69:x:131:LEU:HD11	2.01	0.43
69:x:742:TYR:HA	69:x:782:VAL:HG11	1.99	0.43
1:a:103:ILE:HG23	1:a:108:PHE:HB2	1.99	0.43
1:a:111:GLU:OE2	1:a:111:GLU:O	2.37	0.43
1:a:357:LEU:HD12	1:a:359:HIS:HB3	2.00	0.43
1:a:457:PRO:HB3	1:a:512:ARG:HD2	2.01	0.43
2:m:65:LYS:HG3	3:d:147:GLU:CD	2.44	0.43
4:f:188:PHE:CD2	11:n:281:ARG:HD2	2.54	0.43
6:h:70:LEU:HD21	6:h:72:ARG:NH2	2.32	0.43
6:h:182:VAL:HB	7:r:202:ILE:HD12	2.01	0.43
7:r:86:ARG:CZ	12:q:397:SER:CB	2.97	0.43
7:r:150:ARG:CG	7:r:161:GLU:HB2	2.44	0.43
10:k:34:GLU:HB3	12:q:153:LEU:HD22	1.99	0.43
11:n:554:MET:HE3	11:n:554:MET:HB2	1.88	0.43
13:s:152:PHE:C	13:s:154:LEU:N	2.74	0.43
14:u:11:ALA:C	14:u:69:ILE:HD11	2.44	0.43
24:8:184:LEU:HB3	24:8:222:LEU:HD22	2.01	0.43
31:6:609:LYS:O	31:6:610:VAL:HG22	2.19	0.43
33:EA:34:LEU:HD23	33:EA:37:LEU:HD12	2.01	0.43
36:DB:106:PHE:HB2	36:DB:954:TRP:CZ2	2.52	0.43
36:DB:114:VAL:HG11	36:DB:437:HIS:HB2	2.00	0.43
39:DF:400:GLY:O	39:DF:404:ARG:HG2	2.19	0.43
37:Dd:844:ASN:HA	37:Dd:847:GLU:HG2	2.01	0.43
44:Dl:102:LEU:HD13	44:Dl:118:LEU:CD1	2.42	0.43
49:DP:206:GLU:HB3	49:DP:207:PRO:HD3	2.01	0.43
55:PA:375:ILE:HG23	55:PA:666:ARG:HG3	2.00	0.43
55:PA:542:LEU:HD21	55:PA:642:LYS:HA	2.00	0.43
55:PA:922:PHE:HB2	55:PA:1052:ARG:HB2	2.01	0.43
68:w:19:GLU:HA	68:w:25:MET:HG3	1.99	0.43
68:w:389:LEU:HA	68:w:392:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:964:LEU:HD12	68:w:964:LEU:HA	1.89	0.43
70:p:216:ALA:HA	70:p:229:ALA:O	2.19	0.43
1:a:468:ASP:OD1	1:a:468:ASP:O	2.36	0.42
2:m:26:GLN:C	3:d:177:PRO:HB3	2.44	0.42
12:q:102:LEU:HA	12:q:102:LEU:HD23	1.80	0.42
17:c:228:LEU:HD12	17:c:228:LEU:HA	1.86	0.42
21:o:625:VAL:HG23	21:o:634:PHE:HZ	1.84	0.42
21:o:763:LEU:HD11	21:o:775:THR:HG21	2.02	0.42
39:DF:58:MET:HG3	39:DF:66:LEU:HG	2.00	0.42
39:DF:320:ARG:HD2	39:DF:321:PRO:HD3	2.01	0.42
45:Dc:6:SER:HB2	43:Dj:134:VAL:HG13	2.00	0.42
38:De:611:LEU:HB3	38:De:621:ARG:HB2	2.01	0.42
51:BA:242:LEU:HD13	51:BA:295:ARG:HD3	2.01	0.42
58:PD:84:ARG:HD2	58:PD:84:ARG:HA	1.90	0.42
68:w:356:LEU:HD21	68:w:372:LEU:HD11	2.01	0.42
69:x:443:LEU:HD11	69:x:495:ILE:HD12	2.01	0.42
69:x:707:ILE:HD12	69:x:707:ILE:HA	1.88	0.42
1:a:109:TYR:C	1:a:109:TYR:CD1	2.97	0.42
1:a:454:PHE:HE1	1:a:465:VAL:HG23	1.84	0.42
4:f:94:PRO:O	12:q:130:VAL:HG13	2.18	0.42
5:g:24:GLU:C	5:g:27:GLN:NE2	2.77	0.42
5:g:25:ASN:CA	5:g:27:GLN:NE2	2.77	0.42
8:t:76:PHE:CE2	8:t:86:ILE:HG23	2.54	0.42
9:j:45:VAL:O	9:j:49:GLN:HG3	2.19	0.42
10:k:19:ARG:HG3	10:k:58:HIS:CD2	2.53	0.42
10:k:109:ARG:NH1	10:k:109:ARG:HB2	2.34	0.42
11:n:170:PRO:HB3	12:q:22:VAL:CG2	2.45	0.42
11:n:676:ASP:OD1	12:q:593:MET:HE2	2.18	0.42
11:n:908:PRO:HG3	19:b:121:ARG:NH2	2.34	0.42
15:v:82:LEU:HD12	15:v:86:LEU:HD23	2.00	0.42
15:v:131:GLU:CG	15:v:135:TYR:HE2	2.31	0.42
18:e:73:ILE:O	18:e:77:VAL:HG13	2.18	0.42
24:8:183:LEU:HD13	24:8:183:LEU:HA	1.93	0.42
24:8:258:HIS:CB	24:8:264:ALA:HB2	2.50	0.42
29:4:87:THR:HA	29:4:90:LEU:HD12	2.01	0.42
31:6:320:GLN:HB3	31:6:349:VAL:HG13	2.01	0.42
32:7:471:LEU:HB2	32:7:473:PHE:CD1	2.51	0.42
35:DA:410:TRP:CZ3	39:DF:354:ARG:HB2	2.54	0.42
36:DB:922:VAL:O	36:DB:926:ILE:HG13	2.19	0.42
37:DD:940:VAL:O	37:DD:944:LEU:HG	2.18	0.42
38:DE:636:HIS:ND1	38:DE:641:TYR:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:De:468:ASN:HB2	39:Df:129:VAL:HA	2.01	0.42
55:PA:938:LEU:HD22	55:PA:1005:HIS:HD1	1.84	0.42
55:PA:1115:LYS:HB3	55:PA:1116:ASN:H	1.62	0.42
56:PB:119:THR:HG21	56:PB:445:LYS:HE2	2.01	0.42
68:w:18:ILE:HD13	68:w:18:ILE:C	2.44	0.42
68:w:549:LYS:HA	68:w:549:LYS:HD3	1.84	0.42
69:x:177:LEU:HD23	69:x:177:LEU:HA	1.86	0.42
1:a:330:PHE:CZ	1:a:393:VAL:HA	2.54	0.42
1:a:375:PHE:O	1:a:441:GLU:HB2	2.18	0.42
3:d:131:LYS:O	3:d:132:LEU:C	2.61	0.42
4:f:19:SER:O	4:f:22:PRO:HD2	2.20	0.42
4:f:177:VAL:C	11:n:270:GLN:HE21	2.27	0.42
9:j:53:LYS:CD	11:n:60:HIS:CB	2.84	0.42
11:n:153:ALA:HB3	11:n:157:ALA:HB2	2.00	0.42
15:v:85:PHE:CD1	15:v:85:PHE:C	2.97	0.42
21:o:759:ARG:O	21:o:762:GLN:HG3	2.19	0.42
32:7:27:GLU:HB3	32:7:479:ALA:HB1	2.02	0.42
32:7:199:ILE:HD12	32:7:220:LEU:HB2	2.01	0.42
35:DA:715:PRO:HD2	35:DA:739:LEU:HD13	2.01	0.42
36:DB:531:PHE:HE2	36:DB:638:ARG:HB2	1.85	0.42
36:DB:862:GLN:HB3	36:DB:869:SER:HA	2.01	0.42
38:DE:669:LYS:HB2	38:DE:690:ASP:HB3	2.01	0.42
40:DG:9:PRO:HB2	40:DG:10:HIS:H	1.70	0.42
42:DI:32:GLU:HB2	42:DI:35:VAL:HG23	2.01	0.42
46:Dk:205:HIS:CE1	44:Dl:125:ASN:HB2	2.54	0.42
53:X:27:DC:H1'	53:X:28:DA:C8	2.54	0.42
54:Y:8:DA:H4'	54:Y:8:DA:OP1	2.19	0.42
58:PD:15:GLU:HG2	58:PD:23:PRO:HD3	2.00	0.42
60:PF:73:ILE:HD13	60:PF:92:ILE:HB	2.01	0.42
61:PG:13:LEU:HB3	61:PG:18:PHE:HE1	1.85	0.42
68:w:589:LEU:HA	68:w:589:LEU:HD12	1.80	0.42
70:p:182:VAL:HG21	70:p:228:VAL:HG21	2.02	0.42
70:p:194:LYS:HG3	70:p:198:GLN:HB3	2.01	0.42
1:a:66:GLN:O	1:a:68:ALA:N	2.53	0.42
1:a:407:ILE:N	1:a:407:ILE:HD13	2.34	0.42
6:h:32:LYS:HZ3	6:h:40:LEU:CD1	2.26	0.42
6:h:42:TRP:O	6:h:45:VAL:CG2	2.62	0.42
6:h:77:ILE:HD12	12:q:126:THR:HG21	1.97	0.42
9:j:75:ARG:HG3	9:j:80:TYR:CE2	2.43	0.42
10:k:30:THR:HA	10:k:33:LEU:HD12	2.01	0.42
10:k:101:ARG:CZ	10:k:101:ARG:CB	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:545:LEU:HD11	11:n:653:PRO:CB	2.39	0.42
12:q:8:ARG:HD2	12:q:8:ARG:HA	1.87	0.42
17:c:113:TRP:CZ2	19:b:175:HIS:CD2	3.06	0.42
24:8:212:PHE:HZ	24:8:260:ILE:HD12	1.84	0.42
28:3:214:TYR:H	28:3:246:PRO:HB3	1.84	0.42
31:6:310:LEU:HA	31:6:381:TRP:CE3	2.55	0.42
35:DA:786:CYS:HB3	35:DA:938:PHE:CZ	2.54	0.42
35:DA:807:LEU:HD23	35:DA:845:ARG:HG3	2.01	0.42
45:Dc:21:LEU:HD11	45:Dc:23:TRP:CD1	2.54	0.42
44:Dl:141:LYS:HG2	47:Dm:73:MET:HB3	2.00	0.42
53:X:21:DG:N2	54:Y:-20:DT:C2	2.87	0.42
55:PA:416:ALA:O	55:PA:429:LEU:HD12	2.19	0.42
55:PA:892:GLY:HA3	55:PA:1396:ARG:HH11	1.84	0.42
55:PA:1665:SER:O	55:PA:1666:PRO:C	2.61	0.42
56:PB:16:GLU:HG2	56:PB:636:LYS:HD2	2.01	0.42
56:PB:721:ARG:HD3	56:PB:721:ARG:HA	1.82	0.42
56:PB:1062:ARG:CZ	56:PB:1074:PRO:HB3	2.50	0.42
57:PC:43:PRO:HA	57:PC:169:PHE:HA	2.00	0.42
57:PC:153:LEU:HD23	57:PC:153:LEU:HA	1.87	0.42
68:w:95:ARG:HG3	68:w:129:VAL:HG13	2.00	0.42
70:p:35:LEU:HD22	70:p:49:MET:HA	2.01	0.42
1:a:257:VAL:HG23	1:a:305:LEU:HD23	2.02	0.42
2:m:42:TYR:OH	5:g:17:TYR:HB2	2.20	0.42
4:f:118:ARG:HB2	12:q:108:GLU:OE2	2.18	0.42
6:h:72:ARG:HH11	12:q:134:ALA:CB	2.32	0.42
7:r:112:GLU:C	7:r:114:LEU:H	2.28	0.42
9:j:76:ASN:N	9:j:79:LEU:HD12	2.31	0.42
10:k:106:ASP:HA	10:k:109:ARG:HE	1.85	0.42
21:o:719:PRO:N	21:o:720:PRO:HD2	2.34	0.42
22:i:94:PHE:O	22:i:94:PHE:HD1	2.01	0.42
23:0:174:ILE:HG13	23:0:178:LYS:HE3	2.02	0.42
29:4:122:LEU:HA	29:4:122:LEU:HD23	1.81	0.42
29:4:425:ALA:HB1	29:4:431:LEU:HB2	2.00	0.42
29:4:438:LYS:HG2	30:5:38:ILE:HG23	2.00	0.42
30:5:20:LEU:HD21	30:5:53:LEU:HD22	2.01	0.42
35:DA:792:PRO:HB2	35:DA:799:ALA:HB2	2.02	0.42
36:DB:49:VAL:HG21	36:DB:190:PHE:HD2	1.84	0.42
36:DB:637:LEU:HD12	36:DB:637:LEU:HA	1.86	0.42
36:DB:669:LEU:HD22	36:DB:677:SER:HB2	2.01	0.42
38:DE:534:SER:HB2	38:DE:537:LYS:HE3	2.01	0.42
39:Df:224:TYR:O	39:Df:228:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Di:93:LEU:HB3	42:Di:97:ARG:HH21	1.83	0.42
53:X:-5:DG:C2	54:Y:6:DG:C2	2.97	0.42
55:PA:511:THR:HG22	56:PB:1101:GLN:HB3	2.01	0.42
55:PA:962:ASP:HB3	55:PA:1043:ILE:HG12	2.01	0.42
56:PB:1007:ASN:O	56:PB:1011:ILE:HG13	2.18	0.42
61:PG:144:ARG:H	61:PG:169:GLY:H	1.67	0.42
68:w:1097:PHE:HA	68:w:1098:PRO:HD3	1.89	0.42
1:a:56:GLN:O	1:a:59:VAL:HG22	2.20	0.42
2:m:14:ASN:C	5:g:39:LYS:HZ3	2.02	0.42
2:m:117:GLN:HE21	14:u:7:GLN:NE2	2.18	0.42
4:f:34:SER:O	4:f:35:GLU:C	2.62	0.42
4:f:120:LEU:HB2	15:v:52:THR:HA	2.00	0.42
7:r:37:HIS:ND1	15:v:92:PRO:HA	2.35	0.42
10:k:31:VAL:HG23	12:q:157:ALA:CB	2.36	0.42
10:k:115:LEU:HD12	18:e:133:LEU:CD1	2.50	0.42
11:n:530:ILE:HA	11:n:533:LEU:HD12	2.01	0.42
12:q:146:LEU:HD23	12:q:146:LEU:HA	1.86	0.42
13:s:67:LEU:HA	13:s:69:ARG:CZ	2.49	0.42
21:o:715:LEU:HD21	69:x:21:TYR:O	2.19	0.42
25:9:47:PHE:HA	25:9:97:MET:HE1	2.00	0.42
30:5:32:LYS:HE3	36:DB:539:ARG:HE	1.85	0.42
31:6:138:GLU:HA	31:6:141:ARG:HD2	2.00	0.42
31:6:564:ASN:HB3	31:6:567:ALA:HB2	2.02	0.42
33:EA:77:ARG:HB3	33:EA:93:PHE:HB2	2.02	0.42
38:DE:663:ARG:HA	38:DE:663:ARG:HD3	1.88	0.42
44:DL:84:LEU:HD23	44:DL:87:ILE:HD12	2.01	0.42
43:Dj:199:ASP:O	43:Dj:202:PRO:HD2	2.19	0.42
46:Dk:188:ARG:HH11	44:Dl:128:ILE:HG22	1.84	0.42
44:Dl:87:ILE:C	44:Dl:91:PHE:CE2	2.93	0.42
47:Dm:58:GLU:O	47:Dm:62:ILE:HG12	2.18	0.42
53:X:-17:DG:H2'	53:X:-16:DG:C8	2.55	0.42
55:PA:202:TRP:HB2	55:PA:212:LYS:HD3	2.01	0.42
56:PB:318:LEU:HD23	56:PB:336:ILE:HG23	2.01	0.42
68:w:37:LEU:O	68:w:41:LEU:HD13	2.19	0.42
68:w:171:LEU:H	68:w:171:LEU:HG	1.56	0.42
68:w:297:CYS:HA	68:w:298:PRO:HD3	1.89	0.42
69:x:269:MET:O	69:x:273:MET:HG2	2.19	0.42
69:x:273:MET:HE1	69:x:818:LEU:HB2	2.01	0.42
70:p:56:GLN:O	70:p:59:THR:OG1	2.35	0.42
70:p:146:HIS:NE2	70:p:160:SER:OG	2.49	0.42
1:a:305:LEU:HD22	1:a:305:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:124:GLN:HG2	16:z:581:SER:CB	2.47	0.42
6:h:48:SER:O	6:h:51:LEU:HG	2.19	0.42
6:h:51:LEU:HD21	58:PD:76:ASN:OD1	2.19	0.42
7:r:186:MET:HE3	7:r:186:MET:HB3	1.71	0.42
8:t:66:MET:HG2	8:t:78:LEU:CD2	2.50	0.42
10:k:33:LEU:CA	10:k:36:SER:OG	2.63	0.42
11:n:247:LEU:HD21	11:n:250:LEU:HD11	2.01	0.42
11:n:370:LEU:O	11:n:371:GLN:C	2.63	0.42
11:n:707:ASP:CA	21:o:684:ARG:NH2	2.83	0.42
11:n:707:ASP:OD1	11:n:708:CYS:N	2.53	0.42
11:n:751:ASN:OD1	11:n:752:LEU:N	2.52	0.42
14:u:88:ALA:CB	16:z:552:LEU:CD1	2.98	0.42
22:i:89:ALA:O	22:i:93:LYS:HG3	2.19	0.42
29:4:285:ARG:HD2	29:4:285:ARG:HA	1.85	0.42
34:EB:85:MET:HE3	34:EB:85:MET:HB2	1.92	0.42
36:DB:20:PHE:HB3	36:DB:494:SER:HB2	2.02	0.42
36:DB:75:VAL:CG2	36:DB:84:PHE:CD1	3.03	0.42
36:DB:269:CYS:HB3	36:DB:277:LEU:HD22	2.01	0.42
36:DB:671:LYS:H	36:DB:671:LYS:HG3	1.57	0.42
39:DF:279:LEU:HD13	39:DF:279:LEU:HA	1.86	0.42
38:De:766:GLN:H	38:De:766:GLN:HG3	1.54	0.42
39:Df:298:GLU:HG2	39:Df:344:PHE:CD1	2.54	0.42
49:DP:165:LEU:HD13	49:DP:168:ILE:HD11	2.02	0.42
53:X:-11:DG:H5'	54:Y:12:DG:N2	1.97	0.42
55:PA:27:SER:HB3	55:PA:30:GLU:HG2	2.02	0.42
55:PA:1450:PRO:O	55:PA:1451:MET:HB2	2.20	0.42
56:PB:348:LEU:HD12	56:PB:348:LEU:HA	1.86	0.42
56:PB:568:PHE:HB2	56:PB:613:ARG:HG2	2.01	0.42
57:PC:190:ASN:HD22	57:PC:217:GLN:HE21	1.66	0.42
59:PE:164:LYS:HE2	60:PF:110:LEU:HD13	2.02	0.42
67:FA:110:PHE:HB3	67:FA:146:PHE:HB3	2.01	0.42
68:w:237:ILE:HG21	68:w:285:ASN:HB3	2.01	0.42
68:w:1046:ASP:N	68:w:1046:ASP:OD1	2.52	0.42
69:x:68:ILE:HD11	69:x:78:VAL:HG11	2.01	0.42
69:x:591:ALA:HB1	69:x:597:LEU:HD23	2.00	0.42
3:d:164:PRO:HG2	3:d:167:TRP:HD1	1.83	0.42
6:h:121:GLU:HA	6:h:124:LEU:HD12	2.02	0.42
7:r:33:GLU:H	7:r:33:GLU:HG3	1.31	0.42
8:t:66:MET:HG2	8:t:78:LEU:HD21	2.02	0.42
8:t:98:LEU:HD12	8:t:102:PHE:HZ	1.81	0.42
11:n:168:ARG:HD3	11:n:168:ARG:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:u:18:GLN:HE21	16:z:495:SER:HB2	1.84	0.42
18:e:53:GLU:OE2	19:b:187:GLY:O	2.37	0.42
27:2:87:LEU:HD12	27:2:228:TYR:HD2	1.85	0.42
44:DL:106:ARG:HH12	44:DL:115:ASP:H	1.65	0.42
38:De:522:ASP:O	38:De:526:ARG:HG2	2.19	0.42
53:X:-38:DA:H2"	53:X:-37:DG:C8	2.55	0.42
53:X:-28:DT:O5'	53:X:-28:DT:C2'	2.68	0.42
54:Y:-5:DC:H2"	54:Y:-4:DG:C8	2.55	0.42
55:PA:604:ARG:HA	55:PA:604:ARG:HD2	1.79	0.42
55:PA:1053:ARG:HH21	55:PA:1058:PHE:HZ	1.67	0.42
56:PB:254:GLN:H	56:PB:254:GLN:HG3	1.56	0.42
68:w:1005:LEU:HD23	68:w:1005:LEU:HA	1.91	0.42
1:a:408:LEU:HD23	1:a:408:LEU:HA	1.83	0.42
1:a:463:VAL:HG11	1:a:488:ILE:HD12	2.02	0.42
3:d:155:ILE:HD11	3:d:161:VAL:CB	2.43	0.42
12:q:569:ILE:HG22	12:q:582:VAL:HB	2.00	0.42
27:2:315:ALA:N	27:2:316:PRO:HD2	2.34	0.42
31:6:346:LYS:HB3	31:6:346:LYS:HE3	1.86	0.42
32:7:180:LEU:HD21	32:7:195:ALA:HB2	2.01	0.42
35:DA:465:TYR:O	35:DA:466:SER:HB2	2.19	0.42
36:DB:981:LEU:HA	36:DB:981:LEU:HD12	1.69	0.42
37:DD:943:GLN:HG3	38:DE:510:ALA:HB2	2.02	0.42
39:DF:138:ILE:HG22	39:DF:139:GLU:HG3	2.01	0.42
39:DF:263:ILE:HG12	39:DF:285:MET:HE3	2.01	0.42
39:DF:276:LEU:HD12	39:DF:276:LEU:H	1.85	0.42
37:Dd:1070:GLU:O	37:Dd:1071:ARG:HB3	2.19	0.42
49:DP:195:LYS:HB3	52:FB:175:ARG:HG3	2.01	0.42
51:BA:295:ARG:HG2	51:BA:298:ASP:HB3	2.02	0.42
55:PA:1158:LEU:HD13	55:PA:1309:MET:HB2	2.01	0.42
56:PB:789:ASN:HB3	56:PB:795:ILE:HG13	2.01	0.42
67:FA:28:ILE:HD11	67:FA:126:ILE:HD11	2.02	0.42
68:w:442:LYS:HE2	68:w:442:LYS:HB3	1.88	0.42
68:w:470:ASN:OD1	68:w:470:ASN:N	2.52	0.42
4:f:93:ILE:HG12	23:0:237:PRO:CA	2.50	0.42
4:f:177:VAL:CG1	11:n:270:GLN:CG	2.97	0.42
5:g:34:PRO:CB	5:g:35:PRO:HD2	2.47	0.42
9:j:26:VAL:HB	9:j:38:ASN:HD21	1.75	0.42
9:j:85:LEU:O	9:j:89:LEU:HG	2.20	0.42
9:j:99:ILE:HA	9:j:102:MET:SD	2.60	0.42
12:q:149:LYS:CE	15:v:39:THR:O	2.62	0.42
12:q:184:ASN:N	12:q:184:ASN:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:644:SER:HB2	18:e:97:GLN:N	2.35	0.42
14:u:4:ARG:CD	16:z:596:TYR:HA	2.50	0.42
18:e:55:CYS:SG	20:l:52:PHE:HZ	2.43	0.42
21:o:729:TYR:C	21:o:731:ALA:H	2.28	0.42
24:8:164:SER:N	24:8:165:PRO:HD2	2.33	0.42
32:7:14:TYR:HE2	32:7:50:VAL:HG11	1.83	0.42
34:EB:135:GLY:C	34:EB:136:LYS:HD2	2.45	0.42
38:DE:515:LEU:H	38:DE:515:LEU:HG	1.67	0.42
38:DE:673:HIS:CE1	39:DF:59:HIS:HB3	2.55	0.42
46:Dk:136:ARG:HA	46:Dk:136:ARG:HD2	1.89	0.42
51:BA:24:VAL:HG22	51:BA:35:PRO:HG3	2.02	0.42
52:FB:224:ASN:HB3	52:FB:226:LYS:HE2	2.00	0.42
55:PA:282:ASP:HA	55:PA:285:LYS:HE3	2.02	0.42
59:PE:18:MET:HG3	59:PE:32:GLU:HB3	2.02	0.42
60:PF:92:ILE:HA	60:PF:95:LYS:HE3	2.00	0.42
68:w:727:TRP:HB2	68:w:732:LEU:HD13	2.02	0.42
4:f:180:LEU:HD11	11:n:299:PHE:CB	2.46	0.41
6:h:16:LEU:HD22	6:h:16:LEU:HA	1.91	0.41
10:k:79:HIS:CE1	15:v:91:PHE:HE1	2.37	0.41
11:n:945:ASP:N	11:n:945:ASP:OD1	2.53	0.41
12:q:19:VAL:HG22	12:q:22:VAL:HG22	2.01	0.41
12:q:20:HIS:HB3	12:q:31:LEU:HB2	2.01	0.41
15:v:119:LEU:C	15:v:119:LEU:HD13	2.45	0.41
24:8:143:LEU:HD22	24:8:143:LEU:HA	1.91	0.41
26:1:431:ILE:HD11	29:4:74:TRP:HZ2	1.85	0.41
29:4:279:ARG:HD3	29:4:279:ARG:HA	1.82	0.41
31:6:133:THR:HG23	31:6:160:THR:HB	2.02	0.41
31:6:323:SER:HB2	31:6:338:ILE:HG21	2.02	0.41
31:6:634:ARG:HA	31:6:634:ARG:HD2	1.80	0.41
32:7:524:LEU:HD21	32:7:595:ILE:HD11	2.02	0.41
32:7:681:ASP:OD2	32:7:683:ARG:HB2	2.19	0.41
36:DB:69:GLN:O	36:DB:152:LEU:HD23	2.20	0.41
36:DB:215:VAL:HG12	36:DB:322:MET:SD	2.60	0.41
37:DD:1082:ALA:HA	37:DD:1085:LYS:HD2	2.02	0.41
37:DD:1084:LEU:HD21	38:DE:610:ARG:HH12	1.85	0.41
38:DE:588:VAL:HA	38:DE:604:GLY:HA2	2.02	0.41
41:DH:37:LEU:HD23	41:DH:37:LEU:HA	1.80	0.41
38:De:324:LYS:HG3	38:De:326:ASN:OD1	2.20	0.41
38:De:508:LYS:HD3	38:De:512:ASP:HB3	2.00	0.41
38:De:608:VAL:HG12	38:De:624:ALA:HB2	2.01	0.41
39:Df:426:LEU:HG	39:Df:430:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:DP:225:LYS:HD3	49:DP:225:LYS:HA	1.87	0.41
51:BA:25:GLU:HA	51:BA:32:MET:HA	2.02	0.41
52:FB:50:GLY:HA3	52:FB:51:ARG:HH21	1.85	0.41
55:PA:300:ALA:HA	55:PA:303:ILE:HB	2.02	0.41
56:PB:1052:LYS:HE2	56:PB:1052:LYS:HB3	1.84	0.41
58:PD:18:SER:OG	61:PG:82:GLY:HA3	2.20	0.41
68:w:37:LEU:HA	68:w:37:LEU:HD12	1.72	0.41
70:p:273:ARG:HA	70:p:273:ARG:HD2	1.83	0.41
3:d:168:VAL:O	3:d:171:ASP:HB2	2.21	0.41
3:d:175:PRO:C	3:d:176:TYR:O	2.63	0.41
4:f:32:TYR:CD1	4:f:35:GLU:CD	2.97	0.41
5:g:153:PHE:CE2	14:u:107:VAL:C	2.98	0.41
9:j:58:LEU:C	9:j:59:HIS:CG	2.98	0.41
11:n:916:LEU:HD12	11:n:917:ALA:H	1.85	0.41
12:q:596:PHE:HE2	20:l:112:GLU:CG	2.33	0.41
15:v:127:LEU:HD12	15:v:127:LEU:C	2.45	0.41
17:c:114:SER:O	17:c:117:LEU:HG	2.19	0.41
27:2:199:ILE:HG23	27:2:220:HIS:HB2	2.01	0.41
29:4:258:LEU:HD23	29:4:258:LEU:HA	1.90	0.41
32:7:461:LEU:HB3	32:7:464:LEU:HD21	2.01	0.41
36:DB:579:LEU:HD23	36:DB:588:HIS:HB3	1.96	0.41
43:DJ:123:LEU:HD12	43:DJ:123:LEU:HA	1.78	0.41
44:Dl:102:LEU:HA	44:Dl:105:HIS:HD2	1.85	0.41
50:DQ:53:SER:O	50:DQ:54:ARG:HB2	2.20	0.41
52:FB:137:LYS:HE2	52:FB:137:LYS:HB2	1.88	0.41
58:PD:67:TYR:HA	58:PD:70:ARG:NH2	2.35	0.41
59:PE:54:ARG:HD3	59:PE:54:ARG:HA	1.85	0.41
68:w:684:ASN:HD22	68:w:723:THR:HG21	1.85	0.41
68:w:916:ASP:OD1	68:w:916:ASP:N	2.53	0.41
1:a:382:LEU:HD22	1:a:446:SER:HA	2.02	0.41
1:a:402:GLY:O	1:a:405:PRO:HD2	2.21	0.41
5:g:18:ILE:HG23	5:g:22:THR:HG21	2.02	0.41
5:g:138:MET:HE2	5:g:138:MET:HB2	1.78	0.41
6:h:74:GLN:CG	12:q:129:PRO:HB3	2.49	0.41
9:j:96:LYS:HE3	13:s:80:SER:HB2	2.00	0.41
9:j:120:ASP:HB3	9:j:124:TYR:CZ	2.55	0.41
11:n:301:LEU:HD11	11:n:369:PRO:HA	2.01	0.41
11:n:909:GLN:NE2	19:b:114:ASP:OD1	2.53	0.41
15:v:82:LEU:HD13	15:v:86:LEU:HD23	1.92	0.41
15:v:82:LEU:HA	15:v:85:PHE:CE2	2.55	0.41
19:b:157:TYR:N	19:b:158:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:170:SER:HB3	28:3:173:GLN:HB2	2.03	0.41
29:4:160:LEU:HD12	29:4:323:LEU:HD21	2.02	0.41
33:EA:110:MET:O	33:EA:114:ILE:HG13	2.21	0.41
36:DB:270:LEU:HB2	36:DB:273:LEU:HD12	2.01	0.41
36:DB:414:LEU:HB2	36:DB:523:VAL:HG13	2.02	0.41
36:DB:930:LEU:HD12	36:DB:930:LEU:HA	1.80	0.41
39:DF:63:ARG:HD2	39:DF:66:LEU:HA	2.02	0.41
41:DH:45:LEU:HD22	41:DH:50:PHE:HD1	1.84	0.41
37:Dd:895:HIS:HB3	37:Dd:898:VAL:HG23	2.02	0.41
38:De:205:TYR:CZ	38:De:249:LEU:HB3	2.55	0.41
38:De:221:LEU:O	38:De:225:ILE:HG12	2.19	0.41
49:DP:329:TYR:N	49:DP:330:PRO:HD2	2.35	0.41
53:X:-7:DT:H2"	53:X:-6:DC:C6	2.55	0.41
56:PB:257:VAL:HB	56:PB:266:GLU:HB3	2.02	0.41
56:PB:806:PHE:HD1	56:PB:806:PHE:HA	1.69	0.41
56:PB:840:MET:HB2	56:PB:840:MET:HE2	1.82	0.41
57:PC:225:LYS:HD3	57:PC:226:PRO:HD2	2.01	0.41
61:PG:100:GLU:HG3	61:PG:104:MET:O	2.20	0.41
61:PG:147:ILE:HA	61:PG:160:ILE:O	2.20	0.41
62:PH:10:PHE:HB3	62:PH:30:CYS:HB3	2.01	0.41
63:PI:110:LEU:HD12	63:PI:110:LEU:HA	1.79	0.41
69:x:466:ARG:NH2	69:x:512:ILE:O	2.53	0.41
1:a:317:PHE:CD1	1:a:317:PHE:C	2.98	0.41
3:d:144:SER:HB2	12:q:9:ILE:HB	2.02	0.41
9:j:102:MET:HG3	9:j:103:LYS:N	2.35	0.41
11:n:587:LEU:HB2	68:w:36:LYS:HD3	2.01	0.41
11:n:713:GLN:O	11:n:719:THR:HB	2.20	0.41
11:n:904:PHE:CD1	11:n:916:LEU:HD11	2.53	0.41
12:q:633:ARG:HD2	12:q:637:TYR:HE2	1.85	0.41
13:s:65:PHE:CE2	13:s:67:LEU:HD12	2.55	0.41
19:b:159:GLN:O	19:b:163:VAL:HG13	2.20	0.41
24:8:205:GLU:HB2	24:8:211:PRO:HA	2.01	0.41
25:9:111:LEU:HD12	25:9:111:LEU:HA	1.89	0.41
26:1:374:LEU:HD11	28:3:270:VAL:O	2.21	0.41
27:2:145:LEU:HD13	27:2:171:PHE:HE2	1.84	0.41
27:2:201:LEU:HG	27:2:222:ILE:HD12	2.01	0.41
28:3:32:PHE:CZ	28:3:37:CYS:HB2	2.56	0.41
28:3:244:PRO:HA	28:3:245:PRO:HD3	1.93	0.41
29:4:145:VAL:N	29:4:146:PRO:HD2	2.35	0.41
29:4:192:GLU:N	29:4:193:PRO:HD3	2.36	0.41
29:4:274:ARG:HD2	29:4:274:ARG:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:421:LEU:HD12	29:4:421:LEU:HA	1.87	0.41
32:7:122:THR:N	32:7:123:PRO:HD2	2.35	0.41
33:EA:171:LYS:O	33:EA:174:ARG:HG2	2.20	0.41
35:DA:639:LEU:HD11	35:DA:774:ARG:HG2	2.02	0.41
35:DA:791:VAL:HG23	35:DA:935:THR:HG21	2.02	0.41
38:DE:479:THR:HG21	38:DE:555:ARG:HG2	2.02	0.41
39:Df:65:LYS:HA	39:Df:65:LYS:HD2	1.78	0.41
53:X:-1:DT:C4	53:X:0:DC:N4	2.89	0.41
54:Y:4:DA:C2'	54:Y:5:DC:OP2	2.61	0.41
57:PC:23:ILE:HD13	65:PK:101:LEU:HD21	2.03	0.41
57:PC:24:GLU:HG2	57:PC:228:ARG:HA	2.02	0.41
68:w:173:ARG:H	68:w:173:ARG:HG3	1.65	0.41
68:w:213:ARG:HA	68:w:213:ARG:HD3	1.95	0.41
70:p:306:VAL:HG23	70:p:399:LEU:HD13	2.02	0.41
1:a:131:ASN:ND2	1:a:131:ASN:N	2.63	0.41
1:a:420:LEU:HD22	1:a:504:ILE:CG1	2.49	0.41
5:g:57:ARG:HD3	5:g:128:PRO:HG2	2.01	0.41
5:g:143:LYS:HB3	5:g:143:LYS:HZ3	1.85	0.41
7:r:120:GLU:CD	7:r:120:GLU:C	2.88	0.41
8:t:148:VAL:CG2	17:c:218:ASN:HB3	2.51	0.41
9:j:44:ILE:O	9:j:48:LEU:HG	2.19	0.41
9:j:66:GLU:O	9:j:69:GLU:N	2.53	0.41
11:n:202:ARG:HD2	11:n:245:TRP:CZ2	2.54	0.41
11:n:268:SER:HA	11:n:271:ILE:HD12	2.02	0.41
11:n:311:GLN:O	11:n:315:LEU:HG	2.20	0.41
11:n:527:THR:HG23	68:w:42:GLY:HA3	1.92	0.41
11:n:634:MET:HE2	12:q:519:GLN:CD	2.45	0.41
11:n:853:HIS:O	11:n:857:GLU:HG2	2.21	0.41
12:q:523:ASP:HA	12:q:563:ILE:HD12	2.02	0.41
15:v:85:PHE:CD1	15:v:86:LEU:N	2.89	0.41
23:0:76:LYS:HE3	23:0:76:LYS:HB3	1.96	0.41
32:7:663:CYS:HA	32:7:666:ARG:NE	2.36	0.41
36:DB:262:MET:HB3	36:DB:265:VAL:HG23	2.02	0.41
36:DB:881:GLY:HA3	41:DH:218:PRO:HB3	2.02	0.41
38:DE:571:SER:HB2	38:DE:578:LEU:HD11	2.03	0.41
39:DF:289:LEU:O	39:DF:295:LEU:HD11	2.20	0.41
37:Dd:843:VAL:CG1	37:Dd:844:ASN:H	2.29	0.41
37:Dd:885:ILE:CB	44:Dl:96:VAL:CG1	2.98	0.41
39:Df:267:VAL:HG21	39:Df:307:ALA:HB1	2.01	0.41
47:Dm:114:ARG:HA	47:Dm:114:ARG:HD2	1.94	0.41
49:DP:239:ARG:HD2	49:DP:243:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:X:-1:DT:H2"	53:X:0:DC:H5'	2.03	0.41
55:PA:322:LEU:HD12	55:PA:323:PRO:HD2	2.02	0.41
56:PB:193:VAL:HG21	56:PB:482:LEU:HD23	2.02	0.41
60:PF:69:ARG:HD2	60:PF:69:ARG:HA	1.88	0.41
60:PF:75:MET:O	60:PF:76:CYS:HB2	2.20	0.41
62:PH:7:GLU:HG3	62:PH:59:VAL:HG22	2.02	0.41
68:w:10:GLU:OE1	68:w:10:GLU:N	2.53	0.41
68:w:107:LEU:HD22	68:w:118:THR:HG21	2.01	0.41
68:w:361:ALA:HB1	70:p:250:SER:CA	2.51	0.41
68:w:540:ILE:HD13	68:w:540:ILE:HA	1.92	0.41
68:w:559:LEU:HD23	68:w:559:LEU:HA	1.88	0.41
68:w:1183:TRP:HE1	68:w:1190:LEU:HD13	1.85	0.41
1:a:501:CYS:HB2	1:a:502:MET:H	1.56	0.41
1:a:509:ARG:HB2	1:a:509:ARG:HH11	1.77	0.41
4:f:120:LEU:HD22	15:v:51:ALA:HB1	2.02	0.41
5:g:111:ASP:O	5:g:115:LEU:HG	2.20	0.41
7:r:42:LEU:CD1	10:k:75:THR:HG21	2.46	0.41
7:r:101:LEU:HD23	7:r:101:LEU:HA	1.82	0.41
7:r:140:ILE:HD12	7:r:182:VAL:CG1	2.42	0.41
8:t:119:TYR:O	8:t:120:CYS:C	2.64	0.41
9:j:39:GLN:C	9:j:43:PHE:HD2	2.25	0.41
10:k:64:SER:HB2	10:k:68:ARG:NH2	2.35	0.41
11:n:394:HIS:CD2	11:n:399:LYS:HD2	2.56	0.41
12:q:142:GLN:CD	12:q:142:GLN:N	2.78	0.41
12:q:458:PRO:HG3	12:q:533:GLN:NE2	2.28	0.41
15:v:26:ILE:HG22	15:v:27:LYS:N	2.36	0.41
16:z:529:HIS:NE2	16:z:580:ILE:HG21	2.35	0.41
17:c:110:ALA:HB3	19:b:168:ILE:CG2	2.00	0.41
17:c:229:ASP:OD1	17:c:232:SER:OG	2.34	0.41
17:c:299:PHE:C	17:c:301:THR:H	2.29	0.41
24:8:110:THR:HB	24:8:113:HIS:HB2	2.02	0.41
24:8:177:TRP:HZ3	24:8:214:PRO:CB	2.33	0.41
26:1:264:ASN:O	26:1:266:LEU:N	2.54	0.41
27:2:149:LEU:HD13	27:2:189:LEU:HD11	2.02	0.41
32:7:490:LEU:HB3	32:7:668:ILE:HG13	2.03	0.41
35:DA:824:ARG:HB2	35:DA:861:TRP:HB3	2.03	0.41
36:DB:488:PHE:HB3	36:DB:492:MET:H	1.85	0.41
38:DE:684:LEU:HB3	38:DE:696:TRP:CD1	2.56	0.41
38:De:453:LEU:HB2	38:De:454:GLY:H	1.62	0.41
49:DP:263:ASP:HB2	49:DP:309:LYS:HD3	2.01	0.41
55:PA:1382:LEU:HB3	55:PA:1398:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:PA:1460:LEU:HD12	55:PA:1460:LEU:HA	1.93	0.41
56:PB:124:LEU:HD22	56:PB:152:ILE:HD11	2.01	0.41
56:PB:1023:ARG:HA	56:PB:1023:ARG:HD3	1.72	0.41
69:x:7:LYS:HB3	69:x:49:GLN:HE22	1.85	0.41
69:x:579:LEU:HD23	69:x:579:LEU:HA	1.92	0.41
3:d:152:ALA:O	3:d:153:HIS:C	2.63	0.41
4:f:16:VAL:CG1	4:f:104:VAL:HA	2.50	0.41
4:f:77:ILE:HG21	55:PA:1792:PRO:HG3	1.96	0.41
5:g:83:MET:CE	5:g:83:MET:CA	2.98	0.41
8:t:6:VAL:CG2	8:t:141:GLU:HB2	2.46	0.41
8:t:79:PHE:C	8:t:80:GLU:HG3	2.44	0.41
8:t:103:GLN:HE21	8:t:103:GLN:CA	2.27	0.41
9:j:9:GLU:OE2	9:j:55:ARG:HB2	2.21	0.41
10:k:16:ASP:CG	15:v:79:VAL:CG2	2.94	0.41
12:q:613:ASN:O	12:q:616:SER:OG	2.36	0.41
25:9:162:ASN:HA	25:9:163:PRO:HD3	1.93	0.41
29:4:415:GLN:HB2	29:4:439:ARG:HH21	1.85	0.41
32:7:284:GLU:O	32:7:287:ARG:HG2	2.21	0.41
36:DB:67:SER:HG	36:DB:70:CYS:CB	2.32	0.41
36:DB:353:GLN:HA	36:DB:357:CYS:HB2	2.02	0.41
38:DE:672:ILE:H	38:DE:672:ILE:HD12	1.86	0.41
39:DF:122:LEU:H	39:DF:122:LEU:HG	1.48	0.41
44:DL:72:PRO:O	44:DL:73:ASN:HB2	2.19	0.41
38:De:588:VAL:HA	38:De:604:GLY:HA2	2.01	0.41
38:De:694:LEU:HD22	38:De:703:MET:SD	2.60	0.41
39:Df:386:ASP:HA	39:Df:389:LYS:HD3	2.02	0.41
49:DP:240:VAL:O	49:DP:244:LEU:HG	2.20	0.41
52:FB:12:ALA:HA	52:FB:109:ILE:HD11	2.03	0.41
52:FB:42:LYS:HA	67:FA:15:VAL:HA	2.03	0.41
52:FB:223:GLN:HA	52:FB:233:TRP:HA	2.01	0.41
53:X:-5:DG:C2'	53:X:-4:DT:C7	2.98	0.41
55:PA:516:GLN:HA	55:PA:520:MET:HG2	2.01	0.41
55:PA:762:GLU:H	55:PA:762:GLU:HG3	1.54	0.41
56:PB:828:VAL:HG21	66:PL:31:ARG:HG2	2.03	0.41
57:PC:110:ASP:HA	57:PC:155:LYS:HD2	2.02	0.41
58:PD:16:ASP:HB3	61:PG:81:LYS:HB3	2.01	0.41
65:PK:106:ARG:HG2	65:PK:110:LYS:HE2	2.03	0.41
68:w:334:LEU:HD23	68:w:334:LEU:HA	1.92	0.41
69:x:183:LEU:HD21	69:x:974:SER:HB3	2.02	0.41
69:x:303:LEU:HD13	69:x:303:LEU:HA	1.90	0.41
1:a:77:MET:N	1:a:77:MET:SD	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:68:LYS:CE	5:g:50:GLN:NE2	2.64	0.41
2:m:102:ILE:HD11	3:d:174:ARG:HD2	2.02	0.41
2:m:112:ARG:NH1	16:z:598:CYS:O	2.54	0.41
7:r:29:ASP:O	7:r:32:LEU:HB2	2.21	0.41
9:j:102:MET:CE	9:j:106:LYS:HZ1	2.33	0.41
9:j:102:MET:O	9:j:106:LYS:HG3	2.21	0.41
10:k:8:ASN:OD1	10:k:8:ASN:N	2.52	0.41
10:k:87:ARG:NH1	10:k:87:ARG:CG	2.73	0.41
11:n:310:SER:O	11:n:313:LEU:HG	2.21	0.41
11:n:382:ASP:O	11:n:386:VAL:HG22	2.20	0.41
11:n:870:GLN:HG3	21:o:655:THR:HG21	2.03	0.41
12:q:290:HIS:NE2	12:q:294:LYS:CE	2.71	0.41
17:c:70:LEU:HD12	17:c:70:LEU:HA	1.83	0.41
19:b:64:ILE:HA	19:b:64:ILE:HD13	1.79	0.41
22:i:66:LEU:HA	22:i:69:VAL:HB	2.02	0.41
24:8:52:LYS:HD2	24:8:52:LYS:HA	1.87	0.41
24:8:293:LYS:HA	24:8:293:LYS:HD3	1.93	0.41
25:9:174:LEU:HD13	25:9:174:LEU:HA	1.89	0.41
26:1:531:THR:HG21	27:2:294:CYS:HA	2.02	0.41
27:2:255:PRO:HD2	27:2:301:LEU:HD11	2.03	0.41
31:6:444:HIS:HE1	31:6:635:GLN:HA	1.86	0.41
32:7:379:LEU:HD21	32:7:397:LEU:HG	2.03	0.41
33:EA:153:ARG:HD3	33:EA:153:ARG:HA	1.82	0.41
36:DB:290:PHE:CE2	36:DB:381:TRP:HA	2.51	0.41
36:DB:571:LEU:HD12	36:DB:595:LYS:HA	2.03	0.41
36:DB:834:THR:HG21	41:DH:211:PHE:HA	2.02	0.41
36:DB:964:ASP:O	36:DB:965:TRP:HB2	2.20	0.41
38:DE:616:HIS:NE2	42:DI:105:PRO:HG3	2.34	0.41
40:DG:79:THR:HG21	40:DG:82:LYS:HA	2.02	0.41
39:Df:359:PHE:CD1	39:Df:376:SER:HA	2.55	0.41
39:Df:388:ILE:HG12	39:Df:389:LYS:N	2.35	0.41
47:Dm:87:VAL:HG12	47:Dm:91:ARG:HH22	1.86	0.41
51:BA:14:THR:HA	51:BA:20:ASP:HB3	2.03	0.41
53:X:-33:DG:C2	54:Y:34:DG:C2	3.09	0.41
53:X:28:DA:C8	53:X:29:DG:C6	3.09	0.41
54:Y:31:DG:H2"	54:Y:32:DG:C8	2.56	0.41
55:PA:358:ARG:HD3	56:PB:1074:PRO:O	2.21	0.41
55:PA:910:LYS:HE2	55:PA:910:LYS:HB2	1.98	0.41
57:PC:40:ALA:HA	57:PC:170:GLY:HA3	2.02	0.41
59:PE:159:LEU:H	59:PE:159:LEU:HG	1.59	0.41
61:PG:89:VAL:HB	61:PG:99:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:w:1131:LEU:HD13	68:w:1131:LEU:HA	1.87	0.41
1:a:142:LEU:HD12	1:a:142:LEU:HA	1.87	0.41
1:a:221:ASN:HB3	1:a:254:ASN:ND2	2.35	0.41
1:a:361:MET:HE2	1:a:378:LYS:HG2	2.03	0.41
2:m:84:PHE:HB2	11:n:178:ILE:HD11	2.03	0.41
4:f:96:ALA:HA	12:q:130:VAL:HG11	2.03	0.41
6:h:29:PHE:HD2	12:q:102:LEU:HD13	1.85	0.41
7:r:35:LEU:HD13	7:r:35:LEU:O	2.20	0.41
7:r:174:VAL:O	7:r:174:VAL:HG12	2.20	0.41
8:t:98:LEU:HD23	8:t:98:LEU:N	2.36	0.41
8:t:112:THR:CG2	8:t:129:VAL:HG22	2.49	0.41
11:n:138:SER:O	11:n:141:ARG:HG2	2.21	0.41
11:n:567:LYS:HG2	11:n:592:LYS:NZ	2.36	0.41
11:n:573:VAL:HG21	11:n:583:ALA:HB1	2.03	0.41
11:n:731:LEU:HD12	11:n:800:VAL:HG11	2.03	0.41
11:n:794:LEU:HA	11:n:797:PHE:HB3	2.02	0.41
11:n:907:LEU:HD23	11:n:907:LEU:HA	1.90	0.41
11:n:944:PHE:CD2	19:b:101:ARG:NH2	2.89	0.41
12:q:36:MET:O	12:q:39:ASN:N	2.54	0.41
15:v:85:PHE:C	15:v:85:PHE:HD1	2.29	0.41
17:c:180:LEU:HD12	17:c:181:SER:H	1.84	0.41
17:c:258:MET:SD	17:c:258:MET:N	2.84	0.41
21:o:696:SER:HB3	69:x:111:HIS:CE1	2.49	0.41
23:0:46:CYS:SG	23:0:48:GLU:N	2.94	0.41
23:0:192:LEU:HD21	23:0:196:LEU:HD22	2.03	0.41
23:0:204:ARG:O	23:0:207:GLN:HG2	2.21	0.41
26:1:192:ILE:H	26:1:192:ILE:HG12	1.66	0.41
27:2:149:LEU:HD21	27:2:169:ILE:HD11	2.02	0.41
29:4:14:LEU:HD13	29:4:214:TYR:HD1	1.86	0.41
30:5:48:GLU:HG3	30:5:49:LEU:HG	2.03	0.41
31:6:140:LEU:HD23	31:6:140:LEU:HA	1.85	0.41
31:6:353:ALA:O	31:6:357:VAL:HG23	2.20	0.41
32:7:140:SER:H	32:7:303:ALA:HB2	1.85	0.41
32:7:247:MET:HB3	32:7:437:CYS:SG	2.60	0.41
34:EB:120:MET:HA	34:EB:124:LEU:HD12	2.02	0.41
35:DA:941:ALA:HB2	35:DA:948:LEU:HG	2.02	0.41
36:DB:94:CYS:SG	36:DB:954:TRP:CZ2	3.09	0.41
36:DB:218:GLY:N	36:DB:238:LEU:HD13	2.36	0.41
36:DB:230:ARG:H	36:DB:230:ARG:HG3	1.56	0.41
36:DB:806:VAL:HG13	36:DB:826:VAL:HG22	2.03	0.41
38:DE:238:GLN:HE21	38:DE:238:GLN:HB2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DE:264:PHE:O	38:DE:268:HIS:HB3	2.20	0.41
38:DE:321:LEU:HB3	38:DE:330:TRP:HB2	2.02	0.41
38:DE:550:SER:HB3	38:DE:559:LEU:HB3	2.03	0.41
38:DE:693:VAL:HB	38:DE:707:LEU:HB2	2.03	0.41
39:DF:35:THR:CG2	42:DI:71:VAL:HG21	2.49	0.41
39:DF:258:ARG:HA	39:DF:258:ARG:HD3	1.89	0.41
38:De:505:ARG:HA	38:De:532:THR:O	2.20	0.41
38:De:508:LYS:HB3	38:De:512:ASP:HB2	2.03	0.41
44:Dl:102:LEU:CB	44:Dl:115:ASP:HB2	2.51	0.41
49:DP:169:VAL:HG21	53:X:-26:DA:H2	1.81	0.41
50:DQ:335:VAL:HG13	50:DQ:358:MET:HG2	2.02	0.41
53:X:1:DA:N1	54:Y:0:DG:N1	2.68	0.41
55:PA:581:LYS:NZ	62:PH:86:ASP:HA	2.36	0.41
56:PB:237:VAL:HG12	56:PB:372:LEU:HD22	2.03	0.41
56:PB:248:LYS:HG2	67:FA:176:ILE:O	2.20	0.41
56:PB:779:ILE:HB	56:PB:963:PRO:HA	2.01	0.41
68:w:274:LEU:O	68:w:333:HIS:NE2	2.40	0.41
68:w:301:GLU:HG3	68:w:347:ALA:HB1	2.03	0.41
68:w:844:ASN:HA	68:w:847:ILE:HG22	2.02	0.41
68:w:850:LEU:HD23	68:w:889:LEU:HD13	2.03	0.41
1:a:76:ALA:C	1:a:78:THR:N	2.79	0.41
1:a:106:ASP:HA	1:a:127:HIS:HB3	2.03	0.41
1:a:321:LEU:HD21	1:a:407:ILE:CB	2.50	0.41
1:a:351:ASP:O	1:a:351:ASP:CG	2.63	0.41
2:m:108:TYR:CE2	11:n:168:ARG:NH1	2.89	0.41
2:m:116:GLN:HB3	16:z:594:LEU:HD21	1.96	0.41
4:f:77:ILE:HG13	4:f:78:LEU:N	2.36	0.41
4:f:180:LEU:CD2	11:n:299:PHE:O	2.69	0.41
5:g:142:GLN:HE21	5:g:146:ARG:HE	1.68	0.41
6:h:39:ARG:O	6:h:39:ARG:CG	2.69	0.41
8:t:62:LEU:HB2	8:t:80:GLU:HG2	2.02	0.41
8:t:92:ASP:O	8:t:93:VAL:C	2.64	0.41
11:n:368:LYS:HZ3	11:n:368:LYS:HG2	1.68	0.41
11:n:689:PRO:O	11:n:690:CYS:HB2	2.21	0.41
11:n:903:CYS:HB3	11:n:904:PHE:H	1.67	0.41
12:q:379:ILE:HD13	12:q:379:ILE:HA	1.90	0.41
12:q:566:ALA:HB1	12:q:583:ARG:HD3	2.03	0.41
16:z:583:ASP:HB2	16:z:590:ARG:HG2	2.03	0.41
17:c:70:LEU:O	19:b:60:TYR:OH	2.36	0.41
17:c:281:CYS:HB3	17:c:284:CYS:HB2	1.87	0.41
23:0:139:LYS:HE3	23:0:139:LYS:HB3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:407:ILE:HD12	26:1:407:ILE:HA	1.72	0.41
27:2:85:LEU:HD12	27:2:85:LEU:HA	1.83	0.41
35:DA:1190:VAL:HG22	40:DG:162:VAL:HG13	2.02	0.41
45:Dc:23:TRP:CZ3	43:Dj:193:TYR:HB3	2.56	0.41
37:Dd:910:LEU:HD11	44:Dl:88:ALA:HB2	2.02	0.41
39:Df:308:VAL:O	39:Df:312:ILE:HG13	2.20	0.41
43:Dj:162:PHE:O	43:Dj:166:ILE:HG13	2.21	0.41
52:FB:170:LYS:HE2	52:FB:170:LYS:HB3	1.91	0.41
53:X:17:DT:H2"	53:X:18:DC:C6	2.55	0.41
55:PA:34:MET:HA	56:PB:1138:ARG:HG2	2.03	0.41
55:PA:640:LEU:HD23	55:PA:640:LEU:HA	1.92	0.41
55:PA:871:VAL:HB	55:PA:1088:GLY:HA3	2.03	0.41
55:PA:934:LEU:HG	55:PA:938:LEU:HB2	2.03	0.41
56:PB:403:LEU:HD12	56:PB:403:LEU:HA	1.83	0.41
57:PC:149:LEU:HD21	57:PC:152:LYS:HE3	2.02	0.41
61:PG:13:LEU:HB3	61:PG:18:PHE:CE1	2.56	0.41
64:PJ:13:ILE:H	64:PJ:13:ILE:HG13	1.63	0.41
68:w:847:ILE:HD12	68:w:847:ILE:HA	1.97	0.41
70:p:284:LYS:HB3	70:p:356:LEU:HD11	2.03	0.41
3:d:103:ARG:NH1	22:i:128:LYS:HB2	2.36	0.40
5:g:98:ARG:HH11	13:s:72:PRO:HB2	1.86	0.40
7:r:194:LYS:HA	7:r:197:VAL:O	2.21	0.40
10:k:35:LEU:HD22	12:q:154:ALA:HB2	2.02	0.40
11:n:278:VAL:HG11	11:n:295:CYS:SG	2.58	0.40
11:n:569:TYR:CD1	11:n:590:GLN:HB2	2.56	0.40
11:n:647:MET:HG2	11:n:651:ASN:HD21	1.85	0.40
11:n:793:HIS:HD2	11:n:794:LEU:HG	1.86	0.40
11:n:907:LEU:HD21	19:b:118:LEU:CA	2.50	0.40
14:u:75:SER:OG	14:u:76:LEU:N	2.54	0.40
17:c:60:LEU:HD23	17:c:60:LEU:HA	1.85	0.40
29:4:145:VAL:HG13	29:4:245:LEU:HD13	2.02	0.40
29:4:265:LEU:HD12	29:4:265:LEU:HA	1.87	0.40
30:5:24:ASP:HB2	30:5:33:PHE:HB3	2.03	0.40
32:7:494:ILE:HD13	32:7:684:PHE:HB3	2.03	0.40
33:EA:141:ALA:HA	33:EA:144:LEU:HD12	2.02	0.40
37:DD:1085:LYS:NZ	44:DL:83:MET:CE	2.83	0.40
38:DE:684:LEU:HB3	38:DE:696:TRP:HD1	1.86	0.40
38:DE:689:THR:HA	38:DE:713:THR:HG23	2.03	0.40
38:DE:710:HIS:NE2	38:DE:728:SER:HB2	2.36	0.40
38:DE:785:PHE:CZ	38:DE:791:VAL:HG22	2.56	0.40
45:Dc:34:LEU:HD12	45:Dc:34:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Dd:885:ILE:CG1	44:Dl:96:VAL:HG11	2.51	0.40
37:Dd:1079:LEU:HA	37:Dd:1079:LEU:HD23	1.79	0.40
38:De:251:LEU:HB3	38:De:260:ALA:HB2	2.03	0.40
55:PA:963:ARG:NH2	55:PA:967:ARG:HH21	2.20	0.40
55:PA:966:LEU:HD11	55:PA:1043:ILE:HG21	2.04	0.40
55:PA:1794:SER:O	55:PA:1795:PRO:C	2.64	0.40
56:PB:607:ILE:H	56:PB:607:ILE:HG13	1.51	0.40
68:w:427:CYS:O	68:w:431:HIS:ND1	2.40	0.40
68:w:916:ASP:O	68:w:920:LYS:NZ	2.50	0.40
69:x:101:MET:HB3	69:x:101:MET:HE2	1.87	0.40
69:x:166:GLU:O	69:x:170:SER:OG	2.34	0.40
1:a:359:HIS:HD2	1:a:361:MET:H	1.68	0.40
1:a:361:MET:HE3	1:a:376:LEU:HB2	2.02	0.40
1:a:367:LEU:CD1	1:a:509:ARG:NH1	2.82	0.40
1:a:424:CYS:CA	1:a:505:PRO:HG3	2.48	0.40
2:m:116:GLN:HG3	16:z:595:PRO:HD3	2.04	0.40
4:f:59:HIS:HA	24:8:108:VAL:HA	2.03	0.40
5:g:34:PRO:HB2	5:g:35:PRO:CD	2.48	0.40
5:g:145:GLN:O	5:g:149:THR:HG23	2.21	0.40
6:h:86:ASP:H	6:h:99:VAL:HG12	1.85	0.40
6:h:147:CYS:HB2	15:v:41:LYS:CB	2.43	0.40
7:r:47:GLU:CD	7:r:47:GLU:N	2.71	0.40
7:r:50:THR:O	7:r:50:THR:OG1	2.31	0.40
7:r:51:PHE:O	7:r:51:PHE:CG	2.74	0.40
8:t:16:SER:O	8:t:19:GLN:N	2.54	0.40
9:j:102:MET:HE2	9:j:106:LYS:HZ2	1.86	0.40
10:k:106:ASP:HA	10:k:109:ARG:NE	2.35	0.40
11:n:192:LEU:HD12	11:n:192:LEU:HA	1.91	0.40
11:n:202:ARG:HH21	11:n:240:ASP:HA	1.86	0.40
11:n:379:PRO:HB3	11:n:411:GLN:HE22	1.86	0.40
11:n:944:PHE:O	11:n:945:ASP:C	2.64	0.40
12:q:149:LYS:HG3	15:v:42:ILE:CG1	2.48	0.40
12:q:430:LYS:HG2	12:q:471:TYR:OH	2.21	0.40
12:q:599:ASN:OD1	12:q:599:ASN:C	2.65	0.40
19:b:67:LEU:HD12	19:b:67:LEU:HA	1.91	0.40
21:o:762:GLN:NE2	68:w:26:PHE:CE2	2.89	0.40
21:o:772:LEU:HA	21:o:775:THR:HG22	2.02	0.40
23:0:77:LYS:HD2	23:0:109:LEU:HD23	2.02	0.40
23:0:131:ASP:O	23:0:134:GLN:HG2	2.21	0.40
28:3:232:LEU:N	28:3:233:PRO:HD2	2.37	0.40
30:5:38:ILE:H	30:5:38:ILE:HG13	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:7:223:LYS:HE3	32:7:227:ARG:HE	1.86	0.40
32:7:395:SER:N	32:7:396:PRO:HD2	2.37	0.40
33:EA:136:PHE:HB2	33:EA:144:LEU:HD11	2.02	0.40
37:DD:956:GLN:HB3	37:DD:983:ARG:HH21	1.86	0.40
41:DH:224:LEU:HD23	41:DH:224:LEU:HA	1.89	0.40
42:DI:99:ARG:HD3	42:DI:99:ARG:HA	1.91	0.40
39:Df:342:LYS:HE2	39:Df:342:LYS:HB3	1.87	0.40
39:Df:402:ARG:NH1	39:Df:424:GLN:HB2	2.37	0.40
53:X:12:DA:H2"	53:X:13:DA:C8	2.56	0.40
55:PA:687:ILE:HD12	55:PA:687:ILE:HA	1.80	0.40
55:PA:1473:LEU:H	55:PA:1473:LEU:HD12	1.86	0.40
56:PB:310:VAL:HG22	67:FA:164:TRP:CZ2	2.56	0.40
67:FA:109:LYS:HD2	67:FA:149:LEU:HD22	2.03	0.40
67:FA:125:TYR:HB3	67:FA:137:ALA:HB1	2.02	0.40
68:w:16:GLU:HA	68:w:19:GLU:CD	2.47	0.40
69:x:42:LEU:HD12	69:x:42:LEU:HA	1.94	0.40
69:x:162:LEU:HD23	69:x:165:LEU:HD12	2.03	0.40
69:x:169:LEU:HD13	69:x:169:LEU:HA	1.92	0.40
69:x:305:TRP:O	69:x:309:THR:HG23	2.21	0.40
70:p:97:LEU:HD11	70:p:179:TRP:HB3	2.03	0.40
1:a:433:ASP:HB3	1:a:437:LEU:HG	2.03	0.40
1:a:498:VAL:CG2	1:a:507:THR:HG22	2.51	0.40
4:f:181:LEU:HD11	11:n:270:GLN:CD	2.46	0.40
5:g:30:LEU:O	5:g:30:LEU:CG	2.70	0.40
6:h:33:LEU:HD23	6:h:40:LEU:HD22	1.99	0.40
9:j:99:ILE:CG2	9:j:103:LYS:HE3	2.51	0.40
10:k:88:LYS:NZ	12:q:303:LEU:CD2	2.84	0.40
11:n:904:PHE:HZ	11:n:1213:SER:HA	1.86	0.40
11:n:949:LEU:HD23	11:n:949:LEU:HA	1.89	0.40
14:u:110:ARG:HH22	22:i:141:PHE:HB3	1.87	0.40
17:c:16:GLN:HB3	17:c:73:LEU:HD21	2.02	0.40
20:l:36:ILE:O	20:l:40:THR:HG23	2.21	0.40
21:o:715:LEU:HD23	21:o:715:LEU:HA	1.71	0.40
23:0:121:LYS:HA	23:0:124:ILE:CD1	2.52	0.40
24:8:269:LEU:HA	24:8:269:LEU:HD22	1.81	0.40
25:9:219:SER:HB3	25:9:256:ARG:HH12	1.86	0.40
31:6:296:ASP:HB3	31:6:299:ASN:HB2	2.03	0.40
32:7:425:THR:HA	32:7:426:PRO:HD3	1.90	0.40
36:DB:418:PHE:CE1	36:DB:436:LYS:HA	2.56	0.40
38:DE:466:PHE:HB2	38:DE:796:ALA:HA	2.02	0.40
37:Dd:893:GLU:HG2	44:Dl:110:THR:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:De:717:LEU:HD23	38:De:717:LEU:HA	1.86	0.40
51:BA:107:MET:HE2	51:BA:107:MET:HB3	1.95	0.40
56:PB:626:LEU:HD11	56:PB:698:ILE:HA	2.02	0.40
56:PB:713:PHE:N	56:PB:714:PRO:HD3	2.37	0.40
68:w:10:GLU:HB3	68:w:14:LYS:CE	2.50	0.40
68:w:18:ILE:O	68:w:18:ILE:CG1	2.69	0.40
68:w:80:TYR:CD1	68:w:121:LEU:HD22	2.56	0.40
68:w:394:PRO:C	70:p:171:PHE:CZ	2.93	0.40
69:x:47:LEU:HD23	69:x:47:LEU:HA	1.82	0.40
69:x:289:CYS:SG	69:x:313:ILE:HG13	2.61	0.40
69:x:671:GLU:HG2	69:x:687:PHE:CD1	2.56	0.40
69:x:794:ASP:HB3	69:x:797:LYS:HB2	2.02	0.40
69:x:925:GLN:NE2	69:x:958:VAL:O	2.51	0.40
1:a:322:GLN:O	1:a:323:ASN:C	2.64	0.40
1:a:463:VAL:HG21	1:a:488:ILE:HD11	2.04	0.40
8:t:66:MET:HE3	8:t:194:MET:HB2	2.02	0.40
9:j:123:LYS:HG2	13:s:65:PHE:CZ	2.57	0.40
11:n:287:LYS:N	11:n:288:PRO:HD3	2.36	0.40
11:n:301:LEU:HB3	11:n:361:ILE:HD11	2.04	0.40
11:n:402:ILE:HD11	12:q:327:VAL:HA	2.00	0.40
11:n:485:ASP:OD1	11:n:485:ASP:N	2.51	0.40
11:n:544:ARG:CZ	11:n:716:ASN:HA	2.51	0.40
11:n:658:ARG:HH22	68:w:21:ALA:CA	2.28	0.40
11:n:838:VAL:O	11:n:838:VAL:HG23	2.21	0.40
21:o:729:TYR:OH	21:o:768:SER:OG	2.40	0.40
23:0:281:GLN:HE21	24:8:244:PRO:HD3	1.86	0.40
24:8:219:LEU:HD12	24:8:219:LEU:HA	1.88	0.40
28:3:143:TYR:O	28:3:146:ARG:HG3	2.21	0.40
29:4:337:ARG:HB3	31:6:62:ARG:HH21	1.85	0.40
31:6:363:VAL:HG22	31:6:439:ILE:HD12	2.02	0.40
32:7:213:LEU:HD12	32:7:213:LEU:HA	1.87	0.40
32:7:417:ILE:HG21	32:7:632:ILE:HG12	2.03	0.40
35:DA:602:PHE:HZ	35:DA:668:PRO:HB3	1.87	0.40
36:DB:75:VAL:HG11	36:DB:128:ILE:HD13	2.03	0.40
37:DD:950:LEU:HD22	37:DD:950:LEU:HA	1.90	0.40
38:DE:235:GLU:HG2	38:DE:309:ILE:HG13	2.02	0.40
38:DE:369:LYS:HD3	38:DE:369:LYS:HA	1.84	0.40
38:DE:707:LEU:HD21	38:DE:768:LEU:HD12	2.02	0.40
39:DF:377:ILE:HD13	39:DF:377:ILE:HA	1.94	0.40
39:Df:396:LEU:HD21	39:Df:450:ALA:HA	2.04	0.40
48:DO:30:PRO:O	48:DO:31:GLN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:X:26:DG:C2'	53:X:27:DC:H5'	2.49	0.40
55:PA:102:LYS:HE2	55:PA:1444:ALA:HB1	2.04	0.40
55:PA:353:ASN:O	55:PA:357:LYS:HE3	2.21	0.40
55:PA:367:ILE:HB	55:PA:484:LEU:HD21	2.03	0.40
55:PA:560:VAL:HG21	55:PA:586:TRP:HB2	2.03	0.40
55:PA:602:CYS:HB2	55:PA:655:ILE:HG13	2.03	0.40
55:PA:1484:MET:HE3	55:PA:1484:MET:HB3	2.00	0.40
56:PB:470:LEU:HD21	56:PB:478:THR:HG23	2.03	0.40
56:PB:759:VAL:HG12	56:PB:999:ALA:HB2	2.04	0.40
56:PB:1172:MET:HE3	56:PB:1172:MET:HB2	1.94	0.40
59:PE:55:ARG:HD2	59:PE:55:ARG:HA	1.93	0.40
68:w:11:GLU:O	68:w:15:THR:N	2.54	0.40
68:w:248:LEU:HD23	68:w:248:LEU:HA	1.83	0.40
68:w:361:ALA:HB1	70:p:250:SER:CB	2.49	0.40
68:w:711:TRP:CD1	68:w:711:TRP:H	2.39	0.40
70:p:311:LEU:HD13	70:p:339:TRP:CE2	2.57	0.40
1:a:383:PRO:CA	69:x:92:LEU:CD2	2.60	0.40
1:a:398:PHE:O	1:a:398:PHE:CG	2.74	0.40
6:h:162:GLU:HB3	6:h:163:SER:H	1.68	0.40
7:r:129:PHE:O	7:r:129:PHE:CD2	2.74	0.40
9:j:99:ILE:HA	9:j:102:MET:CG	2.50	0.40
9:j:116:VAL:HG13	14:u:67:LYS:HZ1	1.85	0.40
10:k:43:ARG:NH1	10:k:43:ARG:HB3	2.37	0.40
10:k:92:MET:HG3	12:q:377:LEU:HD21	2.02	0.40
11:n:154:ILE:CB	11:n:155:PRO:CD	2.98	0.40
11:n:199:LEU:HD23	11:n:199:LEU:HA	1.88	0.40
11:n:586:LEU:HD23	11:n:587:LEU:HD22	2.02	0.40
12:q:458:PRO:O	12:q:459:GLN:HB2	2.21	0.40
14:u:76:LEU:H	14:u:76:LEU:HG	1.60	0.40
19:b:164:ILE:O	19:b:168:ILE:HG12	2.22	0.40
19:b:181:CYS:SG	20:l:82:LEU:CD2	3.10	0.40
24:8:62:GLU:HG3	24:8:156:PHE:H	1.85	0.40
25:9:129:LEU:HD13	25:9:129:LEU:HA	1.91	0.40
29:4:440:LEU:HD23	29:4:440:LEU:HA	1.85	0.40
31:6:582:GLY:HA2	31:6:610:VAL:HA	2.04	0.40
32:7:115:LEU:HD12	32:7:192:TYR:HD1	1.86	0.40
34:EB:166:ILE:HG22	34:EB:168:LEU:H	1.85	0.40
36:DB:86:TYR:HB2	36:DB:126:LEU:HD13	2.02	0.40
36:DB:232:LYS:HB3	36:DB:232:LYS:HE3	1.67	0.40
36:DB:608:ASN:CB	36:DB:657:ARG:HG3	2.50	0.40
38:DE:611:LEU:HB3	38:DE:621:ARG:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DF:145:ILE:HG13	39:DF:148:ASN:H	1.87	0.40
43:Dj:214:PRO:HB2	43:Dj:217:PHE:CZ	2.57	0.40
53:X:-3:DC:H2"	53:X:-2:DC:C6	2.56	0.40
55:PA:400:ASP:O	55:PA:403:GLN:HG3	2.22	0.40
55:PA:1184:THR:OG1	55:PA:1190:GLN:HB2	2.21	0.40
56:PB:742:VAL:HG23	56:PB:743:ARG:HG3	2.03	0.40
58:PD:76:ASN:O	58:PD:80:ILE:HG13	2.22	0.40
60:PF:59:LYS:HE2	60:PF:59:LYS:HB3	1.94	0.40
61:PG:97:LEU:HD13	61:PG:97:LEU:HA	1.90	0.40
68:w:707:ILE:HG23	68:w:713:LYS:HD3	2.03	0.40
68:w:805:GLN:HE22	68:w:809:ARG:HE	1.69	0.40
68:w:1147:ASN:OD1	68:w:1218:HIS:NE2	2.54	0.40
70:p:206:LEU:HD23	70:p:206:LEU:HA	1.99	0.40
70:p:313:LYS:HB3	70:p:337:LEU:HD23	2.04	0.40
70:p:444:VAL:HG22	70:p:452:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	a	457/1581 (29%)	421 (92%)	29 (6%)	7 (2%)	8 38
2	m	110/131 (84%)	106 (96%)	4 (4%)	0	100 100
3	d	154/270 (57%)	143 (93%)	6 (4%)	5 (3%)	3 24
4	f	163/246 (66%)	142 (87%)	15 (9%)	6 (4%)	2 22
5	g	164/233 (70%)	145 (88%)	10 (6%)	9 (6%)	1 17
6	h	188/268 (70%)	167 (89%)	12 (6%)	9 (5%)	2 18
7	r	189/208 (91%)	176 (93%)	10 (5%)	3 (2%)	7 37
8	t	189/212 (89%)	166 (88%)	15 (8%)	8 (4%)	2 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	j	120/135 (89%)	110 (92%)	6 (5%)	4 (3%)	3 24
10	k	110/117 (94%)	99 (90%)	9 (8%)	2 (2%)	6 34
11	n	980/1454 (67%)	877 (90%)	86 (9%)	17 (2%)	7 36
12	q	540/651 (83%)	474 (88%)	53 (10%)	13 (2%)	4 29
13	s	69/244 (28%)	60 (87%)	7 (10%)	2 (3%)	3 26
14	u	103/144 (72%)	93 (90%)	8 (8%)	2 (2%)	6 33
15	v	132/200 (66%)	119 (90%)	10 (8%)	3 (2%)	5 30
16	z	93/600 (16%)	84 (90%)	7 (8%)	2 (2%)	5 31
17	c	245/311 (79%)	232 (95%)	13 (5%)	0	100 100
18	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6 33
19	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14 48
20	l	120/178 (67%)	115 (96%)	5 (4%)	0	100 100
21	o	152/788 (19%)	138 (91%)	10 (7%)	4 (3%)	4 28
22	i	56/146 (38%)	54 (96%)	1 (2%)	1 (2%)	6 34
23	0	304/309 (98%)	285 (94%)	15 (5%)	4 (1%)	9 41
24	8	297/346 (86%)	290 (98%)	7 (2%)	0	100 100
25	9	285/323 (88%)	279 (98%)	6 (2%)	0	100 100
26	1	399/548 (73%)	336 (84%)	53 (13%)	10 (2%)	4 29
27	2	327/395 (83%)	315 (96%)	10 (3%)	2 (1%)	21 58
28	3	259/308 (84%)	257 (99%)	2 (1%)	0	100 100
29	4	447/462 (97%)	431 (96%)	12 (3%)	4 (1%)	14 48
30	5	52/71 (73%)	50 (96%)	2 (4%)	0	100 100
31	6	602/782 (77%)	585 (97%)	14 (2%)	3 (0%)	24 61
32	7	732/760 (96%)	704 (96%)	23 (3%)	5 (1%)	18 54
33	EA	175/439 (40%)	163 (93%)	12 (7%)	0	100 100
34	EB	170/291 (58%)	161 (95%)	4 (2%)	5 (3%)	3 26
35	DA	534/1872 (28%)	523 (98%)	9 (2%)	2 (0%)	30 65
36	DB	959/1199 (80%)	932 (97%)	25 (3%)	2 (0%)	43 76
37	DD	153/1085 (14%)	148 (97%)	4 (3%)	1 (1%)	18 54
37	Dd	154/1085 (14%)	152 (99%)	2 (1%)	0	100 100
38	DE	540/800 (68%)	524 (97%)	16 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	De	531/800 (66%)	514 (97%)	16 (3%)	1 (0%)	43 76
39	DF	404/677 (60%)	393 (97%)	9 (2%)	2 (0%)	24 61
39	Df	399/677 (59%)	394 (99%)	4 (1%)	1 (0%)	36 70
40	DG	139/349 (40%)	137 (99%)	2 (1%)	0	100 100
41	DH	207/310 (67%)	199 (96%)	5 (2%)	3 (1%)	9 39
42	DI	118/264 (45%)	116 (98%)	1 (1%)	1 (1%)	16 52
42	Di	119/264 (45%)	118 (99%)	1 (1%)	0	100 100
43	DJ	86/218 (39%)	84 (98%)	2 (2%)	0	100 100
43	Dj	91/218 (42%)	90 (99%)	1 (1%)	0	100 100
44	DL	73/161 (45%)	68 (93%)	2 (3%)	3 (4%)	2 20
44	Dl	105/161 (65%)	104 (99%)	0	1 (1%)	12 46
45	Dc	125/929 (14%)	122 (98%)	1 (1%)	2 (2%)	7 37
46	Dk	96/211 (46%)	93 (97%)	3 (3%)	0	100 100
47	Dm	85/124 (68%)	82 (96%)	3 (4%)	0	100 100
48	DO	95/109 (87%)	91 (96%)	2 (2%)	2 (2%)	5 32
49	DP	175/339 (52%)	170 (97%)	4 (2%)	1 (1%)	21 58
50	DQ	118/307 (38%)	115 (98%)	2 (2%)	1 (1%)	16 52
51	BA	247/316 (78%)	244 (99%)	3 (1%)	0	100 100
52	FB	218/249 (88%)	210 (96%)	7 (3%)	1 (0%)	24 61
55	PA	1460/1970 (74%)	1415 (97%)	38 (3%)	7 (0%)	24 61
56	PB	1128/1174 (96%)	1104 (98%)	22 (2%)	2 (0%)	43 76
57	PC	253/275 (92%)	252 (100%)	1 (0%)	0	100 100
58	PD	127/142 (89%)	127 (100%)	0	0	100 100
59	PE	207/210 (99%)	204 (99%)	2 (1%)	1 (0%)	24 61
60	PF	77/127 (61%)	76 (99%)	0	1 (1%)	9 41
61	PG	169/172 (98%)	165 (98%)	4 (2%)	0	100 100
62	PH	146/150 (97%)	144 (99%)	2 (1%)	0	100 100
63	PI	112/125 (90%)	111 (99%)	1 (1%)	0	100 100
64	PJ	62/67 (92%)	61 (98%)	1 (2%)	0	100 100
65	PK	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
66	PL	42/58 (72%)	42 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	FA	130/517 (25%)	126 (97%)	4 (3%)	0	100	100
68	w	1332/1368 (97%)	1261 (95%)	65 (5%)	6 (0%)	24	61
69	x	876/989 (89%)	820 (94%)	51 (6%)	5 (1%)	21	58
70	p	400/841 (48%)	367 (92%)	32 (8%)	1 (0%)	36	70
All	All	20999/34555 (61%)	19990 (95%)	829 (4%)	180 (1%)	16	48

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	67	LYS
1	a	331	GLU
4	f	25	ASN
4	f	35	GLU
4	f	36	ARG
5	g	31	ALA
6	h	100	PHE
6	h	130	ARG
6	h	161	SER
8	t	99	LYS
9	j	61	ILE
9	j	64	PRO
11	n	154	ILE
11	n	1196	PRO
11	n	1255	PRO
11	n	1266	THR
11	n	1326	PRO
12	q	131	SER
12	q	288	SER
12	q	393	PRO
12	q	398	ALA
12	q	399	PRO
13	s	158	PRO
15	v	42	ILE
23	0	7	PRO
23	0	237	PRO
26	1	264	ASN
26	1	276	PRO
26	1	278	ASP
26	1	287	PRO
26	1	292	SER
27	2	268	LYS

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Mol	Chain	Res	Type
29	4	135	GLN
31	6	421	TRP
32	7	307	ASN
32	7	463	PRO
34	EB	171	ILE
35	DA	498	PRO
36	DB	366	ASP
37	DD	876	ALA
39	DF	442	PRO
44	DL	73	ASN
55	PA	1652	PRO
55	PA	1654	SER
60	PF	76	CYS
68	w	51	LEU
69	x	54	PRO
1	a	334	PRO
1	a	430	LEU
5	g	29	GLY
6	h	37	TYR
7	r	45	ASN
8	t	165	LEU
11	n	169	LEU
11	n	254	VAL
11	n	1351	PRO
12	q	395	PRO
12	q	419	ASN
15	v	139	SER
16	z	544	THR
18	e	146	ILE
21	o	714	ASP
31	6	610	VAL
31	6	622	VAL
32	7	36	GLY
32	7	308	PRO
34	EB	134	ASP
36	DB	427	PRO
48	DO	52	VAL
50	DQ	320	VAL
55	PA	1669	PRO
68	w	32	ASP
68	w	1196	CYS
69	x	485	PRO

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Mol	Chain	Res	Type
69	x	566	GLU
1	a	487	LEU
3	d	144	SER
3	d	146	GLU
4	f	139	TYR
5	g	39	LYS
5	g	41	SER
6	h	41	THR
8	t	120	CYS
9	j	60	ASP
11	n	165	SER
11	n	1206	PRO
12	q	91	SER
12	q	420	SER
12	q	458	PRO
14	u	81	SER
21	o	709	LYS
22	i	139	CYS
26	1	280	GLY
26	1	520	ASN
34	EB	212	VAL
44	DL	114	LYS
45	Dc	117	ALA
56	PB	467	SER
68	w	1203	MET
69	x	484	LYS
70	p	250	SER
1	a	208	VAL
3	d	143	ILE
4	f	138	ARG
5	g	20	GLU
5	g	26	ILE
6	h	170	LYS
7	r	94	GLY
7	r	153	VAL
8	t	47	HIS
8	t	109	LYS
11	n	265	LEU
11	n	528	HIS
11	n	1355	PRO
12	q	127	LEU
12	q	134	ALA

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Mol	Chain	Res	Type
18	e	147	ASN
19	b	100	GLN
23	0	233	ILE
26	1	279	GLU
26	1	369	VAL
34	EB	225	VAL
39	DF	66	LEU
41	DH	129	VAL
45	Dc	100	PRO
39	Df	93	PRO
48	DO	84	VAL
52	FB	38	GLY
55	PA	1662	PRO
68	w	128	GLY
3	d	178	THR
4	f	61	ASN
5	g	74	HIS
8	t	129	VAL
10	k	79	HIS
10	k	81	GLY
11	n	264	ALA
11	n	1343	PRO
13	s	153	ARG
14	u	83	ALA
15	v	51	ALA
16	z	540	LEU
21	o	721	LEU
23	0	192	LEU
29	4	129	TRP
34	EB	174	ALA
44	DL	112	GLU
38	De	510	ALA
69	x	564	SER
6	h	99	VAL
11	n	229	GLU
12	q	89	GLN
26	1	512	ILE
29	4	384	PRO
41	DH	163	PRO
44	Dl	60	LYS
49	DP	207	PRO
55	PA	1659	PRO

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Mol	Chain	Res	Type
56	PB	231	PRO
68	w	361	ALA
5	g	137	VAL
11	n	150	PRO
41	DH	140	ARG
1	a	75	PRO
8	t	172	ALA
21	o	716	PRO
35	DA	504	PRO
55	PA	1795	PRO
3	d	176	TYR
6	h	42	TRP
6	h	98	PRO
8	t	17	VAL
9	j	76	ASN
29	4	189	GLU
32	7	291	GLY
42	DI	85	SER
55	PA	462	PRO
5	g	14	PRO
27	2	259	ILE
59	PE	77	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	387/1391 (28%)	322 (83%)	65 (17%)	2 12
2	m	102/115 (89%)	102 (100%)	0	100 100
3	d	138/230 (60%)	98 (71%)	40 (29%)	0 3
4	f	144/223 (65%)	122 (85%)	22 (15%)	3 14
5	g	157/215 (73%)	126 (80%)	31 (20%)	1 9
6	h	168/225 (75%)	126 (75%)	42 (25%)	0 4
7	r	168/183 (92%)	126 (75%)	42 (25%)	0 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	t	166/178 (93%)	136 (82%)	30 (18%)	2 11
9	j	113/124 (91%)	108 (96%)	5 (4%)	25 48
10	k	94/98 (96%)	45 (48%)	49 (52%)	0 0
11	n	689/1272 (54%)	654 (95%)	35 (5%)	21 44
12	q	461/577 (80%)	383 (83%)	78 (17%)	2 12
13	s	31/208 (15%)	27 (87%)	4 (13%)	4 18
14	u	78/119 (66%)	66 (85%)	12 (15%)	2 14
15	v	122/173 (70%)	88 (72%)	34 (28%)	0 3
16	z	89/512 (17%)	74 (83%)	15 (17%)	2 12
17	c	231/280 (82%)	225 (97%)	6 (3%)	40 60
18	e	94/152 (62%)	94 (100%)	0	100 100
19	b	102/163 (63%)	92 (90%)	10 (10%)	7 26
20	l	116/155 (75%)	116 (100%)	0	100 100
21	o	141/697 (20%)	139 (99%)	2 (1%)	59 71
22	i	61/133 (46%)	42 (69%)	19 (31%)	0 2
23	0	209/283 (74%)	194 (93%)	15 (7%)	13 36
24	8	259/299 (87%)	225 (87%)	34 (13%)	4 18
25	9	252/296 (85%)	224 (89%)	28 (11%)	6 22
26	1	176/484 (36%)	162 (92%)	14 (8%)	11 33
27	2	279/352 (79%)	251 (90%)	28 (10%)	7 25
28	3	234/272 (86%)	219 (94%)	15 (6%)	16 40
29	4	387/399 (97%)	355 (92%)	32 (8%)	10 32
30	5	48/64 (75%)	42 (88%)	6 (12%)	4 19
31	6	533/688 (78%)	487 (91%)	46 (9%)	10 31
32	7	616/664 (93%)	565 (92%)	51 (8%)	10 32
33	EA	163/373 (44%)	148 (91%)	15 (9%)	8 29
34	EB	155/261 (59%)	143 (92%)	12 (8%)	12 34
35	DA	488/1665 (29%)	441 (90%)	47 (10%)	8 27
36	DB	876/1083 (81%)	790 (90%)	86 (10%)	7 26
37	DD	144/815 (18%)	134 (93%)	10 (7%)	14 38
37	Dd	146/815 (18%)	138 (94%)	8 (6%)	19 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	DE	478/657 (73%)	435 (91%)	43 (9%)	9 30
38	De	475/657 (72%)	420 (88%)	55 (12%)	5 21
39	DF	324/574 (56%)	295 (91%)	29 (9%)	9 30
39	Df	322/574 (56%)	307 (95%)	15 (5%)	23 46
40	DG	133/322 (41%)	117 (88%)	16 (12%)	5 20
41	DH	181/270 (67%)	170 (94%)	11 (6%)	17 41
42	DI	106/235 (45%)	101 (95%)	5 (5%)	23 46
42	Di	107/235 (46%)	104 (97%)	3 (3%)	38 59
43	DJ	79/154 (51%)	76 (96%)	3 (4%)	29 51
43	Dj	83/154 (54%)	82 (99%)	1 (1%)	63 73
44	DL	70/141 (50%)	64 (91%)	6 (9%)	10 31
44	Dl	98/141 (70%)	94 (96%)	4 (4%)	27 49
45	Dc	113/833 (14%)	106 (94%)	7 (6%)	16 40
46	Dk	87/182 (48%)	84 (97%)	3 (3%)	32 55
47	Dm	80/106 (76%)	75 (94%)	5 (6%)	16 40
48	DO	84/98 (86%)	75 (89%)	9 (11%)	6 23
49	DP	153/293 (52%)	143 (94%)	10 (6%)	15 40
50	DQ	111/269 (41%)	105 (95%)	6 (5%)	20 44
51	BA	214/268 (80%)	197 (92%)	17 (8%)	11 33
52	FB	196/218 (90%)	179 (91%)	17 (9%)	9 31
55	PA	1303/1748 (74%)	1163 (89%)	140 (11%)	6 23
56	PB	993/1027 (97%)	887 (89%)	106 (11%)	6 23
57	PC	234/252 (93%)	218 (93%)	16 (7%)	14 38
58	PD	108/126 (86%)	91 (84%)	17 (16%)	2 14
59	PE	191/192 (100%)	174 (91%)	17 (9%)	9 30
60	PF	69/111 (62%)	60 (87%)	9 (13%)	4 18
61	PG	147/153 (96%)	125 (85%)	22 (15%)	3 15
62	PH	129/131 (98%)	118 (92%)	11 (8%)	10 31
63	PI	103/112 (92%)	93 (90%)	10 (10%)	8 26
64	PJ	53/56 (95%)	51 (96%)	2 (4%)	29 51
65	PK	106/106 (100%)	101 (95%)	5 (5%)	23 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
66	PL	41/55 (74%)	38 (93%)	3 (7%)	13 36
67	FA	117/448 (26%)	115 (98%)	2 (2%)	53 68
68	w	1202/1232 (98%)	1181 (98%)	21 (2%)	53 68
69	x	787/864 (91%)	769 (98%)	18 (2%)	44 63
70	p	353/736 (48%)	347 (98%)	6 (2%)	53 68
All	All	18247/29966 (61%)	16589 (91%)	1658 (9%)	11 29

All (1658) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	77	MET
1	a	93	HIS
1	a	106	ASP
1	a	107	MET
1	a	108	PHE
1	a	109	TYR
1	a	111	GLU
1	a	128	HIS
1	a	131	ASN
1	a	133	VAL
1	a	135	CYS
1	a	145	LYS
1	a	160	LEU
1	a	162	ASN
1	a	167	ASN
1	a	173	MET
1	a	201	ASP
1	a	214	ARG
1	a	226	VAL
1	a	232	LEU
1	a	246	ASN
1	a	253	MET
1	a	254	ASN
1	a	258	THR
1	a	259	ILE
1	a	267	LYS
1	a	278	HIS
1	a	297	VAL
1	a	305	LEU
1	a	309	GLN

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Mol	Chain	Res	Type
1	a	325	THR
1	a	327	ILE
1	a	329	LEU
1	a	333	GLN
1	a	335	THR
1	a	339	LEU
1	a	348	LEU
1	a	357	LEU
1	a	367	LEU
1	a	373	CYS
1	a	376	LEU
1	a	384	ASP
1	a	388	LEU
1	a	391	THR
1	a	400	HIS
1	a	421	ILE
1	a	430	LEU
1	a	432	GLU
1	a	433	ASP
1	a	434	SER
1	a	437	LEU
1	a	438	LEU
1	a	441	GLU
1	a	443	CYS
1	a	445	LEU
1	a	446	SER
1	a	467	MET
1	a	470	GLN
1	a	472	SER
1	a	479	LEU
1	a	481	LYS
1	a	501	CYS
1	a	504	ILE
1	a	509	ARG
1	a	514	LYS
3	d	26	THR
3	d	27	ARG
3	d	28	GLU
3	d	31	LEU
3	d	34	LEU
3	d	44	LEU
3	d	62	GLU

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Mol	Chain	Res	Type
3	d	63	ASN
3	d	64	GLN
3	d	65	VAL
3	d	68	LEU
3	d	69	LEU
3	d	71	HIS
3	d	72	ARG
3	d	76	PHE
3	d	77	GLN
3	d	78	GLU
3	d	79	LEU
3	d	80	MET
3	d	81	LYS
3	d	84	LEU
3	d	86	GLN
3	d	88	LYS
3	d	89	ILE
3	d	93	MET
3	d	111	GLN
3	d	119	GLN
3	d	121	LEU
3	d	127	GLN
3	d	129	LYS
3	d	135	ILE
3	d	137	LYS
3	d	147	GLU
3	d	150	LYS
3	d	151	TYR
3	d	154	ARG
3	d	159	ASN
3	d	168	VAL
3	d	179	ASP
3	d	187	LEU
4	f	16	VAL
4	f	24	LEU
4	f	26	SER
4	f	28	SER
4	f	29	VAL
4	f	30	LEU
4	f	36	ARG
4	f	42	ASP
4	f	43	ARG

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Mol	Chain	Res	Type
4	f	47	ASN
4	f	49	VAL
4	f	50	VAL
4	f	51	LYS
4	f	53	GLN
4	f	56	THR
4	f	57	LEU
4	f	60	LEU
4	f	61	ASN
4	f	62	GLN
4	f	63	MET
4	f	120	LEU
4	f	132	GLU
5	g	11	LEU
5	g	15	MET
5	g	17	TYR
5	g	18	ILE
5	g	19	LYS
5	g	25	ASN
5	g	28	GLU
5	g	30	LEU
5	g	33	LYS
5	g	39	LYS
5	g	45	PHE
5	g	54	LEU
5	g	55	ILE
5	g	64	ILE
5	g	72	PHE
5	g	74	HIS
5	g	83	MET
5	g	92	LEU
5	g	95	ILE
5	g	103	ILE
5	g	110	GLU
5	g	112	LEU
5	g	122	LEU
5	g	127	ARG
5	g	138	MET
5	g	139	MET
5	g	143	LYS
5	g	162	GLU
5	g	163	MET

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Mol	Chain	Res	Type
5	g	166	ASN
5	g	174	ASP
6	h	3	ARG
6	h	7	GLN
6	h	15	LEU
6	h	16	LEU
6	h	17	SER
6	h	18	GLN
6	h	19	VAL
6	h	22	LEU
6	h	23	LYS
6	h	30	ILE
6	h	32	LYS
6	h	33	LEU
6	h	34	GLU
6	h	37	TYR
6	h	39	ARG
6	h	46	LEU
6	h	48	SER
6	h	51	LEU
6	h	52	LEU
6	h	53	SER
6	h	56	LEU
6	h	59	LEU
6	h	66	GLU
6	h	88	ASP
6	h	89	LEU
6	h	91	ARG
6	h	92	GLN
6	h	97	VAL
6	h	100	PHE
6	h	101	SER
6	h	102	HIS
6	h	110	ARG
6	h	111	THR
6	h	112	LYS
6	h	139	GLN
6	h	141	GLN
6	h	143	LEU
6	h	154	ILE
6	h	157	GLU
6	h	170	LYS

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Mol	Chain	Res	Type
6	h	178	THR
6	h	191	LEU
7	r	16	ILE
7	r	17	ASN
7	r	18	MET
7	r	22	LEU
7	r	29	ASP
7	r	31	SER
7	r	32	LEU
7	r	33	GLU
7	r	36	ILE
7	r	37	HIS
7	r	38	ARG
7	r	39	LEU
7	r	52	LEU
7	r	54	HIS
7	r	56	MET
7	r	60	LEU
7	r	69	VAL
7	r	88	LEU
7	r	98	ARG
7	r	114	LEU
7	r	115	THR
7	r	116	ASP
7	r	118	LEU
7	r	119	MET
7	r	120	GLU
7	r	121	MET
7	r	124	ARG
7	r	125	MET
7	r	134	HIS
7	r	143	ILE
7	r	144	MET
7	r	169	VAL
7	r	171	LEU
7	r	186	MET
7	r	193	LEU
7	r	194	LYS
7	r	196	LEU
7	r	197	VAL
7	r	200	GLU
7	r	201	LYS

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Mol	Chain	Res	Type
7	r	202	ILE
7	r	206	ARG
8	t	1	MET
8	t	13	GLU
8	t	17	VAL
8	t	19	GLN
8	t	24	LEU
8	t	63	MET
8	t	67	HIS
8	t	78	LEU
8	t	79	PHE
8	t	80	GLU
8	t	81	ASN
8	t	84	CYS
8	t	85	LEU
8	t	89	THR
8	t	98	LEU
8	t	109	LYS
8	t	110	ILE
8	t	124	VAL
8	t	138	ILE
8	t	142	VAL
8	t	143	GLU
8	t	147	CYS
8	t	149	VAL
8	t	154	TRP
8	t	157	LEU
8	t	158	LEU
8	t	179	ARG
8	t	195	GLU
8	t	196	LEU
8	t	200	ILE
9	j	20	ARG
9	j	62	THR
9	j	63	VAL
9	j	121	MET
9	j	123	LYS
10	k	8	ASN
10	k	10	ARG
10	k	11	LEU
10	k	12	ARG
10	k	14	LEU

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Mol	Chain	Res	Type
10	k	15	GLU
10	k	18	GLU
10	k	19	ARG
10	k	21	ILE
10	k	25	LEU
10	k	26	GLN
10	k	32	ILE
10	k	33	LEU
10	k	34	GLU
10	k	35	LEU
10	k	36	SER
10	k	37	LYS
10	k	40	THR
10	k	42	GLU
10	k	43	ARG
10	k	44	LEU
10	k	45	LEU
10	k	48	GLN
10	k	53	THR
10	k	56	VAL
10	k	57	GLN
10	k	58	HIS
10	k	60	GLU
10	k	64	SER
10	k	67	ILE
10	k	75	THR
10	k	82	SER
10	k	83	SER
10	k	86	SER
10	k	87	ARG
10	k	88	LYS
10	k	90	CYS
10	k	91	GLN
10	k	92	MET
10	k	94	LEU
10	k	96	ARG
10	k	97	VAL
10	k	101	ARG
10	k	102	LEU
10	k	103	LYS
10	k	104	LEU
10	k	107	VAL

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Mol	Chain	Res	Type
10	k	109	ARG
10	k	114	MET
11	n	149	LEU
11	n	154	ILE
11	n	166	TYR
11	n	168	ARG
11	n	169	LEU
11	n	188	LYS
11	n	195	LEU
11	n	197	GLN
11	n	202	ARG
11	n	206	THR
11	n	212	LEU
11	n	229	GLU
11	n	252	ILE
11	n	253	LEU
11	n	254	VAL
11	n	255	GLU
11	n	261	ASP
11	n	265	LEU
11	n	266	VAL
11	n	267	HIS
11	n	273	PHE
11	n	274	ILE
11	n	276	GLN
11	n	277	LEU
11	n	289	LEU
11	n	305	LEU
11	n	359	ILE
11	n	366	VAL
11	n	367	SER
11	n	368	LYS
11	n	522	LEU
11	n	523	SER
11	n	528	HIS
11	n	530	ILE
11	n	532	ASN
12	q	7	VAL
12	q	16	GLU
12	q	19	VAL
12	q	22	VAL
12	q	28	GLU

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Mol	Chain	Res	Type
12	q	29	THR
12	q	31	LEU
12	q	34	LEU
12	q	36	MET
12	q	91	SER
12	q	92	LEU
12	q	93	TRP
12	q	95	TRP
12	q	98	VAL
12	q	100	ASN
12	q	103	ARG
12	q	107	THR
12	q	109	MET
12	q	110	CYS
12	q	111	VAL
12	q	112	LEU
12	q	115	VAL
12	q	116	LEU
12	q	118	ILE
12	q	120	ARG
12	q	122	LYS
12	q	123	LYS
12	q	124	PHE
12	q	125	MET
12	q	128	ASP
12	q	130	VAL
12	q	131	SER
12	q	132	GLN
12	q	133	ASP
12	q	135	LEU
12	q	138	LYS
12	q	139	GLN
12	q	143	THR
12	q	144	LEU
12	q	145	GLN
12	q	146	LEU
12	q	147	ILE
12	q	149	LYS
12	q	153	LEU
12	q	159	ILE
12	q	161	LEU
12	q	165	GLU

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Mol	Chain	Res	Type
12	q	166	ARG
12	q	168	THR
12	q	169	LYS
12	q	171	VAL
12	q	172	THR
12	q	184	ASN
12	q	186	GLU
12	q	187	LEU
12	q	188	LEU
12	q	195	LYS
12	q	428	LEU
12	q	430	LYS
12	q	431	ILE
12	q	432	ILE
12	q	434	GLN
12	q	438	ILE
12	q	440	LEU
12	q	441	ARG
12	q	442	SER
12	q	443	ARG
12	q	447	THR
12	q	448	ILE
12	q	451	LEU
12	q	518	GLU
12	q	629	LYS
12	q	631	GLU
12	q	633	ARG
12	q	646	LEU
12	q	647	SER
12	q	649	CYS
12	q	651	LEU
13	s	67	LEU
13	s	83	LEU
13	s	84	ILE
13	s	85	THR
14	u	20	CYS
14	u	26	LEU
14	u	27	GLN
14	u	80	GLU
14	u	107	VAL
14	u	109	TYR
14	u	110	ARG

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Mol	Chain	Res	Type
14	u	113	MET
14	u	115	LEU
14	u	117	LYS
14	u	118	ILE
14	u	119	GLN
15	v	15	LEU
15	v	26	ILE
15	v	35	GLU
15	v	42	ILE
15	v	43	GLU
15	v	46	THR
15	v	50	ARG
15	v	52	THR
15	v	53	GLN
15	v	61	MET
15	v	69	VAL
15	v	70	ARG
15	v	81	ASP
15	v	82	LEU
15	v	83	LYS
15	v	84	GLN
15	v	85	PHE
15	v	86	LEU
15	v	92	PRO
15	v	99	ASP
15	v	104	GLN
15	v	110	GLU
15	v	111	GLU
15	v	116	LEU
15	v	118	THR
15	v	119	LEU
15	v	120	ARG
15	v	123	ILE
15	v	125	ILE
15	v	130	LEU
15	v	131	GLU
15	v	132	GLU
15	v	133	GLU
15	v	138	SER
16	z	492	ARG
16	z	528	LEU
16	z	530	VAL

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Mol	Chain	Res	Type
16	z	540	LEU
16	z	544	THR
16	z	547	VAL
16	z	551	ASP
16	z	564	ASN
16	z	567	GLN
16	z	572	ASN
16	z	579	CYS
16	z	582	LEU
16	z	585	HIS
16	z	591	LEU
16	z	599	LEU
17	c	36	LYS
17	c	44	THR
17	c	45	LEU
17	c	72	ARG
17	c	73	LEU
17	c	77	VAL
19	b	57	VAL
19	b	74	LEU
19	b	82	LEU
19	b	92	GLN
19	b	99	ILE
19	b	103	ASP
19	b	122	LEU
19	b	126	CYS
19	b	127	LEU
19	b	132	ASP
21	o	715	LEU
21	o	721	LEU
22	i	70	HIS
22	i	72	ILE
22	i	86	ASP
22	i	87	LEU
22	i	88	ASN
22	i	90	LEU
22	i	95	GLN
22	i	100	LEU
22	i	101	ILE
22	i	102	SER
22	i	115	GLN
22	i	117	GLN

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Mol	Chain	Res	Type
22	i	118	LEU
22	i	119	GLN
22	i	121	LEU
22	i	122	ARG
22	i	128	LYS
22	i	136	LYS
22	i	138	LEU
23	0	6	CYS
23	0	7	PRO
23	0	46	CYS
23	0	68	VAL
23	0	71	GLU
23	0	72	VAL
23	0	175	LEU
23	0	196	LEU
23	0	197	LEU
23	0	208	LEU
23	0	251	LEU
23	0	254	GLU
23	0	260	VAL
23	0	272	LEU
23	0	288	THR
24	8	18	LEU
24	8	22	GLN
24	8	26	VAL
24	8	36	GLN
24	8	38	VAL
24	8	56	ASN
24	8	57	ARG
24	8	58	THR
24	8	66	LEU
24	8	96	THR
24	8	100	VAL
24	8	103	LYS
24	8	107	LEU
24	8	108	VAL
24	8	112	SER
24	8	132	TRP
24	8	134	LEU
24	8	143	LEU
24	8	166	ASN
24	8	173	VAL

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Mol	Chain	Res	Type
24	8	174	VAL
24	8	182	GLU
24	8	189	MET
24	8	205	GLU
24	8	206	LEU
24	8	219	LEU
24	8	231	THR
24	8	260	ILE
24	8	262	SER
24	8	267	ASP
24	8	269	LEU
24	8	287	THR
24	8	292	MET
24	8	307	LEU
25	9	3	HIS
25	9	7	GLN
25	9	8	LYS
25	9	40	VAL
25	9	41	LEU
25	9	56	LEU
25	9	94	ASN
25	9	100	HIS
25	9	102	ARG
25	9	122	SER
25	9	126	VAL
25	9	134	LEU
25	9	136	GLN
25	9	153	GLN
25	9	158	LEU
25	9	165	ARG
25	9	167	PHE
25	9	171	LEU
25	9	174	LEU
25	9	181	LEU
25	9	186	ILE
25	9	188	ARG
25	9	204	TYR
25	9	227	THR
25	9	245	LEU
25	9	266	ARG
25	9	273	LEU
25	9	279	ARG

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Mol	Chain	Res	Type
26	1	190	SER
26	1	191	ASP
26	1	192	ILE
26	1	193	ILE
26	1	211	VAL
26	1	216	THR
26	1	232	ARG
26	1	407	ILE
26	1	415	THR
26	1	430	THR
26	1	440	LEU
26	1	521	LEU
26	1	525	ILE
26	1	535	LYS
27	2	62	TYR
27	2	66	ASP
27	2	69	ARG
27	2	70	THR
27	2	71	MET
27	2	76	LEU
27	2	85	LEU
27	2	90	TYR
27	2	104	ILE
27	2	109	THR
27	2	118	THR
27	2	171	PHE
27	2	174	LEU
27	2	182	ILE
27	2	185	LEU
27	2	194	ILE
27	2	201	LEU
27	2	207	VAL
27	2	234	HIS
27	2	250	ILE
27	2	323	HIS
27	2	328	LEU
27	2	333	GLU
27	2	336	LEU
27	2	345	CYS
27	2	372	ASP
27	2	375	VAL
27	2	379	LEU

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Mol	Chain	Res	Type
28	3	15	VAL
28	3	64	ILE
28	3	124	ILE
28	3	131	THR
28	3	132	LEU
28	3	173	GLN
28	3	187	GLN
28	3	195	VAL
28	3	217	VAL
28	3	255	CYS
28	3	257	CYS
28	3	258	HIS
28	3	261	LEU
28	3	262	ILE
28	3	287	THR
29	4	34	LEU
29	4	47	GLU
29	4	71	VAL
29	4	73	LEU
29	4	75	VAL
29	4	109	ILE
29	4	161	HIS
29	4	162	PHE
29	4	168	SER
29	4	184	LEU
29	4	188	THR
29	4	196	ILE
29	4	205	LEU
29	4	215	PHE
29	4	221	GLN
29	4	264	HIS
29	4	265	LEU
29	4	271	VAL
29	4	284	THR
29	4	290	LEU
29	4	300	THR
29	4	314	ARG
29	4	325	ILE
29	4	334	MET
29	4	373	HIS
29	4	375	VAL
29	4	383	LEU

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Mol	Chain	Res	Type
29	4	386	THR
29	4	403	PHE
29	4	440	LEU
29	4	441	MET
29	4	442	VAL
30	5	16	MET
30	5	24	ASP
30	5	32	LYS
30	5	38	ILE
30	5	39	ASP
30	5	60	LEU
31	6	92	VAL
31	6	93	TYR
31	6	103	ILE
31	6	121	TYR
31	6	123	LEU
31	6	152	ILE
31	6	160	THR
31	6	161	VAL
31	6	185	ILE
31	6	276	MET
31	6	277	ILE
31	6	278	GLU
31	6	289	TYR
31	6	297	PHE
31	6	308	ILE
31	6	332	ARG
31	6	349	VAL
31	6	355	CYS
31	6	369	VAL
31	6	371	VAL
31	6	385	ASP
31	6	389	ILE
31	6	401	ILE
31	6	437	LEU
31	6	449	LYS
31	6	472	ARG
31	6	473	GLU
31	6	488	LEU
31	6	504	LYS
31	6	517	GLU
31	6	526	LYS

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Mol	Chain	Res	Type
31	6	530	ARG
31	6	534	TYR
31	6	547	LEU
31	6	554	ARG
31	6	555	ASN
31	6	558	ILE
31	6	568	LEU
31	6	598	HIS
31	6	601	LYS
31	6	603	ASN
31	6	608	SER
31	6	619	GLU
31	6	621	ASN
31	6	676	ARG
31	6	690	ILE
32	7	8	LEU
32	7	17	ILE
32	7	20	GLU
32	7	24	TYR
32	7	25	MET
32	7	46	THR
32	7	49	THR
32	7	50	VAL
32	7	52	LEU
32	7	77	VAL
32	7	113	LYS
32	7	121	VAL
32	7	143	ARG
32	7	147	GLN
32	7	155	CYS
32	7	199	ILE
32	7	200	LEU
32	7	213	LEU
32	7	220	LEU
32	7	237	HIS
32	7	239	ILE
32	7	251	LEU
32	7	266	LEU
32	7	273	ILE
32	7	349	VAL
32	7	361	LEU
32	7	367	ILE

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Mol	Chain	Res	Type
32	7	373	ARG
32	7	385	THR
32	7	387	GLU
32	7	415	THR
32	7	416	ILE
32	7	417	ILE
32	7	418	ILE
32	7	427	THR
32	7	432	ILE
32	7	444	ILE
32	7	457	THR
32	7	463	PRO
32	7	466	ILE
32	7	481	PHE
32	7	485	LEU
32	7	490	LEU
32	7	504	ILE
32	7	530	VAL
32	7	571	THR
32	7	577	THR
32	7	595	ILE
32	7	650	ASP
32	7	654	PHE
32	7	678	VAL
33	EA	43	VAL
33	EA	59	LEU
33	EA	121	SER
33	EA	124	ARG
33	EA	128	LYS
33	EA	131	VAL
33	EA	133	SER
33	EA	135	THR
33	EA	153	ARG
33	EA	154	CYS
33	EA	157	CYS
33	EA	161	VAL
33	EA	164	ASP
33	EA	187	ILE
33	EA	190	LEU
34	EB	77	VAL
34	EB	97	LEU
34	EB	132	VAL

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Mol	Chain	Res	Type
34	EB	136	LYS
34	EB	139	PHE
34	EB	188	GLN
34	EB	194	ARG
34	EB	204	ASN
34	EB	209	GLN
34	EB	218	LYS
34	EB	223	VAL
34	EB	224	THR
35	DA	348	LEU
35	DA	357	GLU
35	DA	396	LEU
35	DA	403	LEU
35	DA	405	VAL
35	DA	414	ILE
35	DA	470	ILE
35	DA	477	TYR
35	DA	479	ARG
35	DA	481	GLU
35	DA	487	ASP
35	DA	491	MET
35	DA	493	ARG
35	DA	495	LEU
35	DA	496	GLU
35	DA	500	LEU
35	DA	502	LEU
35	DA	509	LEU
35	DA	511	LEU
35	DA	588	ILE
35	DA	620	LEU
35	DA	628	LEU
35	DA	639	LEU
35	DA	661	GLU
35	DA	667	THR
35	DA	675	ASP
35	DA	678	LEU
35	DA	680	LEU
35	DA	721	GLU
35	DA	722	THR
35	DA	723	VAL
35	DA	776	LEU
35	DA	809	VAL

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Mol	Chain	Res	Type
35	DA	828	GLU
35	DA	848	LEU
35	DA	849	CYS
35	DA	863	VAL
35	DA	951	THR
35	DA	966	VAL
35	DA	968	ILE
35	DA	1052	ARG
35	DA	1053	PHE
35	DA	1055	VAL
35	DA	1058	HIS
35	DA	1165	LEU
35	DA	1180	VAL
35	DA	1203	GLU
36	DB	24	ARG
36	DB	49	VAL
36	DB	66	ASN
36	DB	72	ILE
36	DB	77	ILE
36	DB	114	VAL
36	DB	125	GLU
36	DB	130	VAL
36	DB	134	LEU
36	DB	136	LYS
36	DB	138	VAL
36	DB	140	GLU
36	DB	143	VAL
36	DB	149	ASN
36	DB	166	VAL
36	DB	177	VAL
36	DB	201	THR
36	DB	220	LEU
36	DB	221	VAL
36	DB	229	MET
36	DB	230	ARG
36	DB	232	LYS
36	DB	233	THR
36	DB	286	GLU
36	DB	288	PHE
36	DB	309	ILE
36	DB	314	VAL
36	DB	316	VAL

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Mol	Chain	Res	Type
36	DB	323	SER
36	DB	324	ILE
36	DB	335	ILE
36	DB	355	PHE
36	DB	365	SER
36	DB	414	LEU
36	DB	418	PHE
36	DB	430	HIS
36	DB	431	LEU
36	DB	435	ILE
36	DB	449	PHE
36	DB	454	HIS
36	DB	484	SER
36	DB	486	GLN
36	DB	487	LYS
36	DB	492	MET
36	DB	494	SER
36	DB	501	SER
36	DB	510	VAL
36	DB	566	VAL
36	DB	583	GLU
36	DB	625	LEU
36	DB	626	LEU
36	DB	636	VAL
36	DB	637	LEU
36	DB	646	ASP
36	DB	670	GLU
36	DB	671	LYS
36	DB	674	THR
36	DB	678	ARG
36	DB	684	ILE
36	DB	693	ARG
36	DB	695	ARG
36	DB	697	SER
36	DB	699	CYS
36	DB	709	MET
36	DB	712	THR
36	DB	753	MET
36	DB	760	LEU
36	DB	763	VAL
36	DB	764	HIS
36	DB	784	ASN

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Mol	Chain	Res	Type
36	DB	785	ARG
36	DB	786	LYS
36	DB	787	ASN
36	DB	788	LYS
36	DB	791	ASP
36	DB	810	VAL
36	DB	812	VAL
36	DB	821	ASN
36	DB	846	TYR
36	DB	851	THR
36	DB	916	ASN
36	DB	923	ARG
36	DB	944	LEU
36	DB	945	CYS
36	DB	946	ASN
36	DB	981	LEU
37	DD	873	LEU
37	DD	889	HIS
37	DD	894	LEU
37	DD	899	VAL
37	DD	917	ILE
37	DD	919	GLU
37	DD	920	THR
37	DD	950	LEU
37	DD	981	GLN
37	DD	1062	ASP
38	DE	214	TYR
38	DE	229	LEU
38	DE	235	GLU
38	DE	239	LEU
38	DE	268	HIS
38	DE	270	ASP
38	DE	285	LEU
38	DE	307	LEU
38	DE	326	ASN
38	DE	341	ILE
38	DE	359	LEU
38	DE	377	LEU
38	DE	424	GLN
38	DE	474	THR
38	DE	476	VAL
38	DE	499	VAL

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Mol	Chain	Res	Type
38	DE	507	VAL
38	DE	515	LEU
38	DE	521	ASP
38	DE	523	VAL
38	DE	542	HIS
38	DE	551	PHE
38	DE	559	LEU
38	DE	567	VAL
38	DE	570	TRP
38	DE	572	LEU
38	DE	585	ASN
38	DE	593	PHE
38	DE	629	ASP
38	DE	635	PHE
38	DE	636	HIS
38	DE	653	LEU
38	DE	668	HIS
38	DE	675	LEU
38	DE	696	TRP
38	DE	715	CYS
38	DE	717	LEU
38	DE	718	ARG
38	DE	719	PHE
38	DE	747	LEU
38	DE	761	LEU
38	DE	765	SER
38	DE	785	PHE
39	DF	12	THR
39	DF	55	LEU
39	DF	60	MET
39	DF	63	ARG
39	DF	66	LEU
39	DF	83	LEU
39	DF	90	GLU
39	DF	114	LEU
39	DF	122	LEU
39	DF	129	VAL
39	DF	136	LEU
39	DF	252	LEU
39	DF	253	TYR
39	DF	273	GLN
39	DF	274	ASN

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Mol	Chain	Res	Type
39	DF	279	LEU
39	DF	294	THR
39	DF	297	LEU
39	DF	298	GLU
39	DF	301	VAL
39	DF	304	LEU
39	DF	320	ARG
39	DF	340	ILE
39	DF	377	ILE
39	DF	388	ILE
39	DF	393	LEU
39	DF	411	VAL
39	DF	412	LEU
39	DF	427	LEU
40	DG	30	ARG
40	DG	73	VAL
40	DG	84	THR
40	DG	90	ASP
40	DG	127	GLU
40	DG	128	LYS
40	DG	129	LYS
40	DG	131	ILE
40	DG	141	LYS
40	DG	143	VAL
40	DG	144	ARG
40	DG	145	LYS
40	DG	146	ARG
40	DG	149	ARG
40	DG	150	LYS
40	DG	184	ILE
41	DH	47	GLU
41	DH	59	GLU
41	DH	104	VAL
41	DH	119	ILE
41	DH	135	THR
41	DH	142	HIS
41	DH	153	PHE
41	DH	160	ILE
41	DH	169	VAL
41	DH	175	LEU
41	DH	200	THR
42	DI	60	HIS

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Mol	Chain	Res	Type
42	DI	67	ASP
42	DI	106	LEU
42	DI	119	ARG
42	DI	132	LEU
43	DJ	127	THR
43	DJ	145	GLU
43	DJ	198	GLU
44	DL	56	GLN
44	DL	57	VAL
44	DL	59	THR
44	DL	63	LEU
44	DL	64	GLN
44	DL	113	VAL
45	Dc	12	VAL
45	Dc	33	LEU
45	Dc	44	GLN
45	Dc	62	ILE
45	Dc	96	ILE
45	Dc	106	VAL
45	Dc	124	ILE
37	Dd	860	VAL
37	Dd	863	LEU
37	Dd	894	LEU
37	Dd	899	VAL
37	Dd	917	ILE
37	Dd	929	LYS
37	Dd	1079	LEU
37	Dd	1084	LEU
38	De	208	GLN
38	De	229	LEU
38	De	238	GLN
38	De	239	LEU
38	De	243	LEU
38	De	286	THR
38	De	324	LYS
38	De	328	GLN
38	De	334	GLN
38	De	337	LEU
38	De	369	LYS
38	De	424	GLN
38	De	450	ARG
38	De	451	VAL

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Mol	Chain	Res	Type
38	De	453	LEU
38	De	456	ASP
38	De	465	THR
38	De	470	TYR
38	De	476	VAL
38	De	477	ASP
38	De	509	GLN
38	De	515	LEU
38	De	523	VAL
38	De	542	HIS
38	De	551	PHE
38	De	556	ASN
38	De	570	TRP
38	De	585	ASN
38	De	588	VAL
38	De	592	GLN
38	De	593	PHE
38	De	634	ARG
38	De	635	PHE
38	De	651	VAL
38	De	653	LEU
38	De	662	VAL
38	De	663	ARG
38	De	668	HIS
38	De	675	LEU
38	De	677	PHE
38	De	704	VAL
38	De	719	PHE
38	De	720	SER
38	De	724	GLU
38	De	725	ILE
38	De	746	ASP
38	De	747	LEU
38	De	756	THR
38	De	761	LEU
38	De	766	GLN
38	De	778	THR
38	De	780	VAL
38	De	785	PHE
38	De	786	THR
38	De	790	LEU
39	Df	64	GLN

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Mol	Chain	Res	Type
39	Df	92	ILE
39	Df	104	LEU
39	Df	109	GLU
39	Df	125	VAL
39	Df	214	HIS
39	Df	218	VAL
39	Df	272	VAL
39	Df	303	GLU
39	Df	317	LEU
39	Df	320	ARG
39	Df	337	VAL
39	Df	388	ILE
39	Df	391	LEU
39	Df	403	ILE
42	Di	28	ILE
42	Di	31	TYR
42	Di	39	MET
43	Dj	125	ASP
46	Dk	144	THR
46	Dk	146	VAL
46	Dk	178	GLU
44	Dl	59	THR
44	Dl	66	LEU
44	Dl	74	GLU
44	Dl	144	THR
47	Dm	32	PHE
47	Dm	45	ASP
47	Dm	55	ASP
47	Dm	86	ILE
47	Dm	91	ARG
48	DO	31	GLN
48	DO	52	VAL
48	DO	55	ARG
48	DO	56	VAL
48	DO	59	ARG
48	DO	76	LEU
48	DO	84	VAL
48	DO	88	ILE
48	DO	93	VAL
49	DP	172	VAL
49	DP	176	CYS
49	DP	196	ARG

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Mol	Chain	Res	Type
49	DP	197	PHE
49	DP	204	ILE
49	DP	250	PHE
49	DP	278	GLN
49	DP	300	ILE
49	DP	306	VAL
49	DP	323	GLU
50	DQ	39	LEU
50	DQ	311	GLU
50	DQ	317	GLU
50	DQ	320	VAL
50	DQ	334	VAL
50	DQ	341	LYS
51	BA	36	GLU
51	BA	48	VAL
51	BA	51	GLU
51	BA	120	GLU
51	BA	128	ILE
51	BA	135	VAL
51	BA	138	THR
51	BA	145	VAL
51	BA	173	VAL
51	BA	176	THR
51	BA	177	PHE
51	BA	195	PHE
51	BA	245	VAL
51	BA	270	THR
51	BA	280	VAL
51	BA	286	ARG
51	BA	310	VAL
52	FB	48	THR
52	FB	51	ARG
52	FB	94	THR
52	FB	106	LEU
52	FB	124	TYR
52	FB	137	LYS
52	FB	148	VAL
52	FB	160	GLN
52	FB	174	LYS
52	FB	175	ARG
52	FB	177	ARG
52	FB	193	LYS

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Mol	Chain	Res	Type
52	FB	197	TYR
52	FB	206	THR
52	FB	211	VAL
52	FB	225	VAL
52	FB	235	LEU
55	PA	15	LEU
55	PA	22	GLN
55	PA	38	GLU
55	PA	45	GLU
55	PA	47	THR
55	PA	57	LEU
55	PA	64	VAL
55	PA	65	ILE
55	PA	66	GLU
55	PA	80	GLU
55	PA	90	LEU
55	PA	101	VAL
55	PA	111	CYS
55	PA	114	CYS
55	PA	116	LYS
55	PA	119	VAL
55	PA	130	LEU
55	PA	143	HIS
55	PA	147	LEU
55	PA	198	LEU
55	PA	216	LEU
55	PA	221	VAL
55	PA	236	LEU
55	PA	255	VAL
55	PA	265	VAL
55	PA	273	GLN
55	PA	274	ASP
55	PA	302	VAL
55	PA	309	LEU
55	PA	318	VAL
55	PA	327	ARG
55	PA	329	MET
55	PA	336	LEU
55	PA	350	VAL
55	PA	357	LYS
55	PA	373	LEU
55	PA	375	ILE

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Mol	Chain	Res	Type
55	PA	384	ILE
55	PA	408	ARG
55	PA	476	ILE
55	PA	481	THR
55	PA	484	LEU
55	PA	488	VAL
55	PA	503	LEU
55	PA	509	LEU
55	PA	510	GLU
55	PA	517	GLU
55	PA	521	VAL
55	PA	534	VAL
55	PA	539	GLN
55	PA	621	ILE
55	PA	628	VAL
55	PA	647	THR
55	PA	676	ILE
55	PA	681	LEU
55	PA	685	HIS
55	PA	689	ILE
55	PA	693	ILE
55	PA	705	THR
55	PA	736	THR
55	PA	749	ARG
55	PA	762	GLU
55	PA	791	GLN
55	PA	793	VAL
55	PA	873	VAL
55	PA	879	VAL
55	PA	889	LEU
55	PA	906	LEU
55	PA	908	THR
55	PA	909	LEU
55	PA	921	ARG
55	PA	922	PHE
55	PA	924	TYR
55	PA	972	THR
55	PA	978	VAL
55	PA	1021	VAL
55	PA	1034	GLN
55	PA	1057	GLU
55	PA	1078	GLN

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Mol	Chain	Res	Type
55	PA	1121	VAL
55	PA	1129	ASN
55	PA	1136	THR
55	PA	1144	LEU
55	PA	1157	ILE
55	PA	1158	LEU
55	PA	1161	LEU
55	PA	1182	GLN
55	PA	1185	VAL
55	PA	1186	VAL
55	PA	1193	VAL
55	PA	1195	VAL
55	PA	1198	GLU
55	PA	1201	ASP
55	PA	1204	VAL
55	PA	1206	ARG
55	PA	1226	LEU
55	PA	1243	LEU
55	PA	1246	ILE
55	PA	1279	MET
55	PA	1281	ASP
55	PA	1292	MET
55	PA	1293	LEU
55	PA	1298	LEU
55	PA	1310	HIS
55	PA	1314	THR
55	PA	1325	ASP
55	PA	1337	GLU
55	PA	1341	VAL
55	PA	1362	ILE
55	PA	1405	MET
55	PA	1412	MET
55	PA	1429	LYS
55	PA	1435	THR
55	PA	1441	GLU
55	PA	1456	GLU
55	PA	1468	THR
55	PA	1475	LEU
55	PA	1479	LYS
55	PA	1482	TYR
55	PA	1644	SER
55	PA	1646	THR

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Mol	Chain	Res	Type
55	PA	1647	SER
55	PA	1649	SER
55	PA	1650	TYR
55	PA	1653	THR
55	PA	1654	SER
55	PA	1656	SER
55	PA	1657	TYR
55	PA	1658	SER
55	PA	1661	SER
55	PA	1663	SER
55	PA	1664	TYR
55	PA	1666	PRO
55	PA	1667	THR
55	PA	1678	TYR
55	PA	1791	SER
55	PA	1794	SER
55	PA	1795	PRO
55	PA	1796	SER
55	PA	1798	SER
56	PB	29	VAL
56	PB	42	GLN
56	PB	59	VAL
56	PB	65	ILE
56	PB	67	LEU
56	PB	85	LEU
56	PB	91	ILE
56	PB	93	LEU
56	PB	132	VAL
56	PB	133	ILE
56	PB	142	THR
56	PB	156	LEU
56	PB	193	VAL
56	PB	194	LEU
56	PB	204	THR
56	PB	206	TYR
56	PB	225	LEU
56	PB	235	ILE
56	PB	254	GLN
56	PB	257	VAL
56	PB	259	THR
56	PB	285	LEU
56	PB	289	ILE

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Mol	Chain	Res	Type
56	PB	310	VAL
56	PB	313	GLU
56	PB	330	VAL
56	PB	332	LYS
56	PB	348	LEU
56	PB	353	VAL
56	PB	357	CYS
56	PB	359	THR
56	PB	361	LYS
56	PB	388	TYR
56	PB	403	LEU
56	PB	414	GLU
56	PB	420	GLN
56	PB	423	ILE
56	PB	431	LEU
56	PB	433	LEU
56	PB	453	TRP
56	PB	458	LYS
56	PB	461	GLN
56	PB	463	ARG
56	PB	466	VAL
56	PB	469	VAL
56	PB	509	VAL
56	PB	526	LEU
56	PB	532	ILE
56	PB	541	ILE
56	PB	542	LEU
56	PB	556	ILE
56	PB	597	ILE
56	PB	601	VAL
56	PB	604	ILE
56	PB	607	ILE
56	PB	626	LEU
56	PB	629	GLU
56	PB	631	GLN
56	PB	634	LEU
56	PB	645	GLU
56	PB	648	TYR
56	PB	662	VAL
56	PB	671	GLU
56	PB	673	VAL
56	PB	675	LEU

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Mol	Chain	Res	Type
56	PB	678	THR
56	PB	731	GLN
56	PB	735	VAL
56	PB	737	ILE
56	PB	752	TYR
56	PB	767	LEU
56	PB	782	ILE
56	PB	786	THR
56	PB	806	PHE
56	PB	809	VAL
56	PB	815	LYS
56	PB	823	PHE
56	PB	860	VAL
56	PB	865	VAL
56	PB	889	LYS
56	PB	890	ARG
56	PB	896	LEU
56	PB	901	THR
56	PB	927	ARG
56	PB	1006	VAL
56	PB	1022	LEU
56	PB	1028	LEU
56	PB	1043	ILE
56	PB	1057	ASP
56	PB	1062	ARG
56	PB	1070	LEU
56	PB	1073	GLN
56	PB	1080	ARG
56	PB	1116	VAL
56	PB	1120	ASN
56	PB	1121	LEU
56	PB	1124	ILE
56	PB	1125	MET
56	PB	1130	THR
56	PB	1136	GLU
56	PB	1137	CYS
56	PB	1138	ARG
56	PB	1140	CYS
56	PB	1141	ARG
56	PB	1143	LYS
56	PB	1158	LEU
57	PC	15	THR

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Mol	Chain	Res	Type
57	PC	44	ILE
57	PC	52	ILE
57	PC	76	ASP
57	PC	79	VAL
57	PC	82	LEU
57	PC	88	CYS
57	PC	103	LEU
57	PC	112	THR
57	PC	120	LEU
57	PC	128	ILE
57	PC	177	ASN
57	PC	179	THR
57	PC	193	ARG
57	PC	213	GLU
57	PC	239	LEU
58	PD	15	GLU
58	PD	20	LEU
58	PD	32	LEU
58	PD	39	MET
58	PD	41	LEU
58	PD	42	GLU
58	PD	45	LYS
58	PD	62	MET
58	PD	67	TYR
58	PD	95	PHE
58	PD	103	LEU
58	PD	107	THR
58	PD	110	GLU
58	PD	118	LEU
58	PD	131	LEU
58	PD	135	GLN
58	PD	137	LYS
59	PE	20	LEU
59	PE	29	THR
59	PE	32	GLU
59	PE	38	GLU
59	PE	57	ASP
59	PE	82	VAL
59	PE	84	ILE
59	PE	103	LEU
59	PE	104	ILE
59	PE	108	GLN

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Mol	Chain	Res	Type
59	PE	139	ILE
59	PE	159	LEU
59	PE	165	LEU
59	PE	179	VAL
59	PE	191	VAL
59	PE	193	ILE
59	PE	209	VAL
60	PF	58	THR
60	PF	71	LEU
60	PF	81	VAL
60	PF	83	LEU
60	PF	86	GLU
60	PF	87	THR
60	PF	91	LEU
60	PF	95	LYS
60	PF	116	GLU
61	PG	8	GLU
61	PG	11	ILE
61	PG	13	LEU
61	PG	30	LEU
61	PG	35	GLU
61	PG	37	THR
61	PG	39	THR
61	PG	42	TYR
61	PG	45	VAL
61	PG	48	VAL
61	PG	50	THR
61	PG	76	VAL
61	PG	88	VAL
61	PG	89	VAL
61	PG	97	LEU
61	PG	101	ILE
61	PG	117	MET
61	PG	145	LEU
61	PG	147	ILE
61	PG	148	VAL
61	PG	150	THR
61	PG	152	VAL
62	PH	4	ILE
62	PH	52	LEU
62	PH	63	THR
62	PH	64	LEU

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Mol	Chain	Res	Type
62	PH	66	GLU
62	PH	69	THR
62	PH	72	ASP
62	PH	76	ASN
62	PH	110	THR
62	PH	132	LEU
62	PH	141	VAL
63	PI	12	VAL
63	PI	29	ASP
63	PI	31	GLU
63	PI	53	ILE
63	PI	55	VAL
63	PI	58	ILE
63	PI	62	VAL
63	PI	69	ILE
63	PI	81	THR
63	PI	95	VAL
64	PJ	13	ILE
64	PJ	54	ASP
65	PK	12	LEU
65	PK	27	VAL
65	PK	61	TYR
65	PK	69	HIS
65	PK	94	LEU
66	PL	32	ASP
66	PL	35	ARG
66	PL	53	VAL
67	FA	37	VAL
67	FA	122	THR
68	w	1	MET
68	w	2	GLU
68	w	5	LEU
68	w	7	SER
68	w	10	GLU
68	w	11	GLU
68	w	12	VAL
68	w	17	VAL
68	w	18	ILE
68	w	36	LYS
68	w	37	LEU
68	w	41	LEU
68	w	51	LEU

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Mol	Chain	Res	Type
68	w	130	ASP
68	w	171	LEU
68	w	173	ARG
68	w	205	VAL
68	w	723	THR
68	w	726	ASN
68	w	1130	VAL
68	w	1134	GLN
69	x	4	VAL
69	x	11	LEU
69	x	52	ILE
69	x	54	PRO
69	x	107	ARG
69	x	118	ILE
69	x	239	THR
69	x	359	CYS
69	x	477	TYR
69	x	479	SER
69	x	565	SER
69	x	567	MET
69	x	596	VAL
69	x	686	LYS
69	x	802	MET
69	x	897	LEU
69	x	986	ILE
69	x	989	LEU
70	p	162	VAL
70	p	170	LEU
70	p	228	VAL
70	p	252	LYS
70	p	289	ASP
70	p	401	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (486) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	56	GLN
1	a	87	GLN
1	a	131	ASN
1	a	146	ASN
1	a	162	ASN
1	a	167	ASN

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Mol	Chain	Res	Type
1	a	221	ASN
1	a	254	ASN
1	a	333	GLN
1	a	359	HIS
1	a	399	GLN
1	a	439	GLN
1	a	459	ASN
2	m	26	GLN
2	m	80	GLN
2	m	100	GLN
2	m	106	GLN
2	m	116	GLN
2	m	124	GLN
3	d	90	HIS
3	d	113	GLN
3	d	119	GLN
3	d	127	GLN
3	d	189	GLN
3	d	191	ASN
4	f	38	ASN
4	f	47	ASN
4	f	61	ASN
4	f	62	GLN
4	f	72	HIS
4	f	84	GLN
4	f	87	GLN
4	f	107	GLN
4	f	140	HIS
5	g	25	ASN
5	g	50	GLN
5	g	82	ASN
5	g	88	ASN
5	g	118	HIS
5	g	124	ASN
5	g	165	GLN
5	g	166	ASN
6	h	18	GLN
6	h	65	HIS
6	h	102	HIS
6	h	137	GLN
6	h	144	ASN
8	t	19	GLN

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Mol	Chain	Res	Type
8	t	103	GLN
8	t	180	HIS
8	t	192	GLN
8	t	204	GLN
9	j	11	HIS
9	j	30	GLN
9	j	38	ASN
9	j	92	ASN
10	k	41	ASN
10	k	66	GLN
10	k	77	GLN
10	k	91	GLN
11	n	189	GLN
11	n	201	HIS
11	n	270	GLN
11	n	275	HIS
11	n	304	GLN
11	n	311	GLN
11	n	330	HIS
11	n	410	HIS
11	n	411	GLN
11	n	507	GLN
11	n	590	GLN
11	n	643	HIS
11	n	668	HIS
11	n	669	GLN
11	n	672	GLN
11	n	698	GLN
11	n	716	ASN
11	n	825	ASN
11	n	841	ASN
11	n	848	HIS
11	n	880	ASN
11	n	883	ASN
11	n	909	GLN
12	q	39	ASN
12	q	139	GLN
12	q	142	GLN
12	q	193	HIS
12	q	262	GLN
12	q	290	HIS
12	q	292	GLN

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Mol	Chain	Res	Type
12	q	317	GLN
12	q	367	HIS
12	q	374	ASN
12	q	434	GLN
12	q	437	HIS
12	q	461	GLN
12	q	463	HIS
12	q	492	GLN
12	q	496	ASN
12	q	506	HIS
12	q	532	HIS
12	q	533	GLN
12	q	539	GLN
12	q	547	GLN
12	q	565	ASN
12	q	595	GLN
12	q	611	GLN
12	q	626	GLN
12	q	634	ASN
14	u	7	GLN
14	u	18	GLN
14	u	21	ASN
14	u	97	ASN
15	v	16	GLN
15	v	32	ASN
15	v	53	GLN
15	v	56	GLN
15	v	58	ASN
15	v	89	ASN
16	z	483	ASN
16	z	527	GLN
16	z	549	GLN
16	z	567	GLN
16	z	585	HIS
16	z	592	ASN
17	c	10	ASN
17	c	41	ASN
17	c	237	GLN
17	c	278	GLN
17	c	282	GLN
17	c	306	HIS
17	c	311	GLN

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Mol	Chain	Res	Type
18	e	97	GLN
18	e	132	HIS
18	e	140	GLN
19	b	66	GLN
19	b	129	GLN
19	b	136	HIS
20	l	72	GLN
20	l	102	ASN
21	o	692	ASN
21	o	701	ASN
21	o	753	HIS
22	i	85	GLN
22	i	95	GLN
22	i	117	GLN
23	0	112	ASN
23	0	144	GLN
23	0	249	GLN
23	0	281	GLN
23	0	294	HIS
23	0	298	GLN
24	8	33	ASN
24	8	56	ASN
24	8	86	ASN
24	8	113	HIS
24	8	130	GLN
24	8	166	ASN
25	9	3	HIS
25	9	7	GLN
25	9	27	ASN
25	9	37	ASN
25	9	93	ASN
25	9	100	HIS
25	9	136	GLN
25	9	152	GLN
25	9	155	ASN
25	9	183	ASN
25	9	211	GLN
25	9	281	HIS
26	1	231	HIS
26	1	384	HIS
27	2	52	GLN
27	2	147	ASN

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Mol	Chain	Res	Type
27	2	257	HIS
27	2	324	HIS
27	2	380	HIS
28	3	18	ASN
28	3	31	GLN
28	3	185	GLN
28	3	205	GLN
29	4	458	GLN
30	5	36	GLN
31	6	83	HIS
31	6	377	GLN
31	6	433	GLN
31	6	444	HIS
31	6	497	GLN
31	6	555	ASN
31	6	586	GLN
31	6	603	ASN
31	6	710	GLN
32	7	60	GLN
32	7	154	HIS
32	7	262	ASN
32	7	328	HIS
32	7	452	GLN
32	7	474	HIS
32	7	555	GLN
32	7	562	GLN
32	7	700	HIS
32	7	733	GLN
33	EA	65	ASN
33	EA	143	GLN
33	EA	158	HIS
34	EB	90	GLN
34	EB	158	HIS
34	EB	160	GLN
34	EB	193	ASN
34	EB	204	ASN
34	EB	209	GLN
35	DA	401	ASN
35	DA	472	ASN
35	DA	569	ASN
35	DA	606	HIS
35	DA	693	GLN

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Mol	Chain	Res	Type
35	DA	837	HIS
35	DA	860	ASN
35	DA	896	GLN
35	DA	1073	GLN
36	DB	30	HIS
36	DB	66	ASN
36	DB	100	GLN
36	DB	123	ASN
36	DB	183	GLN
36	DB	235	HIS
36	DB	279	HIS
36	DB	285	HIS
36	DB	353	GLN
36	DB	430	HIS
36	DB	432	HIS
36	DB	450	GLN
36	DB	486	GLN
36	DB	491	HIS
36	DB	509	ASN
36	DB	558	GLN
36	DB	577	HIS
36	DB	584	ASN
36	DB	599	ASN
36	DB	608	ASN
36	DB	644	GLN
36	DB	784	ASN
36	DB	792	ASN
36	DB	823	ASN
36	DB	912	ASN
36	DB	916	ASN
36	DB	924	HIS
36	DB	963	HIS
37	DD	908	GLN
37	DD	912	ASN
37	DD	925	ASN
37	DD	1005	ASN
37	DD	1059	ASN
38	DE	246	HIS
38	DE	294	ASN
38	DE	320	HIS
38	DE	326	ASN
38	DE	328	GLN

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Mol	Chain	Res	Type
38	DE	334	GLN
38	DE	336	HIS
38	DE	351	GLN
38	DE	424	GLN
38	DE	468	ASN
38	DE	542	HIS
38	DE	585	ASN
38	DE	668	HIS
38	DE	766	GLN
39	DF	89	GLN
39	DF	119	ASN
39	DF	221	GLN
39	DF	244	GLN
39	DF	302	HIS
39	DF	316	GLN
40	DG	53	HIS
40	DG	134	HIS
41	DH	145	HIS
41	DH	157	HIS
41	DH	173	GLN
42	DI	38	GLN
42	DI	60	HIS
42	DI	76	GLN
42	DI	98	GLN
42	DI	100	ASN
42	DI	126	ASN
43	DJ	160	GLN
44	DL	105	HIS
44	DL	117	GLN
45	Dc	16	GLN
45	Dc	27	GLN
45	Dc	44	GLN
45	Dc	50	HIS
45	Dc	94	HIS
37	Dd	912	ASN
37	Dd	949	GLN
37	Dd	1069	ASN
37	Dd	1075	HIS
38	De	294	ASN
38	De	334	GLN
38	De	336	HIS
38	De	368	ASN

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Mol	Chain	Res	Type
38	De	424	GLN
38	De	468	ASN
38	De	542	HIS
38	De	556	ASN
38	De	573	GLN
38	De	585	ASN
38	De	626	HIS
38	De	638	ASN
38	De	658	ASN
38	De	668	HIS
38	De	733	ASN
38	De	758	HIS
38	De	782	HIS
39	Df	30	GLN
39	Df	87	HIS
39	Df	119	ASN
39	Df	142	GLN
39	Df	220	GLN
39	Df	254	GLN
39	Df	292	ASN
39	Df	325	ASN
42	Di	81	GLN
43	Dj	160	GLN
43	Dj	173	HIS
46	Dk	186	HIS
46	Dk	205	HIS
44	Dl	64	GLN
44	Dl	73	ASN
44	Dl	105	HIS
44	Dl	148	HIS
48	DO	16	GLN
48	DO	31	GLN
48	DO	54	ASN
48	DO	77	ASN
49	DP	173	ASN
49	DP	193	ASN
49	DP	277	HIS
49	DP	278	GLN
50	DQ	60	HIS
51	BA	140	ASN
52	FB	29	GLN
52	FB	86	GLN

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Mol	Chain	Res	Type
52	FB	91	GLN
52	FB	112	GLN
52	FB	158	ASN
52	FB	181	GLN
52	FB	182	HIS
55	PA	22	GLN
55	PA	96	HIS
55	PA	123	ASN
55	PA	136	GLN
55	PA	181	HIS
55	PA	296	ASN
55	PA	341	GLN
55	PA	410	ASN
55	PA	459	ASN
55	PA	461	GLN
55	PA	465	HIS
55	PA	485	ASN
55	PA	507	GLN
55	PA	529	GLN
55	PA	539	GLN
55	PA	562	ASN
55	PA	590	GLN
55	PA	721	HIS
55	PA	731	ASN
55	PA	739	ASN
55	PA	780	ASN
55	PA	791	GLN
55	PA	804	HIS
55	PA	861	GLN
55	PA	904	GLN
55	PA	1044	HIS
55	PA	1101	GLN
55	PA	1163	HIS
55	PA	1172	ASN
55	PA	1299	GLN
55	PA	1310	HIS
55	PA	1410	HIS
55	PA	1420	ASN
55	PA	1445	HIS
56	PB	23	GLN
56	PB	43	GLN
56	PB	139	GLN

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Mol	Chain	Res	Type
56	PB	197	GLN
56	PB	350	HIS
56	PB	460	HIS
56	PB	518	HIS
56	PB	537	GLN
56	PB	582	GLN
56	PB	639	HIS
56	PB	642	GLN
56	PB	650	ASN
56	PB	683	GLN
56	PB	717	ASN
56	PB	725	GLN
56	PB	731	GLN
56	PB	741	HIS
56	PB	797	ASN
56	PB	817	GLN
56	PB	930	GLN
56	PB	941	GLN
56	PB	986	GLN
56	PB	1009	GLN
56	PB	1021	HIS
56	PB	1053	HIS
56	PB	1094	GLN
56	PB	1115	GLN
57	PC	6	GLN
57	PC	83	GLN
57	PC	157	GLN
57	PC	217	GLN
57	PC	262	GLN
57	PC	268	GLN
58	PD	38	HIS
58	PD	47	GLN
58	PD	93	HIS
58	PD	135	GLN
59	PE	64	HIS
59	PE	71	GLN
59	PE	108	GLN
59	PE	210	GLN
61	PG	4	HIS
61	PG	21	ASN
61	PG	53	ASN
61	PG	139	GLN

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Mol	Chain	Res	Type
62	PH	130	ASN
63	PI	60	HIS
63	PI	84	HIS
63	PI	118	HIS
64	PJ	26	GLN
65	PK	29	ASN
65	PK	89	ASN
66	PL	23	HIS
67	FA	27	ASN
67	FA	53	ASN
67	FA	121	ASN
67	FA	129	GLN
67	FA	141	HIS
68	w	113	GLN
68	w	239	ASN
68	w	295	GLN
68	w	357	HIS
68	w	358	GLN
68	w	378	GLN
68	w	421	HIS
68	w	433	ASN
68	w	438	ASN
68	w	513	ASN
68	w	596	HIS
68	w	616	GLN
68	w	618	HIS
68	w	638	GLN
68	w	726	ASN
68	w	759	ASN
68	w	783	GLN
68	w	851	ASN
68	w	874	HIS
68	w	923	ASN
68	w	972	HIS
68	w	1037	ASN
68	w	1040	GLN
68	w	1059	ASN
68	w	1124	ASN
68	w	1134	GLN
68	w	1320	ASN
69	x	49	GLN
69	x	111	HIS

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Mol	Chain	Res	Type
69	x	214	GLN
69	x	217	GLN
69	x	335	ASN
69	x	361	ASN
69	x	380	ASN
69	x	402	ASN
69	x	404	GLN
69	x	472	ASN
69	x	502	HIS
69	x	544	HIS
69	x	679	GLN
69	x	737	HIS
70	p	63	HIS
70	p	225	ASN
70	p	272	ASN
70	p	400	GLN
70	p	430	HIS
70	p	435	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 17 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
72	SF4	7	1000	32	0,12,12	-	-	-		

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
72	SF4	7	1000	32	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

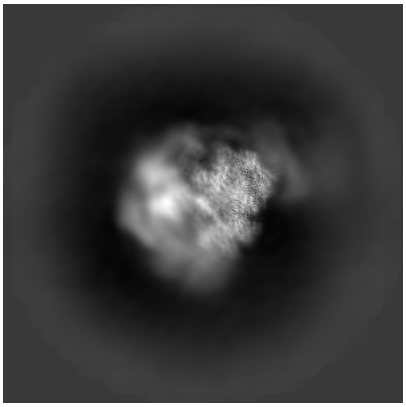
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31207. These allow visual inspection of the internal detail of the map and identification of artifacts.

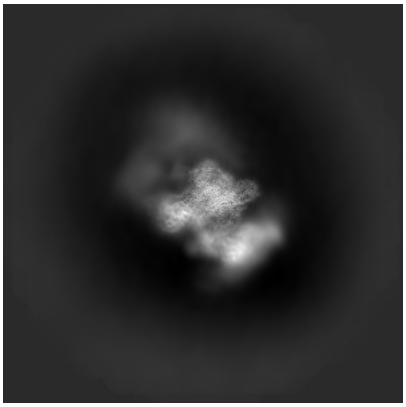
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

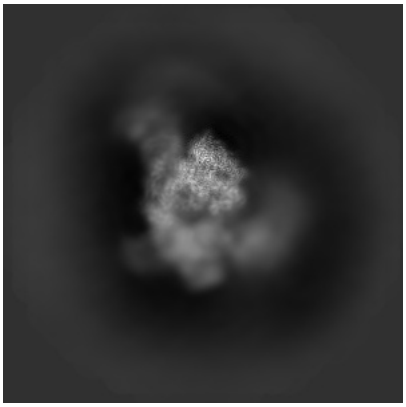
6.1.1 Primary map



X



Y

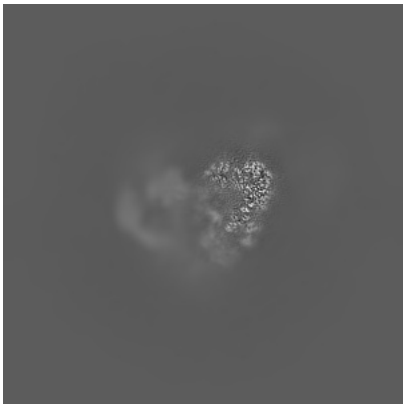


Z

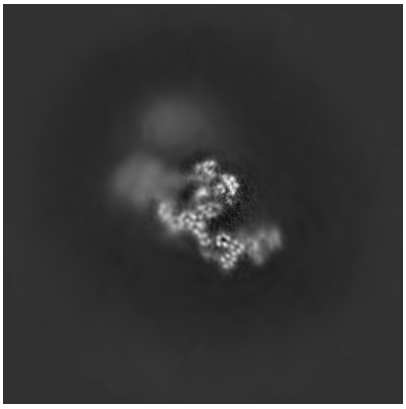
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 240



Y Index: 240

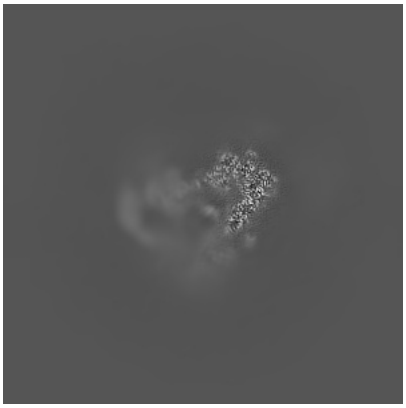


Z Index: 240

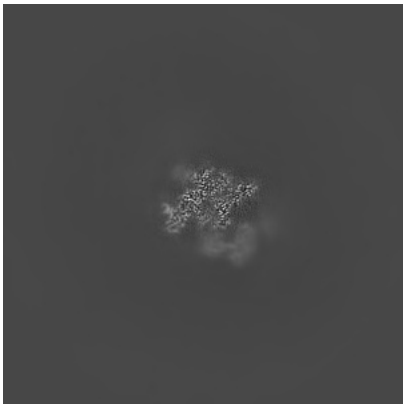
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

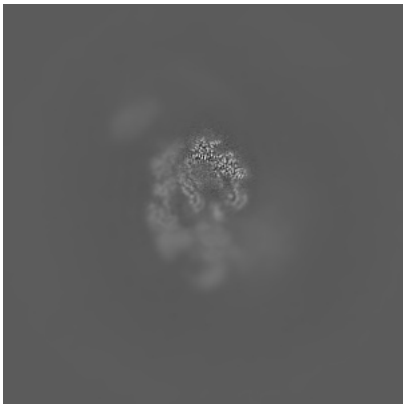
6.3.1 Primary map



X Index: 246



Y Index: 287

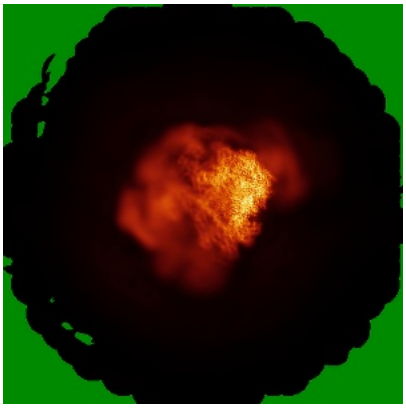


Z Index: 247

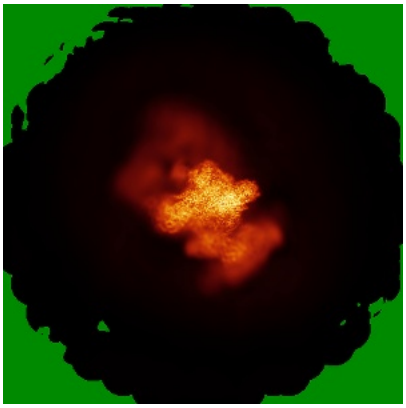
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

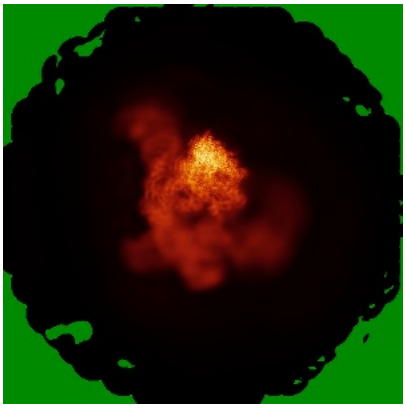
6.4.1 Primary map



X



Y

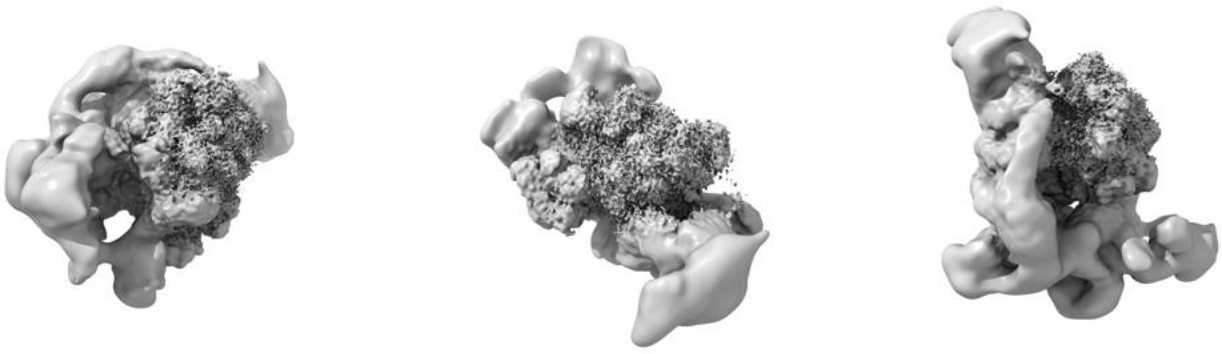


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

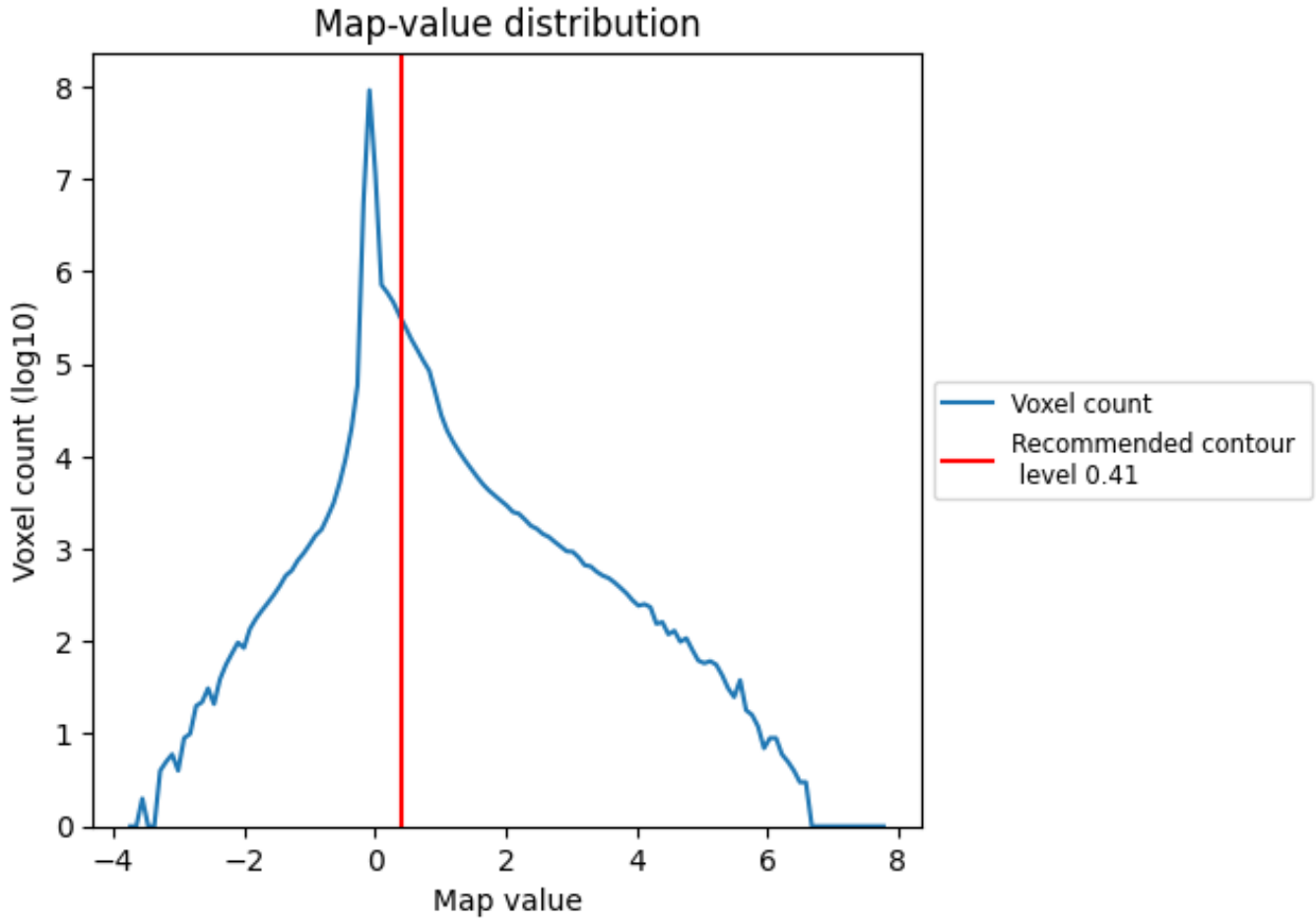
6.6 Mask visualisation (i)

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

7 Map analysis

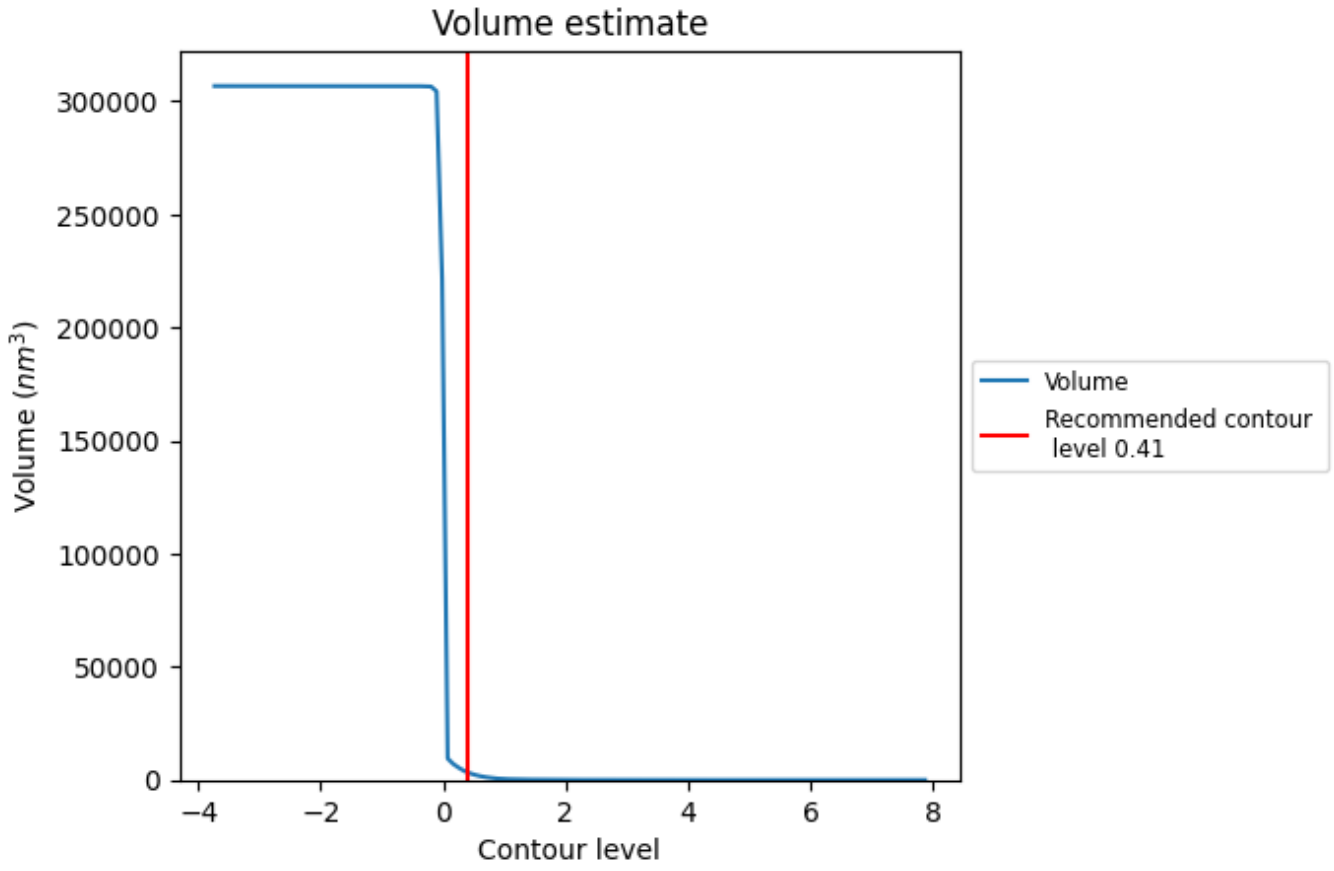
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

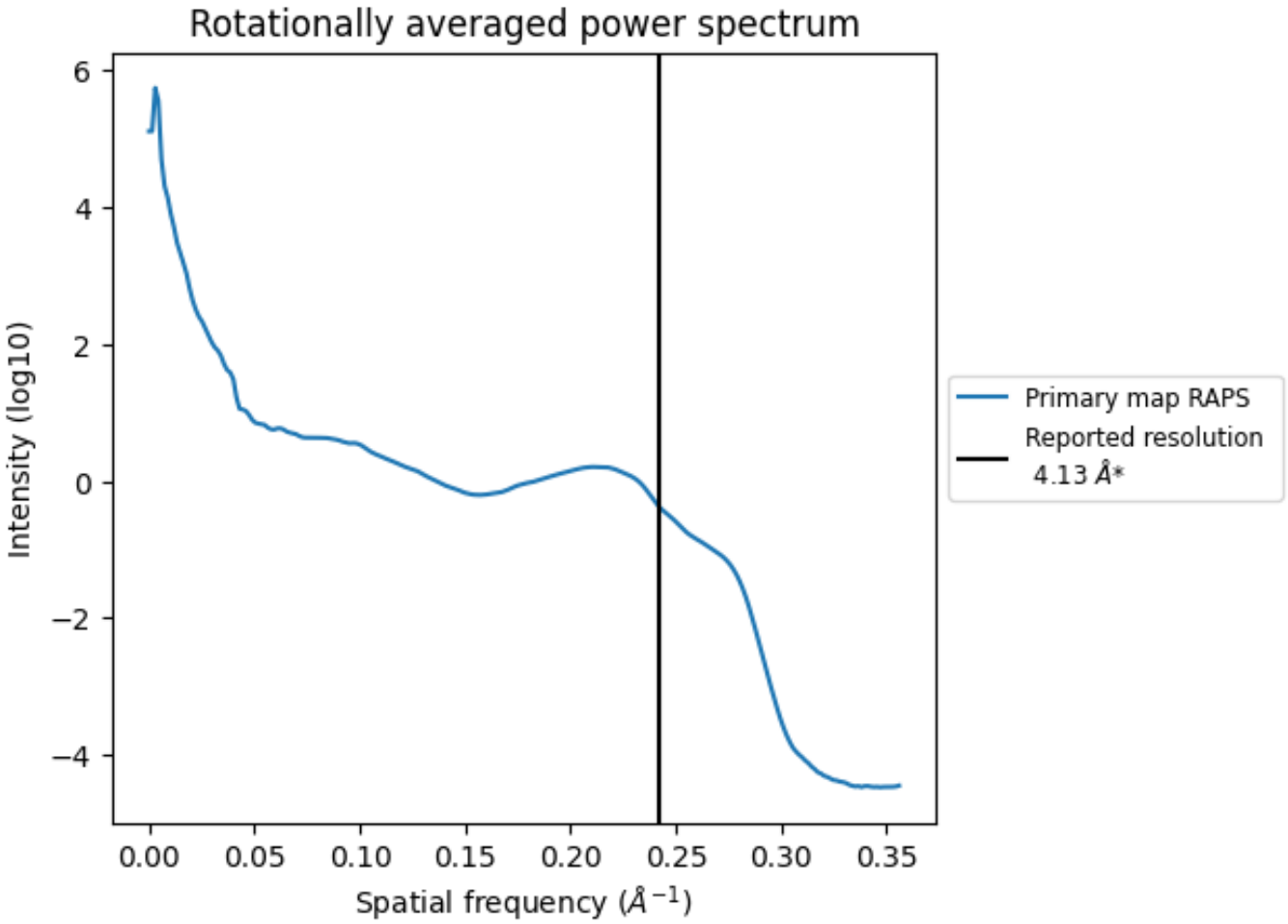
7.2 Volume estimate



The volume at the recommended contour level is 3240 nm^3; this corresponds to an approximate mass of 2927 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 (i)



*Reported resolution corresponds to spatial frequency of 0.242 Å^{-1}

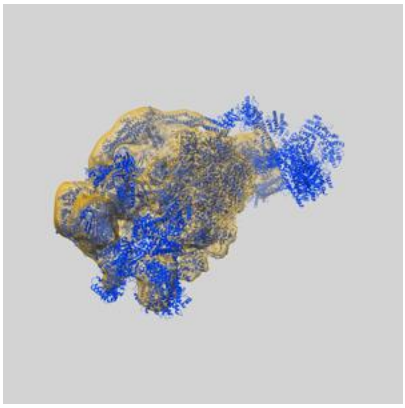
8 Fourier-Shell correlation

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

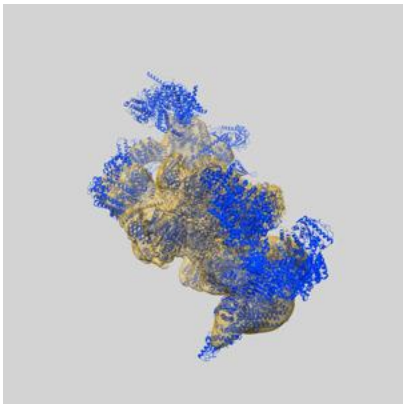
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31207 and PDB model 7ENC. Per-residue inclusion information can be found in section 3 on page 18.

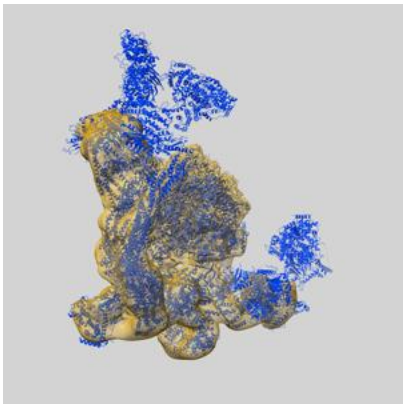
9.1 Map-model overlay



X



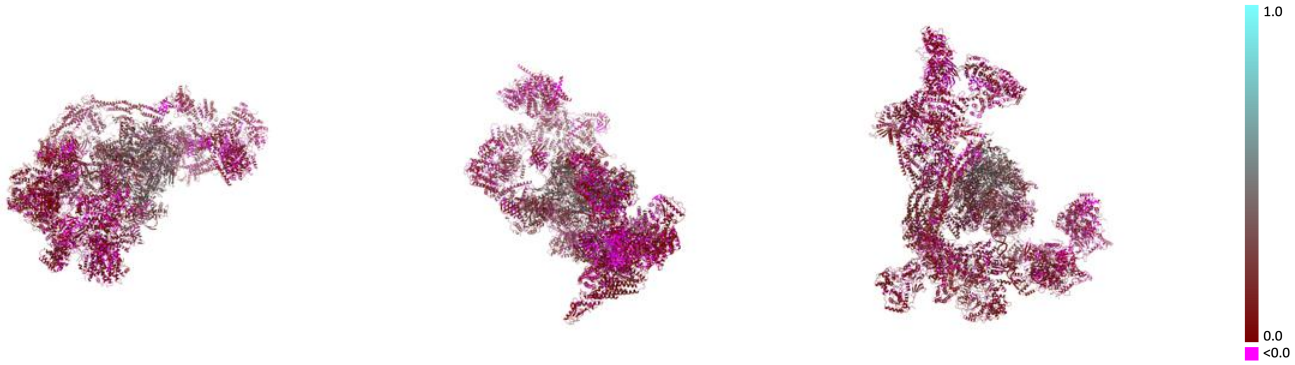
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.41 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.

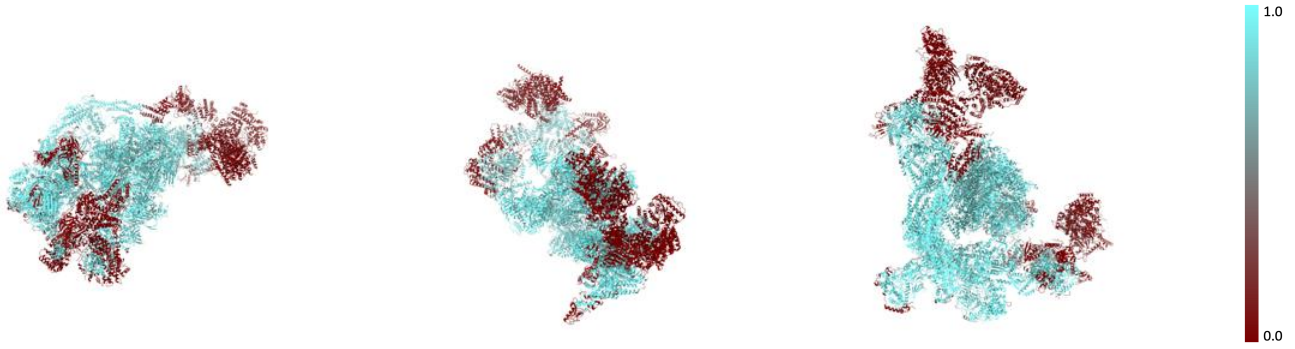
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

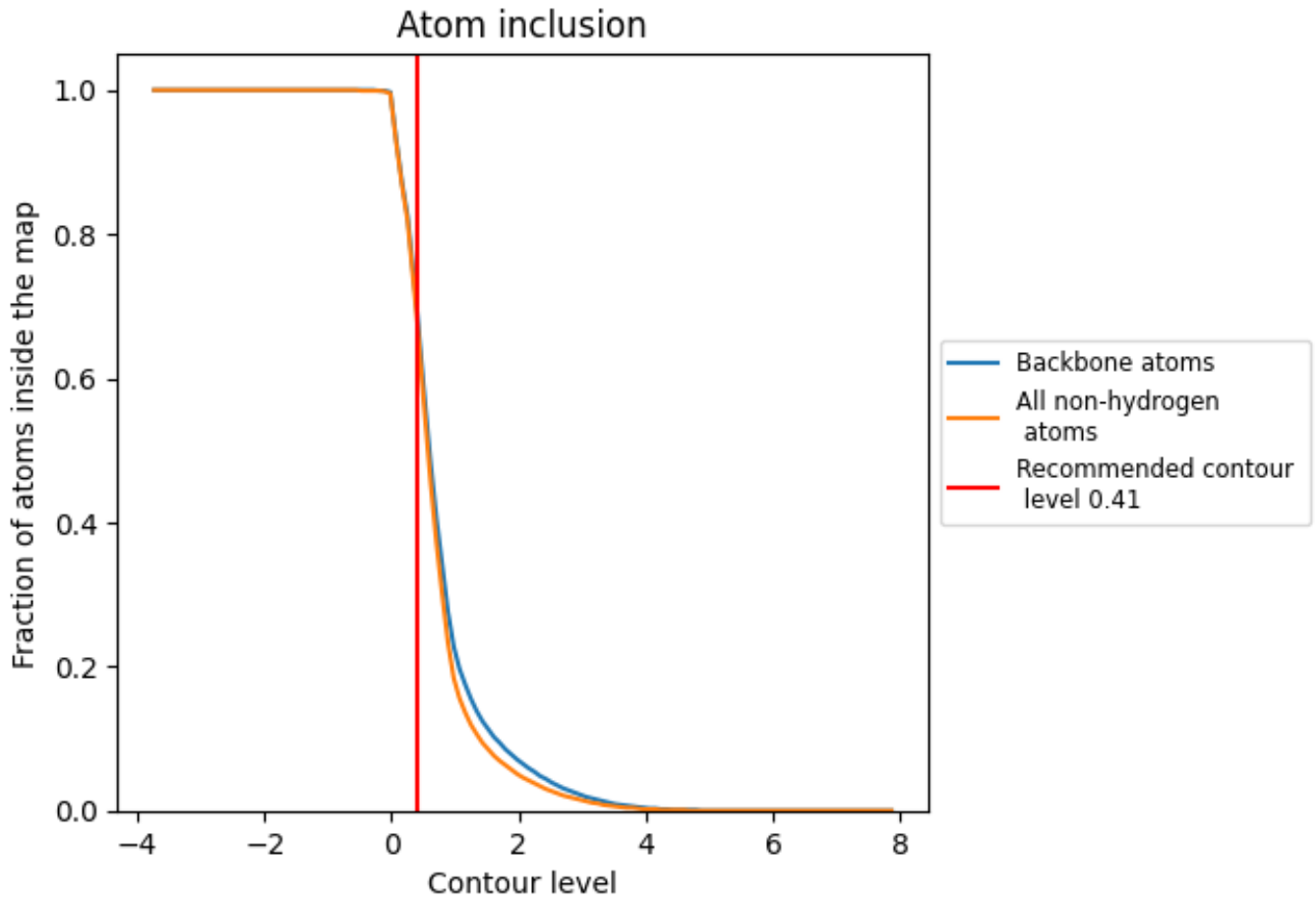
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.41).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 67% 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 (0.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6730	0.1030
0	0.8870	0.0830
1	0.9000	0.0380
2	0.9830	0.0690
3	0.9750	0.0630
4	0.9620	0.0740
5	0.9790	0.0560
6	0.9800	0.0700
7	0.9840	0.0970
8	0.9410	0.0760
9	0.7290	0.0650
BA	0.9130	0.2020
DA	0.2540	0.0410
DB	0.8240	0.0560
DD	0.6080	0.0580
DE	0.6890	0.0520
DF	0.5060	0.0580
DG	0.0200	0.0240
DH	0.6950	0.0550
DI	0.5240	0.0260
DJ	0.5820	0.0500
DL	0.0280	0.0310
DO	0.9350	0.1010
DP	0.9670	0.1650
DQ	0.8710	0.0990
Dc	0.0000	0.0330
Dd	0.0000	0.0140
De	0.0000	0.0180
Df	0.2940	0.0470
Di	0.0000	0.0440
Dj	0.0000	0.0320
Dk	0.0000	-0.0020
Dl	0.0000	0.0200
Dm	0.0000	0.0190
EA	0.9800	0.1020



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Chain	Atom inclusion	Q-score
EB	0.9870	0.1230
FA	0.9480	0.0680
FB	0.9520	0.1150
PA	0.9230	0.2390
PB	0.9390	0.3370
PC	0.9300	0.3250
PD	0.9370	0.1590
PE	0.9560	0.2170
PF	0.8880	0.2560
PG	0.9480	0.1770
PH	0.9240	0.3110
PI	0.9260	0.1450
PJ	0.9090	0.3050
PK	0.8800	0.2840
PL	0.9180	0.2750
X	0.9990	0.1760
Y	0.9950	0.2000
a	0.0030	0.0340
b	0.5510	0.0380
c	0.8450	0.0550
d	0.7480	0.0840
e	0.9600	0.0930
f	0.9870	0.1340
g	0.9810	0.1050
h	0.9870	0.1610
i	0.5010	0.0850
j	0.9190	0.0640
k	0.9560	0.1540
l	0.9170	0.0710
m	0.9990	0.0910
n	0.8740	0.0690
o	0.6690	0.0440
p	0.0000	-0.0260
q	0.9870	0.0940
r	0.9750	0.0870
s	0.9040	0.0620
t	0.9280	0.0540
u	0.9920	0.0930
v	0.9890	0.1300
w	0.0110	0.0280
x	0.0360	0.0360
z	0.8980	0.0450