Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:51 AM UTC

PDB ID	:	7ENA / pdb_00007ena
EMDB ID	:	EMD-31204
Title	:	TFIID-based PIC-Mediator holo-complex in pre-assembled state (pre-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	:	4.07 Å(reported)

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

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

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

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

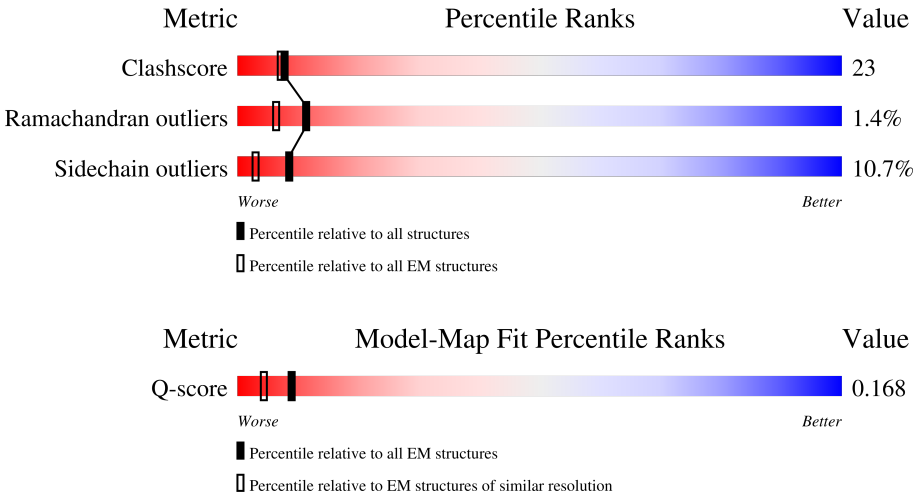
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.07 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	6427 (3.58 - 4.57)

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	0	309	17% 58% 28% 11% ••
2	8	346	8% 34% 34% 17% • 14%
3	9	323	33% 41% 30% 16% • 11%
4	DO	109	• 56% 21% 11% • 11%

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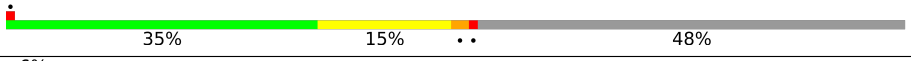
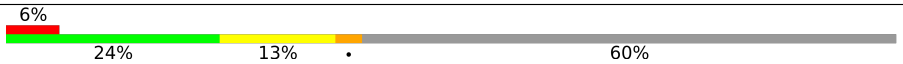
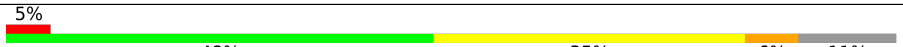
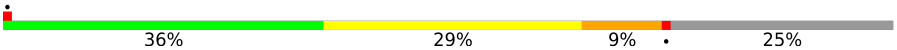
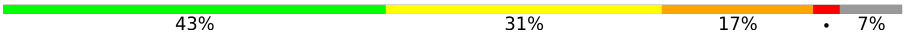
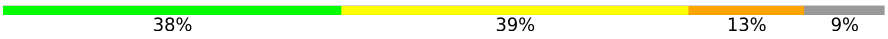
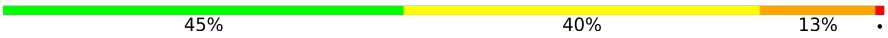
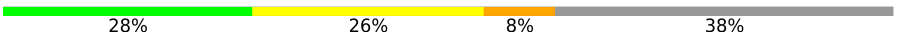
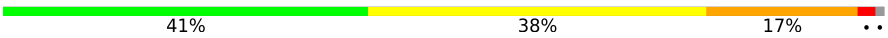
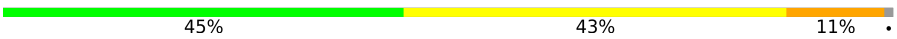
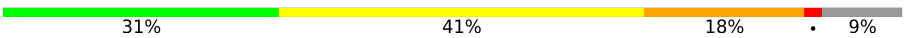
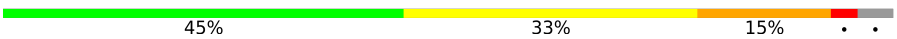
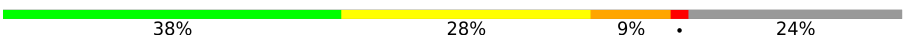
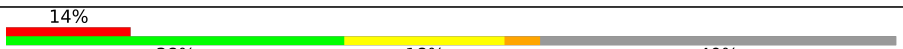
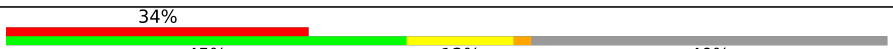
Mol	Chain	Length	Quality of chain
5	DP	339	
6	DQ	307	
7	BA	316	
8	FA	517	
9	FB	249	
10	PA	1970	
11	PB	1174	
12	PC	275	
13	PD	142	
14	PE	210	
15	PF	127	
16	PG	172	
17	PH	150	
18	PI	125	
19	PJ	67	
20	PK	117	
21	PL	58	
22	DA	1872	
23	DB	1199	
24	DD	1085	
24	Dd	1085	
25	DE	800	
25	De	800	
26	DF	677	
26	Df	677	

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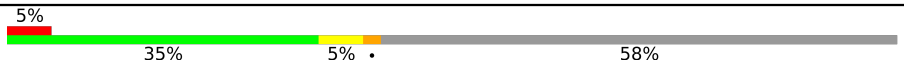
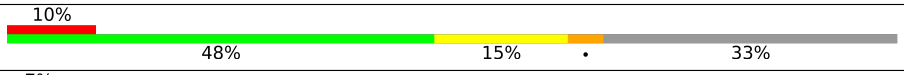
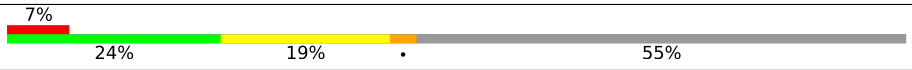
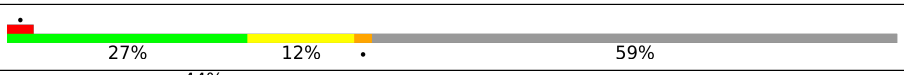
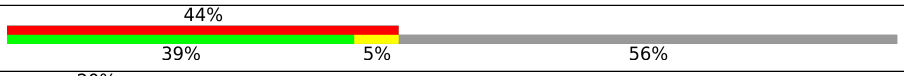
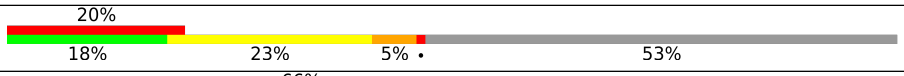
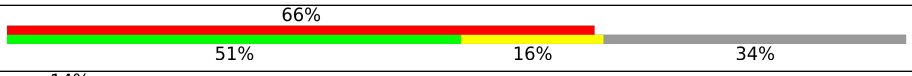
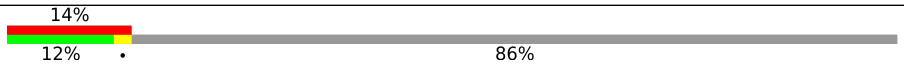
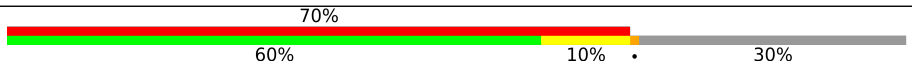
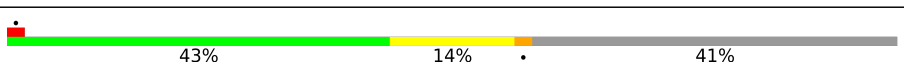
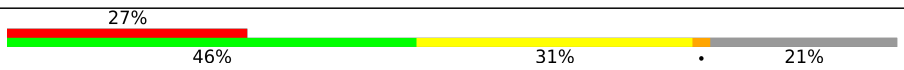
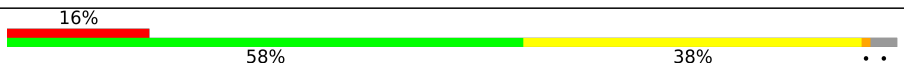
Mol	Chain	Length	Quality of chain
27	DG	349	
28	DH	310	
29	DI	264	
29	Di	264	
30	DJ	218	
30	Dj	218	
31	DL	161	
31	Dl	161	
32	Dc	929	
33	Dk	211	
34	Dm	124	
35	EA	439	
36	EB	291	
37	1	548	
38	2	395	
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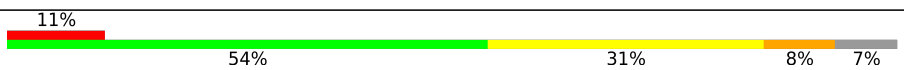
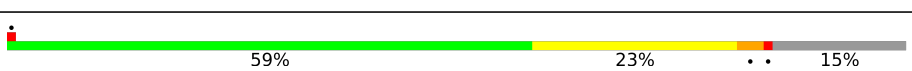
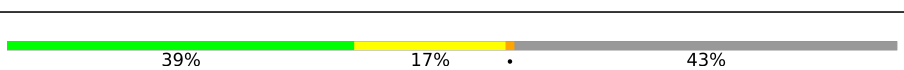
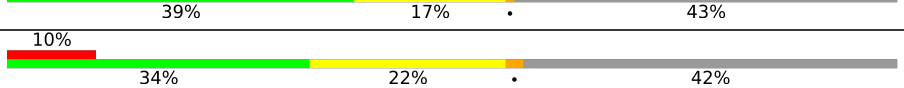
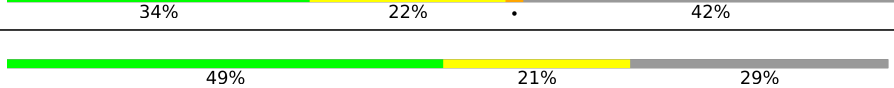
40	4	462	
41	5	71	
42	6	782	
43	7	760	
44	c	311	
45	e	178	
46	b	200	
47	l	178	
48	m	131	

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Mol	Chain	Length	Quality of chain
49	a	1581	11% 17% 9% 70%
50	d	270	23% 28% 7% 41%
51	f	246	34% 29% 32%
52	g	233	33% 31% 6% 29%
53	h	268	34% 28% 8% 29%
54	i	146	14% 31% 5% 50%
55	j	135	36% 49% 6% 10%
56	k	117	26% 42% 28%
57	n	1454	47% 19% 32%
58	o	788	11% 8% 80%
59	q	651	46% 30% 9% 15%
60	r	208	65% 27% 6%
61	s	244	21% 11% 67%
62	t	212	41% 36% 12% 9%
63	u	144	32% 38% 5% 26%
64	v	200	27% 22% 17% 33%
65	z	600	9% 5% 84%
66	x	989	71% 76% 14% 9%
67	w	1368	92% 79% 17%
68	p	841	48% 39% 9% 52%
69	X	69	51% 43% 6%
70	Y	69	48% 48%

2 Entry composition

There are 73 unique types of molecules in this entry. The entry contains 173965 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	306	2255	1404	399	441	11	0	0

- Molecule 2 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	8	299	2378	1535	406	426	11	0	0

- Molecule 3 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	9	287	2307	1477	398	417	15	0	0

- Molecule 4 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 5 is a protein called TATA-box-binding protein.

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

- Molecule 6 is a protein called TFIIA-a.

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

- Molecule 7 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	255	Total	C	N	O	S	0	0
			1959	1226	348	368	17		

- Molecule 8 is a protein called General transcription factor IIF subunit 1.

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

- Molecule 9 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 10 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	PA	1475	Total	C	N	O	S	0	0
			11662	7336	2071	2183	72		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit F.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 19 is a protein called RPB10.

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

- Molecule 20 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 21 is a protein called RPB12.

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

- Molecule 22 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DA	600	Total	C	N	O	S	0	0
			4918	3135	858	897	28		

- Molecule 23 is a protein called Transcription initiation factor TFIID subunit 2.

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

- Molecule 24 is a protein called Transcription initiation factor TFIID subunit 4.

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

- Molecule 25 is a protein called Transcription initiation factor TFIID subunit 5.

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

- Molecule 26 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DF	408	Total	C	N	O	S	0	0
			3109	1970	542	579	18		
26	Df	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 27 is a protein called Transcription initiation factor TFIID subunit 7.

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

- Molecule 28 is a protein called Transcription initiation factor TFIID subunit 8.

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

- Molecule 29 is a protein called Transcription initiation factor TFIID subunit 9.

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

- Molecule 30 is a protein called Transcription initiation factor TFIID subunit 10.

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

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 12.

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

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 3.

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

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 11.

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

- Molecule 34 is a protein called Transcription initiation factor TFIID subunit 13.

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

- Molecule 35 is a protein called General transcription factor IIE subunit 1.

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

- Molecule 36 is a protein called Transcription initiation factor IIE subunit beta.

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

- Molecule 37 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1	433	Total	C	N	O	S	0	0
			3436	2153	602	664	17		

- Molecule 38 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	385	Total	C	N	O	S	0	0
			3024	1909	524	564	27		

- Molecule 39 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	295	Total	C	N	O	S	0	0
			2306	1477	384	426	19		

- Molecule 40 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	457	Total	C	N	O	S	0	0
			3644	2341	641	648	14		

- Molecule 41 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5	66	Total	C	N	O	S	0	0
			522	336	83	100	3		

- Molecule 42 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	652	Total	C	N	O	S	0	0
			5255	3345	898	980	32		

- Molecule 43 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	7	732	Total	C	N	O	S	0	0
			5861	3742	1023	1068	28		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	c	263	Total	C	N	O	S	0	0
			2108	1337	378	382	11		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 28.

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

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 29.

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

- Molecule 47 is a protein called Mediator of RNA polymerase II transcription subunit 30.

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

- Molecule 48 is a protein called Mediator of RNA polymerase II transcription subunit 31.

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

- Molecule 49 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	469	Total	C	N	O	S	0	0
			3585	2283	615	663	24		

- Molecule 50 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	d	158	Total	C	N	O	S	0	0
			1268	791	228	243	6		

- Molecule 51 is a protein called Mediator of RNA polymerase II transcription subunit 6.

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

- Molecule 52 is a protein called Mediator of RNA polymerase II transcription subunit 7.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 53 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	h	190	Total	C	N	O	S	0	0
			1465	913	259	289	4		

- Molecule 54 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	i	73	Total	C	N	O	S	0	0
			605	382	107	110	6		

- Molecule 55 is a protein called Mediator of RNA polymerase II transcription subunit 10.

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

- Molecule 56 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 57 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	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 58 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 59 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	q	555	Total	C	N	O	S	0	0
			4276	2700	767	792	17		

- Molecule 60 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	r	206	Total	C	N	O	S	0	0
			1630	1033	285	294	18		

- Molecule 61 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	s	81	Total	C	N	O	S	0	0
			505	312	91	100	2		

- Molecule 62 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 63 is a protein called Mediator of RNA polymerase II transcription subunit 21.

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

- Molecule 64 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 65 is a protein called Mediator of RNA polymerase II transcription subunit 26.

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

- Molecule 66 is a protein called Mediator of RNA polymerase II transcription subunit 24.

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

- Molecule 67 is a protein called Mediator of RNA polymerase II transcription subunit 23.

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

- Molecule 68 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 16.

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

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

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

- Molecule 70 is a DNA chain called DNA(69-MER).

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

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

Mol	Chain	Residues	Atoms		AltConf
71	0	2	Total	Zn	0
			2	2	
71	BA	1	Total	Zn	0
			1	1	
71	PA	2	Total	Zn	0
			2	2	
71	PB	1	Total	Zn	0
			1	1	
71	PC	1	Total	Zn	0
			1	1	
71	PI	2	Total	Zn	0
			2	2	

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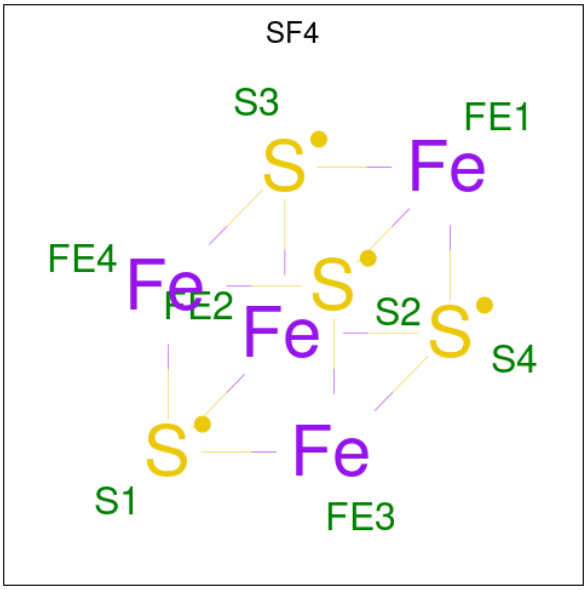
Mol	Chain	Residues	Atoms	AltConf
71	PJ	1	Total Zn 1 1	0
71	PL	1	Total Zn 1 1	0
71	EA	1	Total Zn 1 1	0
71	2	3	Total Zn 3 3	0
71	3	1	Total Zn 1 1	0

- Molecule 72 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 73 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



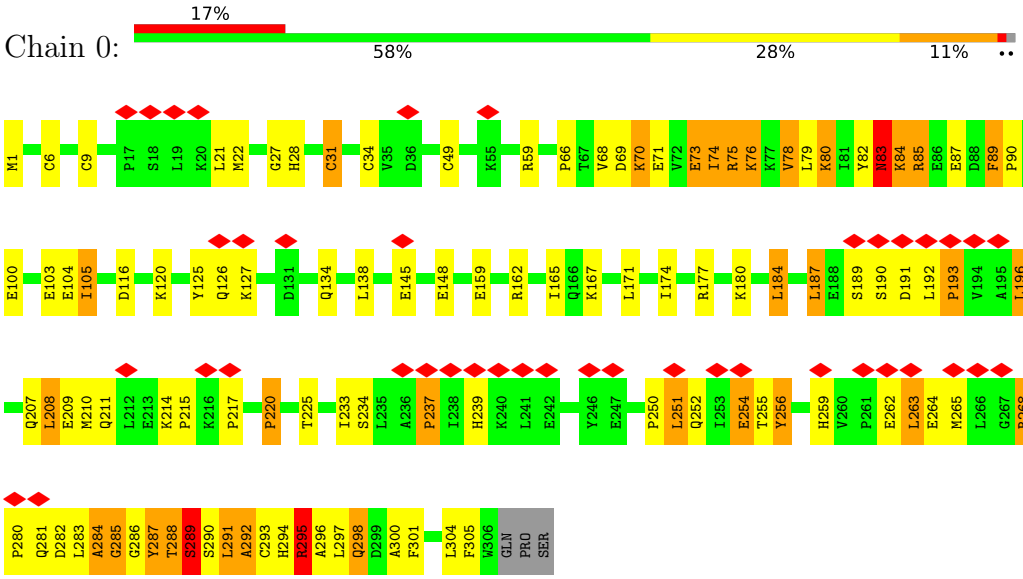
Mol	Chain	Residues	Atoms	AltConf
73	7	1	Total Fe S 8 4 4	0

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.

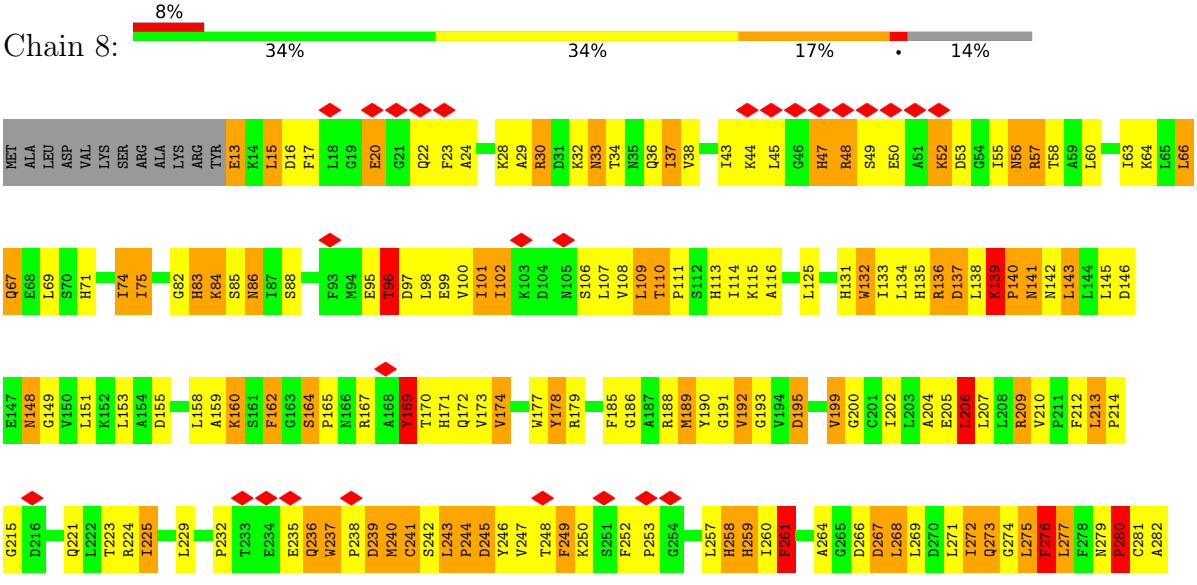
• Molecule 1: CDK-activating kinase assembly factor MAT1

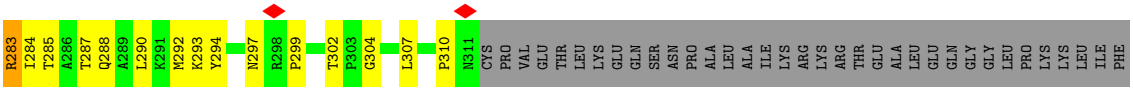
Chain 0:



• Molecule 2: Cyclin-dependent kinase 7

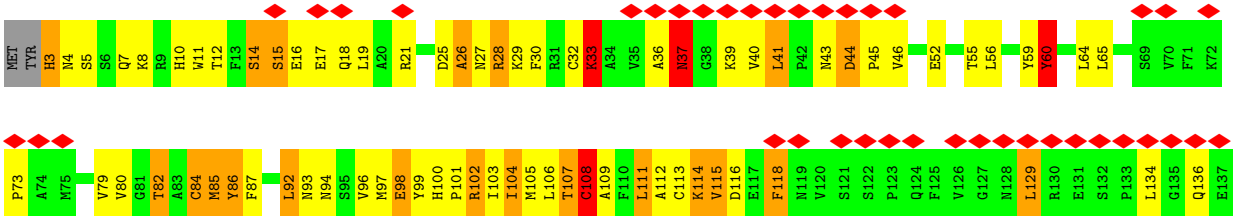
Chain 8:

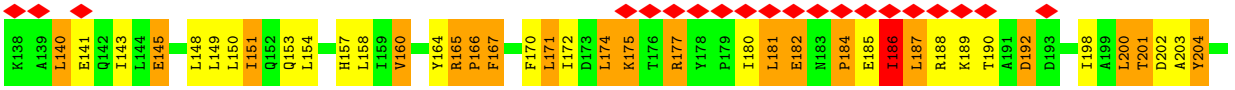


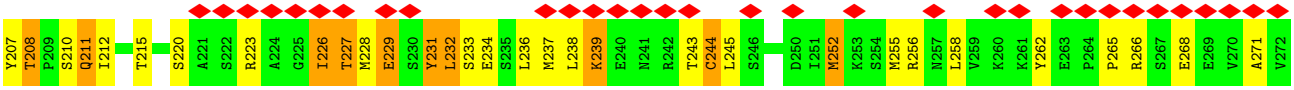


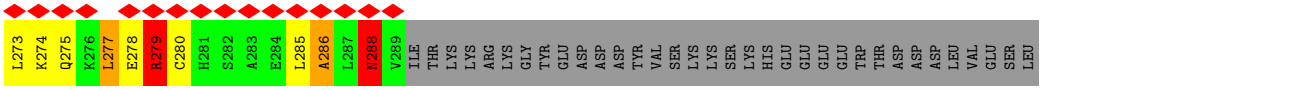
• Molecule 3: Cyclin-H

Chain 9:



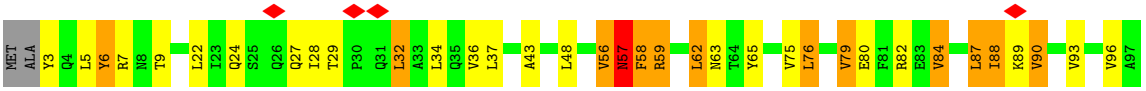






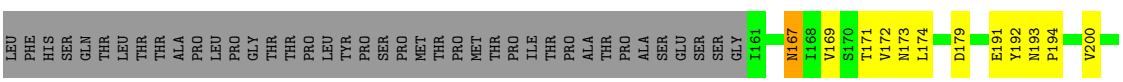
• Molecule 4: Transcription initiation factor IIA subunit 2

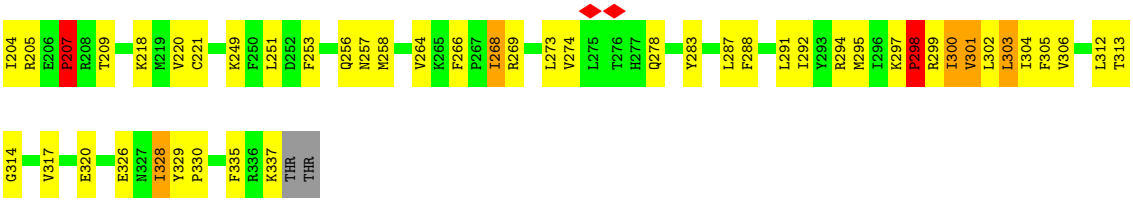
Chain DO:



• Molecule 5: TATA-box-binding protein

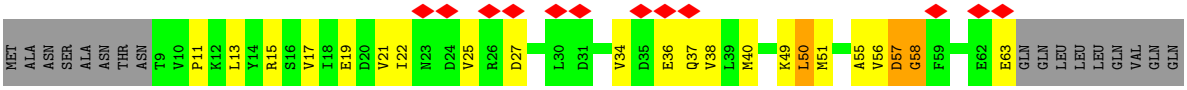
Chain DP:

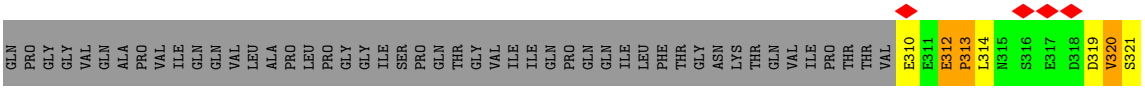


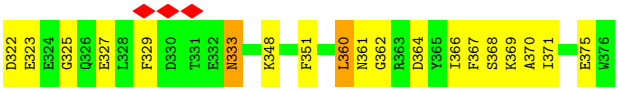


• Molecule 6: TFIIA-a

Chain DQ:

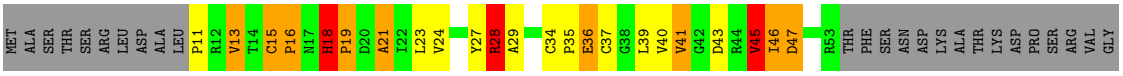


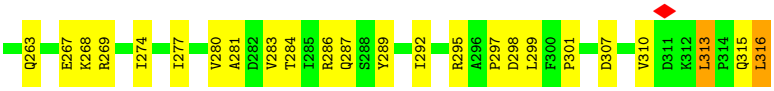




• Molecule 7: Transcription initiation factor IIB

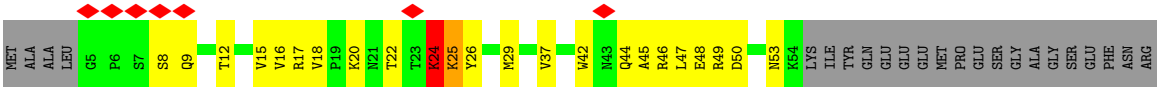
Chain BA:

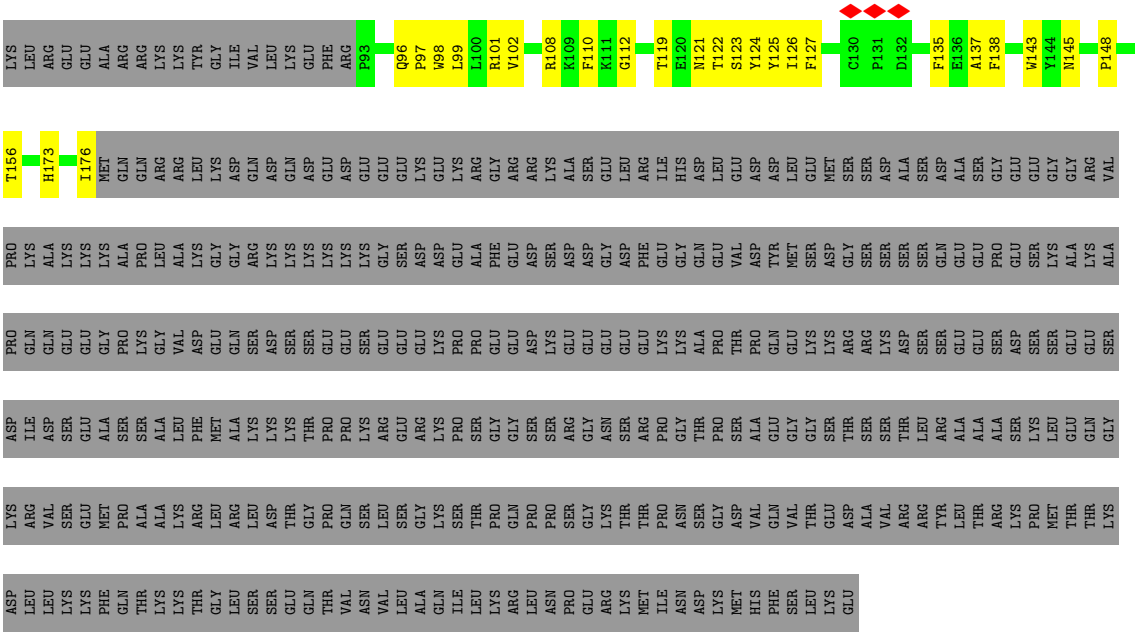




• Molecule 8: General transcription factor IIF subunit 1

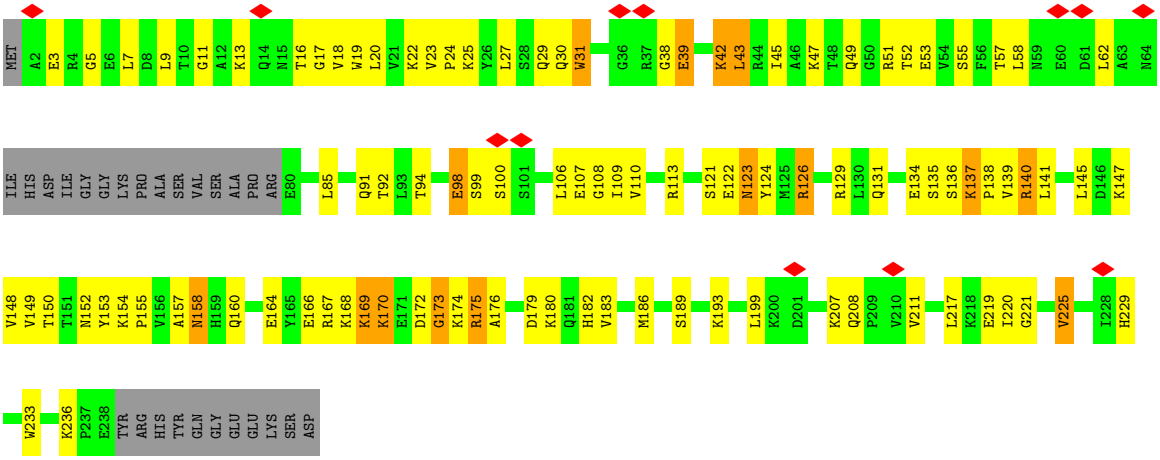
Chain FA:





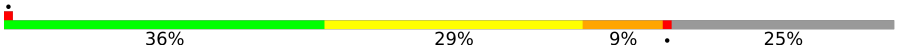
• Molecule 9: General transcription factor IIF subunit 2

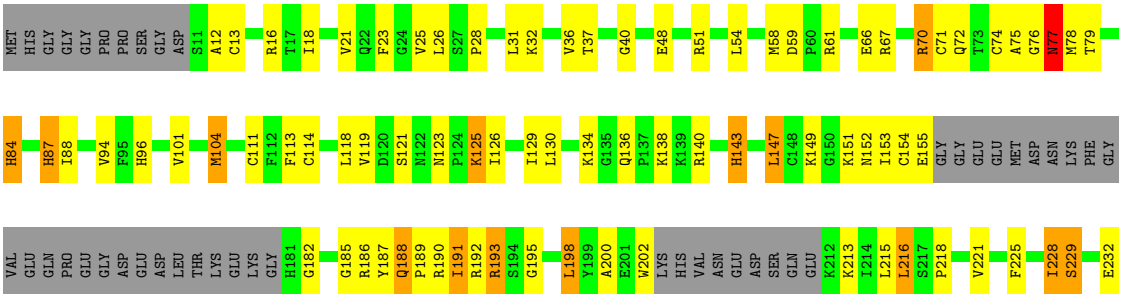
Chain FB:

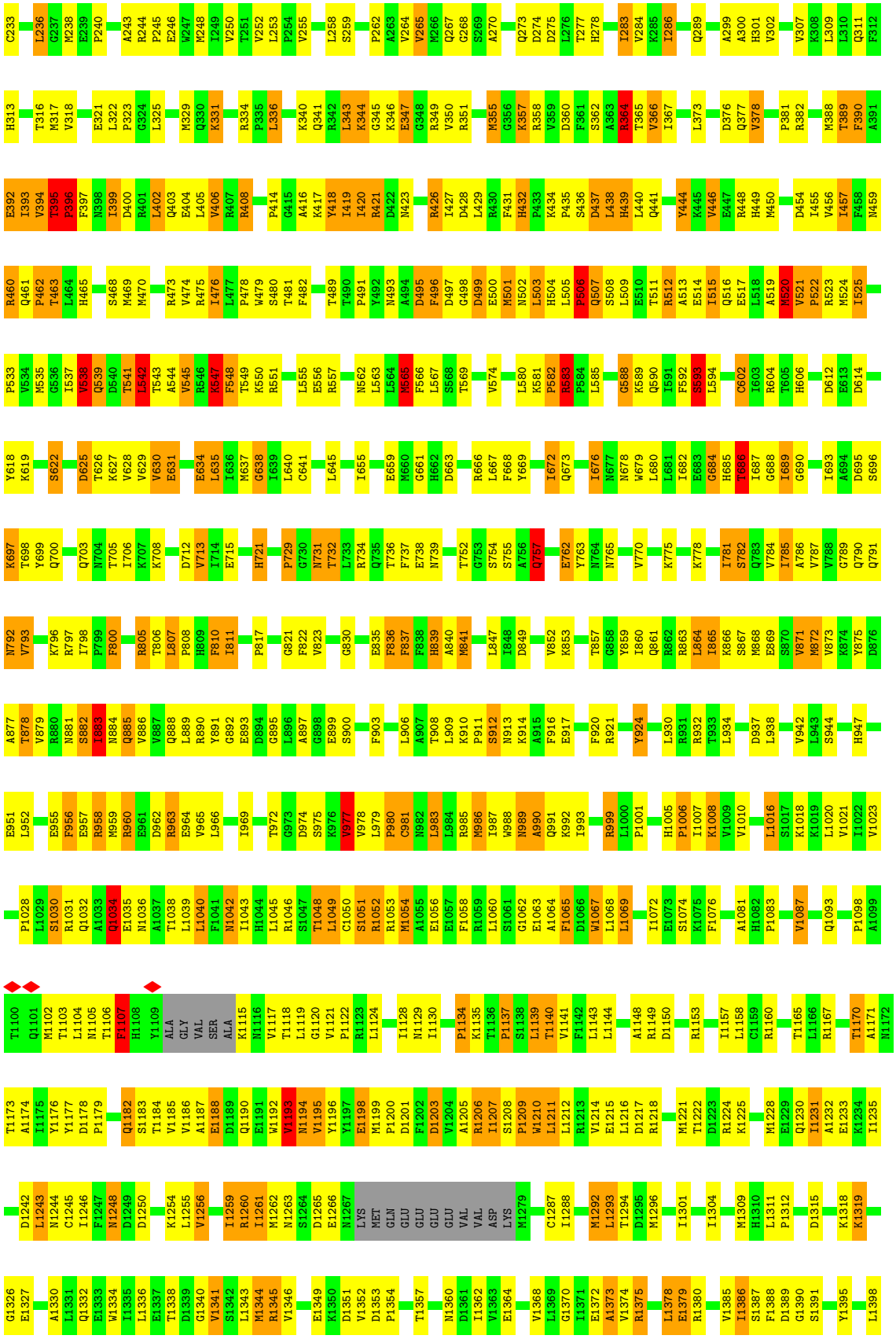


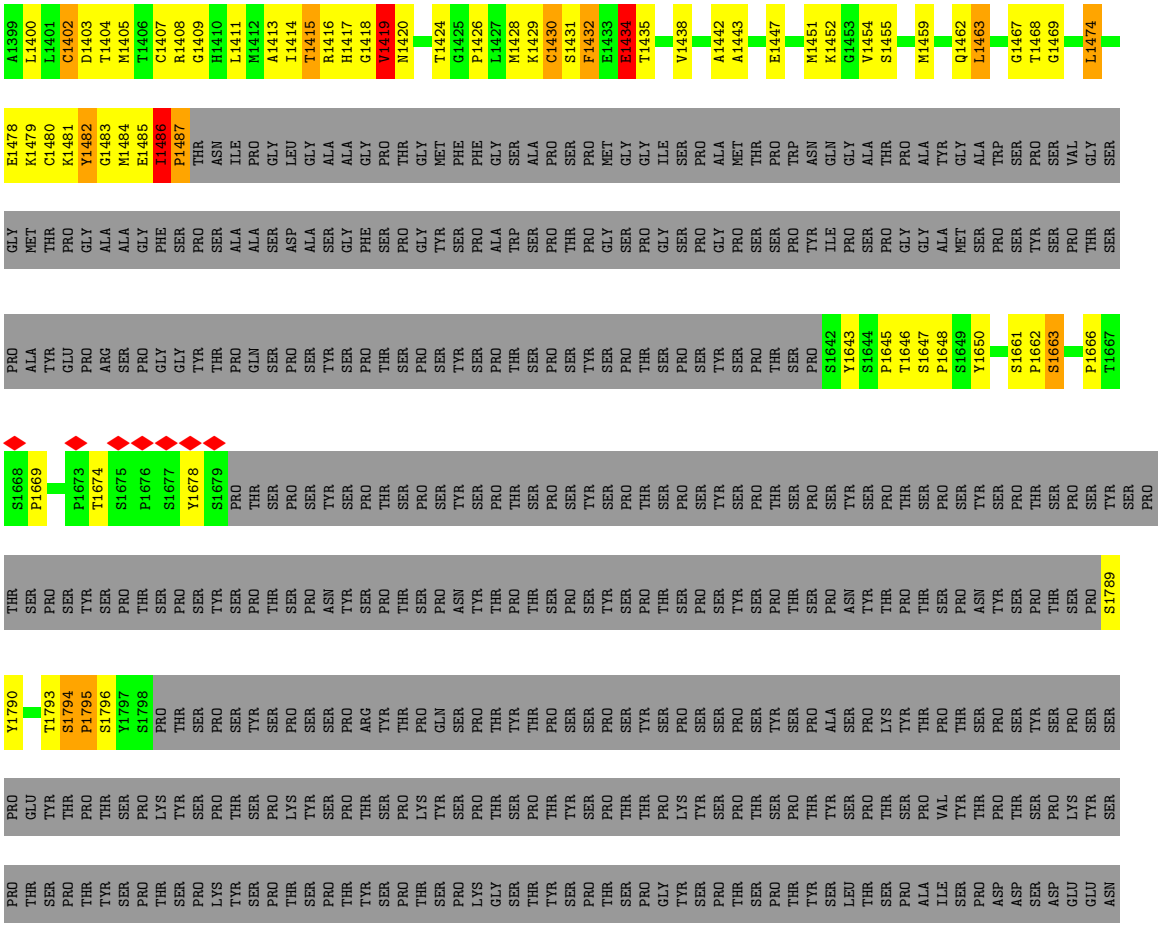
• Molecule 10: RPB1

Chain PA:



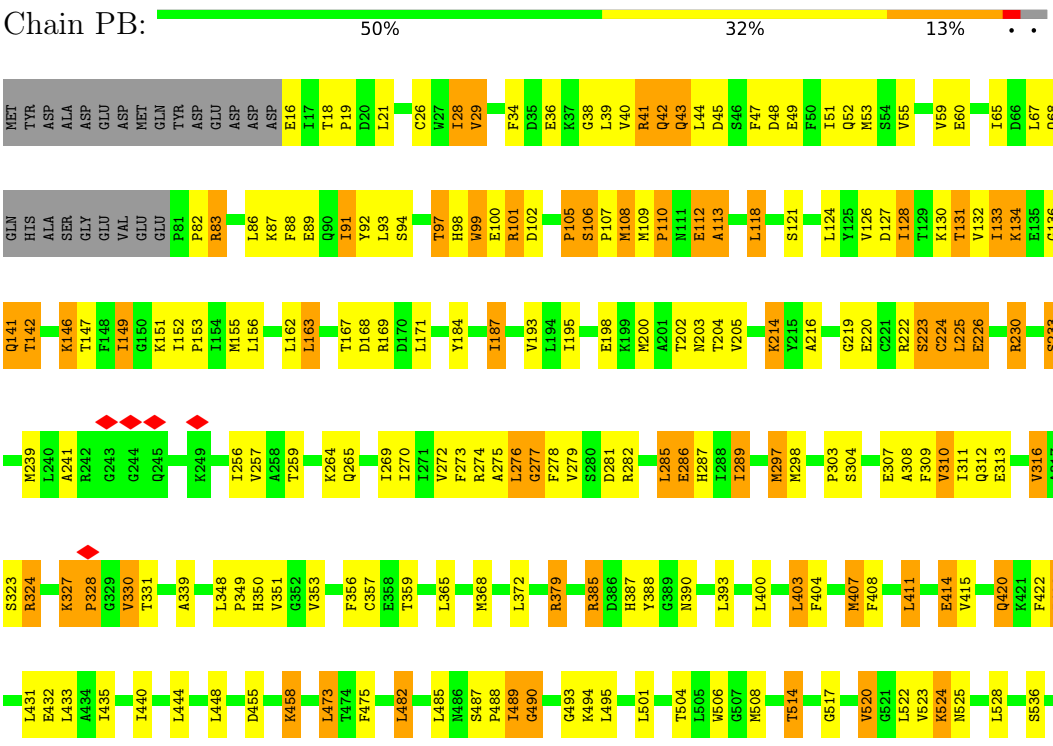


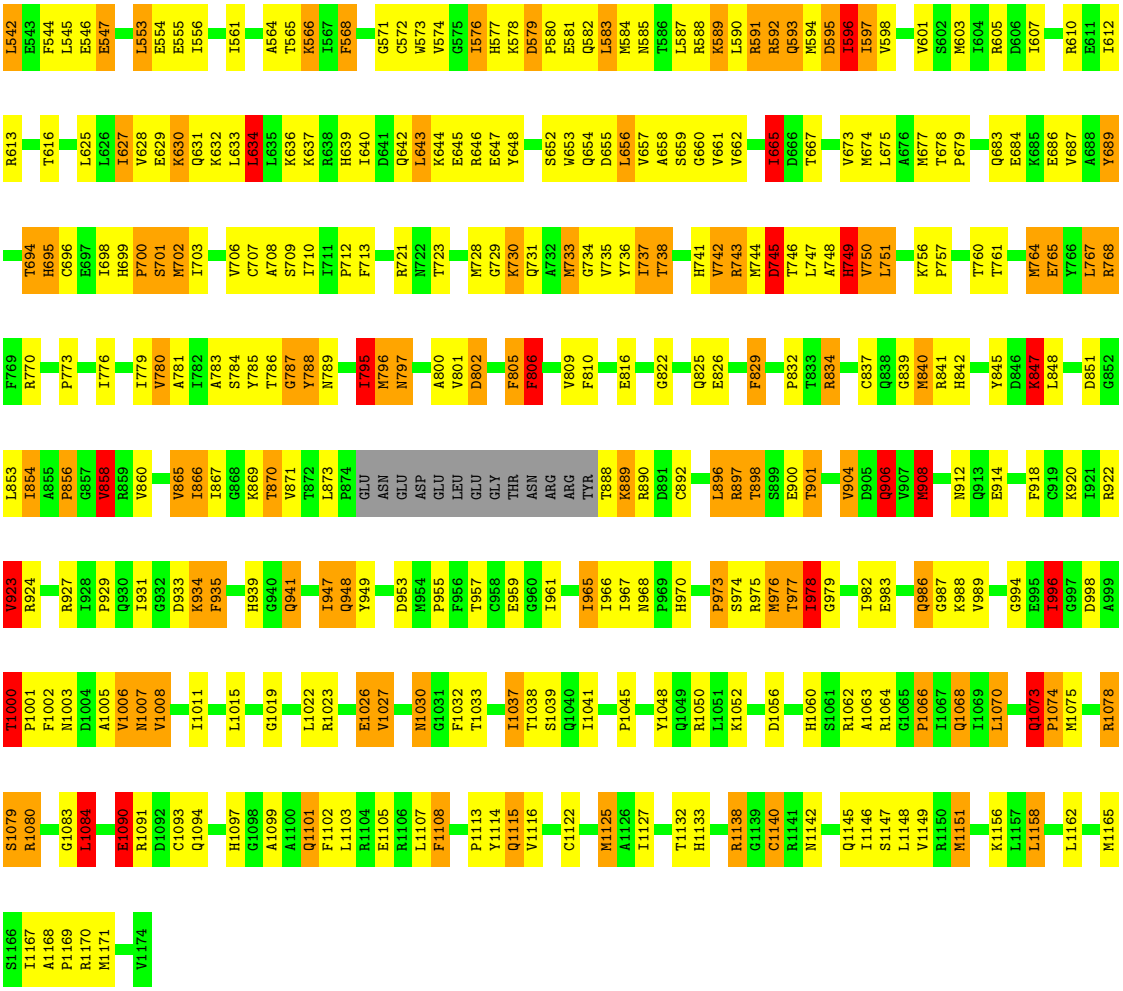




• Molecule 11: DNA-directed RNA polymerase subunit beta

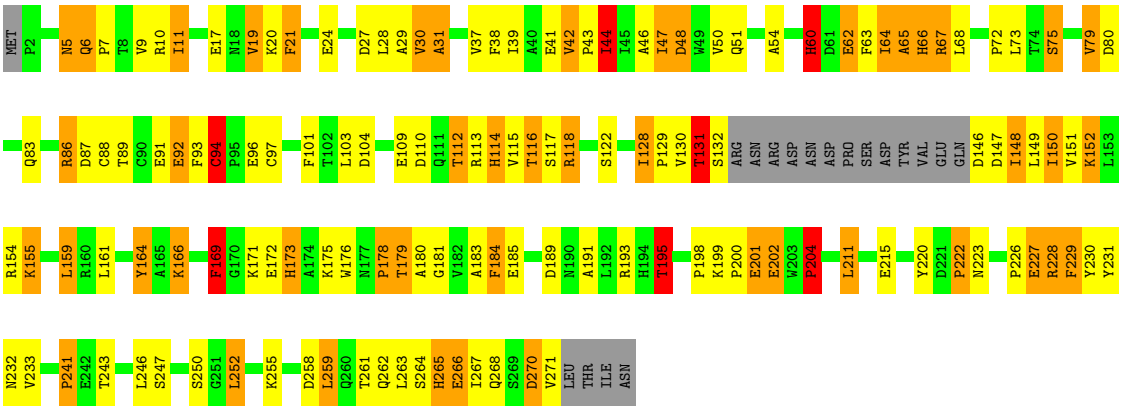
Chain PB:





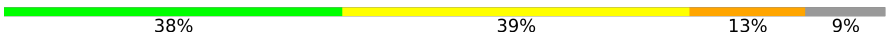
• Molecule 12: DNA-directed RNA polymerase II subunit RPB3

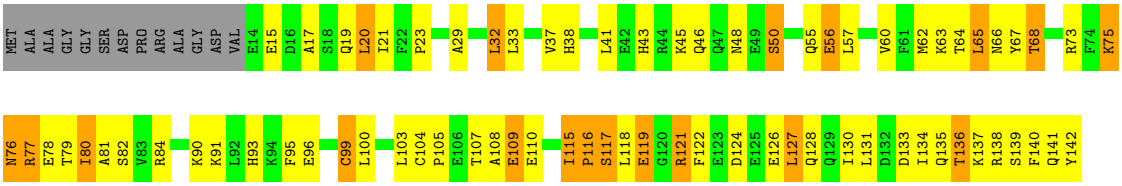
Chain PC:



• Molecule 13: DNA-directed RNA polymerase II subunit RPB4

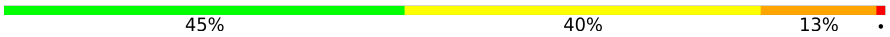
Chain PD:

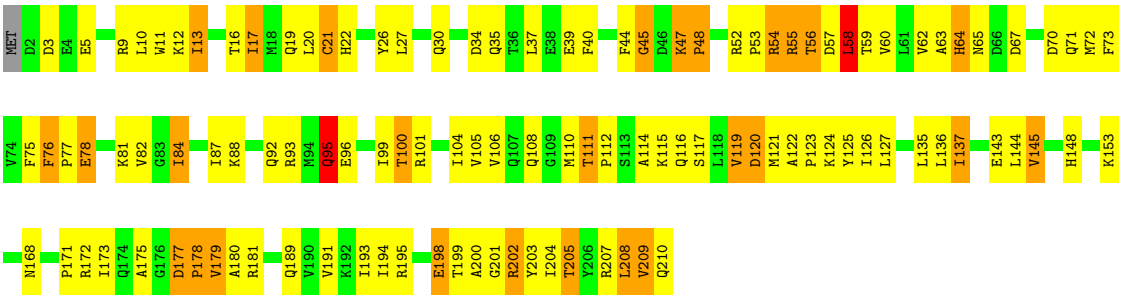




• Molecule 14: DNA-directed RNA polymerase II subunit E

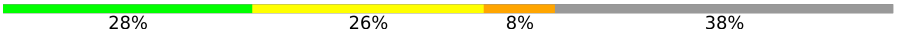
Chain PE:

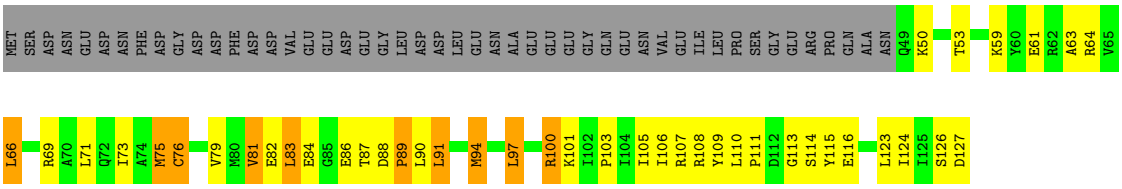




• Molecule 15: DNA-directed RNA polymerase II subunit F

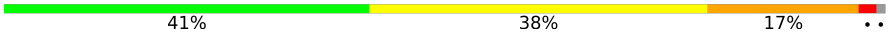
Chain PF:

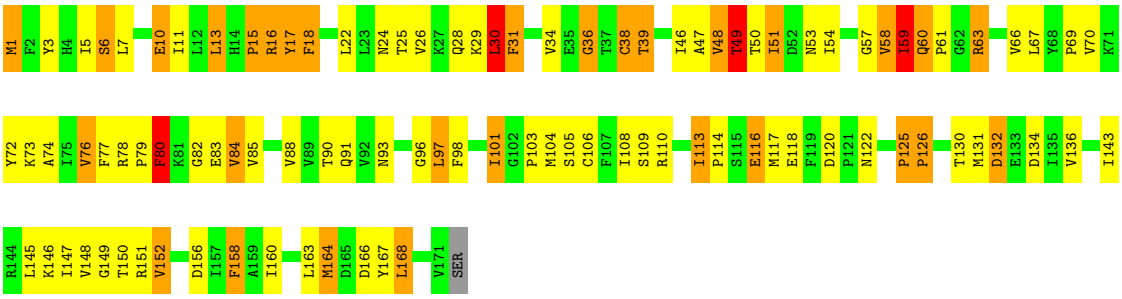




• Molecule 16: DNA-directed RNA polymerase II subunit RPB7

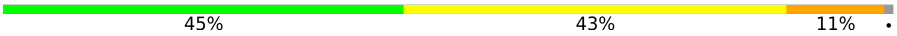
Chain PG:

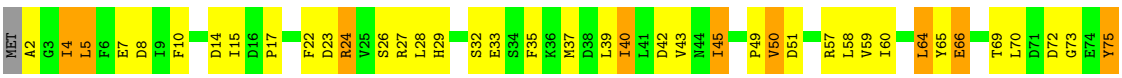




• Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC3

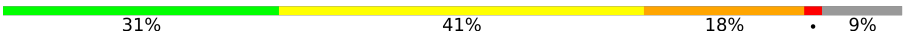
Chain PH:

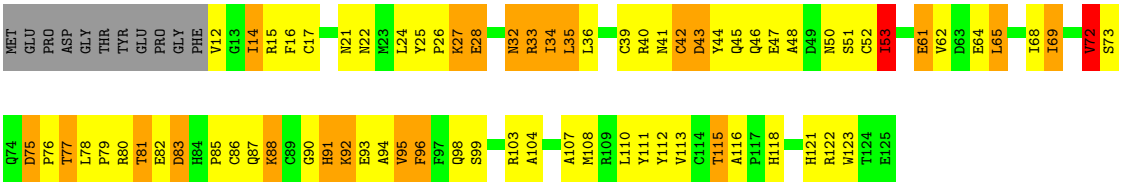




• Molecule 18: DNA-directed RNA polymerase II subunit RPB9

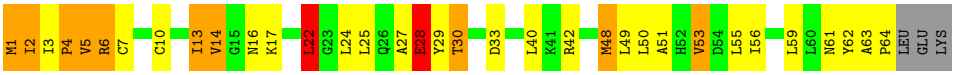
Chain PI:





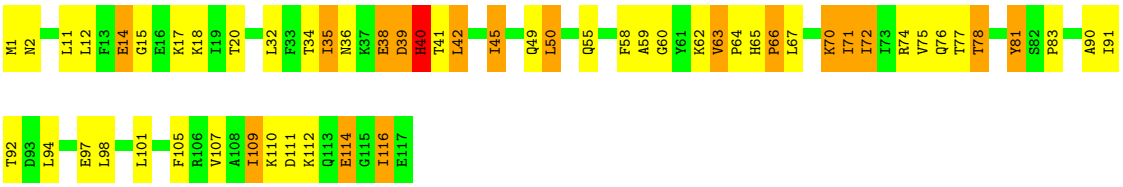
• Molecule 19: RPB10

Chain PJ:



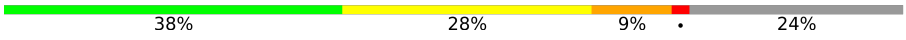
• Molecule 20: RNA_pol_L_2 domain-containing protein

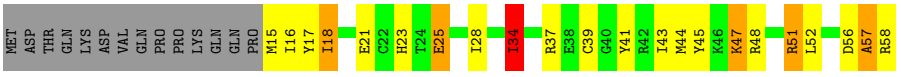
Chain PK:



• Molecule 21: RPB12

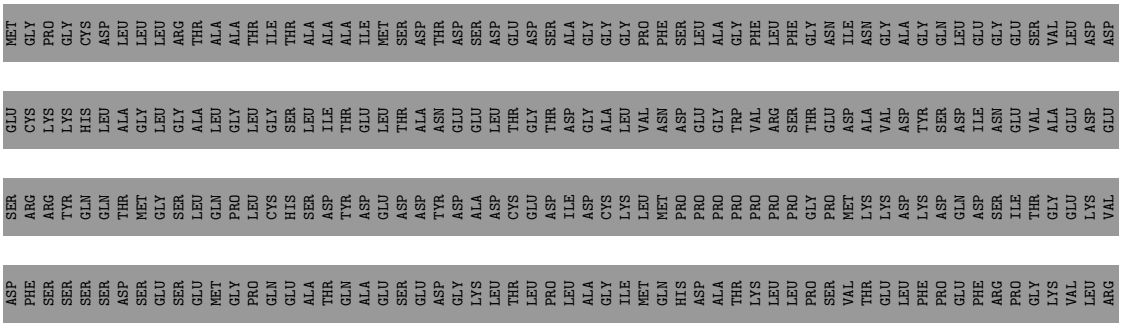
Chain PL:

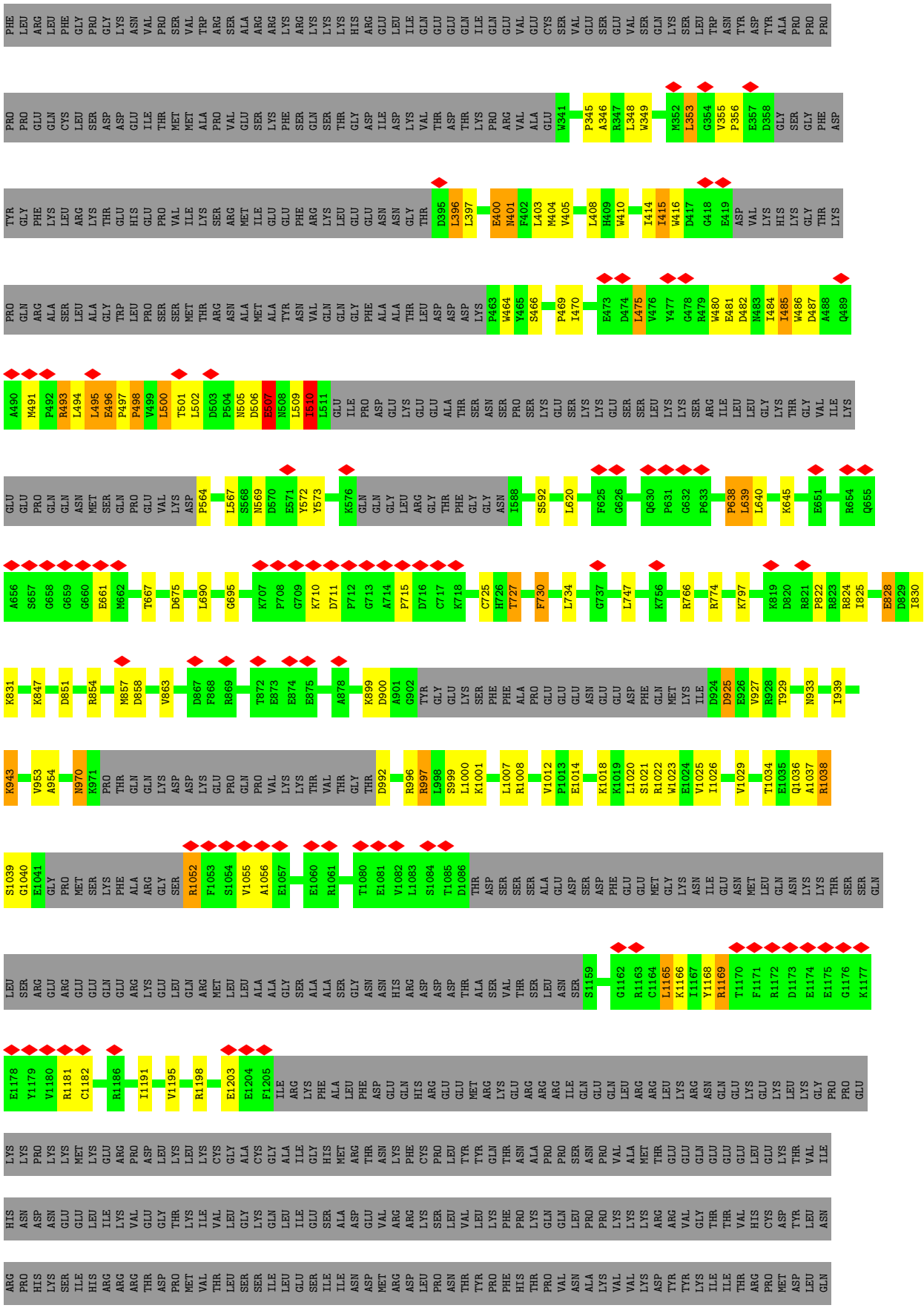


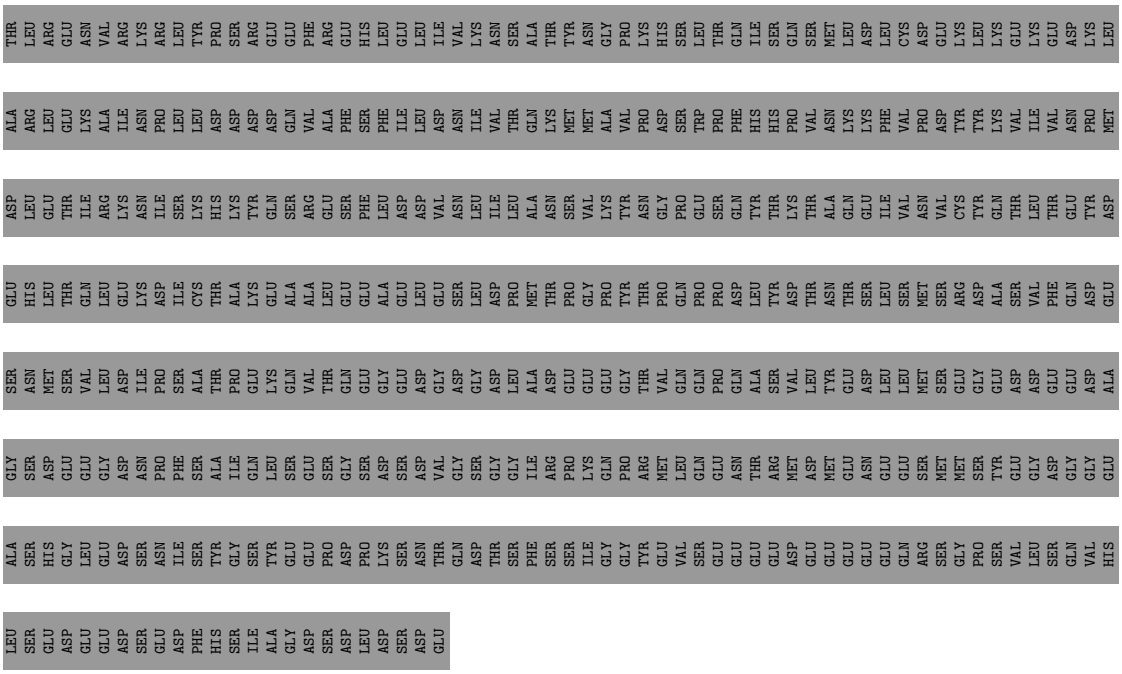


• Molecule 22: Transcription initiation factor TFIID subunit 1

Chain DA:

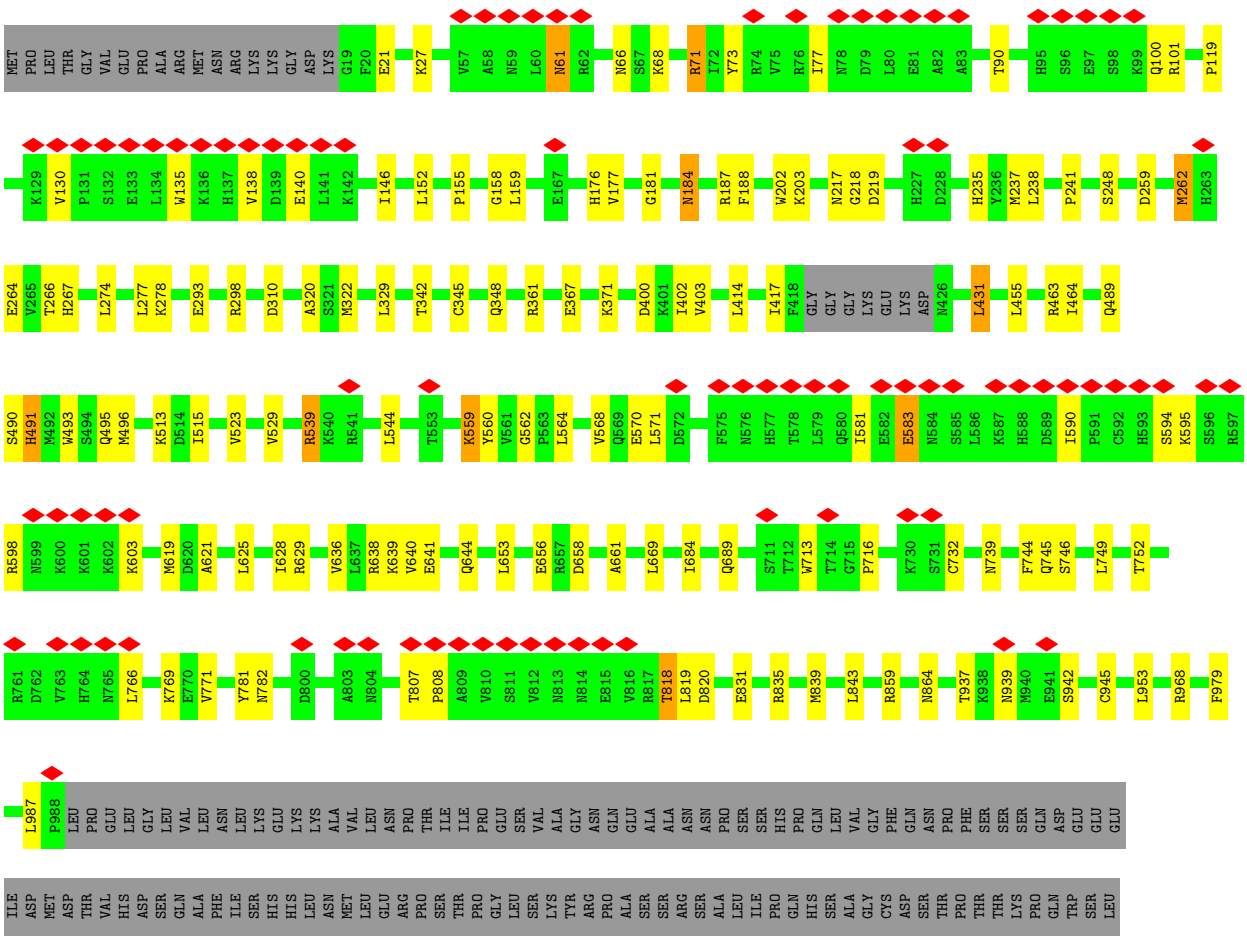


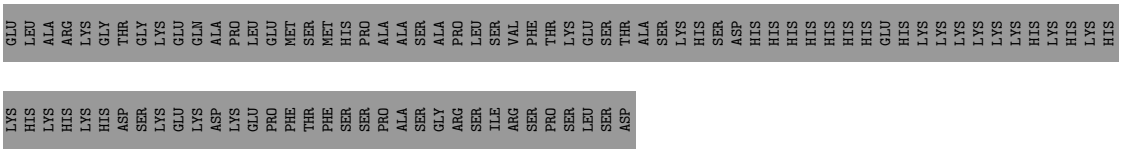




• Molecule 23: Transcription initiation factor TFIID subunit 2

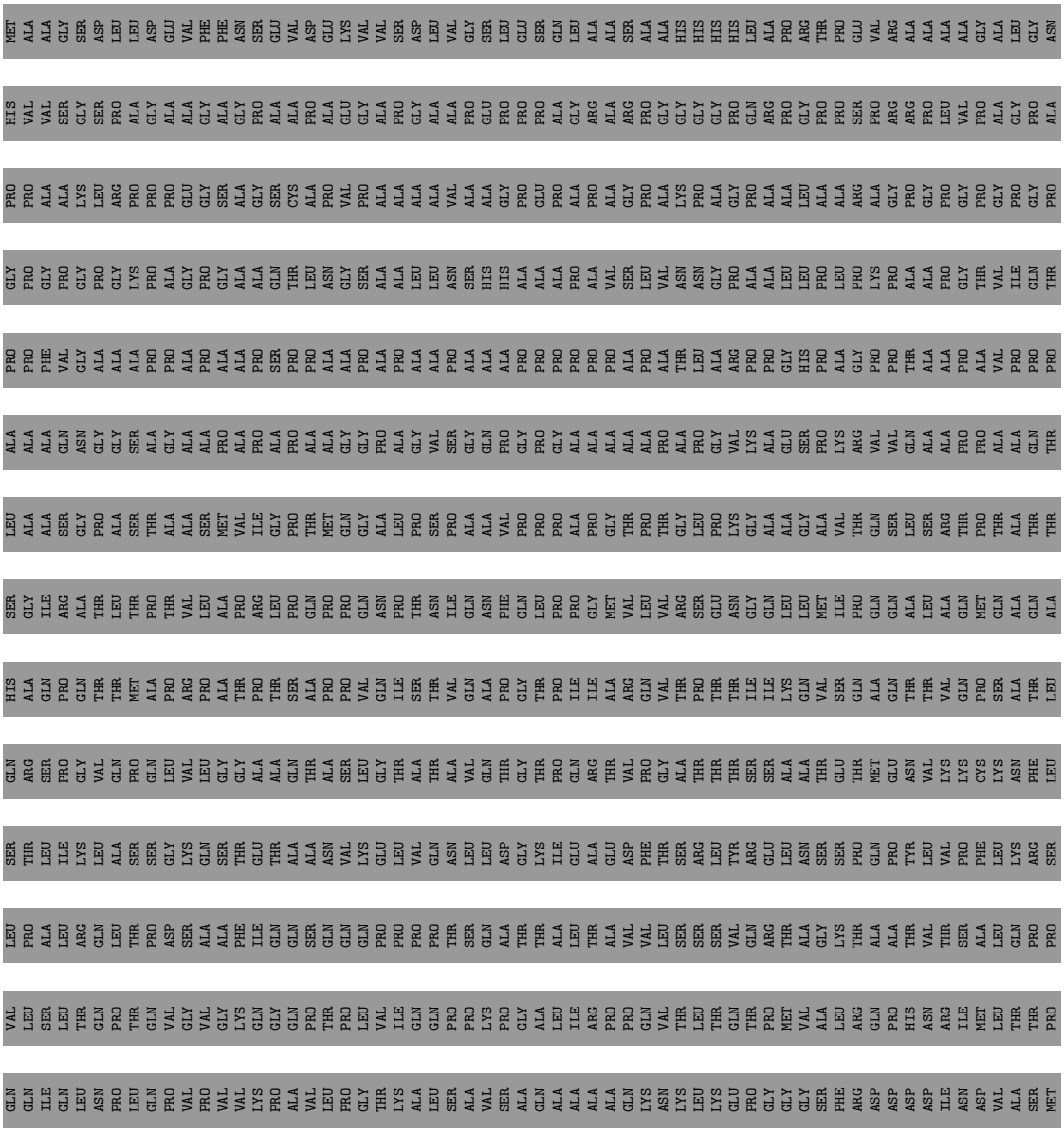
Chain DB:

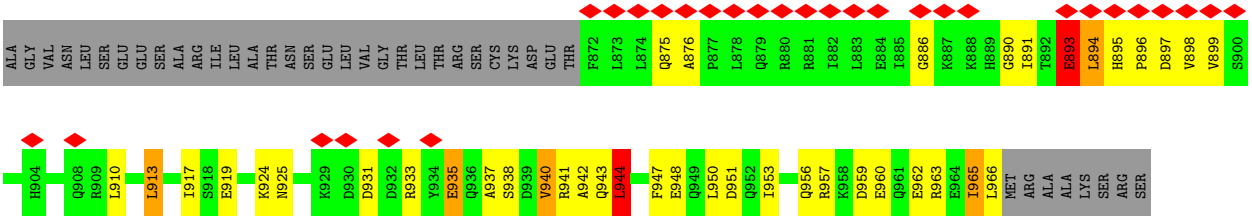


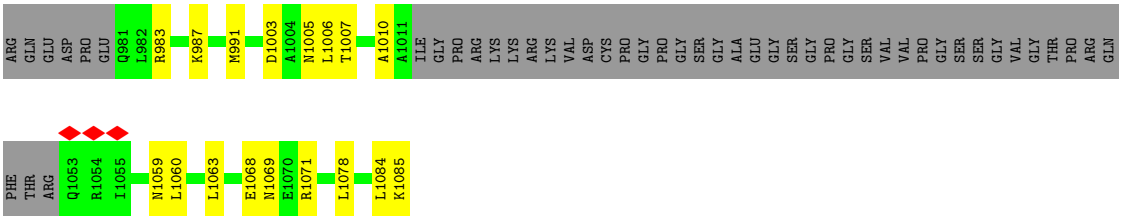


• Molecule 24: Transcription initiation factor TFIID subunit 4

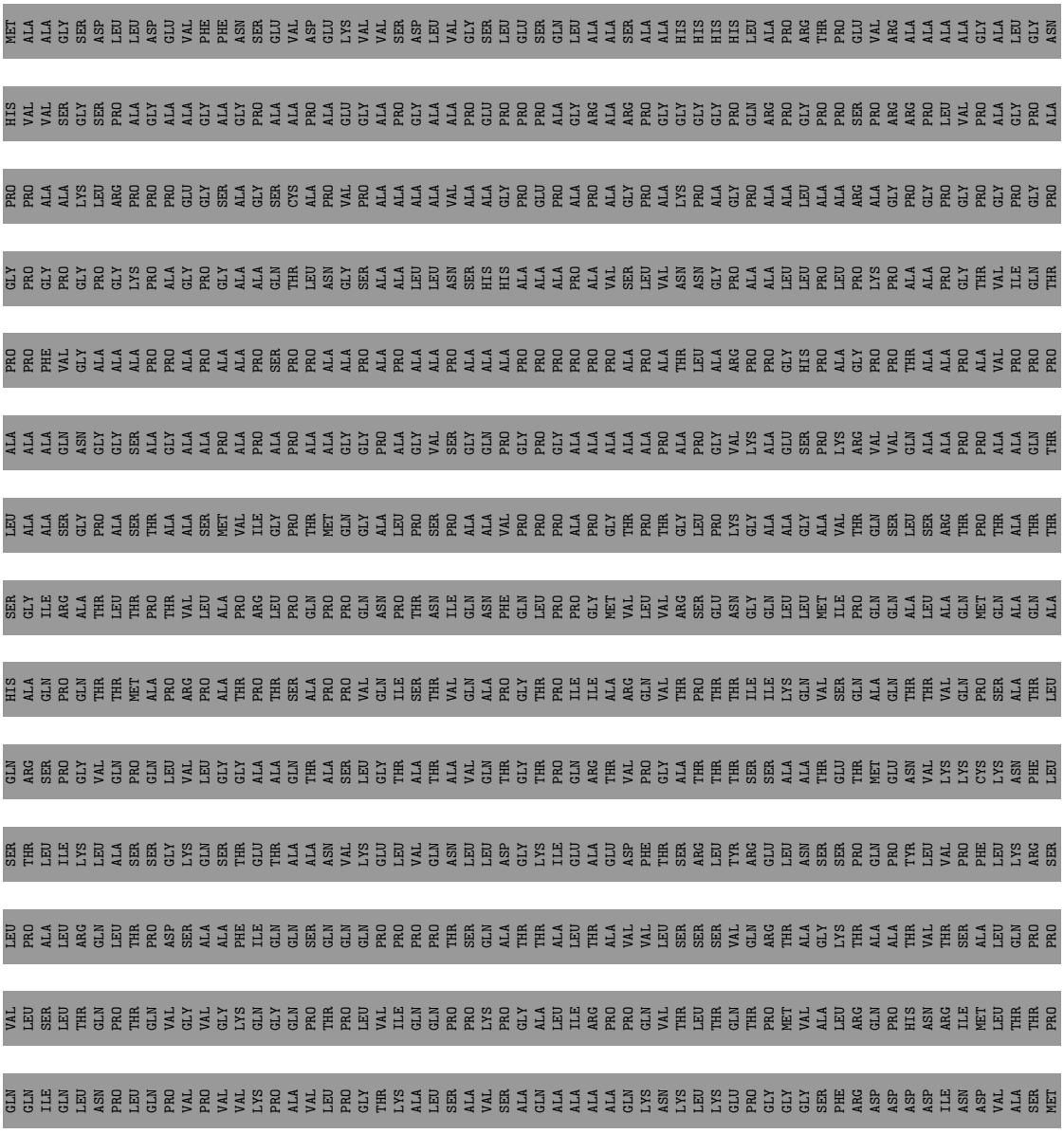
Chain DD: 9% 5% 85%

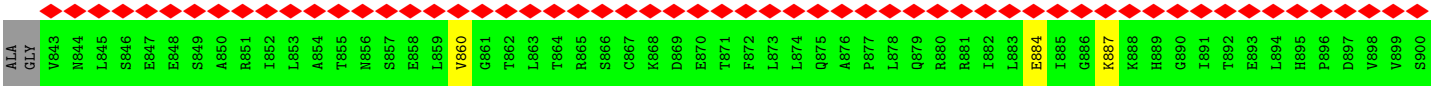


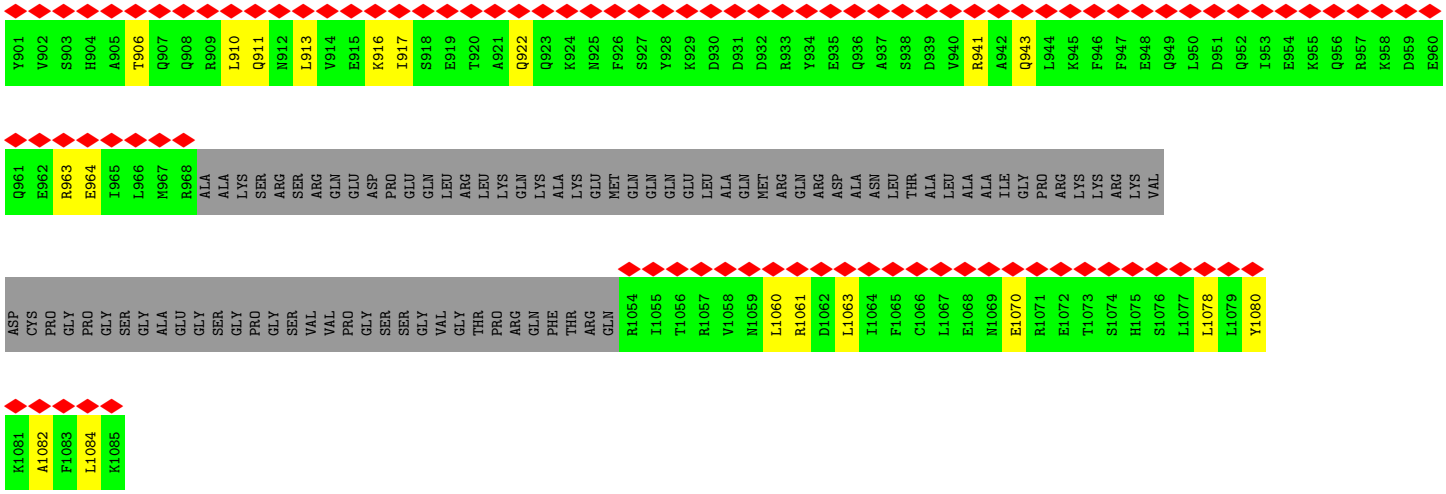




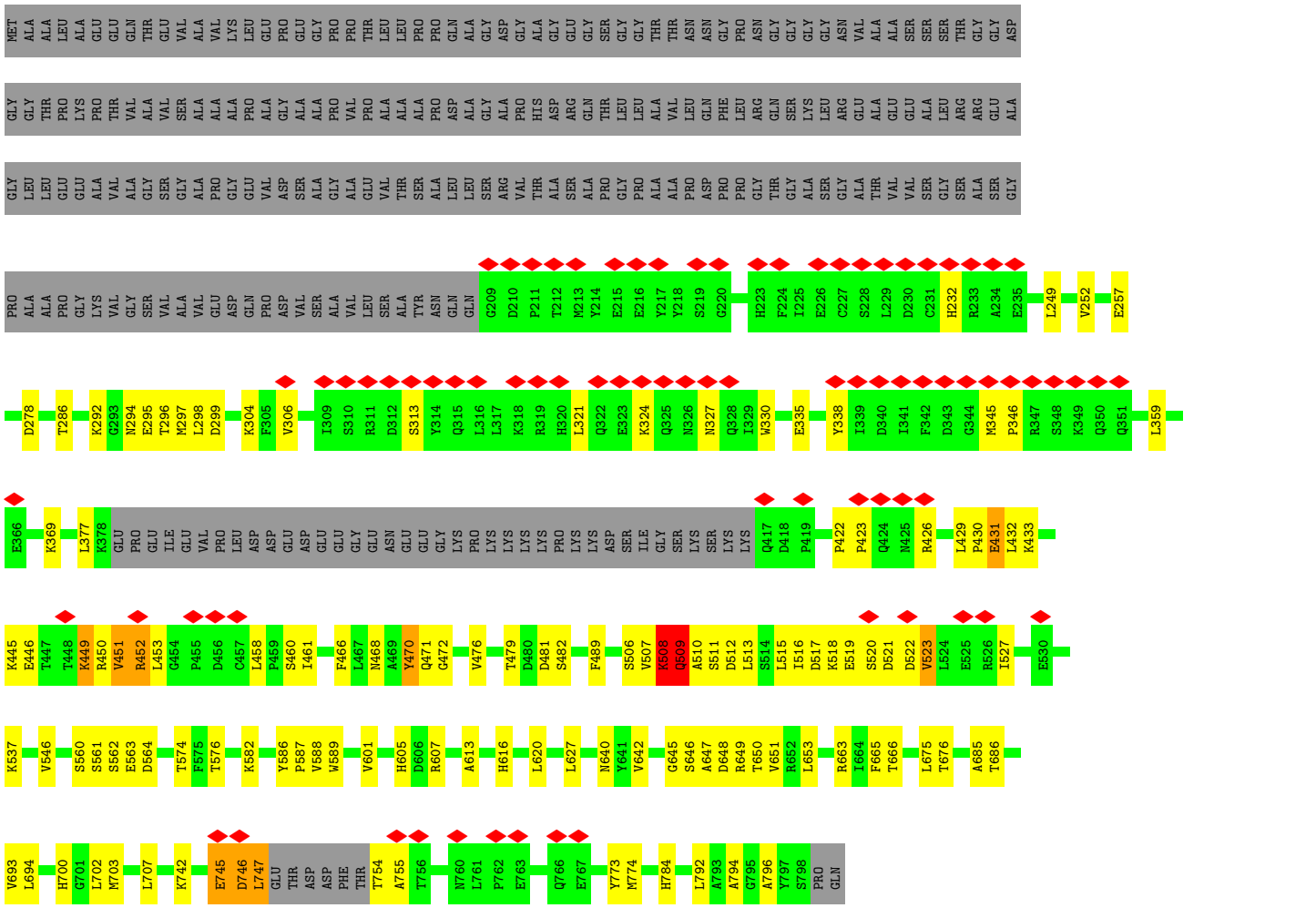
• Molecule 24: Transcription initiation factor TFIID subunit 4



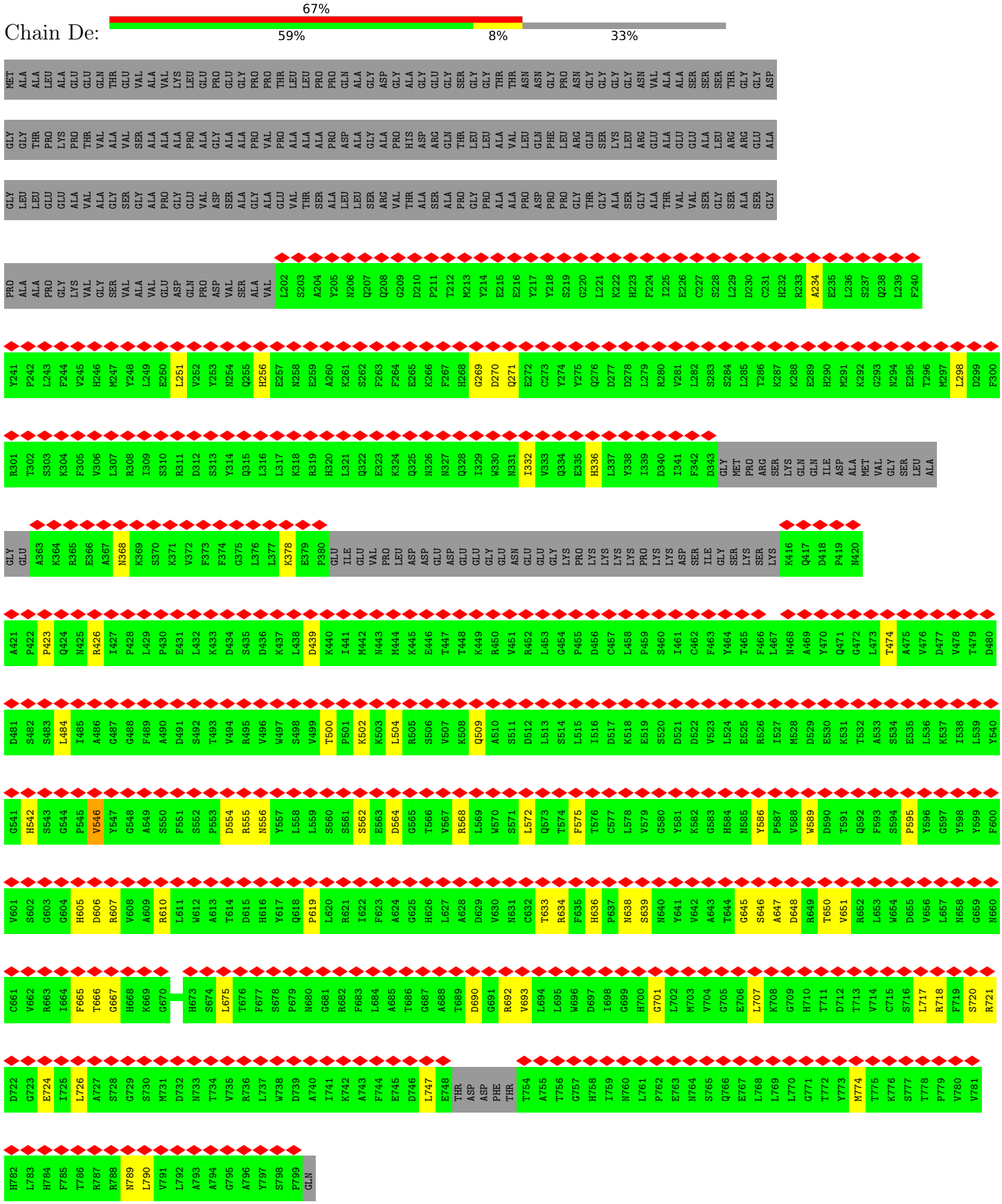




• Molecule 25: Transcription initiation factor TFIID subunit 5

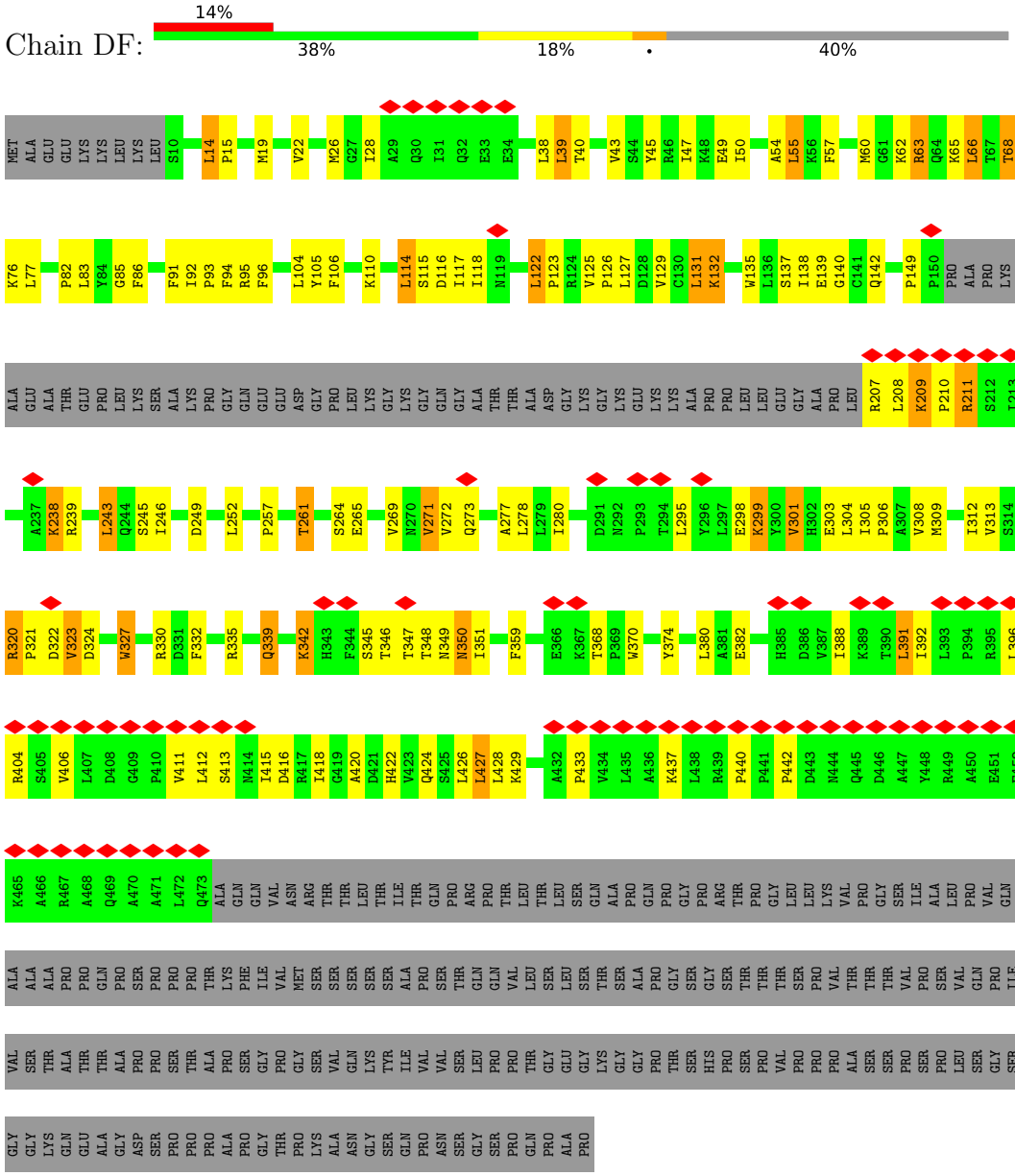


• Molecule 25: Transcription initiation factor TFIID subunit 5



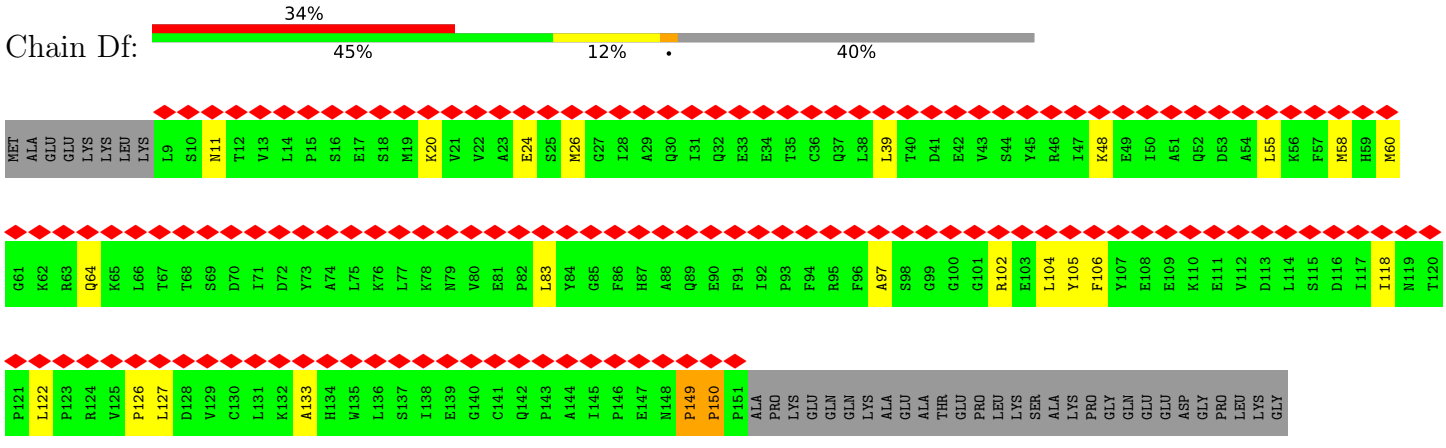
• Molecule 26: Transcription initiation factor TFIID subunit 6

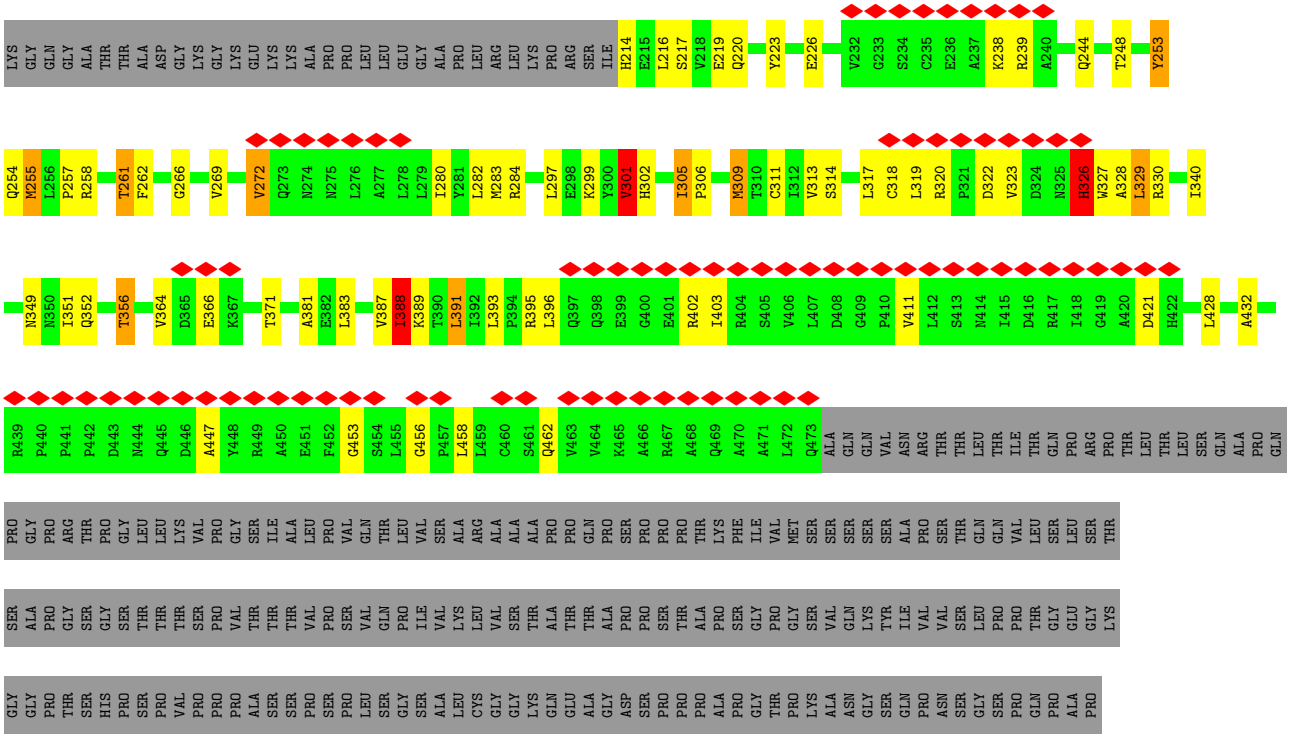
Chain DF:



• Molecule 26: Transcription initiation factor TFIID subunit 6

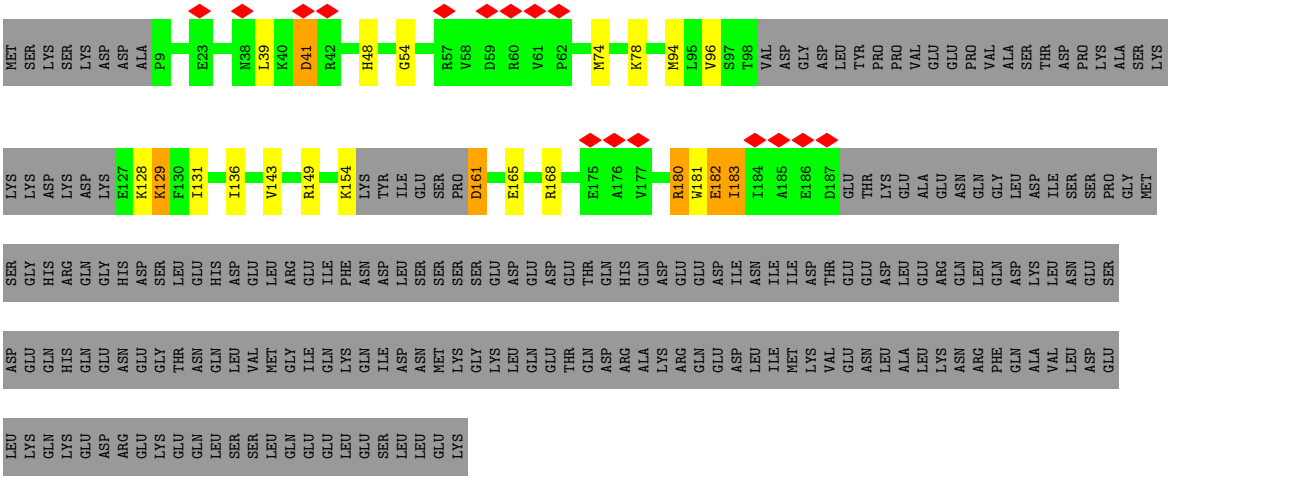
Chain Df:





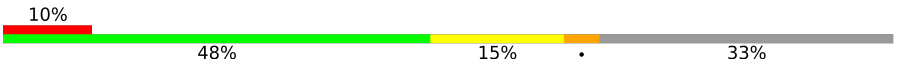
• Molecule 27: Transcription initiation factor TFIID subunit 7

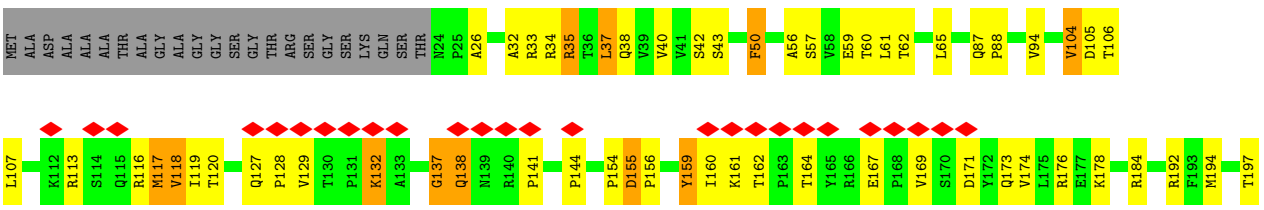
Chain DG:

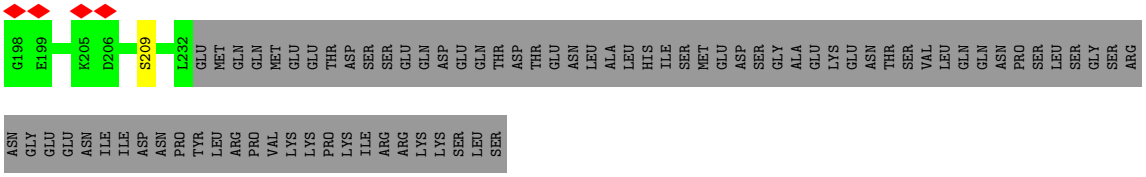


• Molecule 28: Transcription initiation factor TFIID subunit 8

Chain DH:

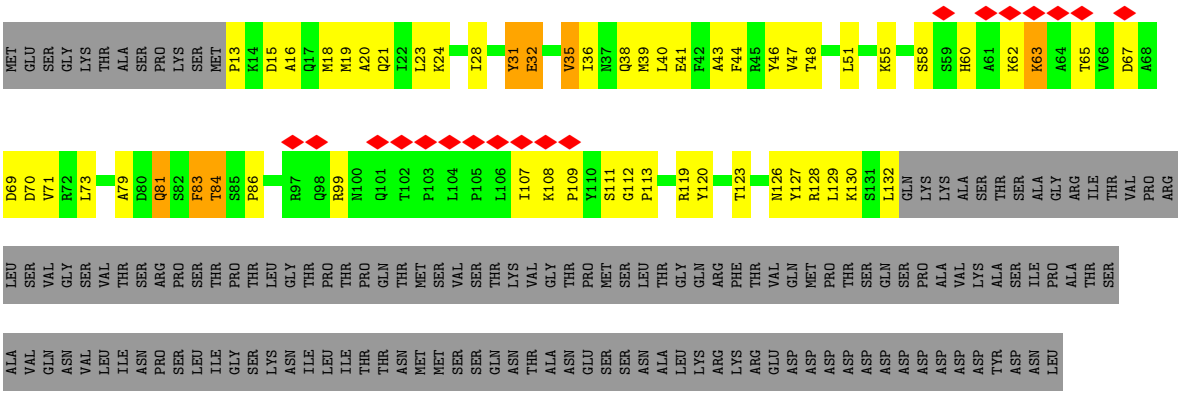






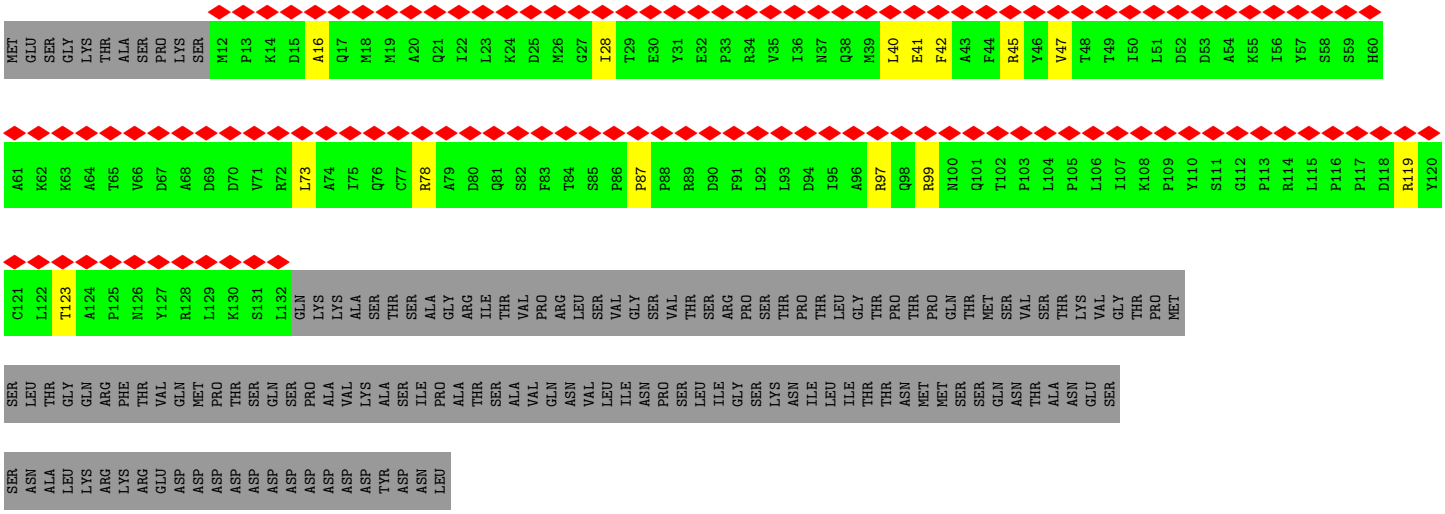
• Molecule 29: Transcription initiation factor TFIID subunit 9

Chain DI:



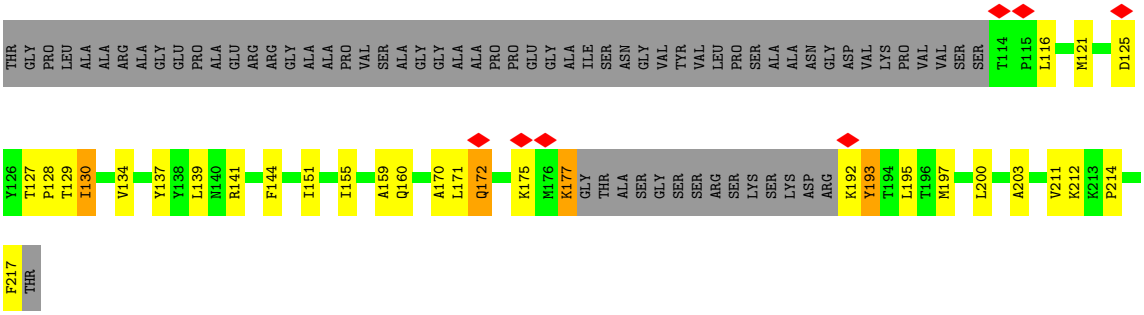
• Molecule 29: Transcription initiation factor TFIID subunit 9

Chain Di:



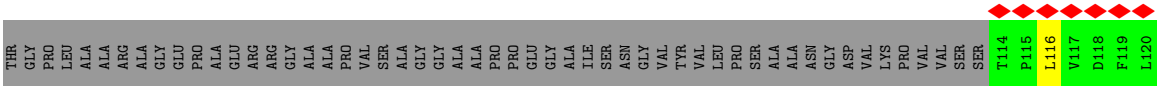
• Molecule 30: Transcription initiation factor TFIID subunit 10

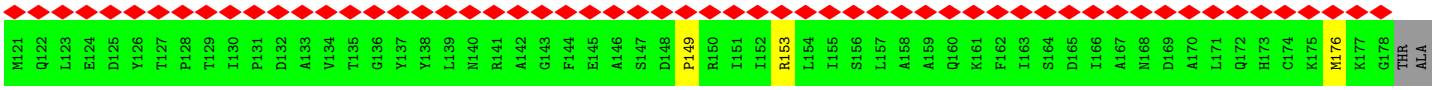
Chain DJ:

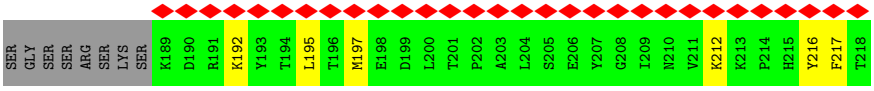


• Molecule 30: Transcription initiation factor TFIID subunit 10

Chain Dj:

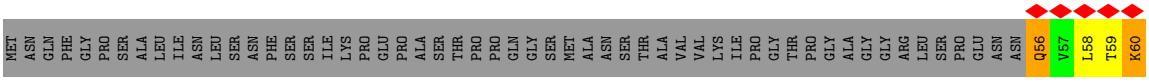


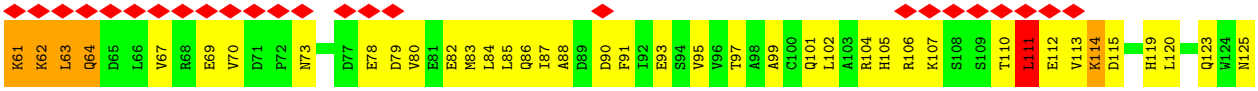


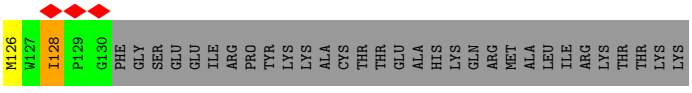


• Molecule 31: Transcription initiation factor TFIID subunit 12

Chain DL:

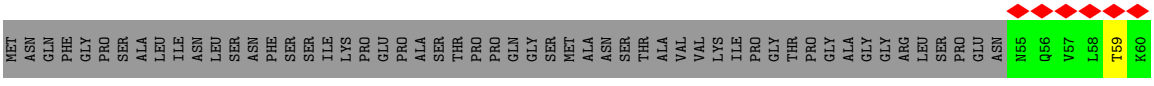


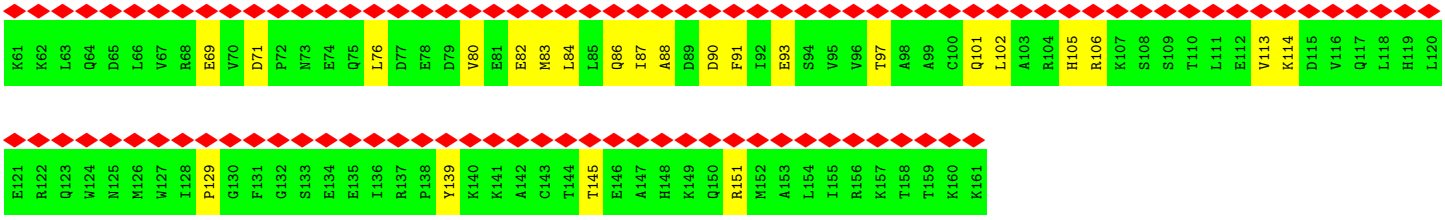




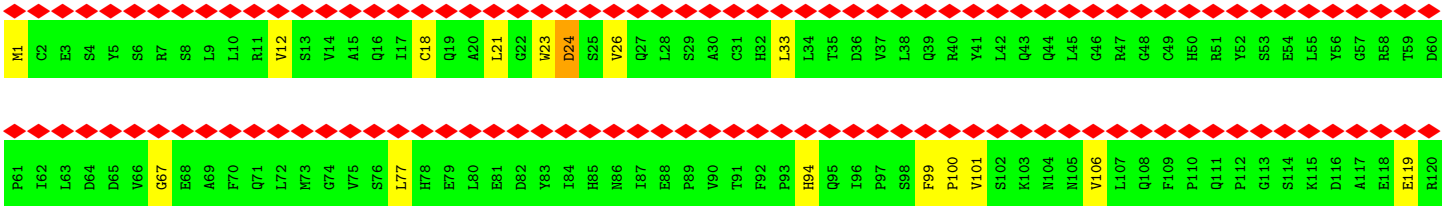
• Molecule 31: Transcription initiation factor TFIID subunit 12

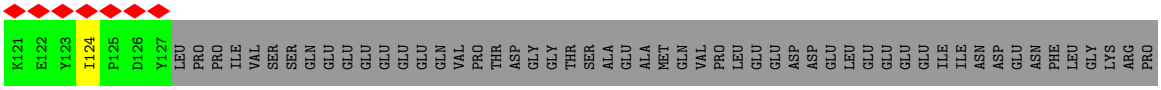
Chain Dl:

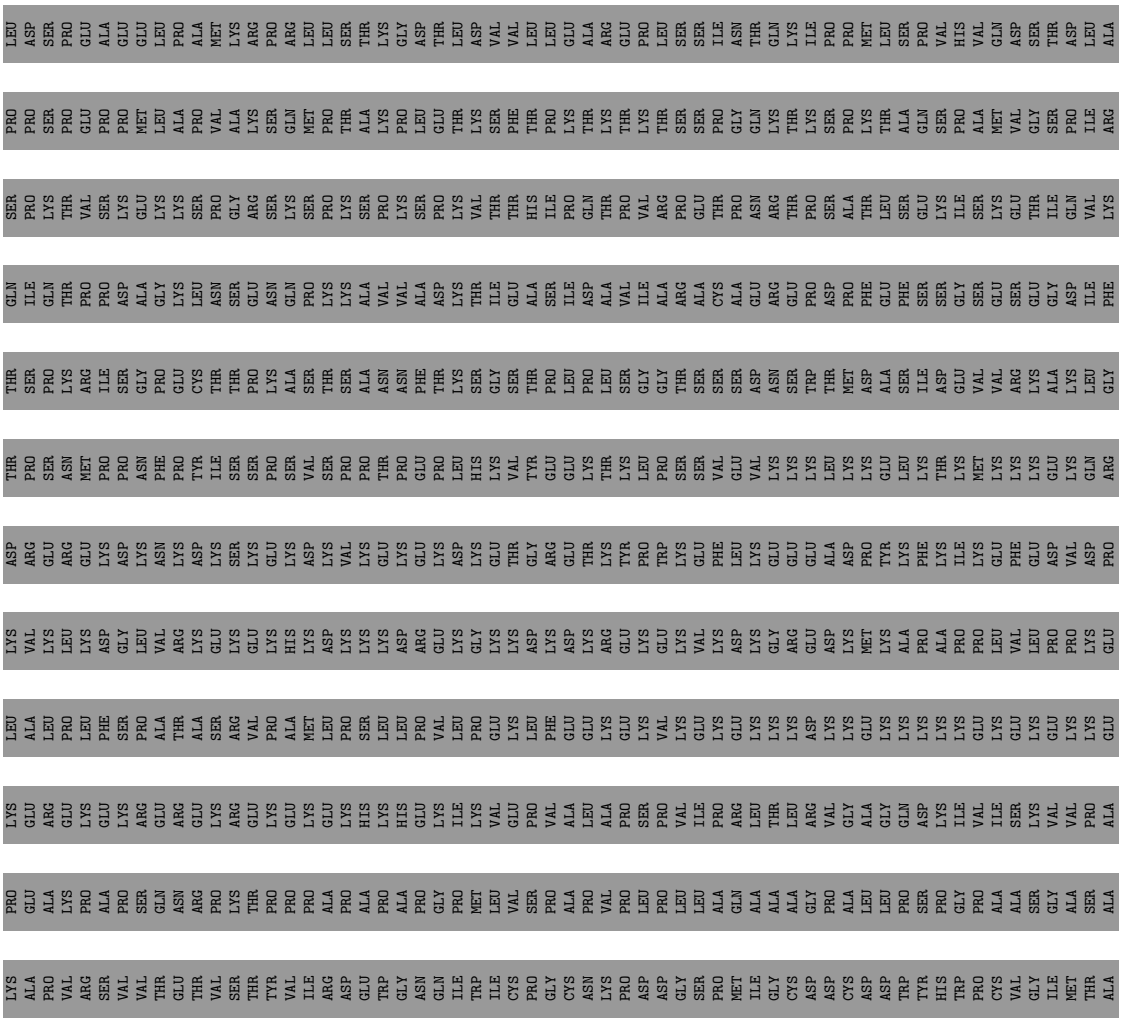




• Molecule 32: Transcription initiation factor TFIID subunit 3

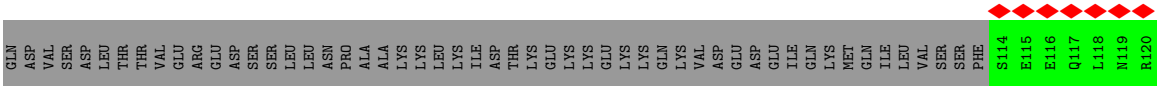


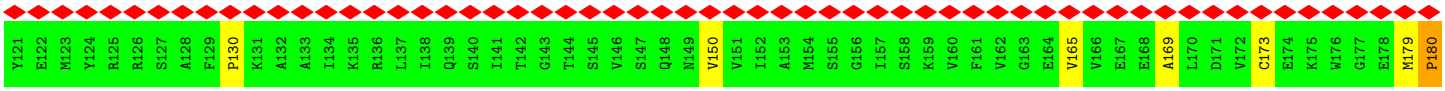


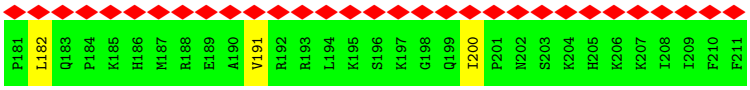


• Molecule 33: Transcription initiation factor TFIID subunit 11

Chain Dk:

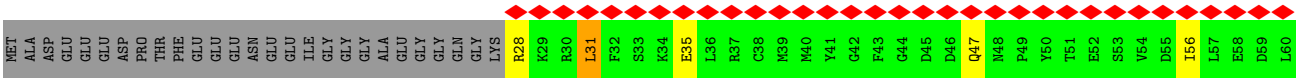


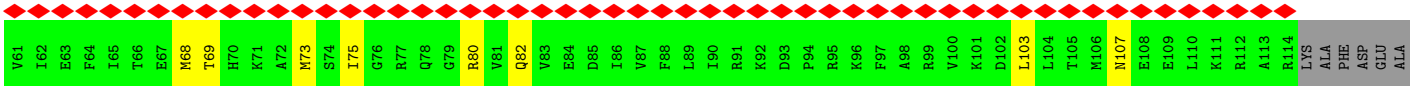




• Molecule 34: Transcription initiation factor TFIID subunit 13

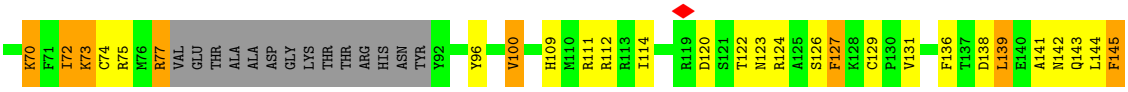
Chain Dm:

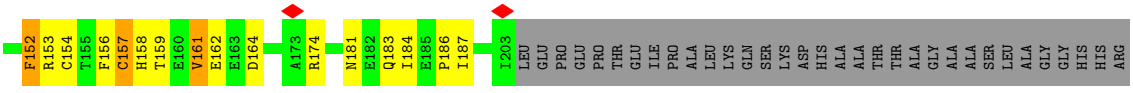


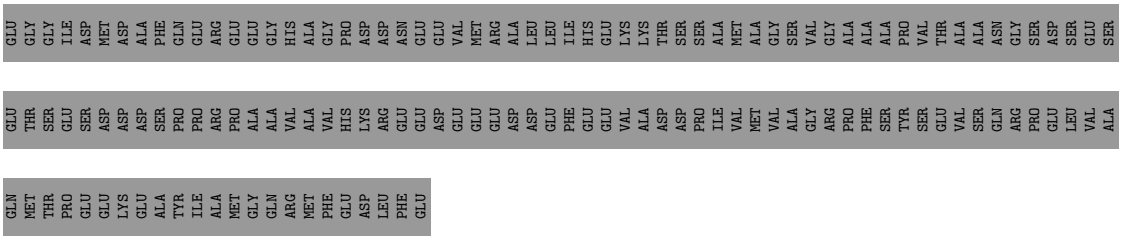


• Molecule 35: General transcription factor IIE subunit 1

Chain EA:

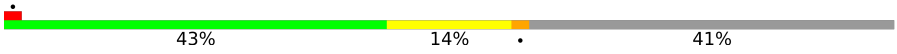


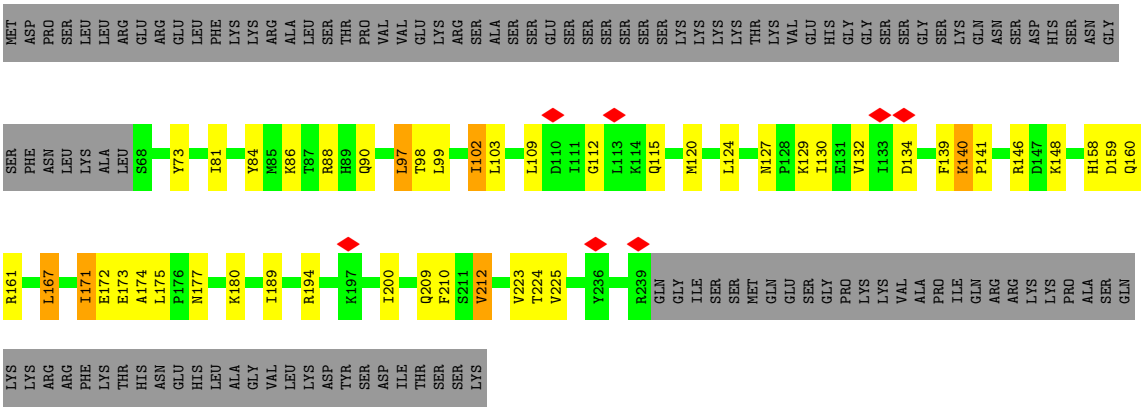




• Molecule 36: Transcription initiation factor IIE subunit beta

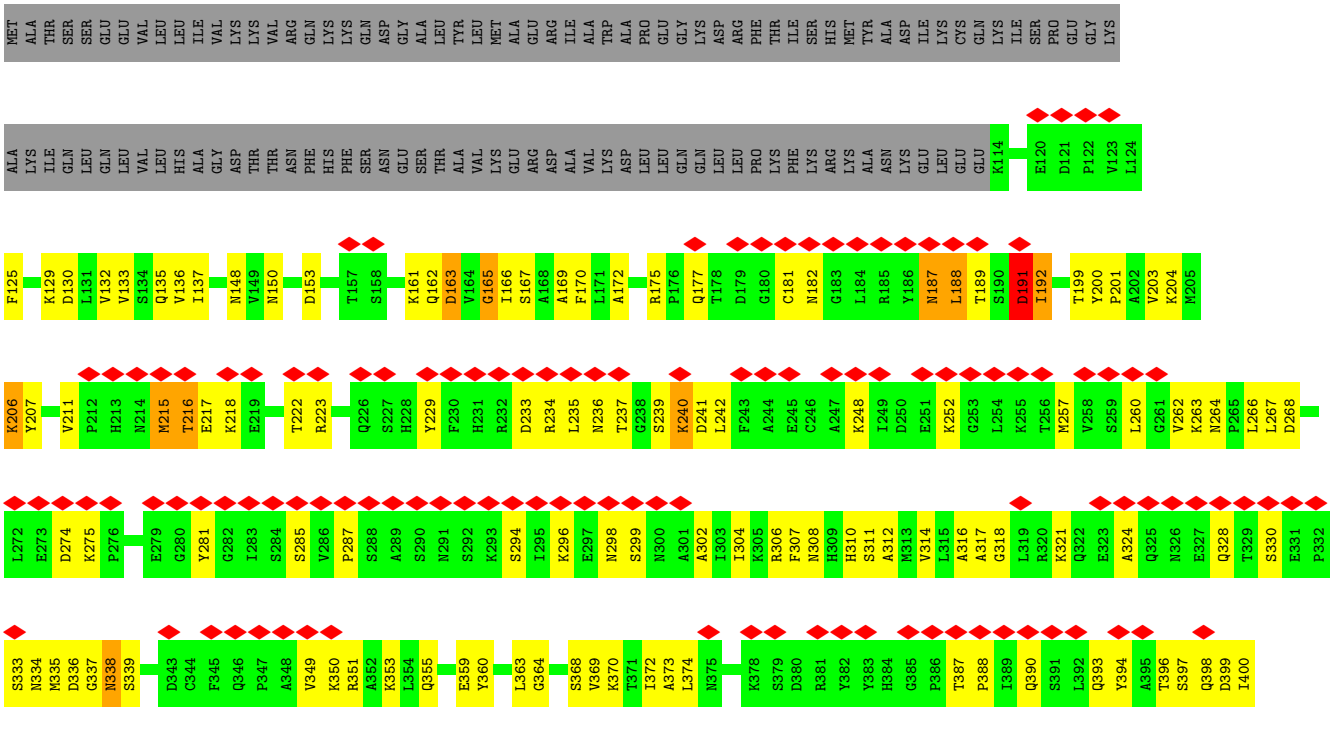
Chain EB:

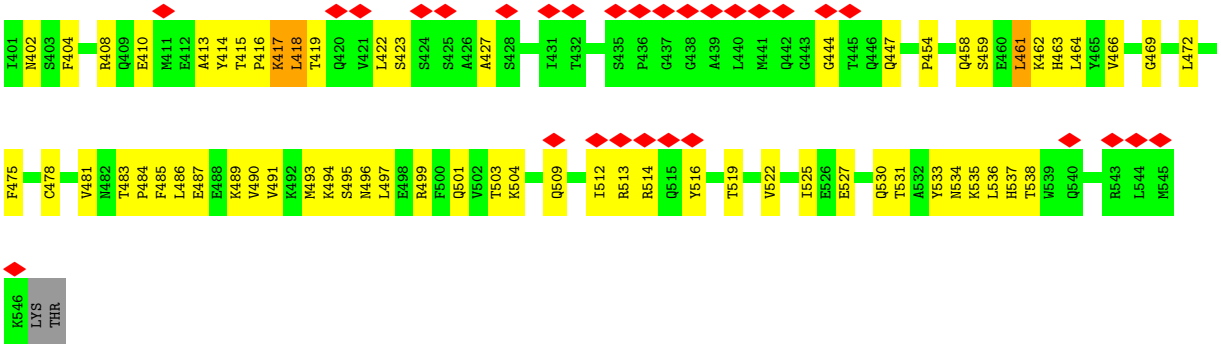




• Molecule 37: General transcription factor IIH subunit 1

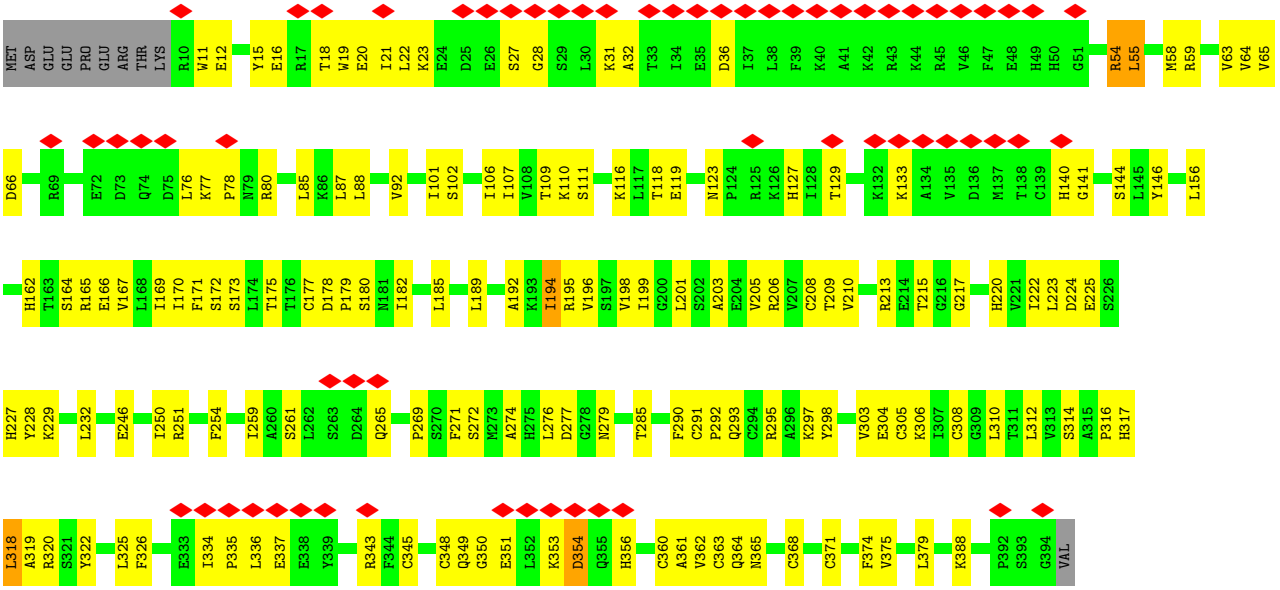
Chain 1:





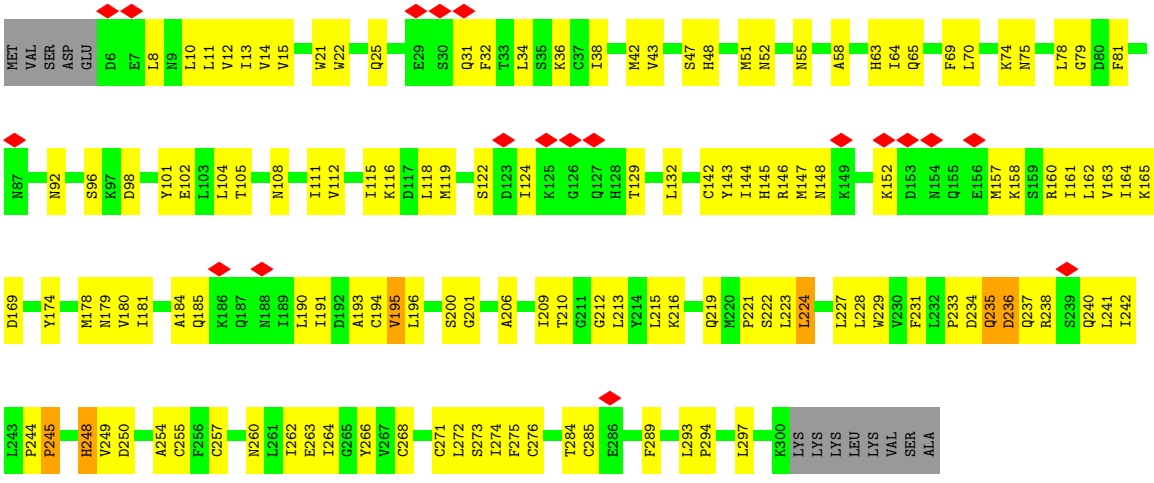
• Molecule 38: General transcription factor IIH subunit 2

Chain 2:



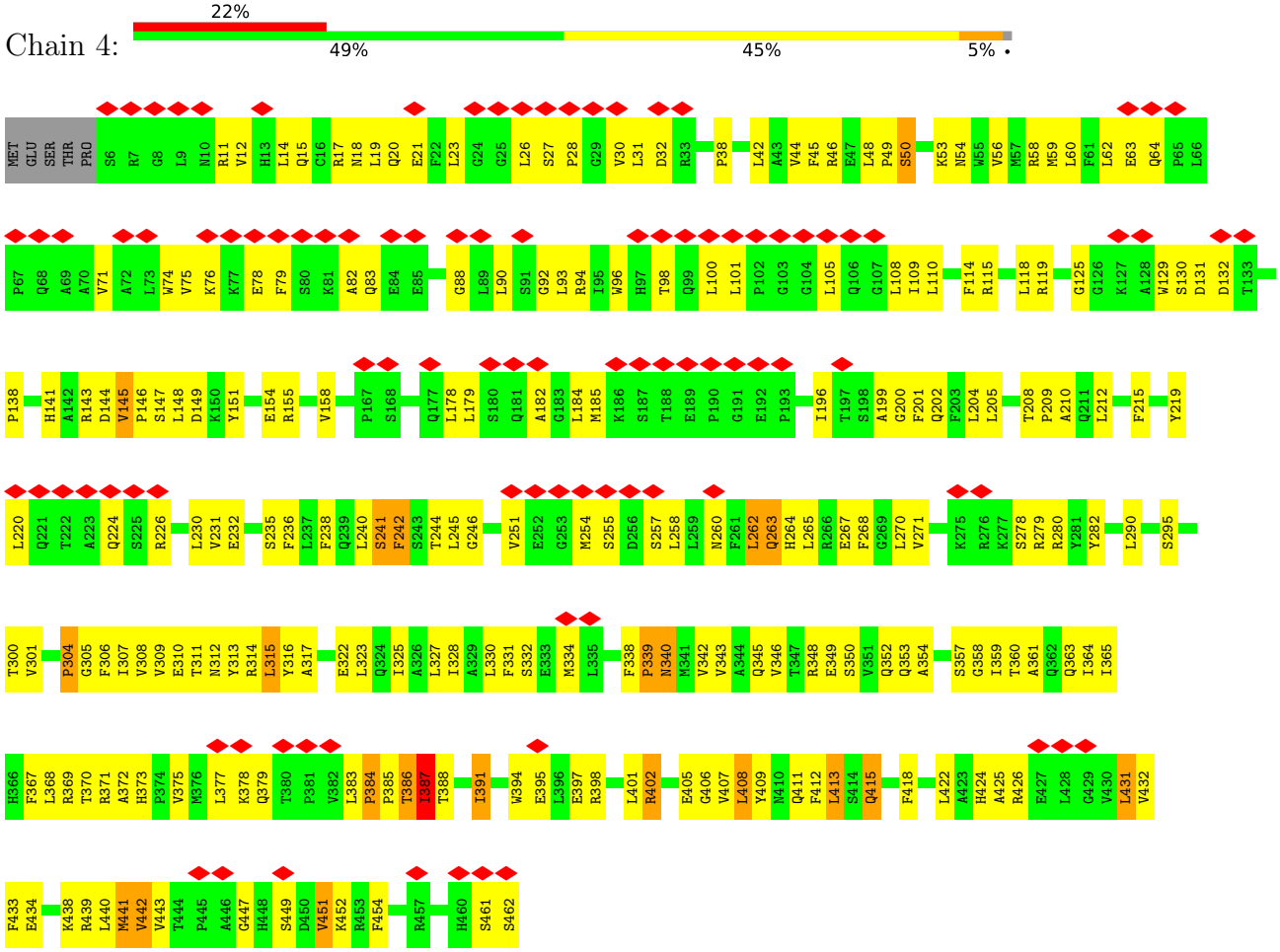
• Molecule 39: General transcription factor IIH subunit 3

Chain 3:



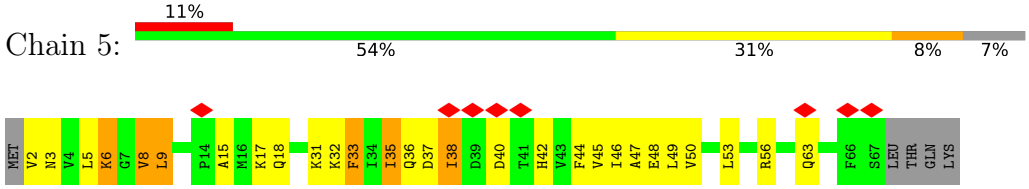
• Molecule 40: General transcription factor IIH subunit 4

Chain 4:



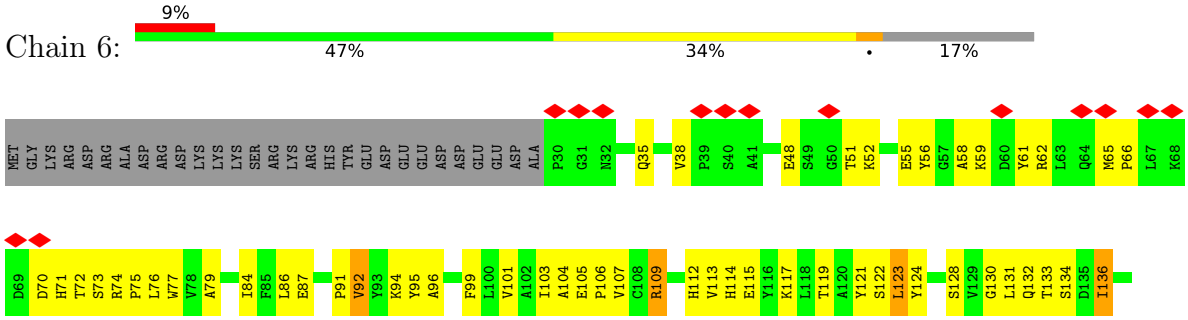
• Molecule 41: General transcription factor IIH subunit 5

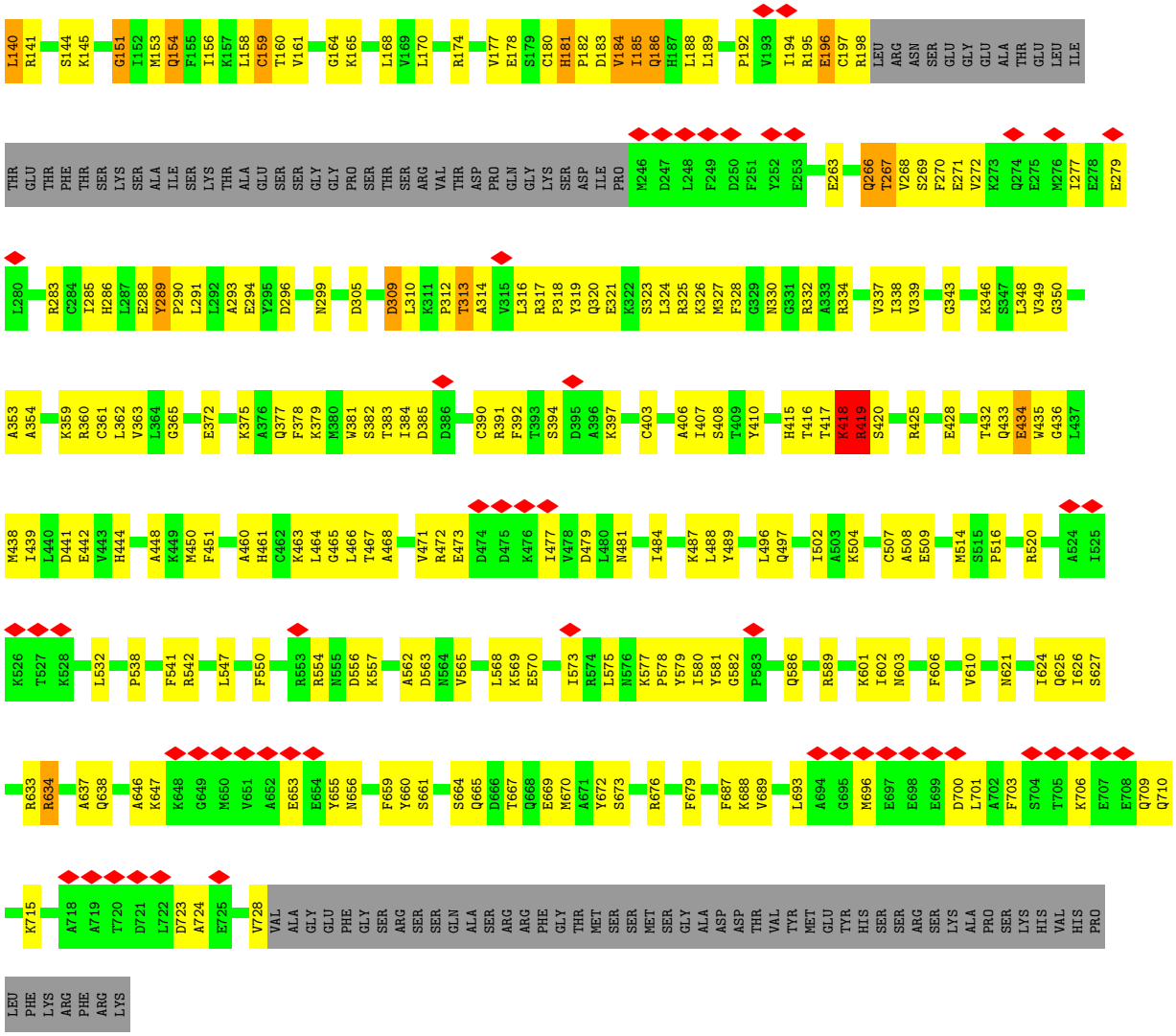
Chain 5:



• Molecule 42: General transcription and DNA repair factor IIH helicase subunit XPB

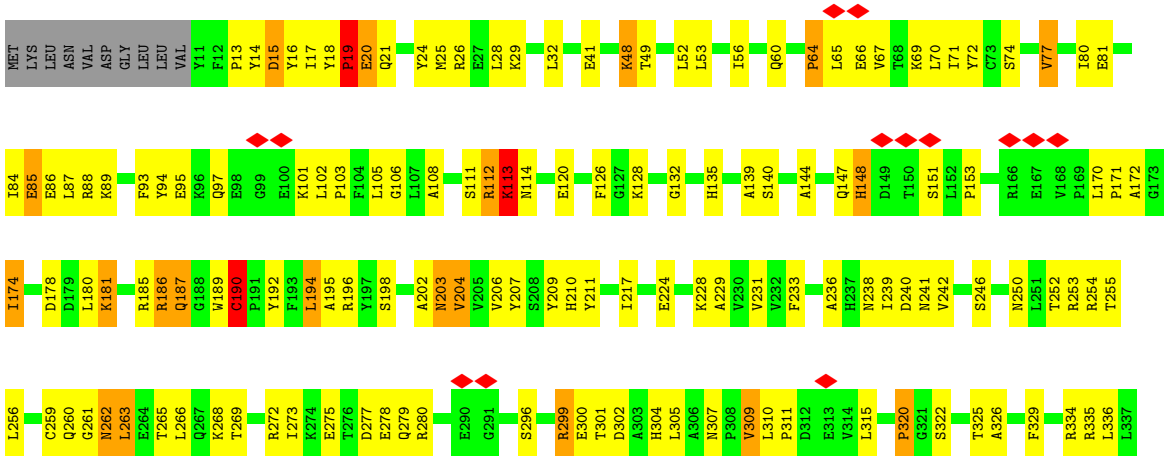
Chain 6:

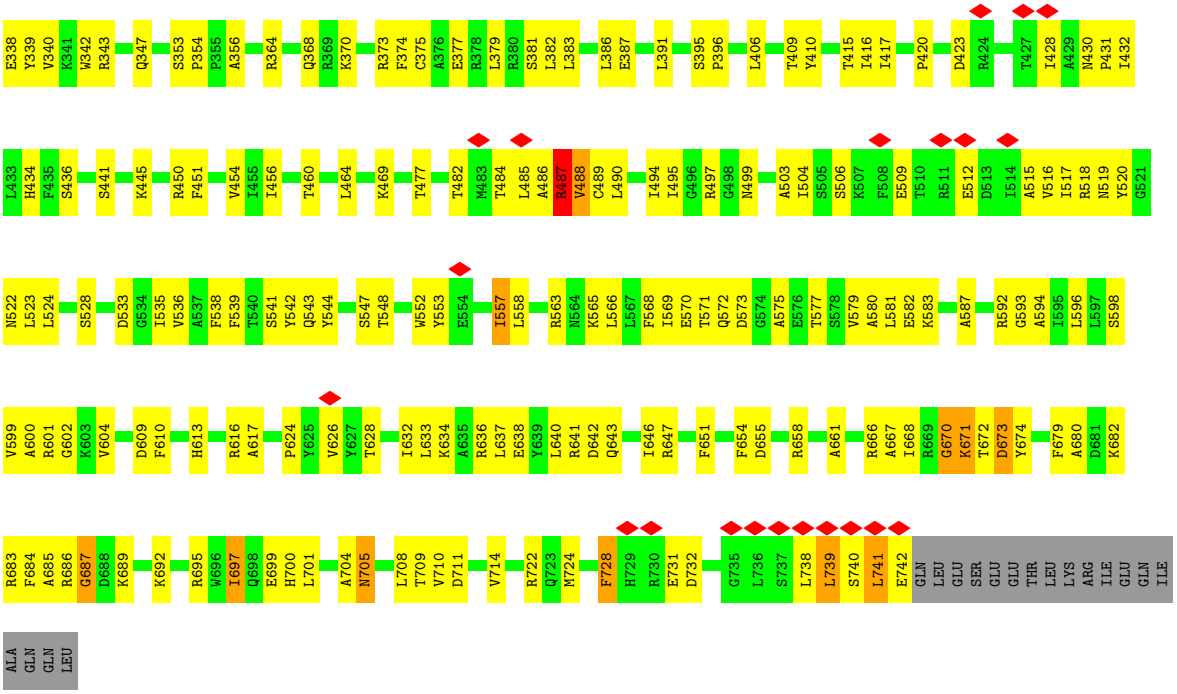




• Molecule 43: General transcription and DNA repair factor IIH helicase subunit XPD

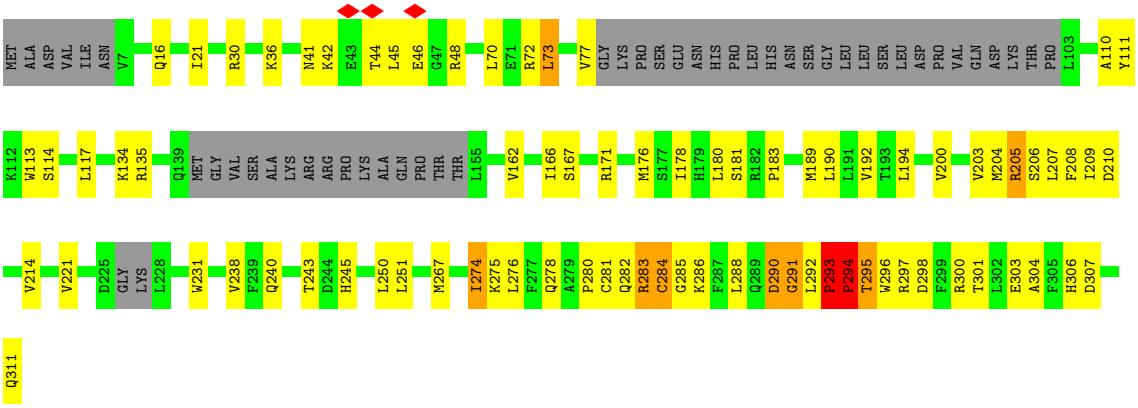
Chain 7:





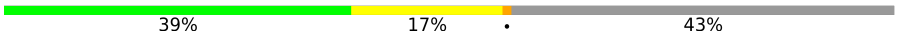
• Molecule 44: Mediator of RNA polymerase II transcription subunit 27

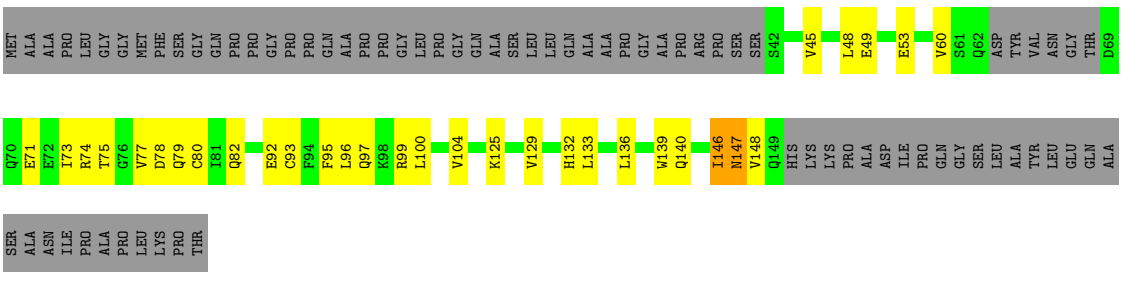
Chain c:



• Molecule 45: Mediator of RNA polymerase II transcription subunit 28

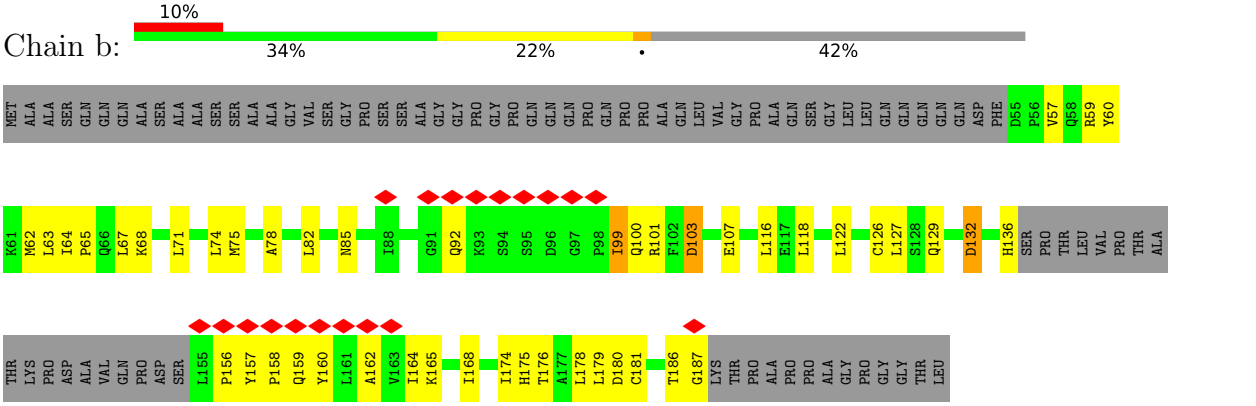
Chain e:





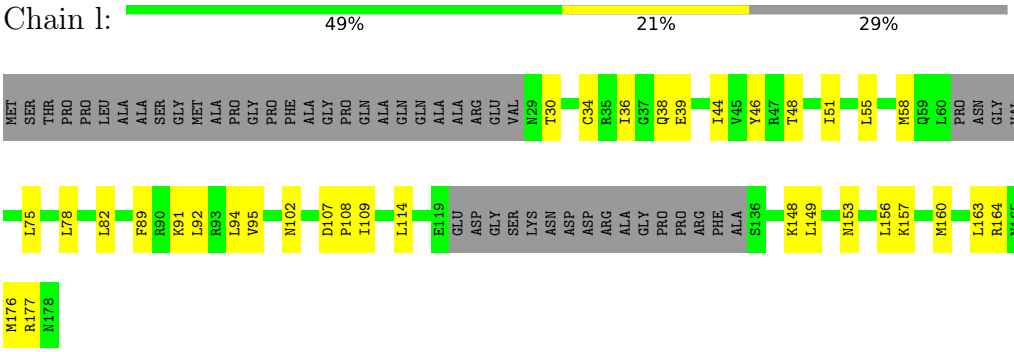
• Molecule 46: Mediator of RNA polymerase II transcription subunit 29

Chain b:



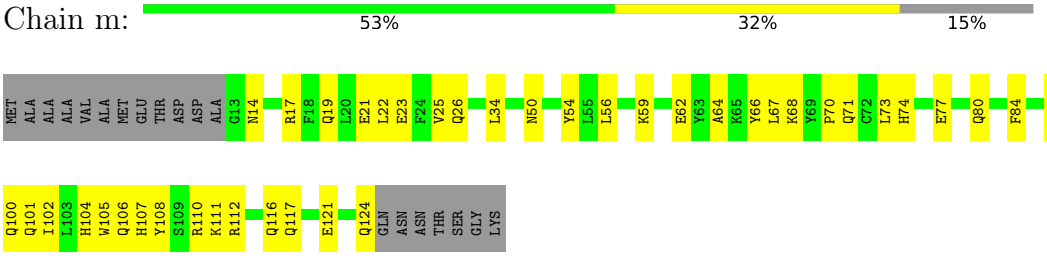
• Molecule 47: Mediator of RNA polymerase II transcription subunit 30

Chain l:



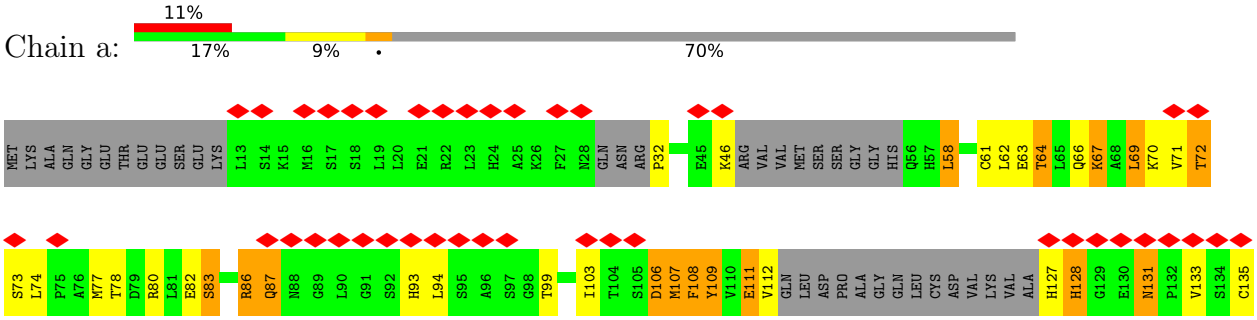
• Molecule 48: Mediator of RNA polymerase II transcription subunit 31

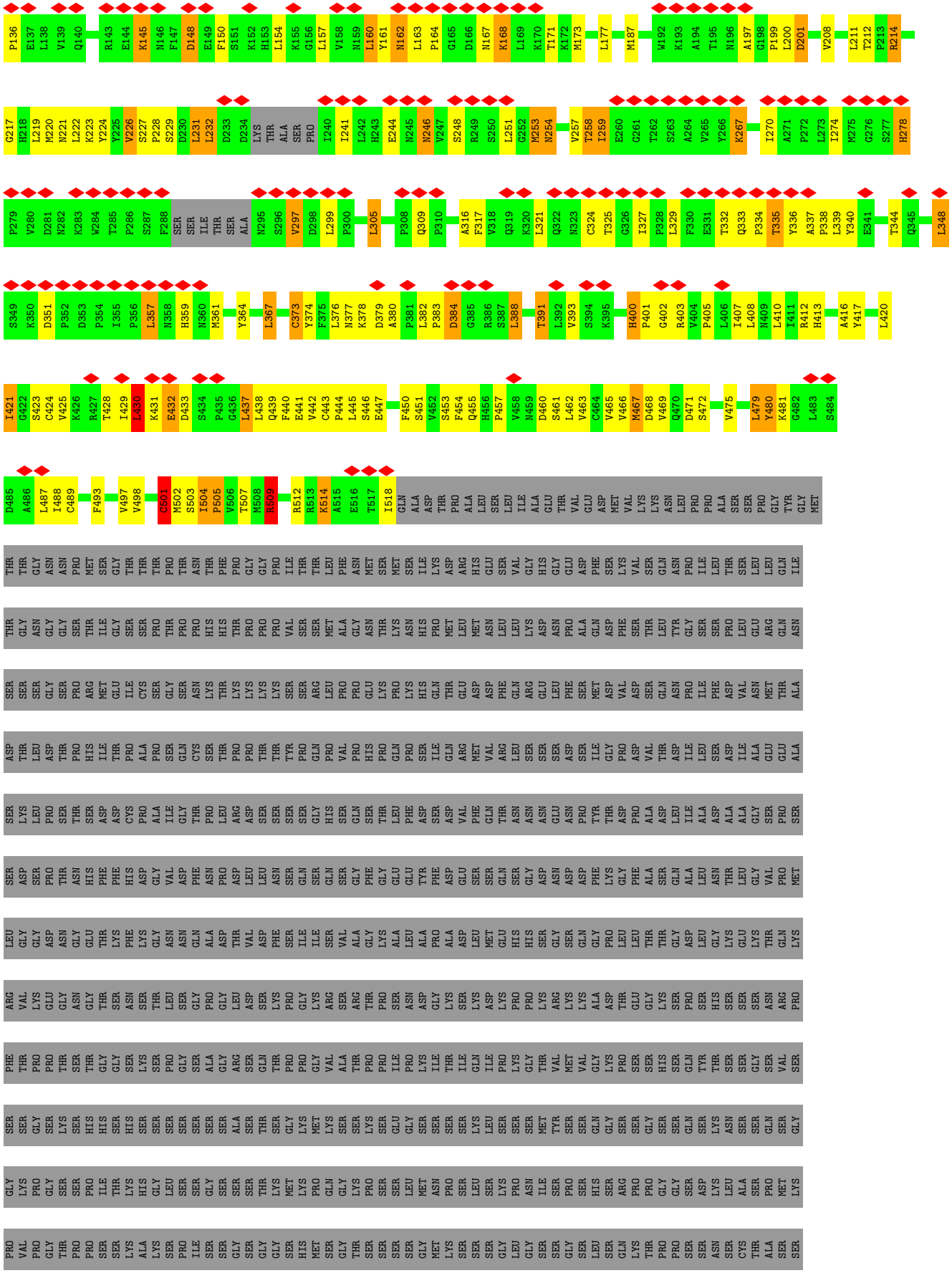
Chain m:

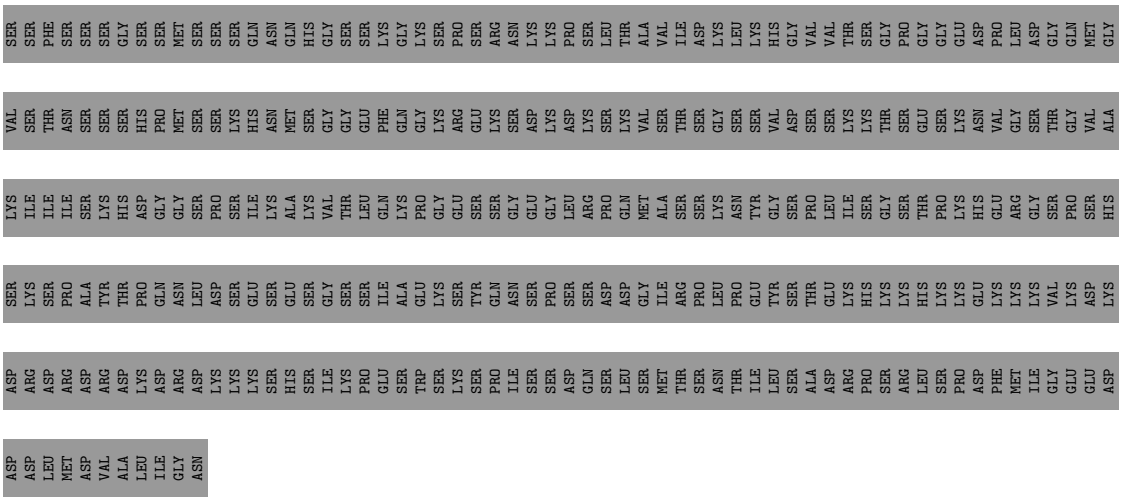


• Molecule 49: Mediator of RNA polymerase II transcription subunit 1

Chain a:

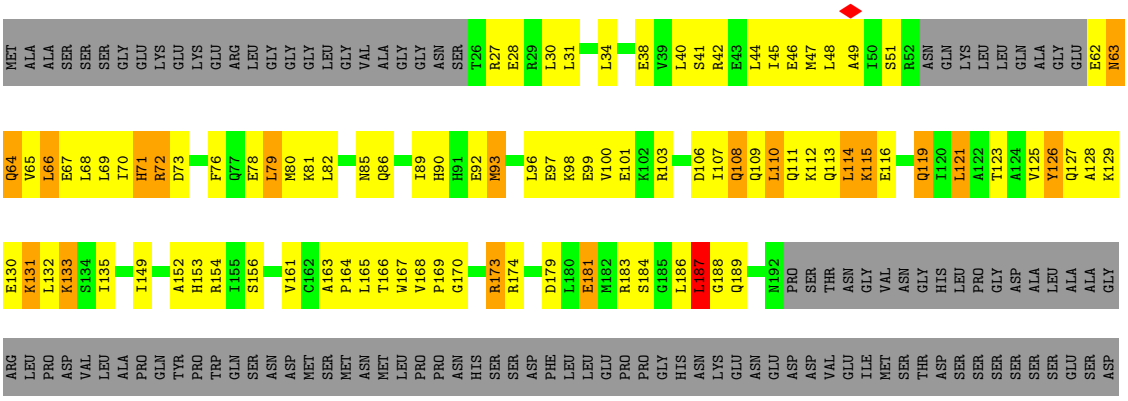



P136 E137 L138 V139 Q140 R143 E144 K145 N146 F147 D148 E149 F150 S151 K152 H153 L154 K155 G156 L157 V158 N159 L160 Y161 N162 L163 P164 G165 D166 N167 K168 L169 K170 T171 K172 M173 L177 M187 W192 K193 A194 T195 N196 A197 G198 P199 L200 D201 V208 L211 T212 P213 R214
G217 H218 L219 M220 N221 L222 K223 Y224 Y225 V226 S227 P228 S229 D230 L231 L232 D233 D234 LYS THR ALA SER PRO T240 I241 L242 H243 E244 N245 N246 V247 S248 R249 S250 L251 G252 M253 N254 V257 T258 I259 E260 C261 T262 S263 A264 V265 Y266 K267 I270 A271 P272 L273 I274 M275 G276 S277 H278
P279 V280 D281 N282 K283 W284 T285 P286 S287 F288 SER SER ILE THR SER ALA N295 S296 V297 D298 L299 P300 L305 P308 Q309 P310 A316 F317 V318 Q319 K320 L321 Q322 N323 C324 T325 G326 I327 P328 L329 F330 E331 T332 Q333 P334 T335 Y336 A337 P338 L339 Y340 E341 T344 Q345 L348
S349 K350 D351 P352 D353 P354 I355 P356 L357 N358 H359 N360 M361 Y364 L367 C373 Y374 F375 L376 N377 K378 D379 A380 P381 L382 P383 D384 G385 R386 S387 L388 T391 L392 V393 S394 K395 H400 P401 G402 R403 V404 P405 L406 I407 L408 N409 L410 I411 R412 H413 A416 Y417 L420
I421 G422 S423 C424 V425 K426 R427 T428 I429 L430 K431 E432 D433 S434 P435 G436 L437 L438 Q439 F440 E441 V442 C443 P444 L445 S446 E447 F450 S451 V452 S453 F454 Q455 H456 P457 V458 N459 D460 S461 L462 V463 C464 V465 V466 M467 D468 V469 Q470 D471 S472 V475 L479 Y480 K481 G482 L483 S484
D485 A486 L487 I488 C489 F493 V497 V498 C501 M502 S503 I504 P505 V506 T507 M508 R509 R512 R513 K514 A515 E516 T517 I518 GLN ALA ASP THR PRO ALA LEU SER LEU ILE ALA GLU THR VAL GLU ASP MET VAL LYS LYS ASN LEU PRO PRO ALA SER SER PRO GLY TYR GLY MET
THR THR GLY ASN ASN PRO MET SER GLY THR THR THR PRO THR ASN THR PHE PRO GLY GLY PRO ILE THR THR LEU PHE ASN MET SER MET SER ILE LYS ASP ARG HIS GLU SER VAL GLY HIS GLY GLU ASP PHE SER LYS VAL SER GLN ASN PRO ILE LEU THR SER LEU LEU GLN ILE
THR GLY ASN GLY GLY SER THR ILE GLY SER SER PRO THR PRO PRO HIS HIS THR PRO PRO PRO VAL SER SER MET ALA ALA GLY ASN THR LYS ASN HIS PRO MET LEU MET ASN LEU LEU LYS ASP ASN PRO ALA GLN ASP PHE SER THR LEU TYR GLY SER SER PRO LEU GLU ARG GLN ASN
SER SER SER GLY SER PRO ARG MET GLU ILE CYS SER GLY SER ASN LYS THR LYS LYS LYS LYS SER SER ARG LEU PRO PRO GLU LYS PRO LYS HIS GLN THR GLU ASP ASP PHE GLN ARG GLU LEU PHE SER MET ASP VAL ASP SER GLN ASN PRO ILE PHE ASP VAL ASN MET THR ALA
ASP THR LEU ASP THR PRO HIS ILE THR PRO ALA PRO SER GLN CYS SER THR PRO PRO THR THR TYR PRO GLN PRO VAL PRO HIS PRO GLN PRO SER ILE GLN ARG MET VAL ARG LEU SER SER SER ASP SER ILE GLY PRO ASP VAL THR ASP ILE LEU SER ASP ILE ALA GLU GLU ALA
SER LYS LEU PRO SER THR SER ASP ASP CYS PRO ALA ILE GLY THR PRO LEU ARG ASP SER SER SER GLY HIS SER GLN SER SER THR LEU PHE ASP SER ASP VAL PHE GLN THR ASN ASN ASN GLU ASN PRO TYR THR ASP PRO ALA ASP ALA ASP ALA ALA GLY SER PRO PRO SER
SER ASP SER PRO THR HIS PHE PHE HIS ASP GLY VAL ASP PHE ASN PRO ASP LEU LEU ASN LEU SER GLY PHE GLY GLU GLU TYR PHE ASP GLU SER SER GLN SER GLY ASP ASN ASP PHE LYS GLY PHE ALA SER GLN ALA ALA LEU ASN THR LEU GLY ASP LEU LEU GLY LYS GLU LYS GLY VAL PRO MET
LEU GLY GLY ASP ASN GLY GLU THR LYS PHE LYS GLY ASN ASN GLN ALA ASP THR VAL ASP PHE SER ILE ILE SER VAL ALA ALA GLY LYS ALA LEU ALA PRO ALA ASP LEU MET GLU HIS HIS SER GLY SER GLN GLY PRO LEU LEU THR THR GLY LYS GLU LYS GLY ASN ASP ASP ASP



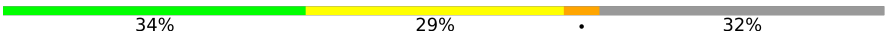
• Molecule 50: Mediator of RNA polymerase II transcription subunit 4

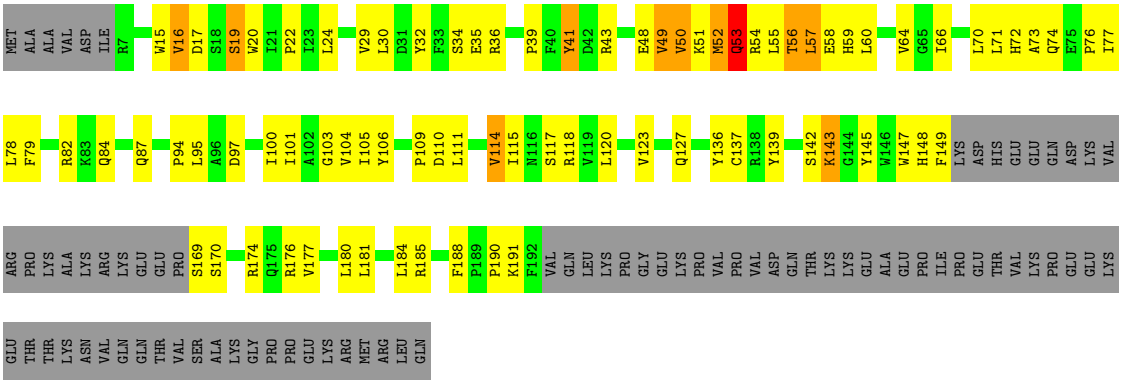
Chain d:



• Molecule 51: Mediator of RNA polymerase II transcription subunit 6

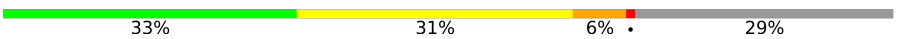
Chain f:

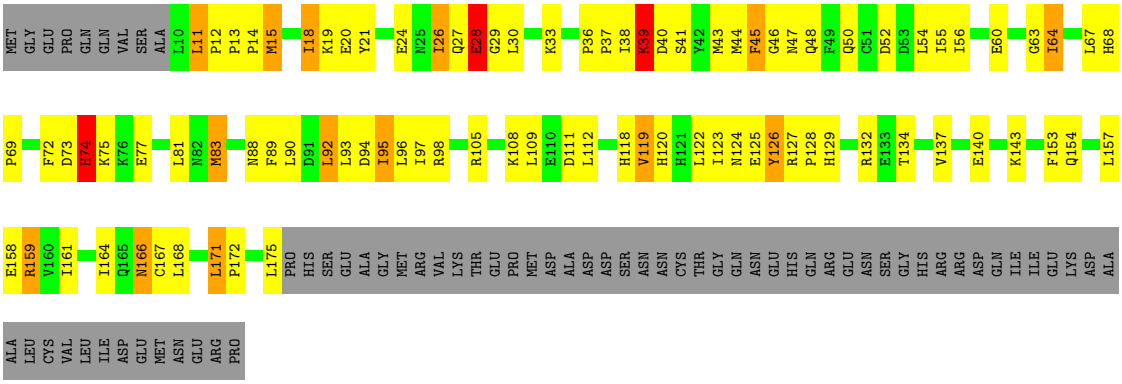




• Molecule 52: Mediator of RNA polymerase II transcription subunit 7

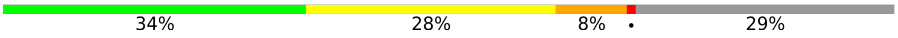
Chain g:

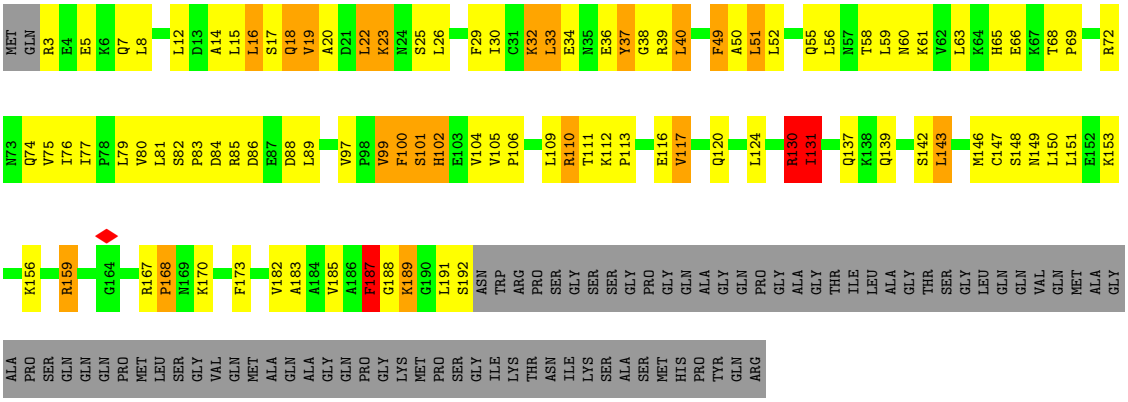




• Molecule 53: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

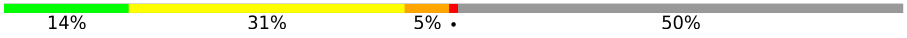
Chain h:

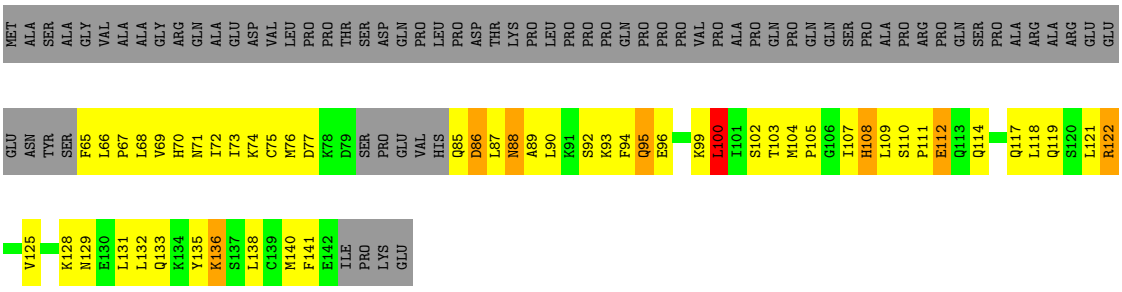




• Molecule 54: Mediator of RNA polymerase II transcription subunit 9

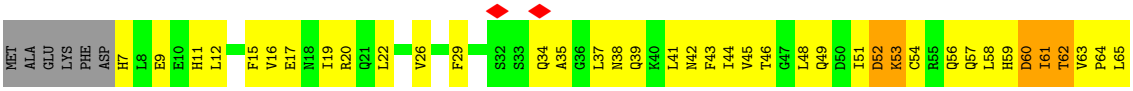
Chain i:

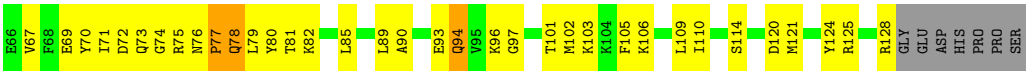




• Molecule 55: Mediator of RNA polymerase II transcription subunit 10

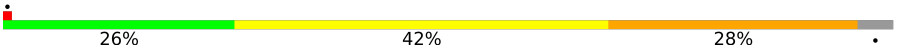
Chain j:

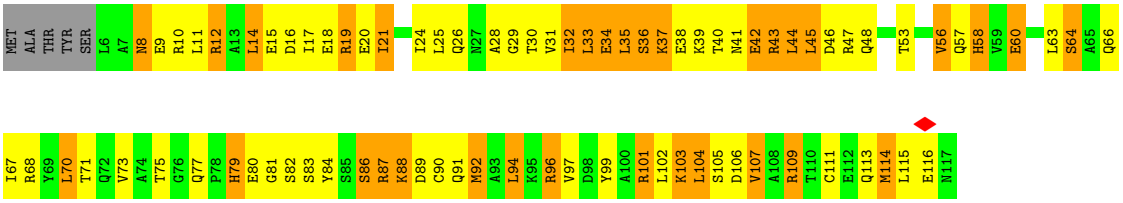




• Molecule 56: Mediator of RNA polymerase II transcription subunit 11

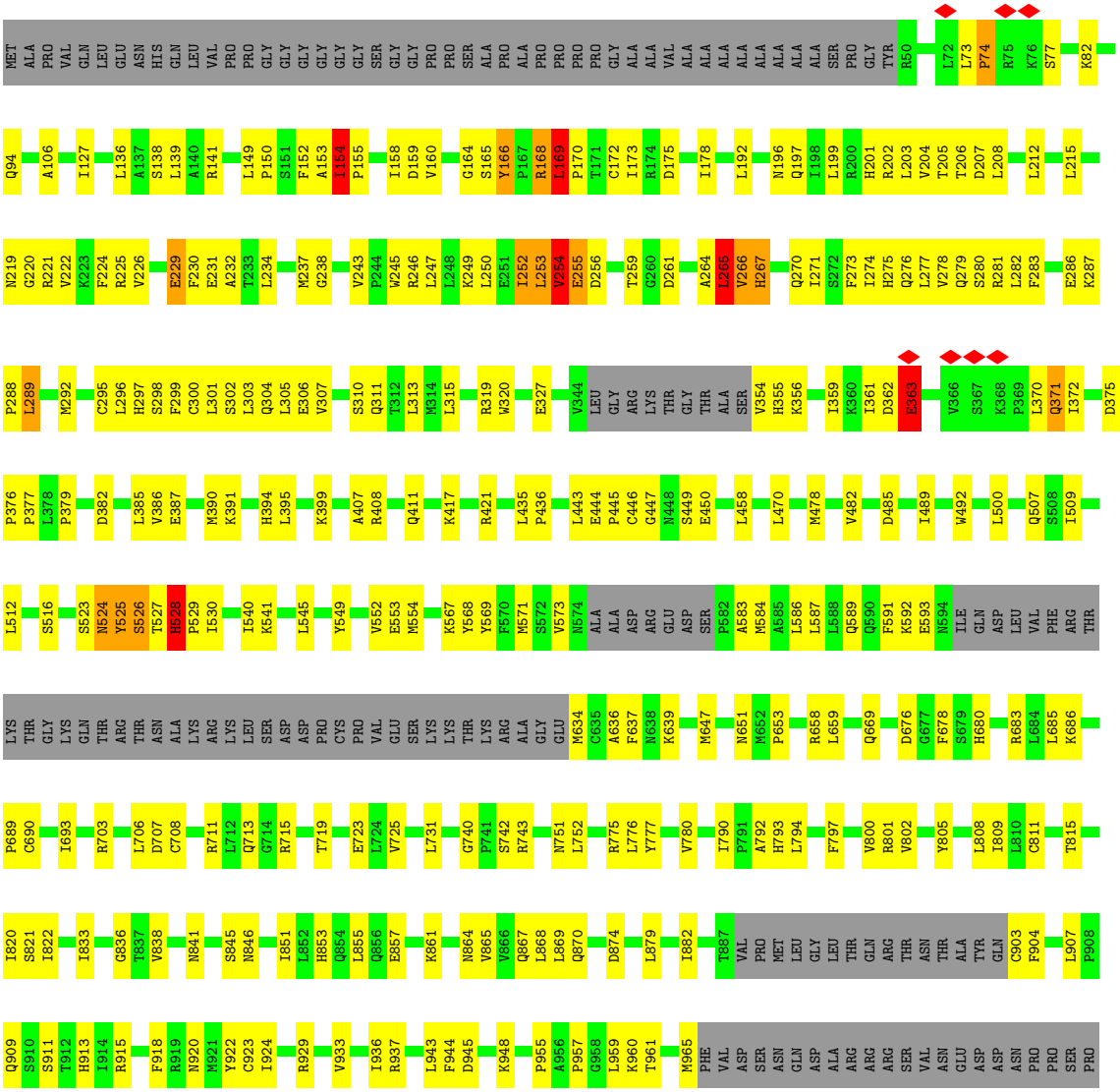
Chain k:

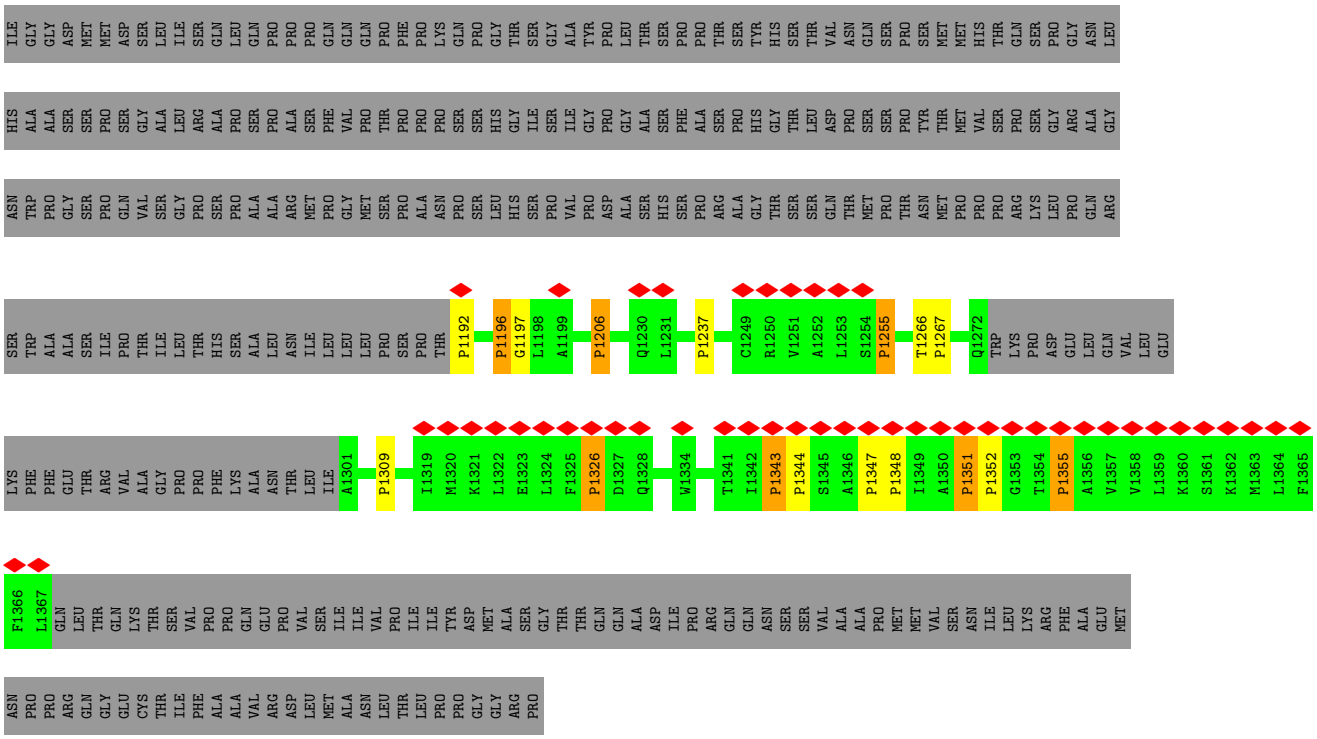




• Molecule 57: Mediator of RNA polymerase II transcription subunit 14

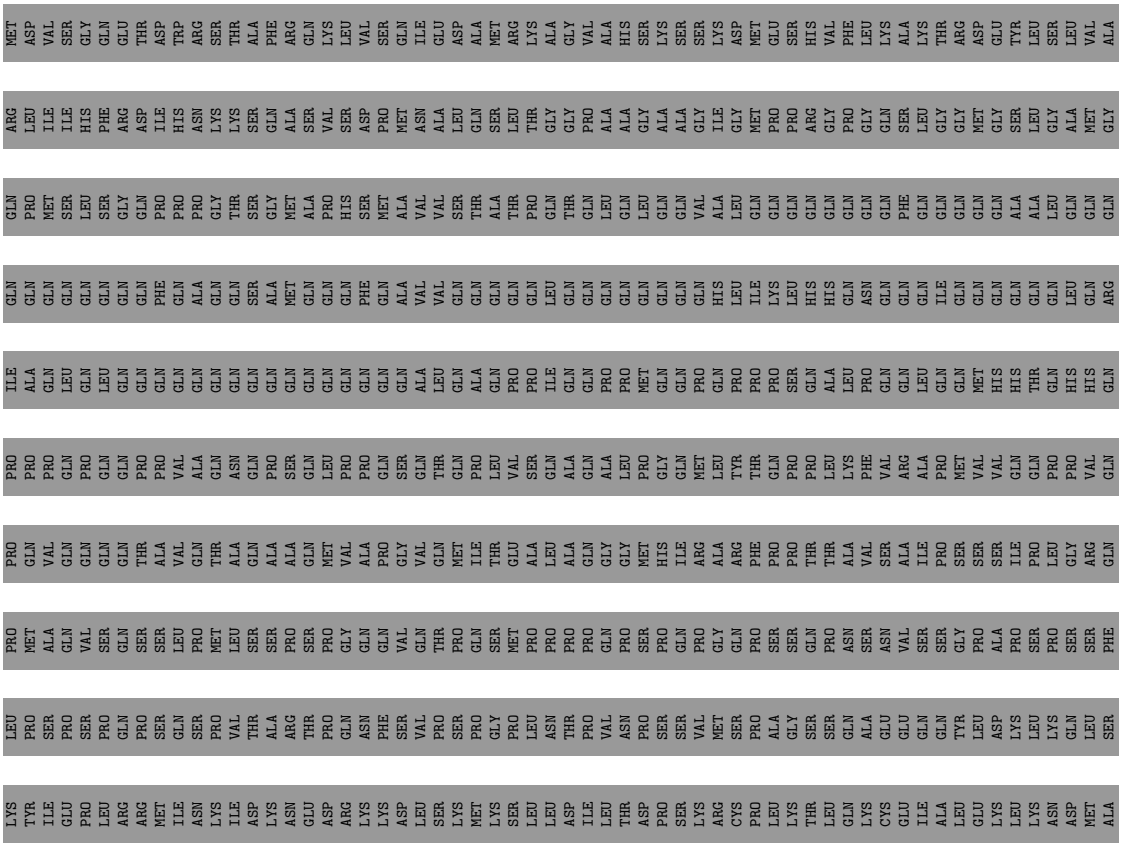
Chain n:

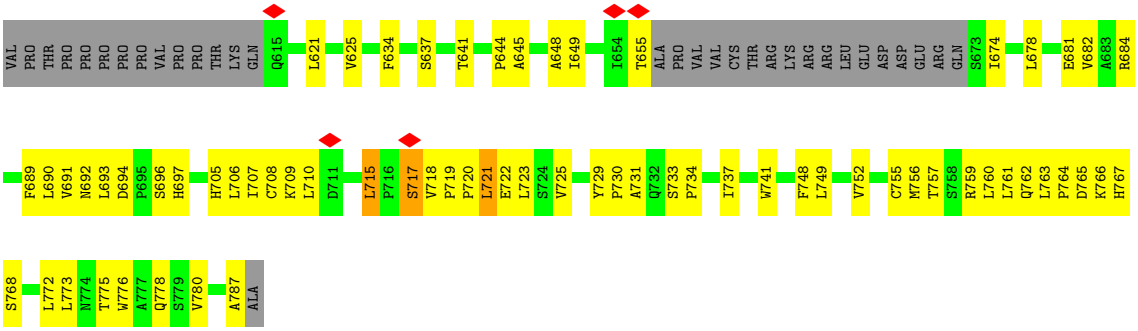




• Molecule 58: Mediator of RNA polymerase II transcription subunit 15

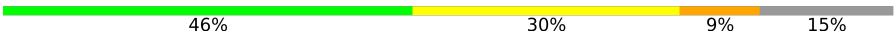
Chain o:

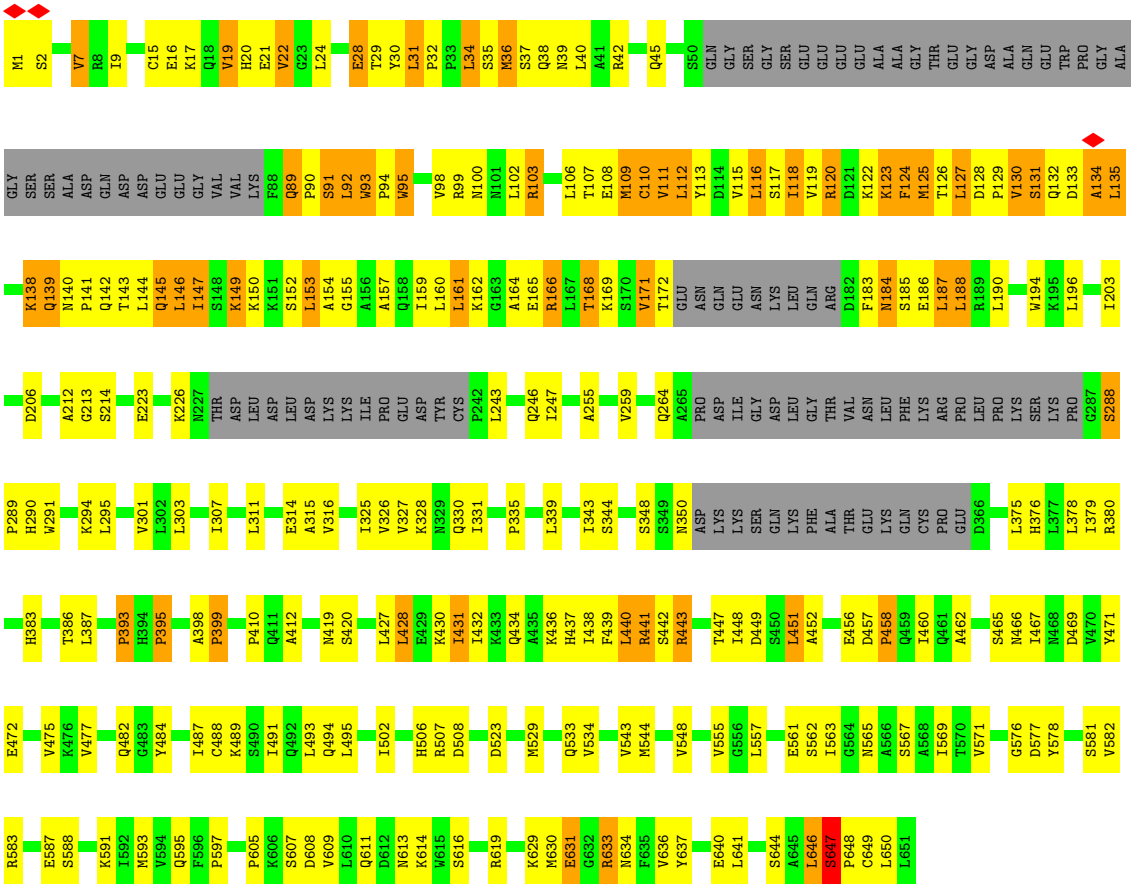




• Molecule 59: Mediator of RNA polymerase II transcription subunit 17

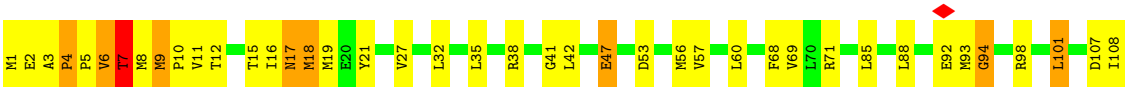
Chain q:





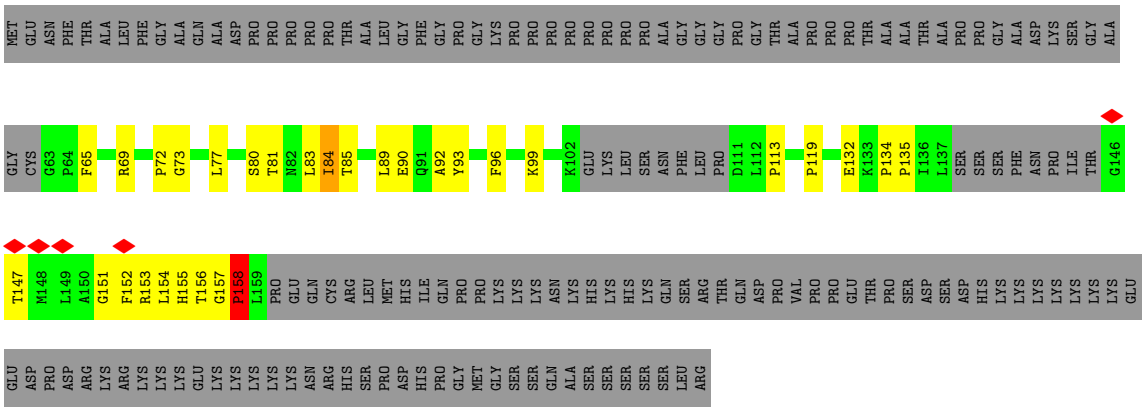
• Molecule 60: Mediator of RNA polymerase II transcription subunit 18

Chain r:



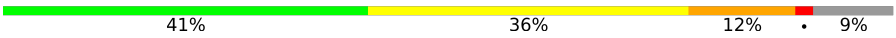
• Molecule 61: Mediator of RNA polymerase II transcription subunit 19

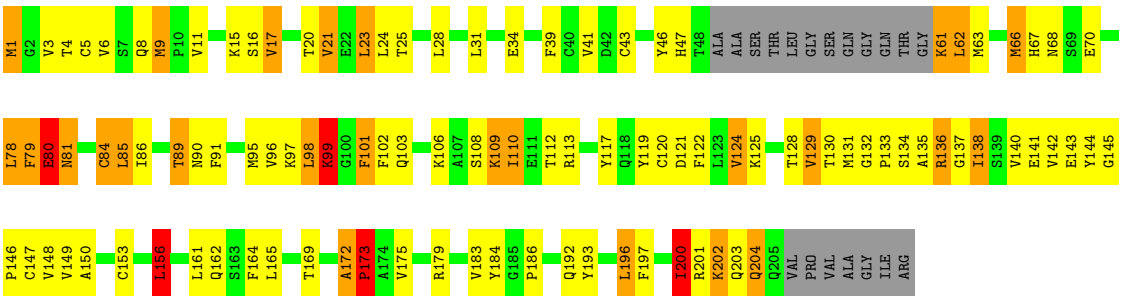
Chain s:



• Molecule 62: Mediator of RNA polymerase II transcription subunit 20

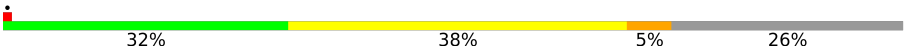
Chain t:

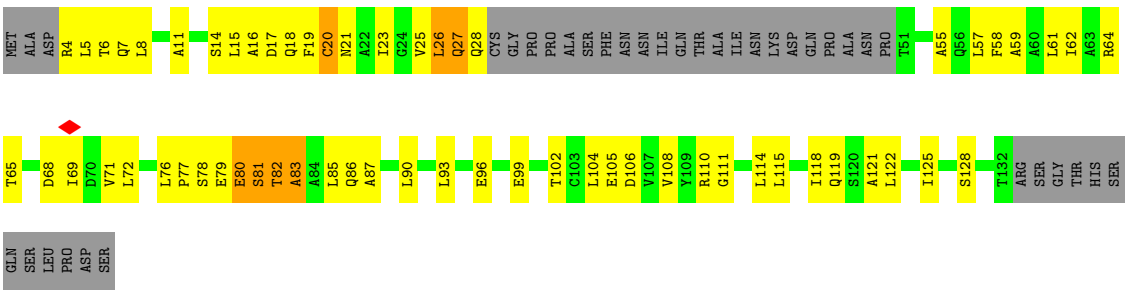




• Molecule 63: Mediator of RNA polymerase II transcription subunit 21

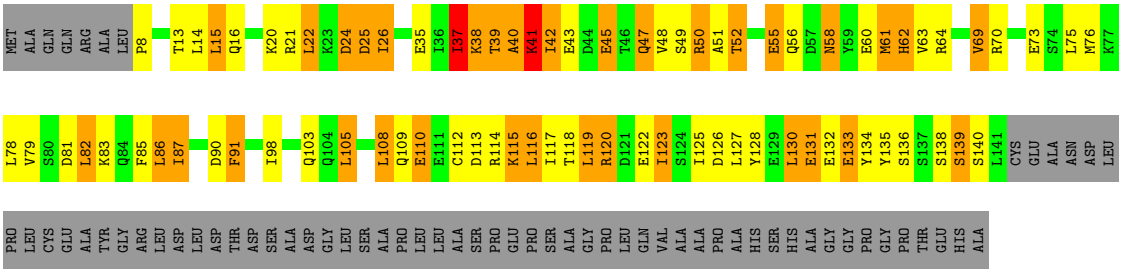
Chain u:





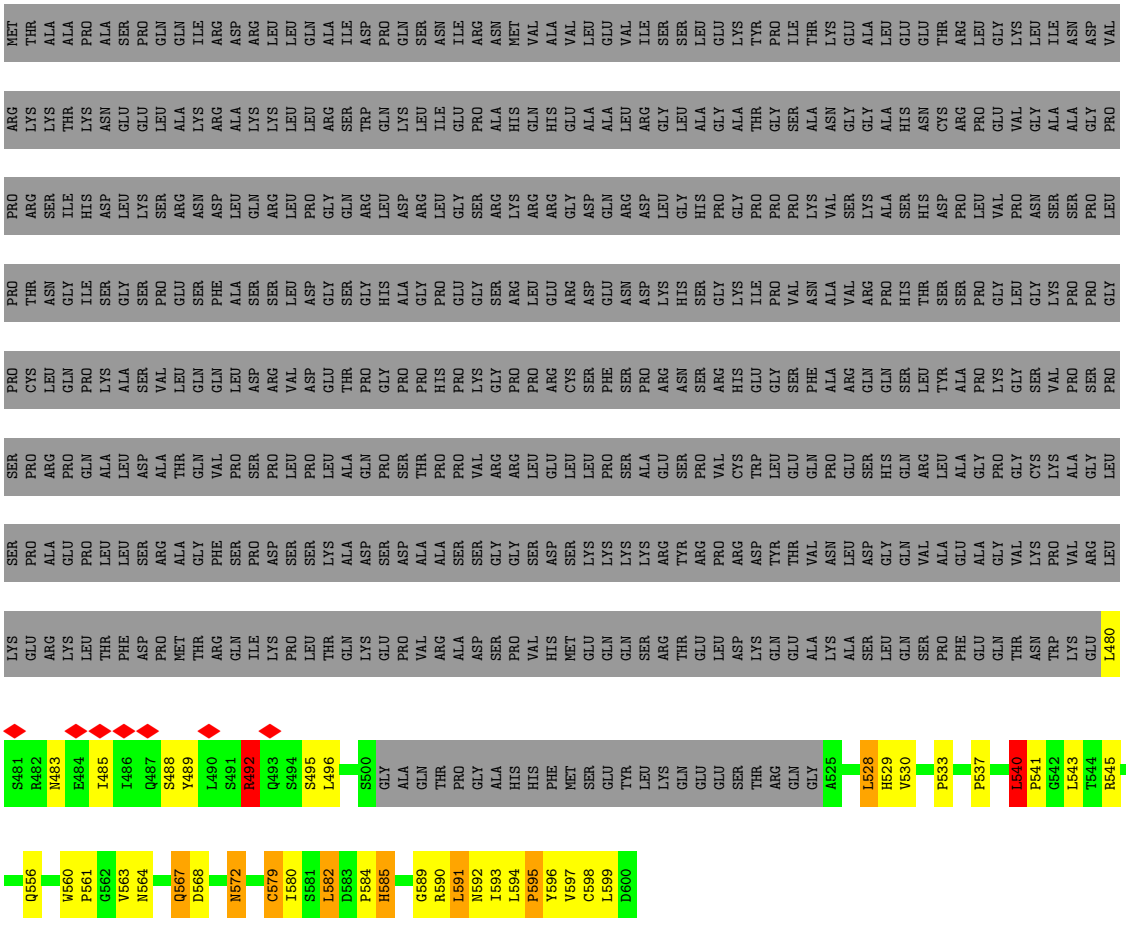
• Molecule 64: Mediator of RNA polymerase II transcription subunit 22

Chain v:



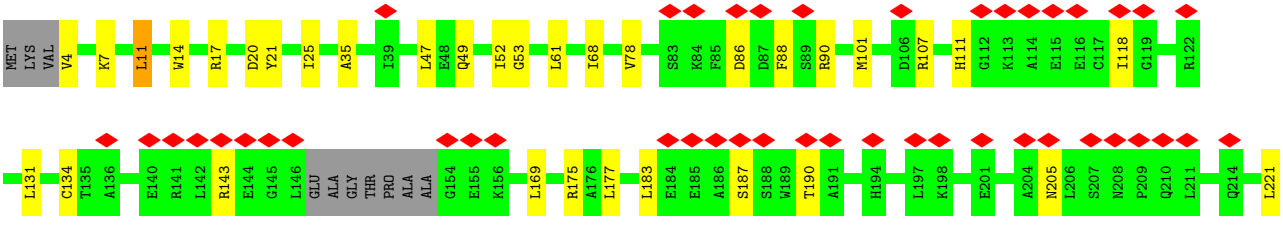
• Molecule 65: Mediator of RNA polymerase II transcription subunit 26

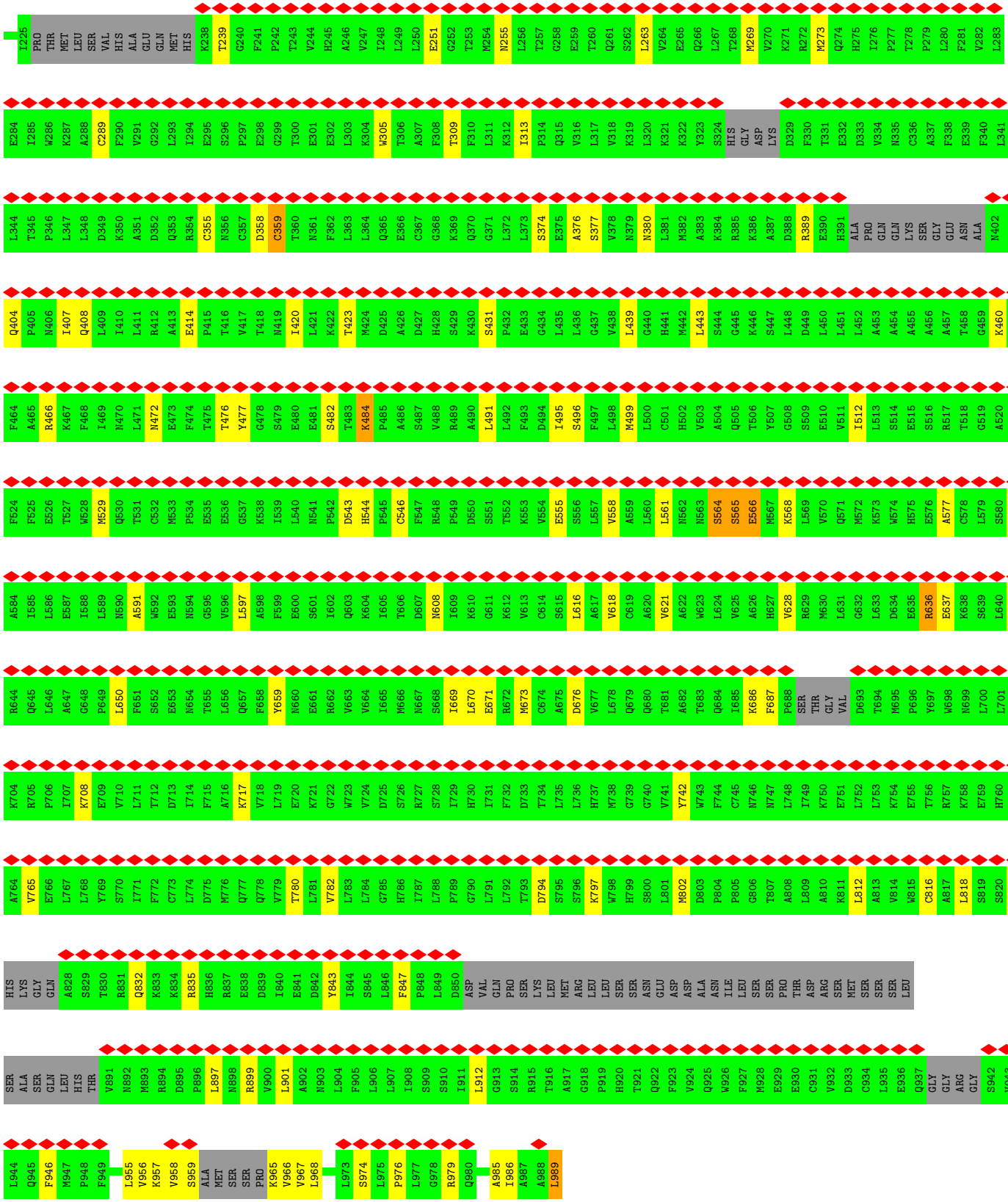
Chain z:



• Molecule 66: Mediator of RNA polymerase II transcription subunit 24

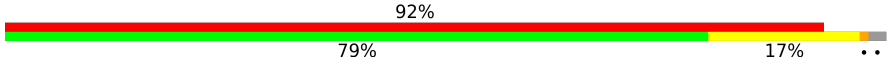
Chain x:

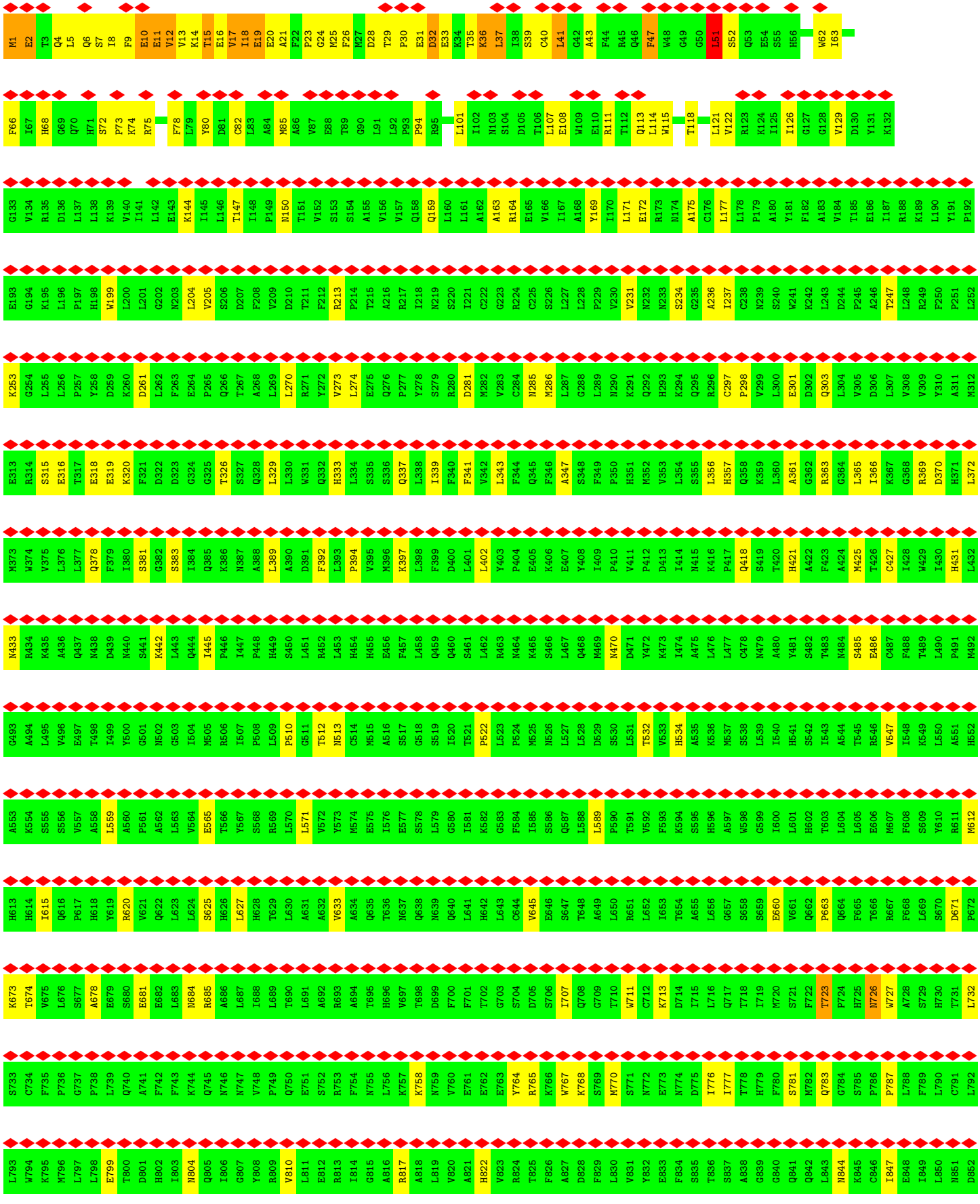


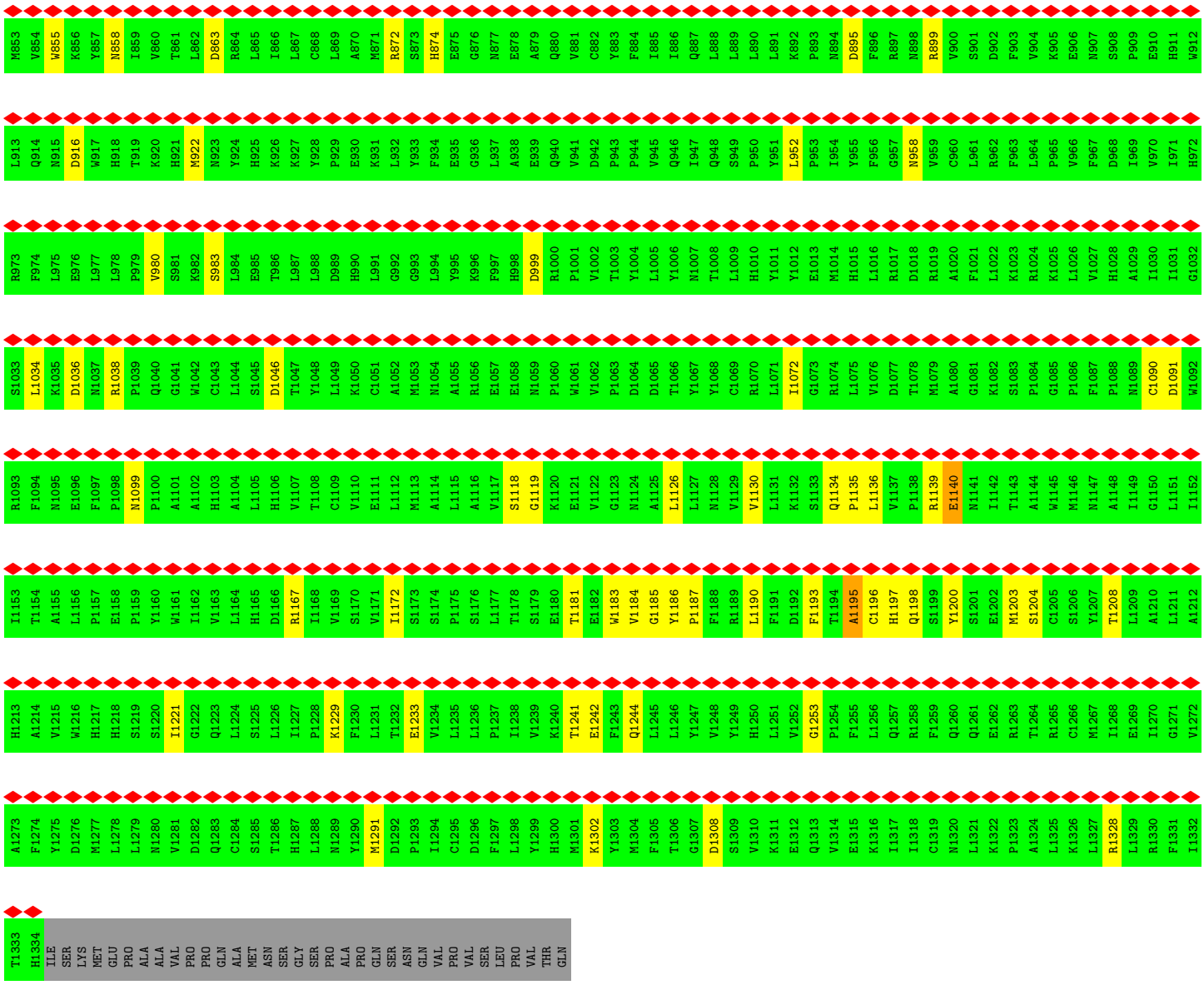


• Molecule 67: Mediator of RNA polymerase II transcription subunit 23

Chain w:

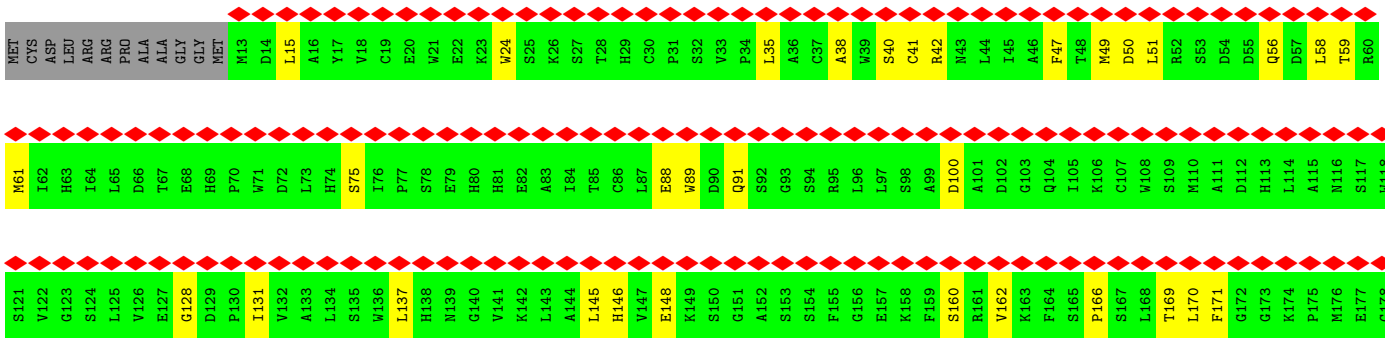


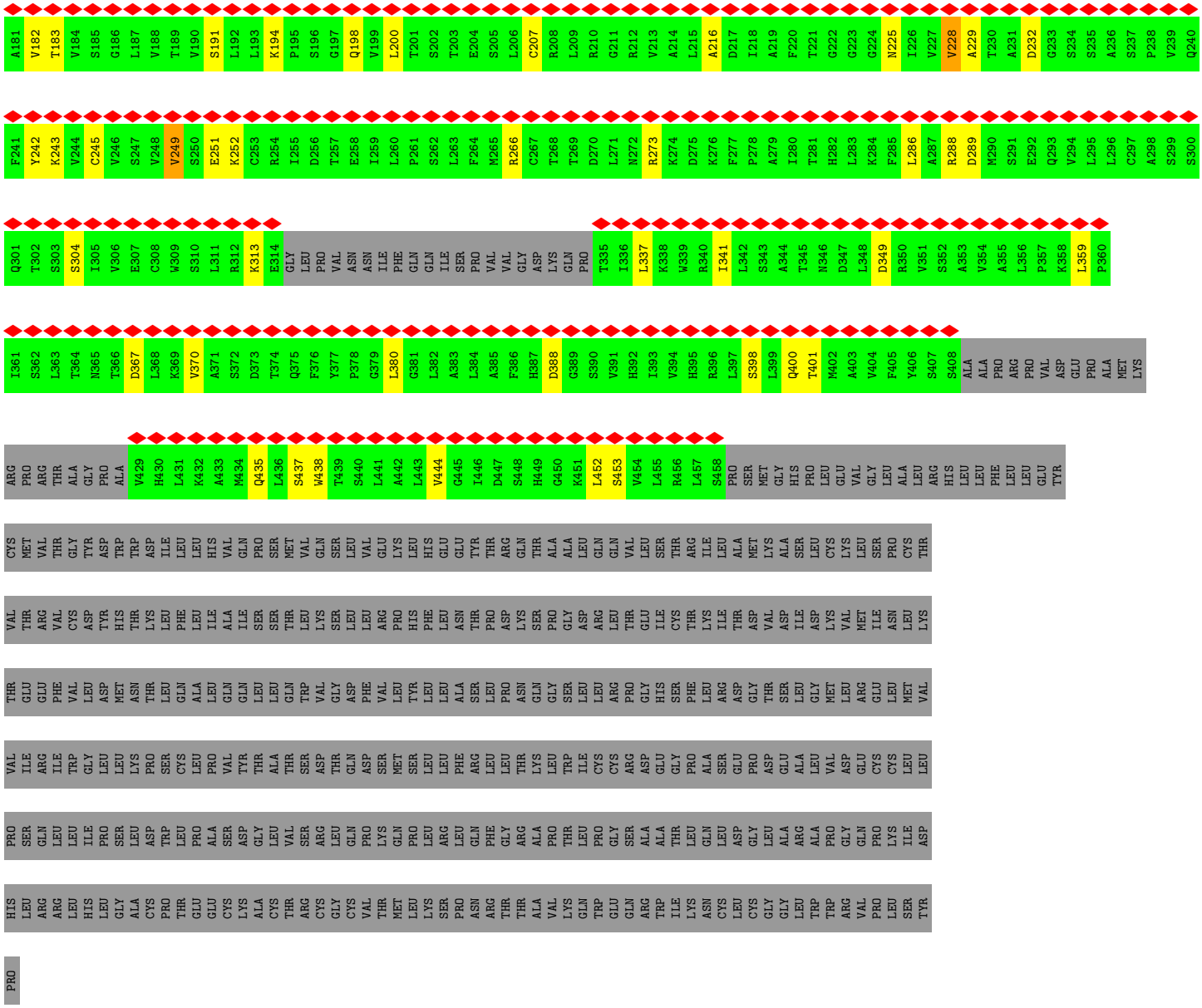

M1 E2 T3 Q4 L5 Q6 S7 I8 F9 E10 E11 V12 V13 K14 T15 E16 V17 I18 E19 E20 A21 F22 P23 G24 M25 F26 M27 D28 T29 P30 E31 D32 E33 K34 T35 K36 L37 I38 S39 C40 L41 G42 A43 F44 R45 Q46 F47 W48 G49 G50 L51 S52 Q53 E54 S55 H56 W62 I63
F66 I67 H68 G69 Q70 H71 S72 P73 K74 R75 F78 L79 Y80 D81 C82 L83 A84 M85 A86 V87 E88 T89 G90 L91 L92 P93 P94 R95 L101 I102 N103 S104 D105 T106 L107 E108 W109 E110 R111 T112 Q113 L114 W115 T118 L121 V122 R123 K124 I125 I126 G127 G128 V129 D130 Y131 K132
G133 V134 R135 D136 L137 L138 K139 V140 I141 L142 E143 K144 I145 L146 T147 I148 P149 N150 T151 V152 S153 S154 A155 V156 V157 Q158 Q159 L160 L161 A162 A163 R164 E165 V166 I167 A168 Y169 I170 L171 E172 R173 N174 A175 C176 L177 L178 P179 A180 Y181 F182 A183 V184 T185 E186 I187 R188 K189 L190 Y191 P192
E193 G194 K195 L196 P197 H198 W199 L200 L201 G202 N203 L204 V205 S206 D207 P208 V209 D210 T211 P212 R213 P214 T215 A216 R217 I218 N219 S220 I221 C222 G223 R224 C225 S226 L227 L228 P229 V230 V231 N232 N233 S234 G235 A236 I237 C238 N239 S240 W241 K242 L243 D244 P245 A246 T247 L248 R249 P250 P251 L252
K253 G254 L255 L256 P257 Y258 D259 K260 D261 L262 F263 E264 P265 Q266 T267 A268 L269 L270 R271 Y272 V273 L274 E275 Q276 P277 Y278 S279 R280 D281 M282 V283 C284 N285 M286 L287 G288 L289 N290 K291 Q292 H293 K294 Q295 R296 C297 P298 V299 L300 E301 D302 Q303 L304 V305 D306 L307 V308 V309 Y310 A311 M312
E313 R314 S315 E316 T317 E318 E319 K320 F321 D322 D323 G324 G325 T326 S327 Q328 L329 L330 W331 Q332 H333 L334 S335 S336 Q337 L338 I339 F340 F341 V342 L343 F344 Q345 F346 A347 S348 F349 P350 H351 M352 V353 L354 S355 L356 H357 Q358 K359 L360 A361 G362 R363 G364 L365 I366 K367 G368 R369 D370 H371 L372
M373 W374 V375 L376 L377 Q378 F379 I380 S381 G382 S383 I384 Q385 K386 N387 A388 L389 A390 D391 F392 L393 P394 V395 M396 K397 L398 F399 D400 L401 L402 Y403 P404 E405 K406 E407 Y408 I409 P410 V411 P412 D413 I414 N415 K416 P417 Q418 S419 T420 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 T707 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 W771 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



• Molecule 68: Isoform 2 of Mediator of RNA polymerase II transcription subunit 16

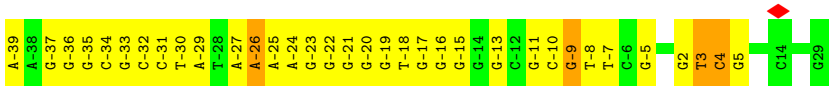
Chain p:





• Molecule 69: DNA (69-MER)

Chain X:



• Molecule 70: DNA(69-MER)

Chain Y:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48654	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	8.884	Depositor
Minimum map value	-4.573	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	674.56, 674.56, 674.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3175, 1.3175, 1.3175	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.89	3/2288 (0.1%)	1.34	29/3101 (0.9%)
2	8	1.01	0/2437	1.65	50/3306 (1.5%)
3	9	1.10	3/2356 (0.1%)	1.72	53/3185 (1.7%)
4	DO	0.84	0/781	1.20	6/1061 (0.6%)
5	DP	0.95	0/1438	1.25	4/1935 (0.2%)
6	DQ	0.79	0/1013	1.12	2/1366 (0.1%)
7	BA	0.70	1/1987 (0.1%)	1.26	22/2684 (0.8%)
8	FA	0.69	0/1130	0.96	0/1528
9	FB	0.84	0/1817	1.17	5/2445 (0.2%)
10	PA	1.12	37/11888 (0.3%)	1.70	214/16066 (1.3%)
11	PB	1.19	39/9243 (0.4%)	1.68	167/12475 (1.3%)
12	PC	1.34	15/2102 (0.7%)	1.88	63/2857 (2.2%)
13	PD	0.90	0/1036	1.80	16/1397 (1.1%)
14	PE	0.89	1/1751 (0.1%)	1.59	22/2366 (0.9%)
15	PF	1.28	3/645 (0.5%)	1.71	10/871 (1.1%)
16	PG	1.01	2/1365 (0.1%)	1.79	22/1853 (1.2%)
17	PH	1.02	0/1207	1.70	25/1628 (1.5%)
18	PI	0.93	0/948	1.72	19/1284 (1.5%)
19	PJ	1.32	2/516 (0.4%)	1.83	13/696 (1.9%)
20	PK	1.30	8/956 (0.8%)	1.75	25/1294 (1.9%)
21	PL	1.09	1/377 (0.3%)	1.56	3/500 (0.6%)
22	DA	0.65	0/5037	0.93	8/6794 (0.1%)
23	DB	0.50	1/7993 (0.0%)	0.71	6/10836 (0.1%)
24	DD	0.86	1/1343 (0.1%)	1.25	4/1795 (0.2%)
24	Dd	0.24	0/1321	0.44	0/1772
25	DE	0.54	1/4469 (0.0%)	0.77	7/6050 (0.1%)
25	De	0.31	0/4433	0.53	0/6004
26	DF	0.79	0/3167	1.12	6/4303 (0.1%)
26	Df	0.56	0/3140	0.86	9/4268 (0.2%)
27	DG	0.71	0/1199	0.94	0/1612
28	DH	0.64	0/1673	0.86	0/2285
29	DI	0.69	1/981 (0.1%)	0.90	2/1332 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	Di	0.23	0/989	0.41	0/1343
30	DJ	0.66	0/736	0.91	0/998
30	Dj	0.24	0/775	0.45	0/1049
31	DL	0.62	0/622	0.98	1/841 (0.1%)
31	Dl	0.34	0/888	0.60	0/1194
32	Dc	0.49	0/1035	0.67	0/1406
33	Dk	0.30	0/799	0.53	1/1070 (0.1%)
34	Dm	0.32	0/733	0.56	0/977
35	EA	0.92	0/1499	1.32	5/2012 (0.2%)
36	EB	0.96	0/1428	1.20	1/1917 (0.1%)
37	1	0.43	1/3502 (0.0%)	0.90	6/4731 (0.1%)
38	2	0.43	0/3094	0.85	4/4188 (0.1%)
39	3	0.48	0/2353	0.96	7/3187 (0.2%)
40	4	0.62	1/3729 (0.0%)	1.04	11/5053 (0.2%)
41	5	0.72	0/528	1.14	3/713 (0.4%)
42	6	0.45	0/5365	0.90	12/7247 (0.2%)
43	7	0.57	3/5984 (0.1%)	0.96	25/8104 (0.3%)
44	c	0.63	0/2146	1.00	14/2899 (0.5%)
45	e	0.19	0/840	0.34	0/1128
46	b	0.75	0/911	1.08	0/1229
47	l	0.18	0/1048	0.36	0/1405
48	m	0.18	0/1010	0.38	0/1359
49	a	0.94	1/3660 (0.0%)	1.33	11/4971 (0.2%)
50	d	0.92	0/1281	1.30	1/1718 (0.1%)
51	f	0.80	1/1359 (0.1%)	1.07	3/1845 (0.2%)
52	g	0.90	0/1411	1.43	4/1901 (0.2%)
53	h	0.92	0/1485	1.31	5/2008 (0.2%)
54	i	0.99	1/612 (0.2%)	1.31	0/815
55	j	0.56	1/1016 (0.1%)	0.84	5/1363 (0.4%)
56	k	0.98	0/885	1.28	0/1190
57	n	0.42	0/7371	0.68	18/10037 (0.2%)
58	o	0.42	0/1256	0.82	1/1724 (0.1%)
59	q	0.68	2/4351 (0.0%)	0.87	5/5886 (0.1%)
60	r	0.93	1/1663 (0.1%)	1.35	7/2241 (0.3%)
61	s	0.84	0/510	1.18	6/694 (0.9%)
62	t	1.08	3/1530 (0.2%)	1.51	13/2066 (0.6%)
63	u	0.48	0/797	0.72	0/1082
64	v	0.97	0/1092	1.42	5/1468 (0.3%)
65	z	0.94	0/781	1.34	2/1067 (0.2%)
66	x	0.56	0/7179	0.70	5/9712 (0.1%)
67	w	0.56	0/11053	0.73	8/15018 (0.1%)
68	p	0.71	0/3191	0.78	2/4333 (0.0%)
69	X	0.60	1/1607 (0.1%)	0.92	6/2481 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
70	Y	0.57	0/1565	0.92	9/2410 (0.4%)
All	All	0.77	135/177706 (0.1%)	1.14	1018/241029 (0.4%)

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	q	264	GLN	C-N	13.59	1.52	1.33
62	t	119	TYR	C-N	11.68	1.48	1.33
59	q	452	ALA	C-N	9.14	1.47	1.33
10	PA	685	HIS	C-O	-8.97	1.14	1.23
11	PB	965	ILE	C-O	-8.96	1.14	1.23
43	7	673	ASP	CA-C	8.75	1.64	1.52
10	PA	456	VAL	C-O	-8.69	1.13	1.23
11	PB	776	ILE	C-O	-8.65	1.14	1.24
12	PC	47	ILE	C-O	-8.38	1.14	1.24
11	PB	797	ASN	C-O	-8.36	1.13	1.24
51	f	110	ASP	C-N	-8.22	1.22	1.33
10	PA	500	GLU	C-O	-7.85	1.15	1.23
55	j	94	GLN	C-N	-7.74	1.24	1.33
20	PK	63	VAL	CA-C	-7.72	1.47	1.53
10	PA	457	ILE	C-O	-7.38	1.15	1.24
10	PA	629	VAL	C-O	-7.35	1.16	1.24
20	PK	35	ILE	C-O	-7.35	1.16	1.24
11	PB	931	ILE	C-O	-7.29	1.16	1.24
1	0	76	LYS	C-O	7.29	1.32	1.24
11	PB	982	ILE	C-O	-7.20	1.16	1.23
10	PA	366	VAL	C-O	-7.20	1.15	1.24
12	PC	43	PRO	C-O	-7.11	1.15	1.23
3	9	244	CYS	C-O	7.02	1.32	1.24
12	PC	233	VAL	C-O	-6.96	1.16	1.24
62	t	136	ARG	C-O	-6.91	1.15	1.23
11	PB	748	ALA	C-O	-6.87	1.16	1.24
11	PB	1045	PRO	C-O	-6.83	1.15	1.24
11	PB	748	ALA	CA-CB	-6.82	1.43	1.53
62	t	89	THR	C-O	6.76	1.32	1.24
10	PA	475	ARG	C-O	-6.75	1.16	1.23
11	PB	665	ILE	C-O	-6.59	1.16	1.24
10	PA	499	ASP	C-O	-6.57	1.15	1.23
12	PC	173	HIS	C-O	-6.56	1.16	1.23
11	PB	856	PRO	N-CA	-6.45	1.39	1.47
10	PA	519	ALA	CA-CB	-6.42	1.44	1.53
10	PA	547	LYS	C-O	-6.39	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	61	ASN	C-O	-6.28	1.18	1.24
10	PA	378	VAL	C-O	-6.26	1.17	1.23
37	1	417	LYS	CA-C	6.21	1.58	1.52
10	PA	545	VAL	C-O	-6.21	1.16	1.24
54	i	100	LEU	C-O	6.20	1.31	1.24
12	PC	31	ALA	CA-CB	-6.15	1.43	1.53
1	0	78	VAL	C-O	-6.15	1.16	1.24
10	PA	840	ALA	CA-CB	-6.12	1.43	1.53
12	PC	19	VAL	C-O	-6.12	1.17	1.24
20	PK	71	ILE	C-O	-6.09	1.17	1.23
10	PA	502	ASN	C-O	-6.09	1.16	1.23
11	PB	949	TYR	C-O	-6.07	1.16	1.23
49	a	501	CYS	N-CA	6.05	1.50	1.46
11	PB	1030	ASN	C-O	-6.02	1.16	1.23
11	PB	749	HIS	C-O	-5.96	1.17	1.24
25	DE	509	GLN	C-O	-5.94	1.16	1.24
11	PB	700	PRO	N-CA	-5.93	1.39	1.47
11	PB	978	ILE	C-O	-5.92	1.17	1.24
3	9	258	LEU	C-O	5.89	1.31	1.24
11	PB	947	ILE	C-O	-5.87	1.17	1.24
12	PC	241	PRO	C-O	-5.87	1.17	1.24
11	PB	795	ILE	C-O	-5.87	1.16	1.23
20	PK	70	LYS	C-O	-5.86	1.17	1.23
15	PF	63	ALA	CA-CB	-5.86	1.43	1.54
10	PA	563	LEU	C-O	-5.85	1.17	1.24
20	PK	60	GLY	C-O	-5.85	1.18	1.23
10	PA	808	PRO	N-CA	-5.81	1.40	1.47
11	PB	781	ALA	CA-CB	-5.81	1.44	1.52
12	PC	50	VAL	C-O	-5.81	1.17	1.24
11	PB	110	PRO	C-O	-5.80	1.16	1.24
11	PB	858	VAL	C-O	-5.78	1.17	1.24
12	PC	178	PRO	N-CA	-5.74	1.40	1.47
10	PA	501	MET	C-O	-5.70	1.16	1.23
10	PA	511	THR	C-O	-5.70	1.17	1.24
43	7	686	ARG	CA-C	5.70	1.59	1.52
10	PA	808	PRO	C-O	-5.68	1.17	1.24
11	PB	187	ILE	C-O	-5.67	1.17	1.24
11	PB	1037	ILE	C-O	-5.66	1.18	1.24
12	PC	183	ALA	C-O	-5.65	1.17	1.24
11	PB	806	PHE	C-O	-5.64	1.16	1.24
24	DD	941	ARG	C-O	5.62	1.31	1.24
20	PK	72	ILE	C-O	-5.60	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	PC	67	ARG	C-O	-5.60	1.17	1.24
29	DI	86	PRO	CA-C	5.59	1.54	1.51
16	PG	15	PRO	N-CA	-5.57	1.40	1.47
10	PA	495	ASP	C-O	-5.55	1.17	1.23
20	PK	62	LYS	C-O	-5.51	1.17	1.24
10	PA	592	PHE	C-O	-5.50	1.17	1.23
10	PA	1387	SER	CA-CB	-5.50	1.45	1.54
10	PA	496	PHE	C-O	-5.50	1.16	1.23
10	PA	520	MET	C-O	-5.50	1.17	1.24
10	PA	454	ASP	C-O	-5.49	1.17	1.23
10	PA	628	VAL	C-O	-5.47	1.18	1.24
12	PC	178	PRO	C-O	-5.45	1.17	1.24
3	9	201	THR	N-CA	5.45	1.52	1.45
11	PB	524	LYS	C-O	-5.44	1.17	1.23
15	PF	89	PRO	N-CA	-5.43	1.40	1.47
11	PB	1074	PRO	C-O	-5.43	1.17	1.23
11	PB	927	ARG	C-O	-5.41	1.17	1.23
10	PA	364	ARG	C-O	-5.39	1.17	1.23
10	PA	622	SER	CA-CB	-5.34	1.45	1.53
40	4	387	ILE	C-O	5.34	1.30	1.24
7	BA	18	HIS	CD2-NE2	-5.33	1.31	1.37
11	PB	110	PRO	N-CA	-5.32	1.40	1.47
15	PF	114	SER	CA-CB	-5.32	1.45	1.53
10	PA	980	PRO	C-O	-5.32	1.17	1.24
11	PB	742	VAL	C-O	-5.30	1.18	1.24
11	PB	701	SER	CA-CB	-5.29	1.45	1.53
10	PA	593	SER	CA-CB	-5.27	1.44	1.53
11	PB	223	SER	CA-CB	-5.25	1.46	1.53
11	PB	787	GLY	C-O	-5.25	1.17	1.24
12	PC	226	PRO	C-O	-5.25	1.18	1.23
11	PB	700	PRO	C-O	-5.25	1.17	1.24
10	PA	583	ARG	N-CA	5.24	1.51	1.46
11	PB	987	GLY	C-O	-5.23	1.17	1.23
11	PB	106	SER	CA-CB	-5.21	1.47	1.54
60	r	4	PRO	C-O	-5.21	1.18	1.24
11	PB	107	PRO	C-O	-5.20	1.17	1.23
10	PA	522	PRO	C-O	-5.18	1.17	1.24
20	PK	18	LYS	C-O	-5.17	1.18	1.24
10	PA	513	ALA	CA-CB	-5.17	1.45	1.53
19	PJ	4	PRO	C-O	-5.17	1.17	1.23
11	PB	1066	PRO	C-O	-5.16	1.17	1.23
1	0	197	LEU	CA-C	5.14	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	X	-26	DA	C1'-N9	-5.14	1.36	1.46
10	PA	630	VAL	C-O	-5.14	1.18	1.24
12	PC	230	TYR	C-O	-5.13	1.17	1.23
16	PG	69	PRO	C-O	-5.13	1.18	1.23
14	PE	145	VAL	N-CA	5.09	1.50	1.46
19	PJ	6	ARG	C-O	-5.09	1.18	1.23
10	PA	689	ILE	C-O	-5.08	1.17	1.24
43	7	262	ASN	CA-C	5.06	1.60	1.52
21	PL	57	ALA	CA-CB	-5.06	1.45	1.53
10	PA	476	ILE	C-O	-5.05	1.18	1.24
11	PB	699	HIS	C-O	-5.05	1.17	1.24
12	PC	66	HIS	C-O	-5.05	1.18	1.24
11	PB	1027	VAL	C-O	-5.04	1.18	1.24
10	PA	782	SER	CA-CB	-5.03	1.45	1.53
11	PB	941	GLN	C-O	-5.01	1.18	1.24

All (1018) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	X	3	DT	P-O3'-C3'	-11.23	103.35	120.20
58	o	719	PRO	N-CA-C	11.13	124.28	110.70
11	PB	982	ILE	N-CA-C	-10.98	101.24	111.45
11	PB	805	PHE	CA-CB-CG	10.80	124.60	113.80
12	PC	63	PHE	N-CA-C	-10.56	99.99	113.72
16	PG	125	PRO	N-CA-C	-10.53	97.86	110.70
1	0	291	LEU	N-CA-C	-10.28	99.88	111.71
60	r	4	PRO	CB-CA-C	10.24	123.41	110.92
3	9	186	ILE	N-CA-C	-10.13	100.29	110.62
12	PC	64	ILE	N-CA-C	-10.13	102.89	111.91
11	PB	977	THR	CB-CA-C	-10.08	97.67	111.88
12	PC	184	PHE	CA-CB-CG	10.02	123.82	113.80
11	PB	689	TYR	N-CA-C	-9.92	100.47	111.28
70	Y	12	DG	C2'-C3'-O3'	-9.91	96.64	111.50
12	PC	30	VAL	N-CA-C	-9.81	100.61	110.62
23	DB	491	HIS	N-CA-C	-9.78	100.62	111.28
60	r	4	PRO	N-CA-C	-9.68	98.89	110.70
12	PC	66	HIS	N-CA-C	-9.49	100.93	111.28
3	9	37	ASN	N-CA-C	-9.48	100.94	111.28
12	PC	63	PHE	CA-CB-CG	9.44	123.24	113.80
11	PB	44	LEU	N-CA-C	-9.39	102.41	112.93
11	PB	1037	ILE	N-CA-C	-9.38	97.58	109.30
10	PA	638	GLY	CA-C-O	-9.35	114.59	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	5	63	GLN	N-CA-C	9.26	121.38	111.28
69	X	-9	DG	C2'-C3'-O3'	-9.19	97.72	111.50
11	PB	1091	ARG	N-CA-C	-9.19	101.60	113.17
19	PJ	56	ILE	N-CA-C	-9.18	100.58	113.07
4	DO	58	PHE	N-CA-C	9.06	120.20	108.24
11	PB	770	ARG	N-CA-C	-9.02	102.44	112.72
18	PI	96	PHE	CA-CB-CG	8.94	122.74	113.80
67	w	19	GLU	N-CA-C	-8.89	101.51	111.82
1	0	197	LEU	N-CA-C	8.87	124.23	113.23
43	7	687	GLY	N-CA-C	8.86	122.78	112.50
49	a	505	PRO	N-CA-C	-8.83	101.73	113.65
49	a	505	PRO	CA-C-N	8.81	132.53	120.46
49	a	505	PRO	C-N-CA	8.81	132.53	120.46
17	PH	124	ARG	CB-CA-C	-8.80	98.91	111.85
11	PB	48	ASP	N-CA-C	-8.80	102.68	113.15
11	PB	596	ILE	CB-CA-C	-8.76	100.76	111.97
12	PC	230	TYR	CA-C-O	-8.73	110.81	121.89
10	PA	729	PRO	CB-CA-C	-8.72	100.56	111.64
11	PB	708	ALA	N-CA-C	-8.69	99.00	112.99
57	n	1343	PRO	N-CA-CB	8.68	111.50	103.08
26	Df	149	PRO	O-C-N	8.66	125.30	121.31
16	PG	49	THR	CB-CA-C	8.62	127.57	110.42
69	X	3	DT	O3'-P-O5'	-8.60	91.09	104.00
11	PB	1093	CYS	N-CA-C	-8.58	102.01	111.36
12	PC	38	PHE	CA-CB-CG	8.54	122.34	113.80
11	PB	1073	GLN	CB-CA-C	8.52	122.07	108.87
14	PE	58	LEU	N-CA-C	-8.48	101.98	111.82
20	PK	63	VAL	N-CA-C	-8.45	99.87	107.56
16	PG	15	PRO	N-CA-C	-8.45	97.96	111.14
57	n	1351	PRO	N-CA-CB	8.44	111.27	103.08
3	9	108	CYS	N-CA-C	-8.43	102.09	111.28
37	1	211	VAL	N-CA-CB	8.42	115.80	110.50
7	BA	23	LEU	CA-C-N	8.40	132.97	120.95
7	BA	23	LEU	C-N-CA	8.40	132.97	120.95
42	6	634	ARG	N-CA-C	8.38	121.47	111.33
10	PA	449	HIS	N-CA-C	-8.32	99.55	110.53
10	PA	661	GLY	N-CA-C	8.30	122.17	110.38
62	t	80	GLU	CB-CA-C	-8.30	107.00	116.54
16	PG	18	PHE	N-CA-C	-8.29	99.83	110.53
10	PA	515	ILE	N-CA-C	-8.24	102.22	110.62
39	3	245	PRO	N-CA-C	-8.19	100.71	110.70
2	8	275	LEU	N-CA-C	-8.12	102.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	PA	659	GLU	CB-CA-C	-8.12	99.96	111.65
44	c	274	ILE	N-CA-C	-8.10	105.59	113.53
11	PB	493	GLY	N-CA-C	-8.10	101.88	111.36
11	PB	923	VAL	N-CA-CB	-8.07	103.50	111.89
12	PC	184	PHE	CA-C-O	-8.06	111.85	121.60
17	PH	23	ASP	N-CA-C	8.05	119.84	111.14
10	PA	113	PHE	CB-CA-C	8.04	121.64	110.06
10	PA	698	THR	CB-CA-C	8.04	124.52	110.85
3	9	184	PRO	CB-CA-C	-8.01	102.19	113.09
37	1	417	LYS	N-CA-C	8.00	123.57	112.93
7	BA	16	PRO	CB-CA-C	-7.95	100.42	113.06
2	8	280	PRO	CB-CA-C	-7.95	99.82	112.21
43	7	686	ARG	N-CA-C	7.93	123.54	113.55
44	c	291	GLY	N-CA-C	-7.93	102.39	112.54
2	8	280	PRO	N-CA-C	-7.93	102.94	113.65
44	c	295	THR	N-CA-C	-7.92	102.61	111.71
62	t	153	CYS	N-CA-C	-7.92	103.52	113.02
57	n	1355	PRO	N-CA-CB	7.91	111.55	103.25
10	PA	1434	GLU	N-CA-C	-7.87	103.75	112.72
10	PA	497	ASP	CA-CB-CG	7.85	120.45	112.60
10	PA	592	PHE	N-CA-C	-7.83	103.95	113.97
13	PD	134	ILE	N-CA-C	-7.83	102.63	110.62
11	PB	802	ASP	N-CA-C	-7.82	103.05	114.39
10	PA	619	LYS	CB-CA-C	-7.79	98.59	110.90
10	PA	396	PRO	CB-CA-C	-7.79	100.06	112.21
11	PB	702	MET	N-CA-C	-7.78	103.10	112.59
16	PG	69	PRO	CB-CA-C	-7.78	100.79	110.98
22	DA	356	PRO	N-CA-C	7.78	124.64	114.68
65	z	595	PRO	CB-CA-C	-7.76	101.45	111.46
10	PA	1390	GLY	N-CA-C	-7.76	104.32	115.64
12	PC	115	VAL	N-CA-C	-7.74	97.25	109.17
10	PA	565	MET	N-CA-C	-7.74	103.84	113.28
57	n	1347	PRO	N-CA-CB	7.72	110.57	103.08
43	7	261	GLY	N-CA-C	7.71	123.34	113.24
13	PD	116	PRO	N-CA-C	-7.71	104.23	113.86
40	4	50	SER	N-CA-C	-7.70	103.91	113.38
70	Y	12	DG	C4'-C3'-O3'	7.69	121.53	110.00
10	PA	1209	PRO	N-CA-C	-7.68	102.85	113.53
16	PG	126	PRO	N-CA-C	-7.66	99.24	111.03
10	PA	1031	ARG	N-CA-C	-7.64	104.48	113.88
57	n	1237	PRO	N-CA-CB	7.61	111.24	103.25
11	PB	276	LEU	N-CA-C	-7.60	102.97	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8	85	SER	N-CA-C	-7.59	102.98	111.71
39	3	245	PRO	CA-C-N	-7.59	110.36	119.84
39	3	245	PRO	C-N-CA	-7.59	110.36	119.84
10	PA	1360	ASN	N-CA-C	-7.58	103.59	112.92
12	PC	265	HIS	N-CA-C	-7.58	103.77	112.87
11	PB	1132	THR	CB-CA-C	-7.58	96.37	110.01
10	PA	635	LEU	N-CA-C	-7.58	98.81	110.10
11	PB	504	THR	CB-CA-C	-7.56	97.73	110.81
2	8	199	VAL	N-CA-C	-7.55	102.92	110.62
4	DO	62	LEU	N-CA-C	7.51	120.68	110.55
42	6	61	TYR	N-CA-C	7.49	122.25	113.18
10	PA	1468	THR	N-CA-C	-7.47	102.36	113.72
10	PA	686	THR	CB-CA-C	-7.47	97.11	109.80
18	PI	81	THR	CB-CA-C	-7.46	95.72	109.46
10	PA	807	LEU	N-CA-C	-7.45	101.51	108.22
2	8	142	ASN	N-CA-C	-7.43	104.69	113.38
42	6	477	ILE	N-CA-C	-7.42	104.62	111.67
44	c	294	PRO	CA-C-N	-7.42	109.59	120.28
44	c	294	PRO	C-N-CA	-7.42	109.59	120.28
20	PK	64	PRO	CB-CA-C	7.42	123.78	112.21
57	n	526	SER	N-CA-C	-7.41	104.24	113.28
11	PB	709	SER	N-CA-C	-7.41	103.37	113.30
1	0	208	LEU	N-CA-C	7.39	120.40	111.82
10	PA	495	ASP	N-CA-C	-7.39	96.11	108.75
57	n	1196	PRO	N-CA-CB	7.38	111.00	103.25
12	PC	44	ILE	CA-C-O	-7.37	114.08	121.45
10	PA	495	ASP	CA-CB-CG	7.37	119.97	112.60
12	PC	252	LEU	N-CA-C	-7.35	103.27	111.28
11	PB	1105	GLU	CB-CA-C	-7.35	99.29	110.90
61	s	156	THR	N-CA-C	-7.35	102.07	113.02
1	0	256	TYR	N-CA-C	-7.33	99.58	110.06
22	DA	640	LEU	N-CA-C	-7.32	103.44	113.18
42	6	313	THR	N-CA-C	7.31	121.24	111.30
16	PG	17	TYR	N-CA-C	-7.30	103.94	112.92
40	4	415	GLN	N-CA-C	7.29	119.22	111.28
11	PB	935	PHE	N-CA-C	-7.28	97.95	109.23
20	PK	116	ILE	N-CA-C	-7.26	103.21	110.62
42	6	277	ILE	N-CA-C	-7.25	106.82	113.71
61	s	134	PRO	N-CA-CB	7.25	110.12	103.08
22	DA	715	PRO	N-CA-C	-7.22	99.91	111.03
55	j	77	PRO	N-CA-C	-7.22	103.49	113.53
70	Y	-4	DG	C2'-C3'-O3'	-7.20	100.70	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	PK	114	GLU	N-CA-C	-7.20	104.37	113.01
10	PA	689	ILE	N-CA-C	-7.18	101.56	111.89
20	PK	18	LYS	CA-C-N	-7.16	113.75	123.14
20	PK	18	LYS	C-N-CA	-7.16	113.75	123.14
26	DF	271	VAL	N-CA-C	-7.16	106.02	112.90
57	n	1255	PRO	N-CA-CB	7.16	110.77	103.25
11	PB	1066	PRO	N-CA-CB	-7.14	96.96	103.31
11	PB	749	HIS	CB-CA-C	-7.14	99.16	110.79
29	DI	86	PRO	CA-C-O	-7.10	115.79	120.90
57	n	1326	PRO	N-CA-CB	7.10	110.70	103.25
10	PA	1795	PRO	N-CA-C	-7.09	99.92	111.77
10	PA	960	ARG	N-CA-C	-7.08	103.56	111.28
69	X	-9	DG	C4'-C3'-O3'	-7.07	99.39	110.00
10	PA	395	THR	CB-CA-C	-7.05	99.05	109.97
2	8	140	PRO	CB-CA-C	-7.04	101.30	113.20
12	PC	43	PRO	CA-C-O	-7.03	113.40	122.12
16	PG	58	VAL	N-CA-C	-7.02	99.90	109.37
67	w	47	PHE	CB-CA-C	7.01	124.14	110.67
10	PA	1430	CYS	N-CA-C	-7.00	104.48	113.16
23	DB	495	GLN	N-CA-C	-6.99	104.76	113.28
11	PB	390	ASN	N-CA-C	-6.97	104.78	112.72
37	1	165	GLY	N-CA-C	-6.96	101.22	113.76
11	PB	703	ILE	N-CA-C	-6.96	105.75	112.29
19	PJ	59	LEU	N-CA-C	-6.96	103.97	113.30
44	c	280	PRO	N-CA-C	6.96	121.50	111.13
18	PI	77	THR	N-CA-C	6.93	118.92	111.36
10	PA	378	VAL	CA-C-O	-6.92	114.40	121.67
11	PB	948	GLN	N-CA-C	-6.92	98.79	109.52
11	PB	845	TYR	N-CA-C	-6.90	104.86	112.72
1	0	284	ALA	N-CA-C	-6.89	103.78	111.71
10	PA	631	GLU	CB-CA-C	-6.88	99.66	110.74
11	PB	1156	LYS	N-CA-C	-6.88	103.78	111.28
11	PB	1007	ASN	N-CA-C	-6.87	101.27	110.55
62	t	137	GLY	CA-C-O	-6.87	114.82	122.24
25	DE	509	GLN	CA-C-N	6.86	129.47	120.28
25	DE	509	GLN	C-N-CA	6.86	129.47	120.28
11	PB	941	GLN	CB-CA-C	-6.85	98.95	110.19
20	PK	71	ILE	CA-C-O	-6.85	114.85	121.63
42	6	309	ASP	N-CA-C	-6.83	99.55	110.14
57	n	1352	PRO	N-CA-CB	6.83	110.42	103.25
2	8	271	LEU	CA-C-N	-6.83	111.82	120.56
2	8	271	LEU	C-N-CA	-6.83	111.82	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	n	1344	PRO	N-CA-CB	6.83	110.42	103.25
10	PA	877	ALA	CA-C-N	-6.82	111.83	121.99
10	PA	877	ALA	C-N-CA	-6.82	111.83	121.99
10	PA	548	PHE	N-CA-C	-6.82	103.78	111.07
12	PC	231	TYR	CA-C-O	-6.81	113.95	121.23
10	PA	752	THR	N-CA-C	-6.80	104.24	112.54
11	PB	616	THR	CB-CA-C	-6.80	100.00	111.02
2	8	136	ARG	CA-C-N	-6.80	113.92	123.03
2	8	136	ARG	C-N-CA	-6.80	113.92	123.03
11	PB	41	ARG	N-CA-C	-6.80	104.86	113.01
10	PA	1137	PRO	N-CA-C	-6.79	100.54	110.80
42	6	159	CYS	N-CA-C	-6.79	105.13	113.41
24	DD	944	LEU	N-CA-C	-6.79	103.88	111.28
11	PB	105	PRO	N-CA-C	-6.78	100.60	111.38
7	BA	112	ARG	N-CA-C	-6.78	103.89	111.28
18	PI	103	ARG	N-CA-C	-6.78	102.03	111.52
10	PA	390	PHE	CA-C-O	-6.76	114.24	121.88
57	n	1192	PRO	N-CA-CB	6.76	110.44	103.00
11	PB	171	LEU	N-CA-C	-6.76	103.92	111.28
1	0	197	LEU	CA-C-O	6.75	127.17	119.27
12	PC	131	THR	N-CA-C	-6.75	103.95	111.71
10	PA	841	MET	N-CA-C	-6.74	103.93	111.28
12	PC	198	PRO	N-CA-C	-6.70	103.89	113.47
10	PA	463	THR	CB-CA-C	-6.70	99.45	109.90
2	8	287	THR	CB-CA-C	-6.69	99.69	110.79
11	PB	923	VAL	CA-C-O	-6.68	113.56	121.64
52	g	14	PRO	N-CA-C	-6.67	100.60	111.21
64	v	24	ASP	N-CA-C	-6.67	104.00	111.28
10	PA	449	HIS	CA-CB-CG	6.67	120.47	113.80
10	PA	963	ARG	N-CA-C	-6.67	104.01	111.28
11	PB	591	ARG	N-CA-C	-6.64	104.04	111.28
17	PH	146	LYS	CA-C-N	-6.63	112.84	122.19
17	PH	146	LYS	C-N-CA	-6.63	112.84	122.19
17	PH	35	PHE	N-CA-C	-6.62	104.92	114.12
33	Dk	180	PRO	N-CA-C	6.60	118.75	110.70
10	PA	28	PRO	N-CA-C	-6.60	104.36	113.53
10	PA	593	SER	N-CA-C	-6.60	105.22	113.20
11	PB	38	GLY	CA-C-O	-6.59	116.95	122.29
3	9	45	PRO	CB-CA-C	-6.58	101.76	112.62
49	a	231	LEU	N-CA-C	-6.58	104.11	111.28
57	n	1206	PRO	N-CA-CB	6.57	110.15	103.25
26	Df	301	VAL	N-CA-C	-6.57	106.28	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	PA	836	PHE	N-CA-C	-6.56	104.13	111.28
14	PE	95	GLN	N-CA-C	-6.55	104.14	111.28
57	n	1267	PRO	N-CA-CB	6.54	110.63	103.23
26	Df	319	LEU	N-CA-C	-6.54	103.98	112.68
11	PB	568	PHE	CA-CB-CG	6.54	120.34	113.80
11	PB	323	SER	N-CA-C	-6.53	104.16	111.28
11	PB	634	LEU	N-CA-C	-6.53	104.24	111.36
10	PA	418	TYR	CA-C-O	-6.53	113.73	121.11
3	9	14	SER	N-CA-C	6.52	119.72	111.69
10	PA	1052	ARG	N-CA-C	-6.52	104.17	111.28
12	PC	200	PRO	CB-CA-C	-6.50	102.62	111.85
40	4	401	LEU	CA-C-O	-6.50	112.76	120.10
11	PB	1000	THR	CB-CA-C	6.49	119.72	109.27
3	9	29	LYS	CA-C-N	-6.48	111.59	120.28
3	9	29	LYS	C-N-CA	-6.48	111.59	120.28
26	Df	326	HIS	N-CA-C	-6.48	104.47	112.38
59	q	395	PRO	N-CA-CB	6.48	110.05	103.25
43	7	673	ASP	CA-C-O	6.47	129.76	120.51
67	w	30	PRO	N-CA-CB	6.47	110.45	103.33
11	PB	1158	LEU	N-CA-C	-6.47	104.23	111.28
18	PI	115	THR	CB-CA-C	-6.46	98.41	109.65
11	PB	108	MET	CB-CA-C	-6.46	102.86	112.09
35	EA	127	PHE	N-CA-C	-6.46	97.75	108.34
43	7	87	LEU	N-CA-C	-6.46	104.88	112.89
51	f	110	ASP	O-C-N	-6.45	115.02	122.89
3	9	82	THR	N-CA-C	-6.45	104.25	111.28
19	PJ	22	LEU	N-CA-C	-6.44	104.26	111.28
1	0	125	TYR	N-CA-C	-6.44	106.63	114.75
12	PC	164	TYR	CA-C-O	-6.44	113.25	120.66
12	PC	65	ALA	N-CA-C	-6.44	104.37	112.93
20	PK	50	LEU	N-CA-C	-6.44	104.27	111.28
2	8	53	ASP	N-CA-C	-6.43	106.15	112.97
62	t	156	LEU	CA-C-N	-6.43	111.66	120.28
62	t	156	LEU	C-N-CA	-6.43	111.66	120.28
11	PB	832	PRO	N-CA-C	-6.43	101.16	111.38
11	PB	796	MET	CA-C-O	-6.42	114.39	121.33
11	PB	490	GLY	N-CA-C	-6.41	103.86	111.36
16	PG	51	ILE	N-CA-CB	-6.41	103.59	111.67
1	0	220	PRO	N-CA-CB	6.41	109.98	103.25
43	7	194	LEU	N-CA-C	-6.41	104.56	112.38
60	r	7	THR	CB-CA-C	6.41	123.18	110.42
11	PB	996	ILE	N-CA-C	-6.40	101.32	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	PA	1001	PRO	N-CA-C	6.40	121.38	111.21
11	PB	898	THR	CB-CA-C	6.40	121.59	109.37
70	Y	21	DC	C4'-C3'-O3'	-6.39	100.41	110.00
26	Df	388	ILE	N-CA-C	-6.39	107.01	113.47
61	s	119	PRO	N-CA-CB	6.39	109.96	103.25
61	s	135	PRO	N-CA-CB	6.37	110.28	103.52
37	1	338	ASN	N-CA-C	-6.37	105.33	113.23
10	PA	84	HIS	CB-CA-C	6.37	121.88	109.33
10	PA	830	GLY	CA-C-O	-6.37	117.84	122.23
10	PA	506	PRO	N-CA-C	-6.36	101.23	111.03
70	Y	-2	DC	C2'-C3'-O3'	6.36	121.04	111.50
7	BA	13	VAL	N-CA-CB	6.36	118.13	110.31
59	q	393	PRO	N-CA-CB	6.35	109.92	103.25
3	9	118	PHE	N-CA-C	-6.35	105.54	113.28
10	PA	1008	LYS	N-CA-C	-6.34	104.36	111.28
16	PG	59	ILE	N-CA-C	-6.34	98.36	107.37
70	Y	-2	DC	P-O3'-C3'	6.34	129.71	120.20
12	PC	270	ASP	N-CA-C	-6.33	104.38	111.28
15	PF	109	TYR	CB-CA-C	-6.33	100.03	109.90
20	PK	20	THR	CB-CA-C	-6.33	102.16	111.77
10	PA	737	PHE	N-CA-C	-6.32	104.39	111.28
10	PA	301	HIS	N-CA-C	-6.31	104.48	111.36
10	PA	713	VAL	N-CA-C	-6.31	104.18	110.62
43	7	85	GLU	N-CA-C	6.31	117.82	111.07
10	PA	1225	LYS	N-CA-C	-6.31	103.22	111.74
12	PC	67	ARG	CB-CA-C	6.31	121.57	110.85
59	q	264	GLN	O-C-N	-6.30	116.88	123.56
10	PA	1354	PRO	N-CA-C	-6.30	107.43	114.92
3	9	232	LEU	N-CA-C	-6.30	104.42	111.28
16	PG	3	TYR	CA-C-O	-6.29	114.28	121.58
11	PB	504	THR	CA-CB-OG1	-6.29	100.17	109.60
11	PB	765	GLU	CB-CA-C	-6.29	99.99	110.68
15	PF	61	GLU	N-CA-C	-6.29	105.65	113.38
43	7	262	ASN	CA-C-O	6.29	127.03	119.43
3	9	103	ILE	CA-C-N	-6.28	111.85	120.46
3	9	103	ILE	C-N-CA	-6.28	111.85	120.46
10	PA	456	VAL	CA-C-O	-6.28	114.73	121.19
15	PF	94	MET	N-CA-C	-6.28	104.54	111.82
11	PB	1140	CYS	N-CA-C	-6.27	105.29	114.39
7	BA	127	ARG	N-CA-C	-6.27	104.44	111.28
10	PA	548	PHE	CA-CB-CG	6.27	120.07	113.80
10	PA	765	ASN	CB-CA-C	6.27	120.81	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	BA	15	CYS	CB-CA-C	-6.27	99.62	109.52
44	c	294	PRO	CB-CA-C	-6.26	101.22	111.56
11	PB	583	LEU	N-CA-C	-6.26	104.45	111.28
19	PJ	14	VAL	N-CA-C	-6.26	106.61	113.43
22	DA	498	PRO	N-CA-CB	6.25	109.81	103.25
25	DE	445	LYS	N-CA-C	-6.25	104.55	111.36
10	PA	419	ILE	CB-CA-C	-6.25	104.34	111.59
16	PG	29	LYS	CA-C-N	-6.25	112.32	120.44
16	PG	29	LYS	C-N-CA	-6.25	112.32	120.44
43	7	673	ASP	N-CA-C	6.25	124.10	110.80
1	0	237	PRO	N-CA-CB	6.24	109.81	103.25
10	PA	538	VAL	N-CA-C	6.23	122.30	109.34
14	PE	178	PRO	CB-CA-C	-6.23	101.80	112.64
49	a	509	ARG	CB-CA-C	-6.23	101.10	110.88
10	PA	496	PHE	CA-C-O	-6.23	114.60	122.63
11	PB	1027	VAL	CB-CA-C	-6.23	102.45	110.98
14	PE	76	PHE	CB-CA-C	-6.23	104.84	110.44
11	PB	933	ASP	CB-CA-C	6.22	119.98	109.84
13	PD	65	LEU	N-CA-C	-6.22	104.50	111.28
11	PB	307	GLU	N-CA-C	-6.22	104.58	111.36
70	Y	3	DG	C2'-C3'-O3'	6.21	120.81	111.50
11	PB	736	TYR	CA-C-O	-6.20	114.31	120.70
11	PB	745	ASP	CA-CB-CG	6.20	118.80	112.60
38	2	325	LEU	N-CA-C	-6.19	106.95	114.75
53	h	168	PRO	N-CA-CB	6.19	109.75	103.25
59	q	399	PRO	N-CA-CB	6.19	109.75	103.25
12	PC	51	GLN	CB-CA-C	-6.19	99.89	110.16
12	PC	265	HIS	CA-CB-CG	6.19	119.99	113.80
49	a	32	PRO	N-CA-CB	6.18	109.80	103.00
3	9	187	LEU	N-CA-C	-6.18	104.46	111.07
17	PH	73	GLY	CA-C-N	-6.18	112.72	122.73
17	PH	73	GLY	C-N-CA	-6.18	112.72	122.73
10	PA	550	LYS	CA-C-O	-6.17	114.33	121.49
10	PA	399	ILE	N-CA-C	-6.16	103.35	111.05
19	PJ	48	MET	N-CA-C	-6.16	104.11	111.69
2	8	268	LEU	N-CA-C	-6.15	104.68	111.82
10	PA	408	ARG	CB-CA-C	-6.15	100.79	110.94
14	PE	202	ARG	CA-C-N	-6.14	114.53	123.00
14	PE	202	ARG	C-N-CA	-6.14	114.53	123.00
26	DF	347	THR	CA-C-N	-6.14	114.33	122.99
26	DF	347	THR	C-N-CA	-6.14	114.33	122.99
10	PA	525	ILE	CA-C-O	-6.13	114.35	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	BA	16	PRO	N-CA-CB	-6.13	96.67	103.23
66	x	35	ALA	CA-C-N	6.13	133.25	121.54
66	x	35	ALA	C-N-CA	6.13	133.25	121.54
11	PB	710	ILE	N-CA-C	-6.13	105.75	112.80
41	5	33	PHE	CA-C-N	-6.12	117.15	122.96
41	5	33	PHE	C-N-CA	-6.12	117.15	122.96
10	PA	956	PHE	N-CA-C	-6.11	104.62	111.28
17	PH	90	TYR	CA-C-N	-6.11	114.73	122.43
17	PH	90	TYR	C-N-CA	-6.11	114.73	122.43
11	PB	931	ILE	N-CA-C	-6.11	98.33	107.37
11	PB	522	LEU	N-CA-C	-6.11	103.99	112.30
10	PA	506	PRO	N-CA-CB	-6.10	97.78	103.27
12	PC	204	PRO	CB-CA-C	-6.10	102.99	110.98
11	PB	411	LEU	N-CA-C	-6.10	104.72	111.36
1	0	295	ARG	CA-C-N	-6.09	112.52	120.44
1	0	295	ARG	C-N-CA	-6.09	112.52	120.44
10	PA	582	PRO	N-CA-C	-6.09	104.76	113.47
12	PC	48	ASP	CA-CB-CG	6.09	118.69	112.60
14	PE	55	ARG	N-CA-C	-6.08	105.10	113.56
57	n	1348	PRO	N-CA-CB	6.08	110.02	103.33
10	PA	1387	SER	N-CA-C	-6.08	106.50	114.04
60	r	6	VAL	N-CA-C	6.08	116.86	110.72
10	PA	358	ARG	CA-C-O	-6.08	114.77	121.58
10	PA	1370	GLY	CA-C-O	-6.07	118.04	122.23
11	PB	870	THR	CB-CA-C	-6.06	101.05	111.23
13	PD	68	THR	N-CA-C	-6.05	104.68	111.28
57	n	74	PRO	N-CA-CB	6.05	109.93	103.39
2	8	287	THR	N-CA-C	-6.05	104.68	111.28
18	PI	118	HIS	CA-C-N	-6.05	115.24	122.44
18	PI	118	HIS	C-N-CA	-6.05	115.24	122.44
20	PK	72	ILE	CA-C-O	-6.05	114.16	120.27
3	9	39	LYS	N-CA-C	-6.05	104.69	111.28
61	s	113	PRO	N-CA-CB	6.05	109.98	103.33
53	h	49	PHE	CB-CA-C	-6.04	101.40	110.88
3	9	82	THR	CB-CA-C	-6.04	100.77	110.79
11	PB	780	VAL	CB-CA-C	-6.04	102.69	111.68
11	PB	736	TYR	CA-CB-CG	6.03	124.75	113.90
2	8	261	PHE	N-CA-C	-6.03	98.91	108.73
3	9	84	CYS	CB-CA-C	-6.03	100.79	110.79
11	PB	303	PRO	N-CA-C	-6.03	104.85	113.47
44	c	290	ASP	N-CA-C	-6.02	105.25	114.16
10	PA	1432	PHE	N-CA-C	6.02	118.42	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	PB	1045	PRO	N-CA-CB	-6.01	96.93	103.25
2	8	240	MET	N-CA-C	-6.01	104.73	111.28
13	PD	121	ARG	N-CA-C	-6.01	104.73	111.28
2	8	96	THR	CB-CA-C	-6.01	98.47	110.42
55	j	94	GLN	O-C-N	-6.00	115.31	122.15
1	0	70	LYS	N-CA-C	-6.00	104.65	111.07
55	j	52	ASP	CA-CB-CG	5.99	118.59	112.60
26	DF	415	ILE	N-CA-C	-5.99	106.90	112.83
2	8	50	GLU	N-CA-C	-5.99	105.82	113.01
62	t	133	PRO	CB-CA-C	-5.99	101.68	111.56
11	PB	743	ARG	N-CA-C	-5.99	102.63	110.53
10	PA	428	ASP	CB-CA-C	-5.98	99.79	109.72
22	DA	822	PRO	N-CA-C	-5.98	100.16	112.47
55	j	60	ASP	CA-C-N	5.98	132.73	121.97
55	j	60	ASP	C-N-CA	5.98	132.73	121.97
3	9	204	TYR	N-CA-C	-5.97	104.77	111.28
10	PA	1072	ILE	N-CA-C	-5.97	104.53	110.62
7	BA	34	CYS	CA-C-N	5.97	125.85	119.28
7	BA	34	CYS	C-N-CA	5.97	125.85	119.28
10	PA	392	GLU	CB-CA-C	-5.96	101.07	110.79
18	PI	65	LEU	N-CA-C	-5.96	104.78	111.28
39	3	236	ASP	N-CA-C	-5.96	105.67	113.12
13	PD	56	GLU	N-CA-C	-5.96	101.84	110.24
10	PA	550	LYS	N-CA-C	-5.96	100.72	109.18
3	9	30	PHE	CB-CA-C	-5.95	100.91	110.79
10	PA	781	ILE	N-CA-C	-5.95	104.55	110.62
6	DQ	368	SER	N-CA-C	-5.95	105.10	112.90
61	s	158	PRO	N-CA-CB	5.95	109.50	103.25
10	PA	757	GLN	CB-CA-C	5.95	120.66	110.79
11	PB	1108	PHE	CA-CB-CG	5.95	119.75	113.80
3	9	274	LYS	CB-CA-C	-5.94	101.55	110.88
7	BA	217	ARG	N-CA-C	5.94	117.76	111.28
44	c	295	THR	CB-CA-C	5.94	121.63	110.63
1	0	285	GLY	N-CA-C	-5.94	107.80	114.40
38	2	55	LEU	N-CA-C	5.94	119.31	110.52
40	4	334	MET	CA-C-N	5.94	132.88	121.54
40	4	334	MET	C-N-CA	5.94	132.88	121.54
12	PC	232	ASN	CB-CA-C	-5.93	102.24	112.44
12	PC	255	LYS	N-CA-C	-5.93	104.73	111.07
52	g	19	LYS	N-CA-C	-5.93	106.38	113.97
10	PA	1193	VAL	N-CA-C	-5.92	104.74	110.72
10	PA	1069	LEU	N-CA-C	-5.92	104.82	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	PA	685	HIS	CA-C-O	-5.92	113.00	120.28
11	PB	788	TYR	N-CA-C	-5.92	106.10	113.15
59	q	410	PRO	N-CA-CB	5.92	110.07	103.44
11	PB	1026	GLU	CA-C-O	-5.91	114.72	121.40
10	PA	1034	GLN	N-CA-C	-5.90	104.85	111.28
23	DB	181	GLY	CA-C-O	-5.90	118.06	122.37
26	Df	255	MET	N-CA-C	-5.89	104.96	114.09
57	n	1309	PRO	N-CA-CB	5.89	110.04	103.44
10	PA	349	ARG	N-CA-C	-5.89	105.95	113.01
62	t	90	ASN	N-CA-C	-5.89	105.94	113.01
3	9	80	VAL	CB-CA-C	-5.88	104.20	112.14
40	4	384	PRO	N-CA-C	5.88	117.88	110.70
14	PE	45	GLY	CA-C-O	-5.88	118.08	122.37
10	PA	924	TYR	N-CA-C	-5.87	106.03	112.72
35	EA	157	CYS	N-CA-C	-5.87	100.93	110.20
1	0	215	PRO	N-CA-CB	5.86	109.78	103.33
49	a	278	HIS	CB-CA-C	5.86	118.78	109.52
3	9	60	TYR	CB-CA-C	5.85	120.80	110.85
10	PA	344	LYS	CB-CA-C	-5.85	103.52	115.28
3	9	19	LEU	CA-C-N	-5.85	112.44	120.28
3	9	19	LEU	C-N-CA	-5.85	112.44	120.28
9	FB	138	PRO	N-CA-C	-5.85	102.08	111.38
20	PK	36	ASN	CA-C-O	-5.84	114.56	121.16
11	PB	1000	THR	N-CA-C	-5.84	102.02	110.08
2	8	253	PRO	N-CA-C	-5.82	105.44	113.53
10	PA	762	GLU	N-CA-C	-5.82	105.83	113.17
62	t	173	PRO	N-CA-CB	-5.82	97.14	103.25
2	8	290	LEU	N-CA-C	-5.82	104.94	111.28
1	0	217	PRO	N-CA-CB	5.82	109.73	103.33
1	0	74	ILE	N-CA-C	-5.81	104.84	110.42
35	EA	152	PHE	CB-CA-C	5.81	119.37	109.72
10	PA	504	HIS	CA-C-O	-5.81	113.93	120.32
19	PJ	51	ALA	CB-CA-C	-5.81	103.31	111.85
2	8	238	PRO	CA-C-O	-5.80	114.83	121.56
3	9	288	ASN	N-CA-C	5.80	118.00	109.24
10	PA	739	ASN	N-CA-C	-5.80	104.96	111.28
10	PA	465	HIS	CA-CB-CG	5.79	119.59	113.80
11	PB	735	VAL	CB-CA-C	5.79	119.09	111.33
11	PB	1097	HIS	N-CA-C	-5.79	105.48	112.54
17	PH	80	ASP	N-CA-C	-5.78	104.76	113.89
13	PD	84	ARG	CB-CA-C	-5.78	101.81	110.88
3	9	202	ASP	N-CA-C	-5.77	106.58	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8	173	VAL	N-CA-C	5.76	116.52	111.56
22	DA	469	PRO	N-CA-C	5.76	121.71	113.47
11	PB	149	ILE	N-CA-C	-5.76	107.89	113.53
19	PJ	4	PRO	CA-C-O	-5.76	114.78	121.34
10	PA	895	GLY	N-CA-C	-5.75	107.38	115.32
11	PB	1050	ARG	CB-CA-C	-5.75	101.53	111.30
52	g	28	GLU	N-CA-C	-5.75	105.58	112.59
10	PA	476	ILE	CA-C-O	-5.75	115.04	121.36
11	PB	339	ALA	N-CA-C	-5.75	105.02	111.28
10	PA	389	THR	CB-CA-C	-5.75	100.03	109.80
10	PA	543	THR	CA-CB-OG1	-5.74	100.98	109.60
2	8	206	LEU	CA-C-N	-5.74	112.64	120.44
2	8	206	LEU	C-N-CA	-5.74	112.64	120.44
2	8	280	PRO	CA-C-N	-5.73	112.60	120.28
2	8	280	PRO	C-N-CA	-5.73	112.60	120.28
11	PB	786	THR	CA-C-N	-5.73	116.66	123.08
11	PB	786	THR	C-N-CA	-5.73	116.66	123.08
2	8	204	ALA	N-CA-C	-5.73	104.94	111.07
11	PB	318	LEU	N-CA-C	-5.73	105.03	111.28
10	PA	989	ASN	N-CA-C	-5.73	105.04	111.28
12	PC	96	GLU	CB-CA-C	5.73	115.50	109.83
3	9	278	GLU	CB-CA-C	-5.72	101.29	110.79
10	PA	462	PRO	CB-CA-C	-5.72	105.31	113.09
12	PC	201	GLU	N-CA-C	5.72	117.60	111.36
35	EA	129	CYS	CB-CA-C	-5.72	103.50	110.08
12	PC	42	VAL	N-CA-C	-5.72	103.35	108.95
3	9	33	LYS	CA-C-N	-5.72	112.62	120.28
3	9	33	LYS	C-N-CA	-5.72	112.62	120.28
14	PE	181	ARG	N-CA-C	-5.72	105.05	111.28
2	8	139	LYS	CB-CA-C	5.71	118.19	109.56
10	PA	1067	TRP	N-CA-C	-5.71	105.05	111.28
11	PB	163	LEU	N-CA-C	-5.71	105.89	112.92
10	PA	507	GLN	CB-CG-CD	-5.71	102.89	112.60
11	PB	797	ASN	CA-CB-CG	5.71	118.31	112.60
10	PA	542	LEU	N-CA-C	-5.70	104.52	112.45
20	PK	36	ASN	CB-CA-C	-5.70	98.94	109.37
40	4	406	GLY	N-CA-C	5.70	117.67	110.38
10	PA	930	LEU	N-CA-C	-5.69	105.08	111.28
3	9	29	LYS	CB-CA-C	-5.69	101.95	110.88
10	PA	672	ILE	N-CA-C	-5.69	104.96	110.42
37	1	418	LEU	N-CA-C	5.69	122.92	110.80
7	BA	19	PRO	N-CA-C	-5.68	100.76	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	PD	128	GLN	N-CA-C	-5.68	105.08	111.28
18	PI	83	ASP	CB-CA-C	-5.68	101.95	110.88
44	c	293	PRO	CB-CA-C	-5.68	103.98	110.92
11	PB	110	PRO	CB-CA-C	-5.68	103.25	112.62
3	9	109	ALA	CA-C-N	-5.68	112.67	120.28
3	9	109	ALA	C-N-CA	-5.68	112.67	120.28
14	PE	13	ILE	N-CA-C	-5.68	104.97	110.42
25	DE	470	TYR	N-CA-C	-5.67	106.33	113.20
11	PB	897	ARG	CA-C-N	-5.67	114.43	122.94
11	PB	897	ARG	C-N-CA	-5.67	114.43	122.94
26	Df	150	PRO	N-CA-C	5.67	117.62	110.70
67	w	1198	GLN	N-CA-C	-5.66	102.14	110.52
10	PA	499	ASP	CA-C-O	-5.66	114.76	121.66
69	X	-7	DT	C2'-C3'-O3'	-5.66	103.01	111.50
44	c	278	GLN	CB-CA-C	-5.65	101.58	110.85
11	PB	748	ALA	CA-C-O	-5.65	114.25	120.30
11	PB	935	PHE	CA-C-O	-5.65	114.50	121.06
13	PD	77	ARG	CB-CA-C	-5.65	101.41	110.79
3	9	271	ALA	CA-C-N	-5.65	113.45	120.56
3	9	271	ALA	C-N-CA	-5.65	113.45	120.56
5	DP	298	PRO	N-CA-C	-5.64	100.85	112.47
1	0	298	GLN	CA-C-N	-5.64	112.72	120.28
1	0	298	GLN	C-N-CA	-5.64	112.72	120.28
11	PB	1074	PRO	N-CA-C	5.64	120.06	111.15
43	7	512	GLU	N-CA-C	-5.64	108.19	114.62
10	PA	903	PHE	CB-CA-C	-5.63	100.87	109.89
40	4	401	LEU	N-CA-C	5.62	118.18	111.71
16	PG	10	GLU	CB-CA-C	5.62	119.45	109.72
25	DE	508	LYS	CA-C-O	-5.62	114.92	120.82
11	PB	257	VAL	CA-C-N	-5.62	114.84	122.77
11	PB	257	VAL	C-N-CA	-5.62	114.84	122.77
10	PA	440	LEU	CA-C-O	-5.62	115.01	121.47
10	PA	557	ARG	CB-CA-C	-5.62	101.47	110.79
25	DE	522	ASP	N-CA-C	-5.62	105.63	112.88
10	PA	1065	PHE	N-CA-C	-5.61	105.16	111.28
16	PG	134	ASP	N-CA-C	-5.61	105.24	111.36
10	PA	951	GLU	N-CA-C	-5.61	105.16	111.28
12	PC	112	THR	CA-C-N	-5.61	115.15	123.11
12	PC	112	THR	C-N-CA	-5.61	115.15	123.11
14	PE	22	HIS	N-CA-C	-5.61	105.17	111.28
3	9	187	LEU	CA-C-N	-5.61	112.97	120.54
3	9	187	LEU	C-N-CA	-5.61	112.97	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	PB	259	THR	N-CA-C	-5.60	103.13	110.53
13	PD	127	LEU	N-CA-C	-5.60	105.07	111.07
16	PG	24	ASN	N-CA-C	-5.60	105.25	111.36
17	PH	75	TYR	CB-CA-C	-5.60	102.17	111.41
11	PB	908	MET	CA-C-O	-5.60	114.59	120.80
20	PK	107	VAL	N-CA-C	-5.59	105.05	110.42
3	9	278	GLU	N-CA-C	-5.59	105.19	111.28
24	DD	948	GLU	N-CA-C	-5.59	105.19	111.28
12	PC	62	GLU	N-CA-C	-5.58	105.06	112.94
17	PH	94	GLY	N-CA-C	5.58	117.71	110.45
11	PB	106	SER	N-CA-CB	-5.58	105.54	111.29
11	PB	1083	GLY	CA-C-O	-5.58	116.44	122.47
40	4	132	ASP	N-CA-C	5.58	122.69	110.80
16	PG	31	PHE	CA-CB-CG	5.58	119.38	113.80
10	PA	449	HIS	CA-C-O	-5.58	115.40	121.87
57	n	525	TYR	CB-CA-C	5.58	118.09	110.06
17	PH	22	PHE	N-CA-C	-5.57	100.62	109.59
3	9	167	PHE	CA-C-N	-5.57	112.82	120.28
3	9	167	PHE	C-N-CA	-5.57	112.82	120.28
10	PA	839	HIS	N-CA-C	-5.57	105.21	111.28
11	PB	568	PHE	CA-C-N	-5.57	115.84	123.14
11	PB	568	PHE	C-N-CA	-5.57	115.84	123.14
19	PJ	24	LEU	N-CA-C	-5.57	105.36	111.82
10	PA	729	PRO	N-CA-CB	-5.57	98.18	103.19
43	7	686	ARG	CA-C-O	5.57	126.07	119.67
19	PJ	61	ASN	N-CA-C	-5.56	106.49	113.28
11	PB	1073	GLN	N-CA-C	-5.56	100.51	109.58
11	PB	1102	PHE	N-CA-C	-5.56	105.22	111.28
39	3	233	PRO	CA-C-N	5.56	132.16	121.54
39	3	233	PRO	C-N-CA	5.56	132.16	121.54
62	t	119	TYR	CA-C-N	5.56	130.64	122.63
62	t	119	TYR	C-N-CA	5.56	130.64	122.63
11	PB	198	GLU	CA-C-O	-5.56	115.50	121.56
10	PA	684	GLY	CA-C-O	-5.56	117.22	122.39
21	PL	45	TYR	CA-C-O	-5.55	114.83	120.71
24	DD	957	ARG	N-CA-C	-5.55	105.31	111.36
10	PA	113	PHE	CA-CB-CG	5.55	119.35	113.80
11	PB	631	GLN	N-CA-C	-5.55	101.94	109.54
20	PK	60	GLY	CA-C-O	-5.55	115.19	121.68
7	BA	11	PRO	N-CA-CB	5.55	109.10	103.00
10	PA	1194	ASN	N-CA-C	-5.55	105.23	111.28
20	PK	64	PRO	N-CA-CB	-5.54	97.40	103.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	PC	150	ILE	CA-C-O	-5.54	114.90	121.05
64	v	37	ILE	CB-CA-C	5.54	119.66	112.24
11	PB	1108	PHE	CB-CA-C	-5.54	99.40	110.42
1	0	289	SER	CA-C-N	-5.53	113.07	120.54
1	0	289	SER	C-N-CA	-5.53	113.07	120.54
2	8	177	TRP	CA-C-N	-5.53	114.95	123.14
2	8	177	TRP	C-N-CA	-5.53	114.95	123.14
3	9	116	ASP	CA-C-N	-5.53	114.65	122.34
3	9	116	ASP	C-N-CA	-5.53	114.65	122.34
18	PI	75	ASP	CB-CA-C	-5.53	100.94	109.62
11	PB	764	MET	N-CA-C	-5.53	104.89	111.69
23	DB	583	GLU	CB-CA-C	-5.52	101.62	110.79
9	FB	157	ALA	N-CA-C	-5.52	100.18	109.07
12	PC	171	LYS	N-CA-C	-5.52	105.42	111.82
11	PB	847	LYS	N-CA-C	-5.52	106.68	113.41
12	PC	166	LYS	N-CA-CB	-5.52	102.06	110.45
17	PH	122	LEU	CA-C-O	-5.52	115.18	121.58
7	BA	307	ASP	N-CA-C	-5.52	106.91	113.97
10	PA	770	VAL	CB-CA-C	-5.51	104.91	111.97
10	PA	432	HIS	N-CA-C	-5.51	101.54	109.48
10	PA	958	ARG	N-CA-C	-5.51	105.27	111.28
25	DE	511	SER	N-CA-C	-5.51	106.64	113.19
11	PB	866	ILE	CA-C-O	-5.50	115.02	120.85
31	DL	112	GLU	CB-CA-C	-5.50	110.21	116.54
14	PE	56	THR	CA-C-O	-5.50	115.18	121.40
11	PB	906	GLN	CA-C-O	-5.50	113.94	120.43
11	PB	734	GLY	N-CA-C	-5.50	103.09	110.56
11	PB	277	GLY	CA-C-N	-5.49	114.71	122.34
11	PB	277	GLY	C-N-CA	-5.49	114.71	122.34
11	PB	1097	HIS	CA-CB-CG	5.49	119.29	113.80
22	DA	638	PRO	CB-CA-C	-5.48	106.41	111.40
66	x	565	SER	CA-C-O	-5.48	115.79	122.64
11	PB	695	HIS	CA-CB-CG	5.48	119.28	113.80
49	a	162	ASN	N-CA-C	-5.48	106.67	113.19
9	FB	100	SER	N-CA-C	-5.47	105.47	111.82
10	PA	508	SER	CA-C-O	-5.47	115.42	121.33
14	PE	198	GLU	N-CA-C	5.47	117.24	111.28
10	PA	1028	PRO	CA-C-O	-5.47	115.00	121.67
12	PC	198	PRO	CB-CA-C	-5.47	104.37	113.06
11	PB	655	ASP	CA-C-N	-5.46	112.96	120.28
11	PB	655	ASP	C-N-CA	-5.46	112.96	120.28
43	7	262	ASN	CB-CA-C	-5.46	100.64	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	DB	264	GLU	N-CA-C	-5.46	106.29	113.17
14	PE	48	PRO	N-CA-C	-5.46	105.94	113.53
10	PA	697	LYS	CB-CA-C	-5.46	102.31	110.88
44	c	205	ARG	N-CA-C	-5.46	106.79	113.50
14	PE	144	LEU	CA-C-N	-5.45	118.66	122.59
14	PE	144	LEU	C-N-CA	-5.45	118.66	122.59
15	PF	81	VAL	CA-C-O	-5.45	116.62	121.09
19	PJ	5	VAL	CA-C-O	-5.45	115.28	120.95
43	7	685	ALA	N-CA-C	5.45	116.90	111.07
22	DA	507	GLU	CA-C-O	-5.45	115.61	121.38
4	DO	6	TYR	N-CA-C	5.44	119.03	112.93
1	0	197	LEU	N-CA-CB	-5.44	101.95	110.44
2	8	137	ASP	N-CA-C	5.44	117.47	108.49
65	z	492	ARG	CB-CA-C	-5.44	102.33	110.88
10	PA	408	ARG	CB-CG-CD	-5.44	98.78	111.30
12	PC	115	VAL	CA-C-O	-5.44	115.84	121.93
11	PB	853	LEU	N-CA-CB	-5.43	102.04	110.57
1	0	83	ASN	N-CA-C	-5.43	105.39	112.23
10	PA	428	ASP	CA-C-O	-5.43	115.22	121.19
10	PA	1340	GLY	CA-C-O	-5.43	117.34	122.39
10	PA	1415	THR	N-CA-C	-5.43	103.73	110.41
10	PA	1373	ALA	CA-C-N	-5.42	113.03	120.46
10	PA	1373	ALA	C-N-CA	-5.42	113.03	120.46
10	PA	444	TYR	CA-C-O	-5.42	114.88	121.28
16	PG	30	LEU	N-CA-CB	5.42	117.86	110.01
20	PK	71	ILE	N-CA-C	-5.42	99.91	108.90
10	PA	859	TYR	CA-C-N	-5.41	113.63	120.56
10	PA	859	TYR	C-N-CA	-5.41	113.63	120.56
10	PA	990	ALA	CA-C-N	-5.41	113.03	120.28
10	PA	990	ALA	C-N-CA	-5.41	113.03	120.28
10	PA	1474	LEU	CA-C-O	-5.41	115.11	121.44
7	BA	246	PRO	N-CA-C	5.40	118.98	110.50
62	t	202	LYS	CA-C-N	-5.39	112.99	120.38
62	t	202	LYS	C-N-CA	-5.39	112.99	120.38
70	Y	-2	DC	C4'-C3'-O3'	-5.39	101.91	110.00
11	PB	1074	PRO	N-CA-CB	-5.39	98.50	103.25
12	PC	229	PHE	N-CA-CB	-5.39	101.59	109.95
20	PK	62	LYS	N-CA-CB	5.39	119.74	110.68
10	PA	1043	ILE	N-CA-C	-5.39	105.12	110.62
12	PC	113	ARG	CB-CA-C	-5.39	102.00	110.79
3	9	177	ARG	CB-CA-C	5.39	120.01	110.85
2	8	276	PHE	CA-C-O	-5.38	114.72	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	PB	1066	PRO	CB-CA-C	5.38	118.40	111.46
18	PI	76	PRO	N-CA-C	-5.38	106.05	113.53
52	g	29	GLY	N-CA-C	-5.38	107.83	115.30
11	PB	749	HIS	CA-CB-CG	5.38	119.18	113.80
35	EA	49	LEU	N-CA-C	-5.38	106.72	113.28
43	7	13	PRO	CA-C-N	5.38	131.81	121.54
43	7	13	PRO	C-N-CA	5.38	131.81	121.54
43	7	558	LEU	CA-C-N	5.37	128.23	120.38
43	7	558	LEU	C-N-CA	5.37	128.23	120.38
2	8	138	LEU	N-CA-C	-5.37	101.90	109.96
11	PB	1030	ASN	CA-C-O	-5.37	115.28	121.19
20	PK	65	HIS	CA-C-O	-5.37	114.23	120.03
60	r	5	PRO	CA-C-O	-5.37	115.29	121.36
10	PA	524	MET	CB-CG-SD	-5.37	96.59	112.70
11	PB	113	ALA	CA-C-N	-5.37	112.67	120.29
11	PB	113	ALA	C-N-CA	-5.37	112.67	120.29
3	9	233	SER	CA-C-O	-5.37	114.86	120.55
17	PH	97	TYR	CB-CA-C	5.37	118.41	109.56
20	PK	78	THR	CB-CA-C	-5.37	99.60	110.17
10	PA	523	ARG	CB-CA-C	-5.36	101.50	110.56
11	PB	21	LEU	N-CA-C	-5.36	105.00	112.30
14	PE	112	PRO	N-CA-C	-5.36	106.08	113.53
49	a	136	PRO	N-CA-C	-5.36	106.07	113.53
17	PH	22	PHE	CA-C-O	-5.36	115.03	120.71
11	PB	387	HIS	CA-CB-CG	5.36	119.16	113.80
43	7	87	LEU	N-CA-CB	5.36	119.13	110.40
10	PA	364	ARG	CB-CG-CD	-5.35	98.98	111.30
18	PI	25	TYR	CB-CA-C	-5.35	100.59	109.15
67	w	1195	ALA	N-CA-C	-5.35	105.56	111.71
10	PA	420	ILE	CA-C-O	-5.35	115.47	121.36
50	d	179	ASP	N-CA-C	-5.35	108.52	114.62
5	DP	207	PRO	N-CA-C	-5.34	101.46	112.47
11	PB	60	GLU	CA-C-N	-5.34	115.23	123.14
11	PB	60	GLU	C-N-CA	-5.34	115.23	123.14
15	PF	116	GLU	N-CA-C	-5.34	102.97	110.50
10	PA	885	GLN	CB-CA-C	-5.34	100.85	109.72
11	PB	805	PHE	CB-CA-C	5.34	120.22	111.41
10	PA	810	PHE	CA-C-O	-5.34	115.74	121.56
2	8	283	ARG	CB-CA-C	5.34	117.84	109.84
11	PB	1101	GLN	CB-CA-C	5.34	119.65	110.79
10	PA	914	LYS	N-CA-C	-5.33	105.47	111.28
12	PC	227	GLU	CA-C-O	-5.33	115.02	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	PE	30	GLN	N-CA-C	-5.33	105.58	111.71
10	PA	506	PRO	CA-C-O	-5.33	115.53	121.23
13	PD	136	THR	CB-CA-C	-5.33	102.51	110.88
12	PC	116	THR	CB-CA-C	-5.33	98.99	111.09
18	PI	72	VAL	N-CA-C	-5.33	106.07	113.00
26	Df	329	LEU	N-CA-C	-5.33	106.48	112.87
49	a	480	TYR	CB-CA-C	5.33	118.82	110.19
10	PA	883	ILE	N-CA-C	-5.33	106.08	113.00
10	PA	77	ASN	CA-CB-CG	5.33	117.93	112.60
12	PC	155	LYS	CB-CA-C	-5.33	101.59	109.90
3	9	112	ALA	CA-C-N	-5.32	113.15	120.28
3	9	112	ALA	C-N-CA	-5.32	113.15	120.28
10	PA	1107	PHE	CB-CA-C	-5.32	101.96	110.79
17	PH	89	GLU	CB-CA-C	-5.32	102.36	111.46
11	PB	986	GLN	CA-C-N	-5.32	114.08	119.98
11	PB	986	GLN	C-N-CA	-5.32	114.08	119.98
3	9	86	TYR	N-CA-C	-5.32	105.49	111.28
2	8	148	ASN	N-CA-C	-5.31	105.49	111.28
3	9	26	ALA	CA-C-N	-5.31	113.16	120.28
3	9	26	ALA	C-N-CA	-5.31	113.16	120.28
3	9	33	LYS	N-CA-C	-5.31	105.49	111.28
10	PA	378	VAL	N-CA-C	-5.31	100.19	108.95
7	BA	15	CYS	N-CA-CB	-5.31	101.65	109.98
10	PA	218	PRO	N-CA-C	-5.31	106.15	113.53
12	PC	204	PRO	CA-C-O	-5.31	115.19	121.67
15	PF	63	ALA	N-CA-C	-5.31	105.93	112.72
60	r	15	THR	CA-C-N	-5.31	113.36	120.95
60	r	15	THR	C-N-CA	-5.31	113.36	120.95
10	PA	980	PRO	N-CA-C	5.31	123.40	112.47
11	PB	659	SER	N-CA-C	-5.30	106.58	113.16
17	PH	121	LEU	CA-C-O	-5.30	115.93	121.55
44	c	221	VAL	N-CA-C	-5.30	106.70	112.80
17	PH	49	PRO	CB-CA-C	-5.30	104.96	111.64
16	PG	36	GLY	CA-C-N	-5.30	113.53	120.95
16	PG	36	GLY	C-N-CA	-5.30	113.53	120.95
3	9	279	ARG	N-CA-C	-5.30	105.51	111.28
10	PA	367	ILE	CA-C-O	-5.30	114.86	120.53
12	PC	222	PRO	N-CA-C	5.30	121.05	113.47
12	PC	19	VAL	CA-C-O	-5.29	114.92	120.27
10	PA	638	GLY	O-C-N	5.29	127.39	122.47
1	0	66	PRO	N-CA-C	-5.29	107.30	114.80
14	PE	93	ARG	N-CA-C	-5.29	105.52	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	PB	1050	ARG	CA-C-O	-5.28	115.42	120.92
11	PB	112	GLU	N-CA-C	-5.28	105.53	111.28
7	BA	21	ALA	CA-C-N	-5.28	116.28	122.93
7	BA	21	ALA	C-N-CA	-5.28	116.28	122.93
40	4	263	GLN	N-CA-C	-5.28	105.64	111.71
10	PA	1006	PRO	N-CA-C	-5.27	106.20	113.53
10	PA	873	VAL	CA-C-O	-5.27	116.11	121.70
5	DP	205	ARG	CB-CA-C	-5.27	101.05	110.70
11	PB	98	HIS	CB-CA-C	-5.27	101.41	110.16
2	8	169	TYR	CB-CA-C	5.27	118.44	109.80
19	PJ	2	ILE	CA-C-O	-5.27	115.70	121.28
10	PA	402	LEU	CA-C-N	-5.26	112.81	120.29
10	PA	402	LEU	C-N-CA	-5.26	112.81	120.29
64	v	25	ASP	CA-C-N	-5.26	113.25	120.46
64	v	25	ASP	C-N-CA	-5.26	113.25	120.46
4	DO	57	ASN	CA-C-O	-5.26	115.10	120.99
17	PH	65	TYR	CA-C-O	-5.26	114.95	120.63
38	2	354	ASP	CA-C-N	5.26	129.59	122.07
38	2	354	ASP	C-N-CA	5.26	129.59	122.07
2	8	177	TRP	N-CA-C	-5.26	105.45	111.07
26	DF	272	VAL	N-CA-C	-5.26	105.26	110.62
42	6	151	GLY	N-CA-C	-5.26	107.75	114.37
29	DI	84	THR	N-CA-C	-5.25	107.04	113.50
19	PJ	40	LEU	N-CA-CB	-5.25	101.34	110.17
20	PK	76	GLN	CB-CA-C	-5.25	101.08	109.75
42	6	140	LEU	N-CA-C	-5.25	106.38	112.89
43	7	368	GLN	CA-C-N	5.25	131.57	121.54
43	7	368	GLN	C-N-CA	5.25	131.57	121.54
70	Y	-2	DC	O3'-P-O5'	5.25	111.88	104.00
10	PA	496	PHE	N-CA-CB	-5.25	104.13	110.53
11	PB	713	PHE	CA-C-O	-5.24	116.85	120.47
16	PG	76	VAL	CA-C-O	-5.24	115.72	121.28
37	1	324	ALA	N-CA-C	5.24	118.56	111.17
9	FB	31	TRP	N-CA-C	5.24	117.74	111.71
42	6	263	GLU	CA-C-N	5.24	131.55	121.54
42	6	263	GLU	C-N-CA	5.24	131.55	121.54
10	PA	566	PHE	CB-CA-C	5.24	118.84	110.09
23	DB	491	HIS	CB-CA-C	5.24	119.49	110.79
10	PA	977	VAL	CA-C-O	-5.24	116.17	121.67
67	w	15	THR	N-CA-C	-5.23	105.64	112.23
2	8	283	ARG	N-CA-C	-5.23	102.55	110.24
12	PC	114	HIS	N-CA-C	-5.23	102.64	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8	173	VAL	CA-C-O	-5.23	115.71	120.73
43	7	20	GLU	CA-C-N	-5.23	112.75	120.28
43	7	20	GLU	C-N-CA	-5.23	112.75	120.28
7	BA	40	VAL	CA-C-O	-5.23	118.08	122.63
11	PB	136	GLY	N-CA-C	-5.23	107.51	115.66
11	PB	1091	ARG	CB-CA-C	-5.22	101.37	110.09
19	PJ	6	ARG	CB-CA-C	-5.22	100.51	109.65
21	PL	17	TYR	CA-C-O	-5.22	115.65	121.81
40	4	315	LEU	N-CA-C	5.22	121.92	110.80
10	PA	594	LEU	N-CA-C	-5.22	106.59	113.12
10	PA	1420	ASN	N-CA-C	-5.22	105.59	111.28
10	PA	307	VAL	N-CA-C	-5.22	105.30	110.62
10	PA	895	GLY	CA-C-N	-5.22	115.52	122.72
10	PA	895	GLY	C-N-CA	-5.22	115.52	122.72
10	PA	1203	ASP	N-CA-C	-5.22	105.77	111.82
10	PA	837	PHE	N-CA-C	-5.21	105.60	111.28
15	PF	69	ARG	N-CA-C	-5.21	105.60	111.28
68	p	380	LEU	CA-C-N	-5.21	118.52	122.33
68	p	380	LEU	C-N-CA	-5.21	118.52	122.33
10	PA	669	TYR	CB-CA-C	-5.21	102.70	110.88
10	PA	1431	SER	CA-C-N	-5.20	116.06	123.03
10	PA	1431	SER	C-N-CA	-5.20	116.06	123.03
2	8	271	LEU	N-CA-C	-5.20	105.61	111.28
10	PA	569	THR	N-CA-CB	-5.20	103.05	110.80
12	PC	173	HIS	CA-CB-CG	5.20	119.00	113.80
14	PE	88	LYS	N-CA-C	-5.19	105.62	111.28
10	PA	1231	ILE	N-CA-C	-5.19	105.32	110.62
18	PI	91	HIS	N-CA-C	-5.19	102.71	110.23
3	9	79	VAL	CA-C-N	-5.19	113.35	120.46
3	9	79	VAL	C-N-CA	-5.19	113.35	120.46
11	PB	805	PHE	CA-C-O	-5.19	115.59	121.66
10	PA	942	VAL	N-CA-C	-5.18	105.33	110.62
11	PB	219	GLY	CA-C-O	-5.18	116.44	121.11
11	PB	941	GLN	CA-C-O	-5.18	114.62	120.32
10	PA	1224	ARG	N-CA-C	-5.18	106.22	112.54
7	BA	126	ASP	CB-CA-C	5.18	119.31	110.56
10	PA	590	GLN	CB-CG-CD	-5.18	103.80	112.60
1	0	263	LEU	CA-C-N	-5.18	114.40	122.42
1	0	263	LEU	C-N-CA	-5.18	114.40	122.42
10	PA	457	ILE	CA-C-O	-5.18	114.73	120.74
12	PC	233	VAL	CA-C-O	-5.18	115.13	121.13
43	7	632	ILE	N-CA-C	-5.18	105.30	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	PC	195	THR	CA-C-N	-5.17	116.15	122.93
12	PC	195	THR	C-N-CA	-5.17	116.15	122.93
10	PA	84	HIS	CA-CB-CG	-5.17	108.63	113.80
10	PA	408	ARG	N-CA-C	-5.17	106.83	112.72
10	PA	344	LYS	O-C-N	5.17	125.36	120.71
51	f	109	PRO	O-C-N	5.17	129.30	123.10
4	DO	58	PHE	CB-CA-C	-5.16	101.52	112.78
11	PB	1115	GLN	CA-C-N	-5.16	115.94	123.06
11	PB	1115	GLN	C-N-CA	-5.16	115.94	123.06
2	8	195	ASP	CA-C-N	-5.16	113.73	120.44
2	8	195	ASP	C-N-CA	-5.16	113.73	120.44
18	PI	108	MET	N-CA-C	-5.16	104.28	110.88
11	PB	1079	SER	CA-C-N	-5.16	114.92	122.40
11	PB	1079	SER	C-N-CA	-5.16	114.92	122.40
1	0	198	LEU	N-CA-C	5.16	121.78	110.80
10	PA	839	HIS	CB-CA-C	-5.16	102.23	110.79
7	BA	45	VAL	CA-C-O	-5.16	114.36	118.90
10	PA	1311	LEU	N-CA-C	-5.15	103.29	109.83
10	PA	1030	SER	N-CA-C	-5.15	105.75	113.89
12	PC	20	LYS	CB-CA-C	-5.15	104.00	112.03
10	PA	1482	TYR	N-CA-C	-5.15	106.83	113.01
21	PL	18	ILE	CA-C-O	-5.15	115.02	120.48
10	PA	1230	GLN	N-CA-C	-5.14	105.56	111.07
64	v	8	PRO	N-CA-CB	5.14	108.66	103.00
3	9	92	LEU	N-CA-C	-5.14	107.01	113.28
20	PK	40	HIS	CA-CB-CG	5.14	118.94	113.80
10	PA	1153	ARG	N-CA-C	-5.14	105.76	111.36
26	DF	299	LYS	N-CA-C	-5.14	106.70	113.17
39	3	152	LYS	N-CA-C	-5.14	106.83	114.64
18	PI	43	ASP	CA-C-N	-5.13	113.58	120.82
18	PI	43	ASP	C-N-CA	-5.13	113.58	120.82
10	PA	836	PHE	CA-CB-CG	5.13	118.93	113.80
11	PB	781	ALA	N-CA-CB	-5.13	102.08	110.95
10	PA	1104	LEU	CA-C-O	-5.13	115.44	120.82
10	PA	602	CYS	CB-CA-C	-5.12	99.54	109.68
10	PA	805	ARG	CA-C-O	-5.12	115.95	121.38
11	PB	1078	ARG	CB-CA-C	-5.12	101.76	113.33
42	6	419	ARG	N-CA-C	-5.12	106.88	113.02
2	8	100	VAL	CA-C-N	-5.12	114.11	120.56
2	8	100	VAL	C-N-CA	-5.12	114.11	120.56
12	PC	166	LYS	CA-C-O	-5.12	115.77	121.81
14	PE	56	THR	N-CA-C	-5.12	101.51	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	PB	703	ILE	CB-CA-C	-5.12	104.87	111.88
49	a	501	CYS	CB-CA-C	-5.12	109.70	117.07
2	8	244	PRO	CB-CA-C	-5.12	104.92	113.06
20	PK	36	ASN	CA-C-N	5.12	129.40	122.19
20	PK	36	ASN	C-N-CA	5.12	129.40	122.19
10	PA	426	ARG	N-CA-CB	-5.11	102.92	110.90
11	PB	934	LYS	N-CA-CB	5.11	117.49	109.97
11	PB	737	ILE	N-CA-C	-5.11	98.71	109.34
17	PH	14	ASP	CA-C-N	-5.11	116.07	121.84
17	PH	14	ASP	C-N-CA	-5.11	116.07	121.84
10	PA	588	GLY	CA-C-N	-5.10	113.44	120.28
10	PA	588	GLY	C-N-CA	-5.10	113.44	120.28
13	PD	80	ILE	N-CA-C	-5.10	105.42	110.62
11	PB	933	ASP	CA-C-O	-5.10	114.88	120.69
1	0	298	GLN	CB-CA-C	-5.10	102.33	110.79
10	PA	800	PHE	N-CA-C	-5.10	102.10	109.59
11	PB	427	LYS	CA-C-O	-5.10	115.15	120.55
69	X	4	DC	P-O3'-C3'	5.10	127.85	120.20
11	PB	947	ILE	N-CA-C	-5.09	98.75	109.34
16	PG	28	GLN	N-CA-C	-5.09	105.73	111.28
11	PB	589	LYS	N-CA-C	-5.09	105.73	111.28
11	PB	422	PHE	CB-CA-C	5.09	119.50	110.85
11	PB	1084	LEU	N-CA-CB	-5.08	103.36	110.38
10	PA	583	ARG	N-CA-CB	5.08	116.44	111.10
12	PC	184	PHE	CB-CA-C	5.08	121.48	111.22
17	PH	95	LYS	CA-C-O	-5.08	115.80	121.23
11	PB	684	GLU	N-CA-C	-5.08	101.35	109.07
12	PC	169	PHE	CA-CB-CG	5.08	118.88	113.80
20	PK	66	PRO	CB-CA-C	-5.08	104.27	111.68
67	w	1140	GLU	CA-CB-CG	5.08	124.25	114.10
10	PA	655	ILE	N-CA-C	-5.08	105.44	110.62
13	PD	81	ALA	N-CA-C	-5.07	105.75	111.28
20	PK	58	PHE	CA-C-O	-5.07	114.51	120.60
2	8	273	GLN	N-CA-C	-5.07	105.75	111.28
10	PA	1051	SER	CA-C-N	-5.07	113.49	120.28
10	PA	1051	SER	C-N-CA	-5.07	113.49	120.28
10	PA	857	THR	CA-C-N	-5.07	113.71	122.83
10	PA	857	THR	C-N-CA	-5.07	113.71	122.83
10	PA	1107	PHE	N-CA-C	-5.07	105.75	111.28
11	PB	1090	GLU	CB-CA-C	-5.07	101.99	110.56
11	PB	224	CYS	CA-C-N	-5.07	114.39	122.29
11	PB	224	CYS	C-N-CA	-5.07	114.39	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	PB	750	VAL	CA-C-O	-5.07	114.45	120.78
11	PB	1079	SER	CA-C-O	-5.07	114.07	120.55
4	DO	9	THR	N-CA-C	-5.06	101.72	109.41
1	0	292	ALA	CA-C-N	-5.06	113.00	120.28
1	0	292	ALA	C-N-CA	-5.06	113.00	120.28
12	PC	152	LYS	CA-C-O	-5.06	116.05	121.56
17	PH	42	ASP	CA-C-O	-5.06	115.24	120.70
43	7	263	LEU	N-CA-C	-5.06	100.03	110.80
2	8	204	ALA	CB-CA-C	-5.05	102.94	110.88
10	PA	732	THR	CB-CA-C	-5.05	99.32	109.68
10	PA	1419	VAL	N-CA-C	-5.05	107.54	112.29
44	c	285	GLY	CA-C-O	-5.05	117.22	122.28
2	8	249	PHE	CA-CB-CG	-5.05	108.75	113.80
10	PA	549	THR	CA-C-O	-5.05	116.11	122.63
53	h	58	THR	N-CA-C	-5.05	105.77	111.28
11	PB	28	ILE	N-CA-C	-5.05	105.62	110.72
24	DD	875	GLN	CA-C-O	-5.05	115.64	121.19
5	DP	167	ASN	CB-CA-C	-5.05	101.22	109.80
9	FB	45	ILE	N-CA-C	5.05	115.03	107.51
10	PA	808	PRO	CB-CA-C	-5.04	104.30	112.62
18	PI	112	TYR	CA-C-O	-5.04	115.46	121.56
10	PA	985	ARG	N-CA-C	-5.04	105.79	111.28
13	PD	29	ALA	CA-C-N	-5.04	115.89	123.00
13	PD	29	ALA	C-N-CA	-5.04	115.89	123.00
13	PD	43	HIS	N-CA-C	-5.04	105.78	111.28
15	PF	103	PRO	CA-C-O	-5.04	115.65	123.16
11	PB	488	PRO	CA-C-N	-5.04	113.31	122.43
11	PB	488	PRO	C-N-CA	-5.04	113.31	122.43
10	PA	512	ARG	CA-C-N	-5.04	113.53	120.28
10	PA	512	ARG	C-N-CA	-5.04	113.53	120.28
51	f	147	TRP	CA-C-O	-5.04	116.44	122.13
10	PA	697	LYS	N-CA-C	-5.04	105.68	111.07
10	PA	1409	GLY	CA-C-N	-5.04	115.39	122.94
10	PA	1409	GLY	C-N-CA	-5.04	115.39	122.94
18	PI	111	TYR	CA-C-O	-5.04	115.18	120.92
10	PA	283	ILE	N-CA-C	-5.03	105.48	110.62
10	PA	685	HIS	CB-CA-C	-5.03	100.84	109.65
15	PF	100	ARG	CA-C-O	-5.03	115.76	121.65
10	PA	763	TYR	CA-C-N	-5.03	113.73	120.82
10	PA	763	TYR	C-N-CA	-5.03	113.73	120.82
10	PA	944	SER	N-CA-C	5.03	116.84	111.36
10	PA	1117	VAL	CA-C-N	-5.03	116.08	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	PA	1117	VAL	C-N-CA	-5.03	116.08	122.77
12	PC	97	CYS	N-CA-C	-5.03	106.07	113.61
62	t	200	ILE	CB-CA-C	-5.03	105.35	112.14
15	PF	116	GLU	CA-C-O	-5.02	116.09	121.56
43	7	299	ARG	N-CA-C	-5.02	106.40	112.88
11	PB	414	GLU	CA-C-N	-5.02	113.58	120.46
11	PB	414	GLU	C-N-CA	-5.02	113.58	120.46
10	PA	1016	LEU	N-CA-C	-5.02	105.81	111.28
11	PB	385	ARG	CA-C-N	-5.02	114.35	122.23
11	PB	385	ARG	C-N-CA	-5.02	114.35	122.23
11	PB	741	HIS	CA-CB-CG	-5.02	108.78	113.80
6	DQ	58	GLY	CA-C-O	-5.01	118.05	122.16
12	PC	37	VAL	N-CA-C	-5.01	105.69	113.16
14	PE	177	ASP	CA-CB-CG	5.01	117.61	112.60
10	PA	1294	THR	N-CA-C	5.01	116.82	111.36
53	h	51	LEU	CA-C-N	-5.01	113.93	120.44
53	h	51	LEU	C-N-CA	-5.01	113.93	120.44
7	BA	166	ILE	N-CA-C	5.01	115.23	110.42
17	PH	51	ASP	CB-CA-C	5.01	120.05	109.79
26	Df	305	ILE	N-CA-CB	5.01	113.87	110.52
67	w	1253	GLY	N-CA-C	5.01	122.55	112.34
2	8	243	LEU	N-CA-CB	-5.00	103.38	110.04
36	EB	112	GLY	CA-C-O	-5.00	117.98	121.88
12	PC	30	VAL	CA-C-N	-5.00	113.64	120.44
12	PC	30	VAL	C-N-CA	-5.00	113.64	120.44
12	PC	51	GLN	CA-C-O	-5.00	114.95	120.30
12	PC	66	HIS	CA-CB-CG	5.00	118.80	113.80
66	x	636	ARG	CA-C-N	5.00	127.23	120.38
66	x	636	ARG	C-N-CA	5.00	127.23	120.38

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	0	2255	0	2006	146	0
2	8	2378	0	2397	191	0
3	9	2307	0	2314	148	0
4	DO	771	0	764	41	0
5	DP	1412	0	1506	97	0
6	DQ	996	0	926	31	0
7	BA	1959	0	1987	118	0
8	FA	1101	0	1065	88	0
9	FB	1788	0	1819	133	0
10	PA	11662	0	11737	501	0
11	PB	9062	0	9110	381	0
12	PC	2059	0	2007	108	0
13	PD	1021	0	979	131	0
14	PE	1720	0	1737	79	0
15	PF	635	0	665	22	0
16	PG	1334	0	1333	76	0
17	PH	1186	0	1147	43	0
18	PI	927	0	859	64	0
19	PJ	507	0	523	22	0
20	PK	937	0	959	33	0
21	PL	372	0	378	11	0
22	DA	4918	0	4854	122	0
23	DB	7796	0	7751	135	0
24	DD	1330	0	1351	70	0
24	Dd	1307	0	1318	21	0
25	DE	4364	0	4244	106	0
25	De	4327	0	4197	46	0
26	DF	3109	0	3045	151	0
26	Df	3081	0	3012	81	0
27	DG	1180	0	1235	16	0
28	DH	1633	0	1621	53	0
29	DI	959	0	969	118	0
29	Di	967	0	977	31	0
30	DJ	720	0	719	70	0
30	Dj	759	0	759	18	0
31	DL	614	0	614	93	0
31	Dl	876	0	893	59	0
32	Dc	1011	0	975	25	0
33	Dk	785	0	818	9	0
34	Dm	724	0	744	12	0
35	EA	1476	0	1487	43	0
36	EB	1404	0	1424	25	0
37	1	3436	0	3403	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	3024	0	2991	128	0
39	3	2306	0	2332	109	0
40	4	3644	0	3687	221	0
41	5	522	0	528	60	0
42	6	5255	0	5247	269	0
43	7	5861	0	5869	252	0
44	c	2108	0	2095	101	0
45	e	832	0	824	70	0
46	b	899	0	908	108	0
47	l	1040	0	1065	65	0
48	m	983	0	968	148	0
49	a	3585	0	3524	348	0
50	d	1268	0	1305	239	0
51	f	1329	0	1302	164	0
52	g	1382	0	1407	224	0
53	h	1465	0	1460	291	0
54	i	605	0	628	226	0
55	j	1001	0	1023	255	0
56	k	879	0	886	226	0
57	n	7241	0	6673	513	0
58	o	1221	0	1212	147	0
59	q	4276	0	4243	528	0
60	r	1630	0	1644	77	0
61	s	505	0	361	74	0
62	t	1499	0	1482	142	0
63	u	792	0	749	247	0
64	v	1083	0	1059	188	0
65	z	765	0	727	115	0
66	x	7050	0	7205	166	0
67	w	10772	0	10832	284	0
68	p	3124	0	3133	58	0
69	X	1429	0	769	119	0
70	Y	1400	0	774	105	0
71	0	2	0	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	PJ	1	0	0	0	0
71	PL	1	0	0	0	0
72	PA	1	0	0	0	0
73	7	8	0	0	0	0
All	All	173965	0	171540	7785	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 23.

All (7785) 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)
50:d:49:ALA:HB2	54:i:76:MET:SD	1.22	1.67
67:w:394:PRO:HA	68:p:171:PHE:CZ	1.29	1.66
49:a:493:PHE:CE2	49:a:514:LYS:HG3	1.29	1.65
54:i:65:PHE:CD1	54:i:99:LYS:HG2	1.16	1.63
52:g:161:ILE:HA	54:i:140:MET:CE	1.15	1.62
49:a:229:SER:CB	49:a:502:MET:HG2	1.14	1.61
13:PD:137:LYS:HE2	53:h:51:LEU:CG	1.17	1.61
12:PC:265:HIS:CE1	62:t:113:ARG:HD2	1.15	1.60
60:r:19:MET:CE	60:r:177:ALA:HA	1.27	1.60
54:i:65:PHE:CE1	54:i:99:LYS:CG	1.75	1.59
13:PD:137:LYS:HE2	53:h:51:LEU:CD1	1.33	1.58
46:b:174:ILE:CD1	47:l:75:LEU:HD21	1.23	1.58
55:j:26:VAL:CG1	55:j:38:ASN:HD21	1.17	1.57
55:j:75:ARG:CB	55:j:80:TYR:CE2	1.82	1.57
49:a:467:MET:CE	49:a:504:ILE:HD11	1.25	1.57
56:k:24:ILE:HG21	59:q:164:ALA:CB	1.35	1.57
56:k:24:ILE:CG2	59:q:164:ALA:HB2	1.08	1.56
49:a:462:LEU:CD2	66:x:11:LEU:HD11	1.29	1.55
49:a:229:SER:HB3	49:a:502:MET:CG	1.29	1.55
29:Di:73:LEU:HD22	31:Dl:105:HIS:CE1	1.04	1.55
52:g:161:ILE:CA	54:i:140:MET:HE1	1.09	1.54
55:j:75:ARG:HB2	55:j:80:TYR:CE2	1.02	1.54
59:q:92:LEU:HD11	59:q:99:ARG:CZ	1.34	1.54
66:x:955:LEU:CD2	66:x:967:VAL:HG21	1.32	1.54
1:0:145:GLU:HG3	53:h:3:ARG:CZ	1.10	1.53
12:PC:265:HIS:CE1	62:t:113:ARG:CD	1.86	1.53
55:j:26:VAL:HG11	55:j:38:ASN:ND2	1.23	1.53
59:q:1:MET:HE3	65:z:541:PRO:CG	1.40	1.51
12:PC:265:HIS:CD2	62:t:113:ARG:HB2	1.42	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:d:121:LEU:CD1	63:u:115:LEU:HB2	1.08	1.50
63:u:81:SER:CB	63:u:85:LEU:HB2	1.05	1.50
67:w:9:PHE:HD2	67:w:66:PHE:CD2	1.23	1.50
55:j:20:ARG:HH11	57:n:94:GLN:CB	1.25	1.50
67:w:9:PHE:CD2	67:w:66:PHE:CD2	1.97	1.50
12:PC:265:HIS:NE2	62:t:113:ARG:CG	1.73	1.50
57:n:359:ILE:CG1	57:n:372:ILE:HD11	1.37	1.49
11:PB:592:ARG:HH11	11:PB:592:ARG:CB	1.25	1.49
56:k:28:ALA:CB	59:q:161:LEU:CD2	1.89	1.49
49:a:462:LEU:HD23	66:x:11:LEU:CD1	1.43	1.49
12:PC:265:HIS:NE2	62:t:113:ARG:CB	1.75	1.48
29:Di:73:LEU:CD2	31:Dl:105:HIS:CE1	1.95	1.48
44:c:110:ALA:CB	46:b:168:ILE:CG2	1.89	1.48
56:k:28:ALA:CB	59:q:161:LEU:HD23	1.44	1.48
50:d:76:PHE:HZ	54:i:65:PHE:CE2	1.29	1.48
64:v:21:ARG:CZ	64:v:78:LEU:CD2	1.92	1.48
49:a:493:PHE:CD2	49:a:514:LYS:CD	1.94	1.47
13:PD:137:LYS:CE	53:h:51:LEU:HG	1.43	1.47
56:k:12:ARG:CB	56:k:66:GLN:HE22	1.27	1.47
57:n:659:LEU:CD2	67:w:17:VAL:HG21	1.39	1.47
69:X:-19:DG:N1	70:Y:19:DC:N4	1.64	1.46
66:x:955:LEU:HD22	66:x:967:VAL:CG2	0.99	1.46
50:d:45:ILE:HG23	54:i:76:MET:CB	1.43	1.46
50:d:126:TYR:CE2	59:q:36:MET:HB3	1.50	1.46
13:PD:137:LYS:HD2	53:h:55:GLN:CB	1.43	1.46
1:0:145:GLU:CG	53:h:3:ARG:NH2	1.77	1.45
55:j:75:ARG:HD2	55:j:80:TYR:CZ	1.51	1.45
59:q:92:LEU:HD11	59:q:99:ARG:NH2	1.15	1.45
50:d:76:PHE:CZ	54:i:65:PHE:CE2	2.04	1.45
56:k:28:ALA:HB1	59:q:161:LEU:CD2	1.40	1.45
13:PD:137:LYS:HB2	53:h:55:GLN:CD	1.43	1.44
1:0:145:GLU:HG3	53:h:3:ARG:NH2	1.22	1.44
63:u:61:LEU:HD11	65:z:496:LEU:CG	1.44	1.44
49:a:462:LEU:CD2	66:x:11:LEU:CD1	1.93	1.44
48:m:104:HIS:CE1	57:n:168:ARG:HG3	1.50	1.43
57:n:659:LEU:HD21	67:w:17:VAL:CG2	1.43	1.43
54:i:65:PHE:CE1	54:i:99:LYS:HG2	0.90	1.43
13:PD:78:GLU:OE1	53:h:51:LEU:CD2	1.66	1.43
13:PD:137:LYS:CE	53:h:51:LEU:CG	1.94	1.43
49:a:413:HIS:HD2	49:a:472:SER:N	1.13	1.43
59:q:9:ILE:CD1	63:u:90:LEU:HD22	1.45	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:PD:137:LYS:CE	53:h:51:LEU:CD1	1.94	1.42
46:b:174:ILE:CG1	47:l:75:LEU:HD21	1.50	1.42
52:g:161:ILE:CG1	54:i:140:MET:HE2	1.46	1.42
50:d:45:ILE:CG2	54:i:76:MET:HB2	1.50	1.42
55:j:75:ARG:HB2	55:j:80:TYR:CD2	1.56	1.41
59:q:9:ILE:HD11	63:u:90:LEU:CD2	1.50	1.41
2:8:259:HIS:NE2	10:PA:1669:PRO:HB3	1.27	1.40
31:Dl:106:ARG:NH1	31:Dl:114:LYS:HE2	1.12	1.40
56:k:24:ILE:CG2	59:q:164:ALA:CB	1.90	1.40
31:DL:101:GLN:O	31:DL:105:HIS:CD2	1.75	1.40
59:q:290:HIS:CE1	59:q:294:LYS:HE3	1.56	1.39
55:j:93:GLU:HG2	61:s:83:LEU:CD1	1.50	1.38
58:o:715:LEU:CD1	66:x:21:TYR:HB2	1.53	1.38
49:a:229:SER:CA	49:a:502:MET:HG2	1.53	1.38
57:n:274:ILE:HD11	57:n:299:PHE:CE1	1.56	1.38
66:x:956:VAL:HG11	66:x:968:LEU:CD1	1.53	1.38
50:d:121:LEU:CD1	63:u:115:LEU:CB	2.02	1.38
57:n:359:ILE:HG12	57:n:372:ILE:CD1	1.54	1.38
50:d:49:ALA:CB	54:i:76:MET:SD	2.13	1.37
59:q:1:MET:N	65:z:540:LEU:CD1	1.87	1.37
63:u:81:SER:CB	63:u:85:LEU:CB	2.01	1.37
64:v:16:GLN:NE2	64:v:20:LYS:HE2	1.07	1.36
50:d:76:PHE:CE2	54:i:65:PHE:CD2	2.13	1.36
60:r:19:MET:HE3	60:r:177:ALA:CA	1.54	1.36
45:e:60:VAL:CG1	46:b:179:LEU:HB2	1.53	1.36
29:Di:73:LEU:HD22	31:Dl:105:HIS:NE2	1.39	1.35
49:a:417:TYR:HD1	49:a:469:VAL:CG2	1.40	1.35
52:g:161:ILE:HG12	54:i:140:MET:CE	1.56	1.35
55:j:20:ARG:HD2	57:n:94:GLN:CA	1.54	1.35
63:u:82:THR:C	63:u:86:GLN:HG3	1.52	1.35
50:d:76:PHE:CZ	54:i:65:PHE:CD2	2.14	1.34
53:h:146:MET:CG	56:k:39:LYS:HZ2	1.38	1.34
54:i:135:TYR:OH	63:u:125:ILE:CB	1.76	1.34
59:q:92:LEU:CD1	59:q:99:ARG:NH2	1.90	1.34
11:PB:592:ARG:HH11	11:PB:592:ARG:CG	1.38	1.34
49:a:455:GLN:HG3	66:x:11:LEU:CD2	1.56	1.34
31:DL:111:LEU:HA	31:DL:114:LYS:NZ	1.39	1.34
63:u:82:THR:C	63:u:86:GLN:CG	1.99	1.34
11:PB:592:ARG:CB	11:PB:592:ARG:NH1	1.91	1.33
51:f:174:ARG:HD3	57:n:267:HIS:CD2	1.64	1.33
60:r:19:MET:CE	60:r:177:ALA:CA	2.06	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:413:HIS:CD2	49:a:472:SER:N	1.96	1.33
58:o:761:LEU:O	67:w:74:LYS:HE3	1.25	1.33
1:0:145:GLU:HG3	53:h:3:ARG:NH1	1.43	1.32
55:j:19:ILE:HG21	55:j:45:VAL:CG2	1.60	1.32
12:PC:265:HIS:NE2	62:t:113:ARG:CD	1.84	1.32
48:m:26:GLN:OE1	52:g:45:PHE:HD2	1.08	1.32
49:a:364:TYR:HB3	49:a:430:LEU:CD1	1.58	1.32
49:a:493:PHE:CE2	49:a:514:LYS:CG	2.12	1.32
10:PA:436:SER:C	62:t:97:LYS:NZ	1.87	1.31
53:h:146:MET:HB2	56:k:39:LYS:NZ	1.46	1.31
56:k:12:ARG:CG	56:k:66:GLN:NE2	1.92	1.31
46:b:181:CYS:SG	47:l:82:LEU:HD13	1.69	1.31
59:q:186:GLU:HG3	59:q:243:LEU:CD2	1.59	1.31
44:c:113:TRP:CH2	46:b:175:HIS:HB2	1.66	1.31
56:k:70:LEU:HD21	64:v:85:PHE:CD1	1.64	1.31
49:a:413:HIS:CD2	49:a:471:ASP:HA	1.65	1.30
52:g:28:GLU:OE2	52:g:30:LEU:HB3	1.26	1.30
57:n:250:LEU:HD21	57:n:275:HIS:CD2	1.67	1.30
46:b:174:ILE:CD1	47:l:75:LEU:CD2	2.08	1.29
55:j:89:LEU:HD11	61:s:93:TYR:CD1	1.67	1.29
59:q:89:GLN:CG	59:q:90:PRO:HD2	1.60	1.29
55:j:20:ARG:HD2	57:n:94:GLN:CB	1.63	1.29
56:k:12:ARG:HB3	56:k:66:GLN:NE2	1.45	1.29
57:n:73:LEU:O	57:n:77:SER:CB	1.80	1.29
11:PB:594:MET:SD	11:PB:658:ALA:HB2	1.73	1.29
30:DJ:171:LEU:HD11	30:DJ:193:TYR:CE1	1.68	1.29
66:x:955:LEU:CD2	66:x:967:VAL:CG2	1.92	1.28
5:DP:218:LYS:HB2	69:X:-23:DG:OP1	1.18	1.28
26:DF:104:LEU:HB3	30:DJ:217:PHE:CE2	1.67	1.28
58:o:715:LEU:CD1	66:x:21:TYR:CB	2.11	1.28
1:0:300:ALA:CB	3:9:166:PRO:HA	1.60	1.28
11:PB:99:TRP:CE3	11:PB:105:PRO:HB3	1.67	1.28
37:1:187:ASN:HB2	37:1:191:ASP:CB	1.63	1.27
54:i:135:TYR:OH	63:u:125:ILE:CA	1.81	1.27
49:a:493:PHE:CD2	49:a:514:LYS:HD2	1.57	1.27
47:l:168:TRP:CD2	59:q:441:ARG:NH1	2.01	1.27
54:i:65:PHE:CD1	54:i:99:LYS:CG	1.94	1.27
49:a:417:TYR:CE1	49:a:450:PHE:CD1	2.23	1.27
24:DD:890:GLY:O	31:DL:104:ARG:NH2	1.66	1.27
50:d:45:ILE:O	54:i:76:MET:HG2	1.22	1.27
53:h:77:ILE:HG13	59:q:126:THR:CB	1.65	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:147:CYS:SG	64:v:41:LYS:HG2	1.75	1.26
1:0:145:GLU:CG	53:h:3:ARG:CZ	2.05	1.26
56:k:17:ILE:CG2	59:q:171:VAL:HG21	1.64	1.26
57:n:245:TRP:HB2	57:n:282:LEU:CD1	1.64	1.26
28:DH:105:ASP:OD1	30:DJ:116:LEU:HD11	1.14	1.26
44:c:110:ALA:CB	46:b:168:ILE:HG23	1.56	1.26
55:j:20:ARG:NH1	57:n:94:GLN:CB	1.96	1.26
69:X:-19:DG:N2	70:Y:19:DC:N3	1.83	1.26
57:n:254:VAL:CG1	57:n:304:GLN:HE21	1.48	1.26
57:n:267:HIS:HB3	57:n:270:GLN:OE1	1.30	1.25
13:PD:137:LYS:CD	53:h:55:GLN:OE1	1.84	1.25
31:Dl:106:ARG:NH1	31:Dl:114:LYS:CE	2.00	1.25
59:q:186:GLU:CG	59:q:243:LEU:CD2	2.12	1.25
45:e:129:VAL:CG1	56:k:111:CYS:SG	2.23	1.25
51:f:185:ARG:HD2	57:n:273:PHE:CZ	1.70	1.25
56:k:87:ARG:HA	64:v:105:LEU:CD1	1.65	1.25
49:a:227:SER:OG	49:a:502:MET:HE2	1.28	1.25
55:j:20:ARG:CD	57:n:94:GLN:HA	1.66	1.25
55:j:69:GLU:O	55:j:73:GLN:HG3	1.34	1.25
48:m:26:GLN:OE1	52:g:45:PHE:CD2	1.89	1.24
48:m:116:GLN:CG	65:z:594:LEU:HG	1.66	1.24
10:PA:436:SER:OG	62:t:97:LYS:CE	1.86	1.23
10:PA:439:HIS:NE2	60:r:19:MET:HB3	1.51	1.23
31:Dl:101:GLN:O	31:Dl:105:HIS:CD2	1.90	1.23
49:a:413:HIS:CD2	49:a:471:ASP:CA	2.20	1.23
5:DP:294:ARG:NH1	69:X:-27:DA:OP1	1.72	1.23
63:u:82:THR:CA	63:u:86:GLN:CG	2.17	1.23
67:w:394:PRO:HA	68:p:171:PHE:CE1	1.74	1.23
11:PB:643:LEU:HD21	11:PB:656:LEU:CD1	1.68	1.22
13:PD:137:LYS:CG	53:h:55:GLN:OE1	1.87	1.22
57:n:274:ILE:CD1	57:n:299:PHE:CZ	2.23	1.22
1:0:209:GLU:OE1	1:0:210:MET:HE2	1.37	1.22
45:e:60:VAL:CG1	46:b:179:LEU:CB	2.17	1.22
57:n:250:LEU:CD2	57:n:275:HIS:CD2	2.21	1.22
29:Di:73:LEU:CD2	31:Dl:105:HIS:NE2	1.95	1.22
53:h:182:VAL:HG21	60:r:202:ILE:CD1	1.68	1.22
61:s:92:ALA:O	61:s:96:PHE:CD2	1.92	1.22
66:x:355:CYS:SG	66:x:407:ILE:CD1	2.28	1.22
40:4:205:LEU:HD23	40:4:367:PHE:CE2	1.74	1.21
66:x:355:CYS:SG	66:x:407:ILE:HD12	1.79	1.21
37:1:483:THR:OG1	37:1:484:PRO:HD3	1.38	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:415:HIS:NE2	70:Y:-12:DT:H5"	1.56	1.21
47:l:168:TRP:CE3	59:q:441:ARG:NH1	2.09	1.21
49:a:228:PRO:HB2	49:a:502:MET:SD	1.78	1.21
59:q:1:MET:N	65:z:540:LEU:HD13	1.54	1.21
70:Y:33:DC:O2	70:Y:34:DG:N7	1.71	1.21
57:n:250:LEU:HD23	57:n:275:HIS:CG	1.73	1.21
5:DP:220:VAL:CG2	69:X:-24:DA:H2"	1.71	1.20
43:7:20:GLU:OE1	43:7:482:THR:HG22	1.41	1.20
58:o:715:LEU:HD13	66:x:21:TYR:CA	1.70	1.20
64:v:16:GLN:NE2	64:v:20:LYS:CE	2.04	1.20
13:PD:137:LYS:HD3	53:h:55:GLN:OE1	1.40	1.20
49:a:467:MET:CE	49:a:504:ILE:CD1	2.18	1.20
2:8:259:HIS:CD2	10:PA:1669:PRO:HB3	1.75	1.20
56:k:12:ARG:HG2	56:k:66:GLN:NE2	1.51	1.20
24:DD:895:HIS:CG	24:DD:896:PRO:HD2	1.76	1.20
5:DP:218:LYS:CB	69:X:-23:DG:OP1	1.88	1.20
11:PB:923:VAL:O	11:PB:923:VAL:CG1	1.86	1.20
31:Dl:106:ARG:HH11	31:Dl:114:LYS:CE	1.54	1.20
55:j:102:MET:CG	63:u:26:LEU:HG	1.72	1.20
55:j:109:LEU:HD23	63:u:59:ALA:HB1	1.24	1.20
63:u:61:LEU:CD1	65:z:496:LEU:HD21	1.71	1.19
55:j:70:TYR:CD1	55:j:80:TYR:HB3	1.75	1.19
10:PA:666:ARG:NH1	10:PA:667:LEU:HD21	1.58	1.19
22:DA:353:LEU:HD21	26:Df:272:VAL:HG21	1.24	1.19
49:a:417:TYR:HE1	49:a:450:PHE:CD1	1.58	1.19
59:q:186:GLU:CG	59:q:243:LEU:HD22	1.70	1.19
12:PC:6:GLN:N	12:PC:6:GLN:HE21	1.41	1.19
58:o:715:LEU:HD11	66:x:21:TYR:CB	1.71	1.19
54:i:65:PHE:HD1	54:i:99:LYS:CD	1.54	1.19
57:n:686:LYS:HZ1	58:o:730:PRO:CD	1.55	1.19
59:q:138:LYS:HB3	59:q:140:ASN:OD1	1.42	1.19
67:w:357:HIS:CE1	67:w:397:LYS:HE2	1.76	1.19
67:w:394:PRO:CA	68:p:171:PHE:CZ	2.25	1.19
11:PB:594:MET:SD	11:PB:658:ALA:CB	2.30	1.18
56:k:21:ILE:HD12	59:q:168:THR:OG1	1.43	1.18
40:4:205:LEU:CD2	40:4:367:PHE:CE2	2.26	1.18
44:c:204:MET:CE	44:c:208:PHE:H	1.56	1.18
10:PA:666:ARG:NH1	10:PA:667:LEU:CD2	2.06	1.18
13:PD:137:LYS:CB	53:h:55:GLN:OE1	1.91	1.18
28:DH:57:SER:HB2	30:DJ:197:MET:SD	1.83	1.18
49:a:413:HIS:CD2	49:a:472:SER:H	1.57	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:FA:122:THR:HG22	9:FB:24:PRO:HA	1.18	1.18
12:PC:6:GLN:N	12:PC:6:GLN:NE2	1.91	1.18
46:b:174:ILE:HD11	47:l:75:LEU:HD21	1.22	1.18
49:a:417:TYR:CD1	49:a:469:VAL:HG21	1.77	1.18
53:h:150:LEU:HD21	56:k:45:LEU:HD11	1.20	1.18
56:k:20:GLU:OE1	64:v:76:MET:SD	2.02	1.18
5:DP:313:THR:HG23	69:X:-27:DA:C4'	1.72	1.18
13:PD:79:THR:OG1	53:h:51:LEU:HD22	1.40	1.18
49:a:417:TYR:CD1	49:a:469:VAL:CG2	2.27	1.18
52:g:90:LEU:CD1	55:j:124:TYR:CE1	2.27	1.18
55:j:102:MET:HG2	63:u:26:LEU:CG	1.74	1.18
45:e:129:VAL:HG21	56:k:114:MET:CE	1.73	1.17
52:g:90:LEU:HD13	55:j:124:TYR:CE1	1.78	1.17
54:i:135:TYR:OH	63:u:125:ILE:N	1.75	1.17
59:q:1:MET:CE	65:z:541:PRO:HG2	1.72	1.17
45:e:60:VAL:HG13	46:b:179:LEU:CB	1.73	1.17
49:a:227:SER:OG	49:a:502:MET:CE	1.90	1.17
51:f:184:LEU:CD2	57:n:299:PHE:HD1	1.56	1.17
59:q:152:SER:HB2	64:v:58:ASN:HA	1.20	1.17
59:q:307:ILE:HG12	59:q:379:ILE:HG13	1.24	1.17
10:PA:436:SER:OG	62:t:97:LYS:NZ	1.77	1.17
55:j:93:GLU:CG	61:s:83:LEU:HD13	1.73	1.17
57:n:197:GLN:OE1	63:u:119:GLN:NE2	1.78	1.17
58:o:762:GLN:HA	67:w:74:LYS:NZ	1.60	1.17
67:w:9:PHE:CD2	67:w:66:PHE:CE2	2.33	1.17
7:BA:280:VAL:HA	70:Y:33:DC:OP2	1.41	1.16
63:u:82:THR:CA	63:u:86:GLN:HG2	1.74	1.16
57:n:169:LEU:HB3	57:n:170:PRO:CD	1.72	1.16
28:DH:105:ASP:OD1	30:DJ:116:LEU:CD1	1.94	1.16
59:q:212:ALA:HA	59:q:387:LEU:HD11	1.18	1.16
44:c:204:MET:HE1	44:c:208:PHE:N	1.59	1.15
50:d:45:ILE:HG12	54:i:73:ILE:HA	1.26	1.15
57:n:192:LEU:HD12	57:n:220:GLY:CA	1.75	1.15
63:u:81:SER:HB3	63:u:85:LEU:CB	1.68	1.15
54:i:68:LEU:HD13	54:i:95:GLN:HG2	1.15	1.15
56:k:17:ILE:CG2	59:q:171:VAL:CG2	2.24	1.15
58:o:715:LEU:HB3	66:x:25:ILE:CG1	1.75	1.15
22:DA:567:LEU:HD13	23:DB:745:GLN:HG2	1.19	1.15
48:m:68:LYS:HD2	52:g:50:GLN:NE2	1.60	1.15
52:g:93:LEU:HD13	55:j:106:LYS:HG2	1.23	1.15
53:h:147:CYS:SG	64:v:41:LYS:CG	2.35	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:274:ILE:CD1	57:n:299:PHE:CE1	2.28	1.15
53:h:146:MET:CB	56:k:39:LYS:NZ	2.08	1.15
56:k:70:LEU:CD2	64:v:85:PHE:CD1	2.29	1.15
56:k:87:ARG:CA	64:v:105:LEU:CD1	2.23	1.15
48:m:104:HIS:CG	57:n:169:LEU:HA	1.81	1.15
49:a:417:TYR:CE1	49:a:450:PHE:CE1	2.35	1.15
49:a:493:PHE:CG	49:a:514:LYS:HD2	1.82	1.15
51:f:174:ARG:HG3	57:n:270:GLN:NE2	1.61	1.15
31:DL:111:LEU:CA	31:DL:114:LYS:HZ2	1.59	1.14
50:d:31:LEU:CD2	54:i:103:THR:HG21	1.76	1.14
56:k:17:ILE:HG21	59:q:171:VAL:CG2	1.77	1.14
56:k:87:ARG:CA	64:v:105:LEU:HD11	1.77	1.14
31:DL:83:MET:SD	31:DL:86:GLN:OE1	2.05	1.14
57:n:686:LYS:HZ3	58:o:730:PRO:CG	1.59	1.14
51:f:184:LEU:CD2	57:n:299:PHE:CD1	2.29	1.14
4:DO:65:TYR:CE1	5:DP:191:GLU:HG2	1.81	1.14
59:q:1:MET:N	65:z:540:LEU:HD12	1.62	1.14
53:h:146:MET:CB	56:k:39:LYS:HZ2	1.60	1.13
56:k:9:GLU:HG3	64:v:86:LEU:HG	1.28	1.13
55:j:75:ARG:CG	55:j:80:TYR:CE2	2.29	1.13
57:n:686:LYS:NZ	58:o:730:PRO:CG	2.11	1.13
10:PA:436:SER:CB	62:t:97:LYS:NZ	2.12	1.13
49:a:467:MET:HE2	49:a:504:ILE:HD11	1.31	1.13
54:i:85:GLN:CG	54:i:86:ASP:H	1.60	1.13
11:PB:592:ARG:NH1	11:PB:592:ARG:HB2	1.56	1.13
50:d:45:ILE:HG22	54:i:76:MET:HE2	1.25	1.13
56:k:87:ARG:N	64:v:105:LEU:HD12	1.62	1.13
4:DO:65:TYR:HE1	5:DP:191:GLU:CG	1.60	1.13
5:DP:220:VAL:CG2	69:X:-24:DA:C2'	2.27	1.12
50:d:31:LEU:HD23	54:i:103:THR:HG21	1.15	1.12
52:g:28:GLU:OE2	52:g:30:LEU:CB	1.97	1.12
59:q:186:GLU:HG3	59:q:243:LEU:HD21	1.19	1.12
42:6:472:ARG:HG3	42:6:473:GLU:HG3	1.28	1.12
50:d:121:LEU:HD13	63:u:115:LEU:CB	1.68	1.12
50:d:165:LEU:HD11	63:u:6:THR:CG2	1.80	1.12
59:q:155:GLY:HA3	64:v:62:HIS:CE1	1.83	1.12
26:DF:71:ILE:HD12	29:DI:38:GLN:HE21	1.03	1.12
42:6:314:ALA:CB	42:6:381:TRP:HD1	1.60	1.12
55:j:75:ARG:CB	55:j:80:TYR:CD2	2.23	1.12
29:DI:60:HIS:CD2	31:DL:106:ARG:HE	1.68	1.12
63:u:18:GLN:HB3	63:u:62:ILE:HG12	1.19	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:w:16:GLU:OE2	67:w:78:PHE:CB	1.97	1.12
8:FA:121:ASN:HA	9:FB:25:LYS:HE2	1.32	1.12
56:k:87:ARG:N	64:v:105:LEU:CD1	2.11	1.12
57:n:254:VAL:HG13	57:n:304:GLN:HE21	1.13	1.12
57:n:686:LYS:NZ	58:o:730:PRO:HG3	1.62	1.12
8:FA:125:TYR:CE2	9:FB:31:TRP:CE3	2.37	1.11
13:PD:137:LYS:CB	53:h:55:GLN:CD	2.21	1.11
48:m:116:GLN:HG3	65:z:594:LEU:HG	1.20	1.11
50:d:121:LEU:HD12	63:u:115:LEU:HB2	1.24	1.11
53:h:77:ILE:O	59:q:126:THR:OG1	1.68	1.11
56:k:28:ALA:CB	59:q:161:LEU:HD21	1.76	1.11
64:v:16:GLN:HE21	64:v:20:LYS:CE	1.59	1.11
64:v:21:ARG:CZ	64:v:78:LEU:HD21	1.69	1.11
1:0:284:ALA:CB	2:8:243:LEU:HD13	1.79	1.11
11:PB:110:PRO:HG2	11:PB:163:LEU:HD11	1.32	1.11
48:m:68:LYS:CD	52:g:50:GLN:HE22	1.61	1.11
49:a:462:LEU:HD21	66:x:11:LEU:CD1	1.77	1.11
59:q:89:GLN:HG2	59:q:90:PRO:CD	1.79	1.11
44:c:110:ALA:CB	46:b:168:ILE:HG21	1.63	1.11
49:a:497:VAL:O	49:a:501:CYS:SG	2.09	1.11
53:h:146:MET:CG	56:k:39:LYS:NZ	2.13	1.11
57:n:265:LEU:HD13	57:n:303:LEU:HD21	1.26	1.11
24:DD:890:GLY:C	31:DL:104:ARG:HH22	1.57	1.11
29:Di:73:LEU:HD22	31:Dl:105:HIS:ND1	1.66	1.11
49:a:229:SER:HB3	49:a:502:MET:HG3	1.33	1.11
55:j:89:LEU:HD21	61:s:93:TYR:CE1	1.86	1.11
10:PA:666:ARG:HH12	10:PA:667:LEU:CD2	1.62	1.10
13:PD:79:THR:HA	53:h:51:LEU:HD21	1.24	1.10
13:PD:137:LYS:CD	53:h:55:GLN:HB2	1.80	1.10
13:PD:137:LYS:NZ	53:h:51:LEU:C	2.09	1.10
48:m:70:PRO:HB2	57:n:166:TYR:OH	1.50	1.10
49:a:321:LEU:HD21	49:a:407:ILE:HG23	1.33	1.10
1:0:284:ALA:HB3	2:8:243:LEU:CD1	1.81	1.10
26:DF:428:LEU:HD13	26:DF:455:LEU:CB	1.81	1.10
51:f:188:PHE:CD2	57:n:295:CYS:SG	2.43	1.10
66:x:955:LEU:HD22	66:x:967:VAL:HG22	1.15	1.10
52:g:93:LEU:HB3	55:j:106:LYS:CE	1.81	1.10
53:h:146:MET:HG2	56:k:39:LYS:HZ2	1.00	1.10
56:k:12:ARG:CG	56:k:66:GLN:HE21	1.56	1.10
56:k:70:LEU:HD21	64:v:85:PHE:CE1	1.85	1.10
67:w:9:PHE:HD2	67:w:66:PHE:CE2	1.67	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:m:62:GLU:HG3	52:g:38:ILE:HD11	1.29	1.10
49:a:467:MET:HE1	49:a:504:ILE:CD1	1.78	1.10
55:j:20:ARG:HD2	57:n:94:GLN:HA	1.12	1.10
46:b:174:ILE:HG12	47:l:75:LEU:HD21	1.33	1.10
49:a:413:HIS:CD2	49:a:471:ASP:C	2.30	1.10
57:n:274:ILE:HD11	57:n:299:PHE:CZ	1.86	1.10
5:DP:301:VAL:HB	69:X:-27:DA:H5"	1.22	1.09
55:j:75:ARG:CD	55:j:80:TYR:CZ	2.35	1.09
55:j:89:LEU:HD11	61:s:93:TYR:CE1	1.86	1.09
58:o:762:GLN:HA	67:w:74:LYS:CE	1.80	1.09
63:u:61:LEU:CD1	65:z:496:LEU:CD2	2.29	1.09
4:DO:65:TYR:CE1	5:DP:191:GLU:CG	2.35	1.09
44:c:110:ALA:HB1	46:b:168:ILE:CG2	1.63	1.09
48:m:102:ILE:CG2	50:d:167:TRP:CH2	2.34	1.09
60:r:19:MET:CE	60:r:177:ALA:CB	2.30	1.09
45:e:129:VAL:HG13	56:k:111:CYS:SG	1.90	1.09
46:b:174:ILE:HG12	47:l:75:LEU:HD11	1.30	1.09
48:m:102:ILE:HG21	50:d:167:TRP:HH2	1.15	1.09
11:PB:99:TRP:HE3	11:PB:105:PRO:CB	1.64	1.09
40:4:205:LEU:CD2	40:4:367:PHE:HE2	1.62	1.09
46:b:174:ILE:HD11	47:l:75:LEU:CD2	1.76	1.09
54:i:85:GLN:HG3	54:i:86:ASP:N	1.53	1.09
57:n:659:LEU:CD1	67:w:14:LYS:HG2	1.81	1.09
58:o:693:LEU:HD22	59:q:608:ASP:HB2	1.15	1.09
29:DI:73:LEU:HD22	31:DL:105:HIS:NE2	1.69	1.08
55:j:19:ILE:HD13	55:j:45:VAL:HG22	1.32	1.08
42:6:289:TYR:H	42:6:290:PRO:HD3	1.07	1.08
49:a:364:TYR:HB3	49:a:430:LEU:HD12	1.26	1.08
50:d:38:GLU:CD	54:i:96:GLU:HG2	1.77	1.08
53:h:74:GLN:NE2	59:q:129:PRO:HB3	1.67	1.08
59:q:7:VAL:HB	63:u:90:LEU:HD11	1.10	1.08
67:w:12:VAL:HG23	67:w:78:PHE:CE2	1.87	1.08
67:w:357:HIS:HE1	67:w:397:LYS:HE2	0.99	1.08
5:DP:173:ASN:ND2	5:DP:218:LYS:HZ3	1.50	1.08
5:DP:314:GLY:HA2	69:X:-26:DA:H5'	1.28	1.08
49:a:412:ARG:HB3	49:a:472:SER:CB	1.83	1.08
24:DD:895:HIS:ND1	24:DD:896:PRO:HD2	1.67	1.08
42:6:359:LYS:NZ	42:6:436:GLY:HA2	1.68	1.08
48:m:104:HIS:NE2	57:n:168:ARG:CD	2.17	1.08
49:a:229:SER:N	49:a:502:MET:SD	2.27	1.08
55:j:19:ILE:HG21	55:j:45:VAL:HG21	1.11	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:j:109:LEU:HD21	63:u:59:ALA:CB	1.84	1.08
59:q:1:MET:HB2	65:z:541:PRO:HG3	1.16	1.08
10:PA:439:HIS:ND1	60:r:92:GLU:OE1	1.86	1.08
31:DL:111:LEU:O	31:DL:114:LYS:HG2	1.54	1.08
31:Dl:102:LEU:HA	31:Dl:105:HIS:HD2	1.19	1.08
55:j:11:HIS:O	55:j:15:PHE:CD2	2.07	1.08
55:j:109:LEU:CD2	63:u:59:ALA:CB	2.32	1.08
56:k:86:SER:C	64:v:105:LEU:HD12	1.78	1.08
56:k:87:ARG:HA	64:v:105:LEU:HD11	1.12	1.08
57:n:686:LYS:HZ1	58:o:730:PRO:HD3	0.93	1.08
58:o:761:LEU:O	67:w:74:LYS:CE	2.01	1.08
23:DB:621:ALA:H	41:5:36:GLN:NE2	1.51	1.07
51:f:174:ARG:CD	57:n:267:HIS:HD2	1.67	1.07
52:g:161:ILE:CB	54:i:140:MET:CE	2.32	1.07
10:PA:436:SER:C	62:t:97:LYS:HZ1	1.52	1.07
12:PC:265:HIS:CD2	62:t:113:ARG:CB	2.27	1.07
49:a:321:LEU:CD2	49:a:407:ILE:HD12	1.84	1.07
60:r:19:MET:HE1	60:r:177:ALA:HA	1.27	1.07
44:c:204:MET:CE	44:c:208:PHE:N	2.14	1.07
48:m:104:HIS:CE1	57:n:168:ARG:CG	2.37	1.07
50:d:45:ILE:HG22	54:i:76:MET:CE	1.83	1.07
53:h:182:VAL:HG21	60:r:202:ILE:HD12	1.20	1.07
57:n:245:TRP:CB	57:n:282:LEU:HD13	1.84	1.07
13:PD:137:LYS:NZ	53:h:51:LEU:HG	1.70	1.07
53:h:150:LEU:HD21	56:k:45:LEU:CD1	1.84	1.07
63:u:61:LEU:CD1	65:z:496:LEU:CG	2.32	1.07
13:PD:137:LYS:CE	53:h:51:LEU:HD12	1.65	1.07
40:4:412:PHE:CE2	40:4:418:PHE:HE1	1.72	1.07
58:o:715:LEU:HB3	66:x:25:ILE:HG13	1.12	1.07
11:PB:628:VAL:HG13	11:PB:632:LYS:O	1.55	1.06
13:PD:133:ASP:CG	53:h:59:LEU:HD22	1.79	1.06
44:c:110:ALA:HB2	46:b:168:ILE:CG2	1.81	1.06
48:m:59:LYS:NZ	48:m:77:GLU:OE2	1.88	1.06
52:g:166:ASN:OD1	52:g:167:CYS:N	1.85	1.06
56:k:12:ARG:CB	56:k:66:GLN:NE2	1.96	1.06
26:DF:15:PRO:HD3	29:DI:18:MET:HG2	1.34	1.06
53:h:77:ILE:HG13	59:q:126:THR:OG1	1.55	1.06
55:j:109:LEU:HD21	63:u:59:ALA:CA	1.83	1.06
55:j:109:LEU:HD21	63:u:59:ALA:HA	1.31	1.06
59:q:92:LEU:CD1	59:q:99:ARG:CZ	2.29	1.06
67:w:16:GLU:OE2	67:w:78:PHE:CG	2.08	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:295:ARG:NH1	3:9:165:ARG:HH21	1.52	1.06
5:DP:294:ARG:HH21	7:BA:196:LYS:HE2	1.18	1.06
32:Dc:67:GLY:HA3	30:Dj:116:LEU:CD1	1.85	1.06
49:a:229:SER:N	49:a:502:MET:CG	2.18	1.06
55:j:93:GLU:HG2	61:s:83:LEU:HD13	1.22	1.06
63:u:61:LEU:HD11	65:z:496:LEU:CD2	1.86	1.06
54:i:65:PHE:HE1	54:i:99:LYS:CB	1.67	1.06
59:q:138:LYS:HD2	59:q:140:ASN:OD1	1.55	1.06
5:DP:173:ASN:CG	5:DP:218:LYS:HZ3	1.63	1.06
7:BA:189:LYS:HD2	69:X:-30:DT:H5'	1.38	1.06
37:1:187:ASN:CB	37:1:191:ASP:HB3	1.86	1.06
50:d:165:LEU:HD11	63:u:6:THR:HG21	1.31	1.06
55:j:75:ARG:HD2	55:j:80:TYR:CE1	1.89	1.06
29:DI:16:ALA:HA	29:DI:40:LEU:HD11	1.34	1.05
45:e:60:VAL:HG13	46:b:179:LEU:HB3	1.33	1.05
55:j:73:GLN:O	55:j:80:TYR:OH	1.73	1.05
45:e:146:ILE:HG22	45:e:147:ASN:H	0.96	1.05
50:d:126:TYR:CE2	59:q:36:MET:CB	2.39	1.05
55:j:9:GLU:HG2	55:j:56:GLN:NE2	1.70	1.05
55:j:109:LEU:CD2	63:u:59:ALA:HB1	1.85	1.05
67:w:12:VAL:HG23	67:w:78:PHE:HE2	0.96	1.05
10:PA:666:ARG:HH12	10:PA:667:LEU:HD21	0.89	1.05
11:PB:643:LEU:HD21	11:PB:656:LEU:HD13	1.08	1.05
29:DI:60:HIS:CD2	31:DL:106:ARG:NE	2.25	1.05
53:h:77:ILE:HG13	59:q:126:THR:CG2	1.85	1.05
59:q:155:GLY:HA3	64:v:62:HIS:HE1	0.94	1.05
5:DP:313:THR:CG2	69:X:-27:DA:O4'	2.05	1.05
42:6:62:ARG:HA	42:6:73:SER:HB2	1.34	1.05
45:e:60:VAL:HG11	46:b:179:LEU:HB2	1.20	1.05
56:k:17:ILE:HG23	59:q:171:VAL:HG21	1.37	1.05
56:k:24:ILE:HG22	59:q:164:ALA:CB	1.78	1.05
5:DP:169:VAL:HB	69:X:-25:DA:C2	1.91	1.05
5:DP:313:THR:HG23	69:X:-27:DA:O4'	1.56	1.05
48:m:102:ILE:CG2	50:d:167:TRP:HH2	1.68	1.05
49:a:380:ALA:HB3	49:a:444:PRO:HD2	1.36	1.05
53:h:72:ARG:NH1	59:q:134:ALA:H	1.54	1.05
55:j:75:ARG:CB	55:j:80:TYR:HE2	1.42	1.05
55:j:93:GLU:CG	61:s:83:LEU:CD1	2.33	1.05
63:u:61:LEU:HD12	65:z:496:LEU:HD21	1.08	1.05
11:PB:99:TRP:HE3	11:PB:105:PRO:HB3	0.92	1.04
11:PB:592:ARG:HH11	11:PB:592:ARG:HB2	1.09	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:PD:137:LYS:CD	53:h:55:GLN:CB	2.32	1.04
29:DI:73:LEU:HD22	31:DL:105:HIS:CE1	1.92	1.04
44:c:204:MET:HE3	44:c:208:PHE:H	1.21	1.04
51:f:180:LEU:HD11	57:n:302:SER:OG	1.53	1.04
53:h:19:VAL:CG1	59:q:113:TYR:HB2	1.88	1.04
53:h:29:PHE:CE2	59:q:102:LEU:HD11	1.92	1.04
50:d:113:GLN:NE2	52:g:167:CYS:SG	2.31	1.04
59:q:149:LYS:CE	64:v:40:ALA:HA	1.87	1.04
59:q:155:GLY:CA	64:v:62:HIS:HE1	1.71	1.04
60:r:19:MET:HE2	60:r:177:ALA:CB	1.86	1.04
54:i:85:GLN:HG3	54:i:86:ASP:OD1	1.56	1.04
56:k:29:GLY:O	56:k:33:LEU:HG	1.55	1.04
56:k:104:LEU:HD21	64:v:123:ILE:HD11	1.39	1.04
63:u:82:THR:HA	63:u:86:GLN:CG	1.82	1.04
10:PA:437:ASP:N	62:t:97:LYS:HZ1	1.56	1.04
50:d:45:ILE:HD11	54:i:73:ILE:N	1.73	1.04
57:n:225:ARG:HB2	57:n:231:GLU:OE1	1.56	1.04
44:c:110:ALA:HB3	46:b:168:ILE:HG21	1.37	1.04
45:e:125:LYS:HE2	64:v:133:GLU:OE2	1.53	1.04
49:a:382:LEU:HD22	49:a:446:SER:HA	1.40	1.04
57:n:267:HIS:CB	57:n:270:GLN:OE1	2.05	1.04
62:t:129:VAL:HG21	62:t:200:ILE:HD12	1.32	1.04
5:DP:313:THR:OG1	69:X:-27:DA:N3	1.89	1.03
25:DE:429:LEU:HB3	25:DE:430:PRO:HD2	1.41	1.03
49:a:441:GLU:OE1	66:x:17:ARG:NH2	1.88	1.03
67:w:8:ILE:O	67:w:12:VAL:HG13	1.58	1.03
9:FB:147:LYS:HG3	9:FB:148:VAL:H	1.23	1.03
58:o:715:LEU:HD13	66:x:21:TYR:CB	1.79	1.03
69:X:-19:DG:C6	70:Y:19:DC:N4	2.27	1.03
13:PD:137:LYS:HE3	53:h:51:LEU:HD12	1.35	1.03
56:k:28:ALA:HB1	59:q:161:LEU:HD21	1.35	1.03
60:r:27:VAL:HG22	60:r:197:VAL:HG11	1.40	1.03
1:0:145:GLU:CD	53:h:3:ARG:HH22	1.67	1.03
40:4:49:PRO:O	40:4:53:LYS:HG3	1.57	1.03
2:8:207:LEU:HD23	51:f:52:MET:CE	1.89	1.03
17:PH:130:ASN:HB3	49:a:46:LYS:HA	1.39	1.03
30:DJ:171:LEU:HD11	30:DJ:193:TYR:HE1	0.88	1.03
46:b:174:ILE:HG12	47:l:75:LEU:CD1	1.89	1.03
50:d:45:ILE:O	54:i:76:MET:CG	2.06	1.03
49:a:417:TYR:HD1	49:a:469:VAL:HG23	1.24	1.02
54:i:65:PHE:CD1	54:i:99:LYS:CD	2.35	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:545:LEU:HD11	57:n:653:PRO:HG3	1.37	1.02
59:q:9:ILE:HG13	63:u:90:LEU:CD1	1.89	1.02
59:q:9:ILE:CG1	63:u:90:LEU:HD13	1.88	1.02
1:0:300:ALA:HB2	3:9:166:PRO:HA	1.04	1.02
8:FA:125:TYR:CE2	9:FB:31:TRP:CZ3	2.47	1.02
37:1:187:ASN:HB2	37:1:191:ASP:HB3	1.06	1.02
55:j:19:ILE:CD1	55:j:45:VAL:HG22	1.89	1.02
57:n:250:LEU:CD2	57:n:275:HIS:CG	2.37	1.02
57:n:686:LYS:NZ	58:o:730:PRO:HD3	1.73	1.02
67:w:16:GLU:OE2	67:w:78:PHE:HB3	1.58	1.02
49:a:413:HIS:NE2	49:a:471:ASP:HA	1.74	1.02
50:d:27:ARG:HD2	54:i:108:HIS:HA	1.40	1.02
59:q:451:LEU:CD1	59:q:529:MET:HE1	1.90	1.02
30:DJ:171:LEU:CD1	30:DJ:193:TYR:HE1	1.72	1.02
49:a:493:PHE:CD2	49:a:514:LYS:HD3	1.87	1.02
50:d:45:ILE:CG1	54:i:73:ILE:HA	1.89	1.02
50:d:121:LEU:HB3	63:u:115:LEU:HD12	1.38	1.02
54:i:65:PHE:HE1	54:i:99:LYS:CG	1.30	1.02
59:q:186:GLU:HG2	59:q:243:LEU:CD2	1.90	1.02
2:8:259:HIS:NE2	10:PA:1669:PRO:CB	2.22	1.01
48:m:101:GLN:HA	57:n:169:LEU:CD2	1.90	1.01
51:f:174:ARG:CG	57:n:270:GLN:NE2	2.23	1.01
51:f:185:ARG:CD	57:n:273:PHE:HZ	1.71	1.01
57:n:266:VAL:CG2	57:n:303:LEU:HD11	1.91	1.01
58:o:691:VAL:O	59:q:607:SER:OG	1.76	1.01
59:q:290:HIS:CE1	59:q:294:LYS:CE	2.43	1.01
13:PD:66:ASN:OD1	64:v:16:GLN:HG2	1.59	1.01
38:2:12:GLU:OE1	42:6:130:GLY:HA3	1.60	1.01
48:m:14:ASN:O	52:g:39:LYS:NZ	1.93	1.01
49:a:109:TYR:CZ	49:a:154:LEU:HD21	1.95	1.01
5:DP:218:LYS:CB	69:X:-23:DG:P	2.48	1.01
10:PA:436:SER:OG	62:t:97:LYS:HE3	1.55	1.01
13:PD:133:ASP:CG	53:h:59:LEU:CD2	2.33	1.01
45:e:129:VAL:HG21	56:k:114:MET:HE2	1.39	1.01
48:m:104:HIS:CD2	57:n:169:LEU:HA	1.94	1.01
49:a:455:GLN:CG	66:x:11:LEU:HD21	1.90	1.01
50:d:31:LEU:HD21	54:i:103:THR:OG1	1.59	1.01
54:i:65:PHE:HA	54:i:99:LYS:HE2	1.42	1.01
54:i:85:GLN:CG	54:i:86:ASP:OD1	2.09	1.01
56:k:86:SER:C	64:v:105:LEU:CD1	2.33	1.01
59:q:212:ALA:HA	59:q:387:LEU:CD1	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:x:956:VAL:HG11	66:x:968:LEU:HD11	1.39	1.01
48:m:56:LEU:HD21	48:m:80:GLN:NE2	1.75	1.01
49:a:493:PHE:CD2	49:a:514:LYS:CG	2.37	1.01
5:DP:220:VAL:HG21	69:X:-24:DA:C2'	1.91	1.01
13:PD:137:LYS:HG2	53:h:51:LEU:HD11	1.42	1.01
45:e:129:VAL:HG12	56:k:111:CYS:SG	2.00	1.01
63:u:83:ALA:O	63:u:87:ALA:N	1.92	1.01
26:DF:104:LEU:CB	30:DJ:217:PHE:CE2	2.42	1.00
52:g:89:PHE:CD1	63:u:19:PHE:CD1	2.49	1.00
56:k:17:ILE:HG21	59:q:171:VAL:HG22	1.40	1.00
13:PD:137:LYS:CG	53:h:51:LEU:HD11	1.91	1.00
50:d:168:VAL:HB	50:d:169:PRO:HD2	1.43	1.00
54:i:140:MET:HG3	54:i:141:PHE:HD1	1.24	1.00
55:j:75:ARG:HD2	55:j:80:TYR:CE2	1.97	1.00
55:j:105:PHE:CE2	55:j:109:LEU:HD11	1.95	1.00
57:n:359:ILE:CG1	57:n:372:ILE:CD1	2.25	1.00
61:s:92:ALA:O	61:s:96:PHE:HD2	1.36	1.00
63:u:4:ARG:NE	65:z:594:LEU:O	1.93	1.00
63:u:81:SER:HB2	63:u:85:LEU:CB	1.76	1.00
64:v:21:ARG:CZ	64:v:78:LEU:HD22	1.83	1.00
1:0:209:GLU:OE1	1:0:210:MET:CE	2.09	1.00
13:PD:137:LYS:CG	53:h:51:LEU:CD1	2.39	1.00
40:4:412:PHE:CE2	40:4:418:PHE:CE1	2.49	1.00
48:m:116:GLN:NE2	65:z:579:CYS:SG	2.34	1.00
50:d:45:ILE:CD1	54:i:73:ILE:N	2.24	1.00
55:j:9:GLU:HG2	55:j:56:GLN:HE22	1.19	1.00
56:k:89:ASP:HB3	64:v:109:GLN:OE1	1.61	1.00
57:n:203:LEU:HD13	57:n:215:LEU:CD1	1.91	1.00
26:DF:47:ILE:HD11	29:DI:43:ALA:HB2	1.39	1.00
52:g:93:LEU:HD22	55:j:106:LYS:HE2	1.38	1.00
52:g:93:LEU:CD2	55:j:106:LYS:HE2	1.91	1.00
52:g:93:LEU:CG	55:j:106:LYS:HE2	1.91	1.00
55:j:19:ILE:CG2	55:j:45:VAL:HG21	1.92	1.00
11:PB:923:VAL:O	11:PB:923:VAL:HG12	1.58	1.00
57:n:252:ILE:HD11	57:n:271:ILE:HG12	1.43	1.00
46:b:174:ILE:HG12	47:l:75:LEU:CD2	1.92	1.00
24:DD:1078:LEU:HD21	31:DL:83:MET:HE3	1.44	0.99
69:X:-36:DG:N1	70:Y:36:DC:N4	2.10	0.99
28:DH:57:SER:CB	30:DJ:197:MET:SD	2.50	0.99
40:4:317:ALA:HA	40:4:340:ASN:O	1.60	0.99
49:a:413:HIS:CG	49:a:471:ASP:HA	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:d:41:SER:HB2	54:i:69:VAL:HG13	1.41	0.99
22:DA:564:PRO:HB2	23:DB:744:PHE:CE2	1.97	0.99
29:DI:23:LEU:HD11	29:DI:39:MET:HE1	1.40	0.99
50:d:45:ILE:HD13	54:i:72:ILE:C	1.86	0.99
51:f:174:ARG:CG	57:n:270:GLN:HE22	1.74	0.99
55:j:105:PHE:CZ	55:j:109:LEU:HD11	1.97	0.99
58:o:715:LEU:CB	66:x:25:ILE:HG13	1.92	0.99
59:q:1:MET:H3	65:z:540:LEU:CD1	1.58	0.99
57:n:359:ILE:CB	57:n:372:ILE:HD11	1.91	0.99
2:8:207:LEU:CD2	51:f:52:MET:CE	2.40	0.99
12:PC:83:GLN:HG2	62:t:204:GLN:OE1	1.62	0.99
1:0:145:GLU:CG	53:h:3:ARG:NH1	2.18	0.99
52:g:93:LEU:CB	55:j:106:LYS:HE2	1.92	0.99
70:Y:8:DA:H2"	70:Y:9:DC:C6	1.98	0.99
42:6:314:ALA:CB	42:6:381:TRP:CD1	2.45	0.99
52:g:93:LEU:HB3	55:j:106:LYS:HE2	1.43	0.99
54:i:72:ILE:CD1	54:i:92:SER:HB2	1.91	0.99
58:o:693:LEU:HD22	59:q:608:ASP:CB	1.93	0.99
63:u:81:SER:HB2	63:u:85:LEU:HB2	1.02	0.99
28:DH:154:PRO:HD2	28:DH:159:TYR:OH	1.63	0.99
46:b:181:CYS:SG	47:l:82:LEU:CD1	2.50	0.99
64:v:21:ARG:NH1	64:v:78:LEU:CD2	2.26	0.99
1:0:287:TYR:CD1	2:8:189:MET:SD	2.56	0.98
48:m:26:GLN:CD	52:g:45:PHE:HD2	1.71	0.98
55:j:26:VAL:CB	55:j:38:ASN:HD21	1.76	0.98
13:PD:137:LYS:HB2	53:h:55:GLN:CG	1.93	0.98
55:j:93:GLU:HG2	61:s:83:LEU:HD11	1.44	0.98
58:o:762:GLN:HA	67:w:74:LYS:HE3	1.43	0.98
69:X:-39:DA:N6	70:Y:39:DT:O4	1.94	0.98
46:b:174:ILE:CG1	47:l:75:LEU:CD2	2.39	0.98
3:9:181:LEU:H	3:9:181:LEU:HD13	1.26	0.98
49:a:493:PHE:HD2	49:a:514:LYS:HD3	1.22	0.98
51:f:16:VAL:HG12	51:f:103:GLY:O	1.60	0.98
63:u:7:GLN:NE2	65:z:594:LEU:HD22	1.77	0.98
70:Y:8:DA:H2'	70:Y:9:DC:C5	1.97	0.98
49:a:455:GLN:HG3	66:x:11:LEU:HD21	1.01	0.98
42:6:314:ALA:HB1	42:6:381:TRP:CD1	1.98	0.98
53:h:77:ILE:C	59:q:126:THR:HG1	1.71	0.98
57:n:169:LEU:HB3	57:n:170:PRO:HD3	1.42	0.98
2:8:207:LEU:HD23	51:f:52:MET:HE1	1.45	0.98
24:DD:940:VAL:HG22	29:DI:123:THR:HG21	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DI:60:HIS:CE1	31:DL:106:ARG:NH2	2.32	0.98
63:u:82:THR:CA	63:u:86:GLN:HG3	1.86	0.98
44:c:204:MET:HE3	44:c:206:SER:O	1.60	0.98
11:PB:923:VAL:O	11:PB:923:VAL:HG13	1.63	0.98
51:f:184:LEU:HD22	57:n:299:PHE:CD1	1.96	0.98
55:j:70:TYR:HD1	55:j:80:TYR:CG	1.82	0.97
67:w:9:PHE:HB3	67:w:66:PHE:HE2	1.27	0.97
8:FA:125:TYR:CD2	9:FB:31:TRP:HZ3	1.80	0.97
10:PA:437:ASP:N	62:t:97:LYS:NZ	2.12	0.97
22:DA:725:CYS:O	22:DA:725:CYS:SG	2.22	0.97
48:m:68:LYS:HD2	52:g:50:GLN:HE22	0.83	0.97
55:j:19:ILE:HD13	55:j:45:VAL:CG2	1.94	0.97
12:PC:6:GLN:HE21	12:PC:6:GLN:H	1.09	0.97
8:FA:121:ASN:O	9:FB:25:LYS:HG3	1.64	0.97
11:PB:592:ARG:HH11	11:PB:592:ARG:HG3	1.26	0.97
32:Dc:77:LEU:CD1	30:Dj:116:LEU:HD23	1.95	0.97
59:q:288:SER:CB	59:q:289:PRO:CD	2.42	0.97
42:6:359:LYS:HZ1	42:6:436:GLY:CA	1.78	0.97
66:x:955:LEU:CG	66:x:967:VAL:HG21	1.93	0.97
12:PC:265:HIS:CE1	62:t:113:ARG:HD3	1.96	0.97
13:PD:137:LYS:HD2	53:h:55:GLN:HB3	1.43	0.97
49:a:227:SER:HG	49:a:502:MET:HE2	1.19	0.97
59:q:149:LYS:HE2	64:v:40:ALA:C	1.89	0.97
64:v:21:ARG:NH1	64:v:78:LEU:HD21	1.79	0.97
49:a:229:SER:N	49:a:502:MET:HG2	1.78	0.97
63:u:82:THR:C	63:u:86:GLN:HG2	1.84	0.97
70:Y:33:DC:C2	70:Y:34:DG:N7	2.33	0.97
13:PD:79:THR:CA	53:h:51:LEU:HD21	1.94	0.97
49:a:493:PHE:CD2	49:a:514:LYS:HG3	1.97	0.97
48:m:100:GLN:HB3	57:n:170:PRO:HG3	1.44	0.96
59:q:89:GLN:CB	59:q:90:PRO:HD2	1.94	0.96
3:9:239:LYS:HZ2	3:9:239:LYS:H	1.02	0.96
10:PA:439:HIS:CG	60:r:92:GLU:OE1	2.19	0.96
46:b:174:ILE:HD13	47:l:75:LEU:HD21	1.43	0.96
49:a:321:LEU:HD22	49:a:407:ILE:HD12	1.43	0.96
45:e:129:VAL:HG21	56:k:114:MET:HE1	1.43	0.96
58:o:715:LEU:HD13	66:x:21:TYR:HA	1.45	0.96
2:8:207:LEU:CD2	51:f:52:MET:HE2	1.96	0.96
7:BA:286:ARG:NH1	7:BA:316:LEU:HD12	1.79	0.96
8:FA:124:TYR:HE1	9:FB:22:LYS:HG3	1.28	0.96
49:a:228:PRO:CB	49:a:502:MET:SD	2.52	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:k:28:ALA:HB2	59:q:161:LEU:HD23	1.43	0.96
57:n:703:ARG:O	59:q:614:LYS:NZ	1.99	0.96
59:q:17:LYS:HE2	59:q:30:TYR:CE2	2.00	0.96
3:9:184:PRO:HB3	3:9:187:LEU:HD12	1.47	0.96
49:a:335:THR:O	49:a:391:THR:CG2	2.12	0.96
50:d:76:PHE:CE2	54:i:65:PHE:HD2	1.73	0.96
59:q:437:HIS:CE1	59:q:472:GLU:N	2.33	0.96
7:BA:189:LYS:HE3	69:X:-29:DA:OP2	1.65	0.96
51:f:185:ARG:HD2	57:n:273:PHE:HZ	1.20	0.96
63:u:61:LEU:HD11	65:z:496:LEU:HG	0.99	0.96
51:f:174:ARG:CD	57:n:270:GLN:HE22	1.78	0.96
55:j:70:TYR:CD1	55:j:80:TYR:CB	2.47	0.96
55:j:120:ASP:O	55:j:124:TYR:HD2	1.48	0.96
53:h:74:GLN:HA	59:q:129:PRO:HA	1.44	0.96
55:j:75:ARG:CD	55:j:80:TYR:CE2	2.49	0.96
59:q:1:MET:H1	65:z:540:LEU:CD1	1.63	0.96
7:BA:189:LYS:HG3	69:X:-29:DA:P	2.05	0.96
45:e:97:GLN:HE22	59:q:649:CYS:H	1.11	0.96
53:h:146:MET:HG2	56:k:39:LYS:NZ	1.77	0.96
57:n:192:LEU:HB3	57:n:219:ASN:O	1.66	0.96
57:n:686:LYS:NZ	58:o:730:PRO:CD	2.25	0.96
37:1:263:LYS:O	43:7:581:LEU:HD21	1.65	0.96
40:4:441:MET:H	41:5:5:LEU:HD23	1.30	0.96
48:m:14:ASN:C	52:g:39:LYS:NZ	2.23	0.96
55:j:26:VAL:CG1	55:j:38:ASN:ND2	1.94	0.96
31:DL:93:GLU:O	31:DL:97:THR:HG23	1.65	0.95
51:f:191:LYS:O	57:n:280:SER:O	1.84	0.95
55:j:39:GLN:O	55:j:43:PHE:CD2	2.19	0.95
45:e:60:VAL:HG11	46:b:179:LEU:CB	1.89	0.95
56:k:12:ARG:HG2	56:k:66:GLN:HE21	0.80	0.95
57:n:587:LEU:HD13	67:w:15:THR:HB	1.47	0.95
58:o:715:LEU:HD11	66:x:21:TYR:HB3	1.48	0.95
49:a:229:SER:CA	49:a:502:MET:CG	2.32	0.95
50:d:121:LEU:HD11	63:u:115:LEU:HB2	1.48	0.95
66:x:355:CYS:SG	66:x:407:ILE:HD11	2.05	0.95
66:x:956:VAL:HG11	66:x:968:LEU:CG	1.95	0.95
37:1:274:ASP:OD2	43:7:126:PHE:HB3	1.67	0.95
52:g:90:LEU:CD1	55:j:124:TYR:HE1	1.74	0.95
50:d:126:TYR:CD2	59:q:36:MET:HB3	2.01	0.95
52:g:93:LEU:HD22	55:j:106:LYS:CE	1.96	0.95
59:q:578:TYR:CD1	59:q:646:LEU:CD1	2.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:u:64:ARG:HG3	65:z:585:HIS:CE1	2.01	0.95
1:0:145:GLU:CG	53:h:3:ARG:HH22	1.57	0.95
52:g:161:ILE:CB	54:i:140:MET:HE1	1.94	0.95
60:r:19:MET:HE2	60:r:177:ALA:HB2	1.47	0.95
25:DE:507:VAL:HB	25:DE:513:LEU:HD21	1.48	0.95
29:DI:60:HIS:NE2	31:DL:106:ARG:NE	2.13	0.95
52:g:89:PHE:CG	63:u:19:PHE:CE1	2.55	0.95
52:g:89:PHE:CG	63:u:19:PHE:CD1	2.55	0.95
69:X:-32:DC:N4	70:Y:32:DG:O6	2.00	0.95
50:d:123:THR:HG22	59:q:37:SER:HB3	1.49	0.94
67:w:9:PHE:CD2	67:w:66:PHE:HD2	1.71	0.94
69:X:-8:DT:N3	70:Y:8:DA:N1	2.14	0.94
8:FA:44:GLN:C	9:FB:9:LEU:HD11	1.91	0.94
67:w:1:MET:N	67:w:1:MET:SD	2.31	0.94
24:DD:1078:LEU:CD2	31:DL:83:MET:HE3	1.98	0.94
42:6:415:HIS:CD2	70:Y:-12:DT:H5"	2.01	0.94
54:i:135:TYR:HH	63:u:125:ILE:N	1.52	0.94
55:j:102:MET:HG2	63:u:26:LEU:HG	0.95	0.94
59:q:7:VAL:CB	63:u:90:LEU:HD11	1.96	0.94
1:0:148:GLU:OE1	53:h:3:ARG:HB2	1.66	0.94
26:DF:71:ILE:HD12	29:DI:38:GLN:NE2	1.81	0.94
50:d:31:LEU:HD21	54:i:103:THR:CB	1.96	0.94
50:d:45:ILE:HG13	54:i:73:ILE:HG12	1.48	0.94
59:q:1:MET:CE	65:z:541:PRO:CG	2.36	0.94
67:w:8:ILE:O	67:w:12:VAL:CG1	2.15	0.94
49:a:455:GLN:CG	66:x:11:LEU:CD2	2.46	0.94
57:n:266:VAL:HG21	57:n:303:LEU:HD11	1.47	0.94
67:w:394:PRO:CA	68:p:171:PHE:CE1	2.47	0.94
37:1:483:THR:OG1	37:1:484:PRO:CD	2.15	0.94
49:a:467:MET:HE2	49:a:504:ILE:CD1	1.92	0.94
50:d:41:SER:CB	54:i:69:VAL:HG13	1.96	0.94
51:f:181:LEU:HD11	57:n:270:GLN:CB	1.96	0.94
53:h:146:MET:HE2	56:k:45:LEU:HD12	1.47	0.94
69:X:-33:DG:N1	70:Y:34:DG:C6	2.35	0.94
12:PC:265:HIS:NE2	62:t:113:ARG:HB2	1.51	0.94
53:h:77:ILE:HG13	59:q:126:THR:HG21	1.49	0.94
55:j:11:HIS:O	55:j:15:PHE:HD2	1.44	0.94
55:j:89:LEU:HD21	61:s:93:TYR:CZ	2.01	0.94
55:j:102:MET:CG	63:u:26:LEU:CG	2.38	0.94
55:j:102:MET:HG3	63:u:26:LEU:HD11	1.46	0.94
57:n:686:LYS:HZ3	58:o:730:PRO:HG3	1.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:o:696:SER:CB	66:x:111:HIS:HE1	1.81	0.94
59:q:89:GLN:HG2	59:q:90:PRO:HD2	1.38	0.94
2:8:143:LEU:O	2:8:143:LEU:HD13	1.67	0.94
13:PD:23:PRO:HD3	16:PG:80:PHE:CZ	2.02	0.94
57:n:254:VAL:CG1	57:n:304:GLN:NE2	2.30	0.94
59:q:9:ILE:HG13	63:u:90:LEU:HD13	0.98	0.94
13:PD:79:THR:OG1	53:h:51:LEU:CD2	2.15	0.94
45:e:146:ILE:HG22	45:e:147:ASN:N	1.78	0.94
51:f:185:ARG:CD	57:n:273:PHE:CZ	2.47	0.94
10:PA:666:ARG:NH1	10:PA:667:LEU:HD23	1.82	0.93
56:k:21:ILE:HG21	59:q:168:THR:OG1	1.68	0.93
50:d:45:ILE:HG23	54:i:76:MET:HB3	1.50	0.93
67:w:9:PHE:CB	67:w:66:PHE:CE2	2.50	0.93
53:h:146:MET:HB2	56:k:39:LYS:HZ3	1.05	0.93
59:q:451:LEU:HD12	59:q:529:MET:HE1	1.49	0.93
2:8:86:ASN:O	2:8:86:ASN:ND2	2.01	0.93
49:a:364:TYR:HB3	49:a:430:LEU:CG	1.96	0.93
23:DB:621:ALA:H	41:5:36:GLN:HE21	1.07	0.93
28:DH:57:SER:OG	30:DJ:200:LEU:HD12	1.69	0.93
57:n:192:LEU:CD1	57:n:220:GLY:CA	2.45	0.93
66:x:956:VAL:HG11	66:x:968:LEU:HD12	1.50	0.93
32:Dc:67:GLY:HA3	30:Dj:116:LEU:HD11	1.48	0.93
43:7:705:ASN:HB2	43:7:708:LEU:HD11	1.48	0.93
50:d:45:ILE:HG23	54:i:76:MET:HB2	0.93	0.93
59:q:89:GLN:CG	59:q:90:PRO:CD	2.38	0.93
42:6:289:TYR:H	42:6:290:PRO:CD	1.82	0.93
46:b:176:THR:HA	46:b:179:LEU:CD2	1.97	0.93
49:a:321:LEU:CD2	49:a:407:ILE:HG23	1.98	0.93
24:DD:1078:LEU:CD2	31:DL:83:MET:CE	2.46	0.93
51:f:185:ARG:HD2	57:n:273:PHE:CE2	2.03	0.93
57:n:545:LEU:HD11	57:n:653:PRO:CG	1.98	0.93
69:X:-33:DG:C6	70:Y:34:DG:O6	2.22	0.93
1:0:148:GLU:OE1	53:h:3:ARG:HD3	1.68	0.93
12:PC:265:HIS:NE2	62:t:113:ARG:HD2	1.56	0.93
13:PD:78:GLU:CD	53:h:51:LEU:HD23	1.92	0.93
31:DL:101:GLN:C	31:DL:105:HIS:CD2	2.47	0.93
67:w:9:PHE:HB3	67:w:66:PHE:CE2	2.04	0.93
11:PB:489:ILE:HG23	11:PB:490:GLY:O	1.69	0.92
13:PD:137:LYS:HE2	53:h:51:LEU:HD11	1.50	0.92
29:DI:28:ILE:HG22	29:DI:31:TYR:HD1	1.30	0.92
42:6:62:ARG:HD3	42:6:75:PRO:HD2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:o:762:GLN:HA	67:w:74:LYS:HZ1	1.30	0.92
59:q:93:TRP:CE3	59:q:93:TRP:HA	2.02	0.92
2:8:239:ASP:HA	2:8:242:SER:HB3	1.51	0.92
44:c:111:TYR:CE1	46:b:136:HIS:CD2	2.57	0.92
63:u:61:LEU:CD1	65:z:496:LEU:HG	1.95	0.92
13:PD:137:LYS:HE2	53:h:51:LEU:HG	0.95	0.92
48:m:56:LEU:CD2	48:m:80:GLN:NE2	2.33	0.92
54:i:135:TYR:CZ	63:u:125:ILE:CB	2.53	0.92
56:k:37:LYS:H	56:k:37:LYS:HE3	1.35	0.92
59:q:149:LYS:CD	64:v:40:ALA:HA	1.99	0.92
5:DP:169:VAL:HB	69:X:-25:DA:H2	1.23	0.92
49:a:493:PHE:HD2	49:a:514:LYS:CD	1.74	0.92
67:w:12:VAL:CG2	67:w:78:PHE:HE2	1.81	0.92
69:X:-19:DG:N1	70:Y:19:DC:C4	2.37	0.92
8:FA:125:TYR:CE2	9:FB:31:TRP:HE3	1.83	0.92
40:4:205:LEU:HD23	40:4:367:PHE:CZ	2.03	0.92
50:d:38:GLU:CG	54:i:96:GLU:HG2	1.99	0.92
40:4:100:LEU:C	40:4:101:LEU:HD12	1.93	0.92
45:e:146:ILE:CG2	45:e:147:ASN:H	1.82	0.92
51:f:174:ARG:HD3	57:n:267:HIS:HD2	0.77	0.92
56:k:87:ARG:HH11	56:k:87:ARG:HG3	1.33	0.92
49:a:412:ARG:HB3	49:a:472:SER:HB3	1.48	0.92
69:X:-5:DG:N2	70:Y:5:DC:N3	2.17	0.92
8:FA:45:ALA:CB	9:FB:9:LEU:HD21	2.00	0.92
26:DF:105:TYR:O	30:DJ:217:PHE:CG	2.23	0.92
46:b:62:MET:HE2	46:b:62:MET:HA	1.52	0.92
50:d:103:ARG:HG2	50:d:103:ARG:HH11	1.34	0.92
8:FA:45:ALA:HB3	9:FB:9:LEU:HD21	1.52	0.91
53:h:146:MET:HG3	56:k:39:LYS:HD2	1.52	0.91
2:8:52:LYS:HA	2:8:52:LYS:HE3	1.51	0.91
42:6:62:ARG:HD3	42:6:75:PRO:CD	2.00	0.91
44:c:111:TYR:CD1	46:b:136:HIS:CD2	2.58	0.91
54:i:72:ILE:HD13	54:i:92:SER:CB	2.00	0.91
48:m:71:GLN:HA	57:n:166:TYR:HE2	1.36	0.91
58:o:761:LEU:C	67:w:74:LYS:HE3	1.94	0.91
29:DI:132:LEU:HD21	30:DJ:121:MET:HE1	1.48	0.91
50:d:45:ILE:CD1	54:i:73:ILE:CA	2.48	0.91
53:h:89:LEU:HD11	59:q:124:PHE:CE2	2.05	0.91
62:t:98:LEU:HB3	62:t:102:PHE:HD1	1.36	0.91
67:w:6:GLN:CA	67:w:62:TRP:HH2	1.83	0.91
10:PA:693:ILE:HD11	11:PB:1008:VAL:HG11	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:417:TYR:CE1	49:a:450:PHE:HD1	1.74	0.91
63:u:83:ALA:CA	63:u:86:GLN:HB2	2.00	0.91
4:DO:65:TYR:HE1	5:DP:191:GLU:HG2	1.15	0.91
12:PC:265:HIS:NE2	62:t:113:ARG:HG3	1.85	0.91
54:i:65:PHE:CE1	54:i:99:LYS:HG3	2.04	0.91
63:u:81:SER:HB3	63:u:85:LEU:HB2	0.93	0.91
1:0:284:ALA:HB3	2:8:243:LEU:HD13	0.94	0.91
13:PD:78:GLU:OE1	53:h:51:LEU:HD23	0.73	0.91
50:d:31:LEU:HD23	54:i:103:THR:CG2	2.00	0.91
50:d:45:ILE:HD11	54:i:73:ILE:HG13	1.51	0.91
51:f:111:LEU:HD13	53:h:76:ILE:HD11	1.51	0.91
59:q:1:MET:HE3	65:z:541:PRO:CB	2.01	0.91
1:0:239:HIS:CB	51:f:87:GLN:NE2	2.34	0.91
57:n:359:ILE:HG23	57:n:372:ILE:CD1	2.01	0.91
5:DP:220:VAL:HG23	69:X:-24:DA:H2"	1.53	0.91
8:FA:124:TYR:CE1	9:FB:22:LYS:HG3	2.05	0.91
58:o:715:LEU:HD13	66:x:21:TYR:HB2	1.42	0.91
8:FA:125:TYR:HE2	9:FB:31:TRP:CE3	1.86	0.90
11:PB:592:ARG:CG	11:PB:592:ARG:NH1	2.10	0.90
49:a:417:TYR:HE1	49:a:450:PHE:HD1	1.07	0.90
28:DH:57:SER:CA	30:DJ:197:MET:SD	2.59	0.90
49:a:412:ARG:CB	49:a:472:SER:HB3	2.00	0.90
49:a:416:ALA:CB	49:a:472:SER:O	2.19	0.90
50:d:45:ILE:CG1	54:i:73:ILE:HG12	2.00	0.90
53:h:77:ILE:N	59:q:126:THR:OG1	2.04	0.90
56:k:28:ALA:HB3	59:q:161:LEU:CD2	2.00	0.90
57:n:203:LEU:HD13	57:n:215:LEU:HD12	1.53	0.90
57:n:253:LEU:O	57:n:255:GLU:HG3	1.70	0.90
58:o:696:SER:HB3	66:x:111:HIS:CE1	2.06	0.90
28:DH:60:THR:HG21	30:DJ:211:VAL:HG23	1.53	0.90
42:6:359:LYS:HZ1	42:6:436:GLY:HA2	1.30	0.90
50:d:76:PHE:HE2	54:i:65:PHE:HD2	1.17	0.90
63:u:82:THR:N	63:u:86:GLN:HG2	1.85	0.90
48:m:14:ASN:C	52:g:39:LYS:HZ1	1.77	0.90
49:a:417:TYR:CB	49:a:469:VAL:HG21	2.02	0.90
55:j:69:GLU:O	55:j:73:GLN:CG	2.19	0.90
57:n:587:LEU:HD13	67:w:15:THR:CG2	2.01	0.90
10:PA:439:HIS:CE1	60:r:19:MET:HB3	2.07	0.90
24:DD:1078:LEU:HD23	31:DL:83:MET:CE	2.01	0.90
53:h:142:SER:OG	56:k:39:LYS:HE3	1.72	0.90
59:q:7:VAL:HB	63:u:90:LEU:CD1	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:140:PRO:HA	2:8:202:ILE:HD11	1.53	0.90
2:8:214:PRO:HD2	2:8:224:ARG:HG2	1.53	0.90
10:PA:439:HIS:NE2	60:r:19:MET:CB	2.34	0.90
13:PD:137:LYS:HD2	53:h:55:GLN:HB2	0.91	0.90
28:DH:60:THR:HG21	30:DJ:211:VAL:CG2	2.02	0.90
56:k:28:ALA:HB1	59:q:161:LEU:HD23	0.97	0.90
13:PD:137:LYS:NZ	53:h:52:LEU:HA	1.87	0.90
40:4:443:VAL:H	41:5:6:LYS:HA	1.36	0.90
57:n:359:ILE:HG12	57:n:372:ILE:HD11	0.91	0.90
59:q:482:GLN:HB3	59:q:634:ASN:HD22	1.35	0.90
64:v:21:ARG:NE	64:v:78:LEU:CD2	2.35	0.90
70:Y:8:DA:C2'	70:Y:9:DC:C5	2.54	0.90
26:DF:105:TYR:O	30:DJ:217:PHE:HB3	1.71	0.90
31:Dl:106:ARG:HH12	31:Dl:114:LYS:HE2	1.11	0.90
53:h:182:VAL:CG2	60:r:202:ILE:HD12	2.01	0.90
58:o:715:LEU:CD2	66:x:21:TYR:HB2	2.00	0.90
1:0:145:GLU:HG2	53:h:3:ARG:NH2	1.83	0.89
7:BA:286:ARG:NH1	69:X:-37:DG:OP2	2.04	0.89
52:g:90:LEU:HD12	55:j:124:TYR:CE1	2.06	0.89
59:q:9:ILE:HG12	63:u:90:LEU:HB2	1.53	0.89
3:9:165:ARG:HB2	3:9:165:ARG:HH11	1.35	0.89
57:n:265:LEU:HD13	57:n:303:LEU:CD2	2.01	0.89
29:DI:132:LEU:HG	30:DJ:121:MET:CE	2.02	0.89
43:7:203:ASN:O	43:7:204:VAL:HG23	1.70	0.89
55:j:20:ARG:CD	57:n:94:GLN:CB	2.50	0.89
56:k:31:VAL:HG23	59:q:157:ALA:HB2	1.52	0.89
57:n:266:VAL:HG21	57:n:303:LEU:CD1	2.02	0.89
2:8:259:HIS:HE2	10:PA:1669:PRO:HB3	1.27	0.89
42:6:314:ALA:HB2	42:6:381:TRP:HD1	1.38	0.89
51:f:94:PRO:HB2	59:q:130:VAL:HG22	1.55	0.89
52:g:28:GLU:OE1	52:g:30:LEU:O	1.90	0.89
53:h:77:ILE:CG1	59:q:126:THR:CB	2.51	0.89
55:j:39:GLN:O	55:j:43:PHE:HD2	1.55	0.89
56:k:70:LEU:CD2	64:v:85:PHE:CE1	2.54	0.89
67:w:13:VAL:HG12	67:w:75:ARG:HG3	1.54	0.89
1:0:192:LEU:HD13	1:0:196:LEU:HD12	1.53	0.89
53:h:142:SER:O	56:k:39:LYS:NZ	2.05	0.89
54:i:72:ILE:CD1	54:i:92:SER:CB	2.50	0.89
57:n:192:LEU:HD12	57:n:220:GLY:HA2	1.52	0.89
42:6:289:TYR:N	42:6:290:PRO:HD3	1.86	0.89
50:d:45:ILE:CG2	54:i:76:MET:CB	2.27	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:g:90:LEU:HD13	55:j:124:TYR:HE1	1.31	0.89
59:q:9:ILE:CG1	63:u:90:LEU:HD22	2.03	0.89
13:PD:133:ASP:OD1	53:h:59:LEU:CD2	2.21	0.89
31:DL:111:LEU:CA	31:DL:114:LYS:NZ	2.26	0.89
48:m:68:LYS:HD3	52:g:45:PHE:CZ	2.08	0.89
50:d:45:ILE:HA	50:d:48:LEU:HD12	1.55	0.89
52:g:93:LEU:HD13	55:j:106:LYS:CG	2.03	0.89
9:FB:16:THR:HG21	9:FB:107:GLU:O	1.73	0.89
50:d:128:ALA:HB1	63:u:108:VAL:HG21	1.55	0.89
59:q:290:HIS:NE2	59:q:294:LYS:HE3	1.87	0.89
63:u:82:THR:O	63:u:86:GLN:HG3	1.73	0.89
11:PB:99:TRP:CE3	11:PB:105:PRO:CB	2.46	0.88
37:1:414:TYR:C	37:1:416:PRO:HD3	1.98	0.88
44:c:111:TYR:CD2	46:b:136:HIS:HD2	1.91	0.88
57:n:172:CYS:SG	59:q:21:GLU:HA	2.12	0.88
49:a:364:TYR:CB	49:a:430:LEU:HG	2.03	0.88
55:j:70:TYR:HD1	55:j:80:TYR:CB	1.85	0.88
63:u:18:GLN:HB3	63:u:62:ILE:CG1	2.03	0.88
22:DA:353:LEU:CD2	26:Df:272:VAL:HG21	2.01	0.88
48:m:23:GLU:OE1	52:g:44:MET:O	1.90	0.88
55:j:17:GLU:O	55:j:20:ARG:HG2	1.74	0.88
57:n:707:ASP:HB2	58:o:684:ARG:HH21	1.38	0.88
24:DD:895:HIS:CG	24:DD:896:PRO:CD	2.56	0.88
24:DD:1071:ARG:HB2	26:DF:91:PHE:CD2	2.08	0.88
49:a:412:ARG:C	49:a:472:SER:HB3	1.99	0.88
10:PA:436:SER:CB	62:t:97:LYS:HZ2	1.80	0.88
10:PA:1176:TYR:CE1	18:PI:52:CYS:HB2	2.09	0.88
11:PB:986:GLN:OE1	11:PB:1011:ILE:HG23	1.74	0.88
48:m:102:ILE:HG21	50:d:167:TRP:CH2	2.03	0.88
55:j:9:GLU:CG	55:j:56:GLN:NE2	2.37	0.88
59:q:290:HIS:HE1	59:q:294:LYS:HE3	1.33	0.88
5:DP:173:ASN:ND2	5:DP:218:LYS:NZ	2.21	0.88
29:DI:132:LEU:HG	30:DJ:121:MET:SD	2.13	0.88
53:h:29:PHE:CE2	59:q:102:LEU:CD1	2.57	0.88
59:q:89:GLN:CD	59:q:90:PRO:HD2	1.97	0.88
59:q:482:GLN:HB3	59:q:634:ASN:ND2	1.88	0.88
6:DQ:55:ALA:O	6:DQ:56:VAL:HG23	1.71	0.88
23:DB:539:ARG:HD2	40:4:408:LEU:HD13	1.55	0.88
52:g:89:PHE:CD1	63:u:19:PHE:HD1	1.87	0.88
55:j:26:VAL:HG11	55:j:38:ASN:HD21	0.75	0.88
55:j:89:LEU:HD11	61:s:93:TYR:HD1	1.34	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:274:ILE:CD1	57:n:299:PHE:CE2	2.57	0.88
3:9:175:LYS:HA	3:9:175:LYS:CE	2.03	0.88
29:Di:73:LEU:HD22	31:Dl:105:HIS:CD2	2.08	0.88
47:l:169:ASP:OD2	56:k:99:TYR:OH	1.90	0.88
48:m:104:HIS:CD2	57:n:169:LEU:CA	2.57	0.88
50:d:31:LEU:CD2	54:i:103:THR:CG2	2.51	0.88
54:i:72:ILE:HD11	54:i:92:SER:HB2	1.54	0.88
48:m:124:GLN:CD	65:z:590:ARG:HB2	1.99	0.88
59:q:149:LYS:CE	64:v:40:ALA:CA	2.52	0.88
64:v:21:ARG:NE	64:v:78:LEU:HD21	1.89	0.88
13:PD:137:LYS:CE	53:h:51:LEU:C	2.45	0.88
51:f:16:VAL:CG1	51:f:103:GLY:O	2.22	0.88
53:h:29:PHE:HE2	59:q:102:LEU:HD11	1.36	0.88
44:c:204:MET:HE1	44:c:208:PHE:C	1.99	0.87
49:a:460:ASP:O	66:x:11:LEU:HD22	1.74	0.87
28:DH:171:ASP:HB3	28:DH:174:VAL:HG12	1.54	0.87
48:m:14:ASN:CB	52:g:39:LYS:HZ1	1.87	0.87
48:m:104:HIS:NE2	57:n:168:ARG:HD3	1.87	0.87
49:a:423:SER:HB2	49:a:503:SER:HB2	1.56	0.87
54:i:65:PHE:HD1	54:i:99:LYS:HD3	1.39	0.87
70:Y:33:DC:H1'	70:Y:34:DG:C8	2.09	0.87
8:FA:125:TYR:CD2	9:FB:31:TRP:CZ3	2.63	0.87
10:PA:439:HIS:HB2	60:r:92:GLU:OE1	1.74	0.87
42:6:91:PRO:HB2	42:6:96:ALA:HB2	1.56	0.87
49:a:423:SER:CB	49:a:503:SER:HB2	2.04	0.87
57:n:237:MET:HE1	59:q:45:GLN:CB	2.03	0.87
50:d:45:ILE:CD1	54:i:73:ILE:HA	2.04	0.87
54:i:85:GLN:HG3	54:i:86:ASP:H	0.73	0.87
31:Dl:102:LEU:HA	31:Dl:105:HIS:CD2	2.08	0.87
49:a:462:LEU:HD21	66:x:11:LEU:CG	2.03	0.87
59:q:437:HIS:HE1	59:q:472:GLU:C	1.81	0.87
13:PD:137:LYS:HZ2	53:h:51:LEU:C	1.77	0.87
29:DI:60:HIS:CE1	31:DL:106:ARG:CZ	2.57	0.87
42:6:35:GLN:CD	42:6:159:CYS:HB3	1.98	0.87
67:w:361:ALA:HB3	68:p:251:GLU:HB3	1.56	0.87
5:DP:220:VAL:HG21	69:X:-24:DA:C1'	2.04	0.87
49:a:413:HIS:CE1	49:a:471:ASP:HA	2.10	0.87
57:n:250:LEU:HD21	57:n:275:HIS:HD2	1.39	0.87
57:n:686:LYS:HZ3	58:o:730:PRO:CB	1.87	0.87
3:9:186:ILE:H	3:9:186:ILE:HD13	1.39	0.87
40:4:100:LEU:O	40:4:101:LEU:HD12	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:467:MET:HE1	49:a:504:ILE:HD11	0.88	0.87
59:q:89:GLN:HG2	59:q:90:PRO:HD3	1.55	0.87
67:w:41:LEU:HD11	67:w:85:MET:HB3	1.56	0.87
44:c:204:MET:CE	44:c:208:PHE:O	2.23	0.86
60:r:19:MET:HE3	60:r:177:ALA:HA	0.89	0.86
50:d:126:TYR:CZ	59:q:36:MET:HB3	2.08	0.86
59:q:120:ARG:HG2	59:q:120:ARG:HH11	1.38	0.86
67:w:13:VAL:CG1	67:w:75:ARG:HG3	2.05	0.86
3:9:175:LYS:HA	3:9:175:LYS:HE3	1.56	0.86
8:FA:121:ASN:CA	9:FB:25:LYS:HE2	2.04	0.86
52:g:74:HIS:HB2	52:g:126:TYR:CD2	2.10	0.86
1:0:295:ARG:HH11	3:9:165:ARG:NH2	1.72	0.86
13:PD:137:LYS:HB2	53:h:55:GLN:OE1	1.64	0.86
49:a:380:ALA:HB3	49:a:444:PRO:CD	2.06	0.86
59:q:578:TYR:CD1	59:q:646:LEU:HD13	2.11	0.86
40:4:408:LEU:HB3	41:5:46:ILE:HD11	1.58	0.86
13:PD:137:LYS:HE3	53:h:51:LEU:C	2.01	0.86
50:d:126:TYR:CZ	59:q:36:MET:CB	2.59	0.86
54:i:140:MET:HG3	54:i:141:PHE:CD1	2.10	0.86
63:u:18:GLN:HE22	63:u:65:THR:CG2	1.88	0.86
64:v:21:ARG:CZ	64:v:78:LEU:HD23	1.99	0.86
40:4:412:PHE:CD2	40:4:418:PHE:CD1	2.63	0.86
49:a:377:ASN:HB3	49:a:442:VAL:O	1.75	0.86
50:d:156:SER:HA	50:d:161:VAL:HG12	1.55	0.86
59:q:139:GLN:NE2	59:q:139:GLN:O	2.08	0.86
63:u:18:GLN:CB	63:u:62:ILE:HG12	2.05	0.86
7:BA:193:ARG:NH2	70:Y:22:DC:OP2	2.09	0.86
11:PB:592:ARG:NH1	11:PB:592:ARG:HG3	1.82	0.86
55:j:93:GLU:HG3	61:s:83:LEU:HD13	1.56	0.86
57:n:245:TRP:HB2	57:n:282:LEU:HD13	0.88	0.86
5:DP:220:VAL:CG2	69:X:-24:DA:H1'	2.05	0.85
10:PA:1262:MET:HB3	10:PA:1265:ASP:HB2	1.57	0.85
29:Di:73:LEU:HD21	31:Dl:105:HIS:NE2	1.89	0.85
50:d:121:LEU:HB3	63:u:115:LEU:CD1	2.06	0.85
50:d:128:ALA:HB1	63:u:108:VAL:CG2	2.06	0.85
56:k:45:LEU:O	56:k:45:LEU:HD22	1.76	0.85
59:q:375:LEU:HD21	59:q:431:ILE:HG13	1.56	0.85
64:v:21:ARG:NH2	64:v:78:LEU:CD2	2.38	0.85
46:b:179:LEU:HD12	46:b:180:ASP:N	1.91	0.85
49:a:229:SER:CB	49:a:502:MET:CG	2.01	0.85
49:a:367:LEU:HD13	49:a:509:ARG:CZ	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:509:ARG:HB2	49:a:509:ARG:NH1	1.89	0.85
57:n:192:LEU:HD12	57:n:220:GLY:HA3	1.57	0.85
57:n:359:ILE:CB	57:n:372:ILE:CD1	2.54	0.85
58:o:762:GLN:CA	67:w:74:LYS:NZ	2.39	0.85
56:k:70:LEU:O	56:k:70:LEU:HD22	1.76	0.85
57:n:226:VAL:HG12	57:n:230:PHE:O	1.76	0.85
29:Di:73:LEU:CD2	31:Dl:105:HIS:CD2	2.60	0.85
42:6:289:TYR:N	42:6:290:PRO:CD	2.40	0.85
52:g:161:ILE:HA	54:i:140:MET:SD	2.16	0.85
57:n:169:LEU:HB3	57:n:170:PRO:HD2	1.56	0.85
52:g:89:PHE:CE1	63:u:19:PHE:HD1	1.95	0.85
53:h:22:LEU:HA	53:h:56:LEU:HD13	1.59	0.85
57:n:192:LEU:CD1	57:n:220:GLY:HA3	2.04	0.85
57:n:230:PHE:CE2	57:n:296:LEU:CB	2.59	0.85
44:c:113:TRP:CH2	46:b:175:HIS:CB	2.57	0.85
49:a:335:THR:O	49:a:391:THR:HG21	1.76	0.85
50:d:38:GLU:HG2	54:i:96:GLU:HG2	1.59	0.85
54:i:105:PRO:HD2	54:i:107:ILE:HG13	1.58	0.85
58:o:715:LEU:HD11	66:x:21:TYR:HB2	1.33	0.85
52:g:161:ILE:CG1	54:i:140:MET:CE	2.22	0.85
29:DI:28:ILE:HG22	29:DI:31:TYR:CD1	2.11	0.85
55:j:39:GLN:OE1	61:s:151:GLY:HA2	1.76	0.85
57:n:73:LEU:O	57:n:77:SER:N	2.09	0.85
57:n:254:VAL:HG11	57:n:304:GLN:HE21	1.42	0.85
9:FB:49:GLN:OE1	9:FB:49:GLN:N	2.08	0.85
17:PH:82:PRO:HB2	17:PH:84:ARG:HG2	1.58	0.85
48:m:70:PRO:HB2	57:n:166:TYR:HH	1.37	0.85
59:q:1:MET:CB	65:z:541:PRO:HG3	2.06	0.85
7:BA:27:TYR:HB3	7:BA:28:ARG:HH11	1.42	0.85
50:d:121:LEU:HD12	63:u:115:LEU:CB	1.87	0.85
51:f:180:LEU:HD13	57:n:302:SER:HB2	1.58	0.85
53:h:23:LYS:NZ	53:h:23:LYS:HB3	1.92	0.85
58:o:765:ASP:OD2	67:w:73:PRO:HD3	1.76	0.85
7:BA:127:ARG:HH21	7:BA:127:ARG:CG	1.90	0.84
8:FA:121:ASN:HA	9:FB:25:LYS:CE	2.06	0.84
24:DD:913:LEU:HD23	31:DL:87:ILE:HD13	1.57	0.84
44:c:30:ARG:HE	57:n:861:LYS:HE3	1.41	0.84
48:m:104:HIS:CD2	57:n:169:LEU:H	1.94	0.84
49:a:416:ALA:HB2	49:a:472:SER:O	1.77	0.84
53:h:18:GLN:HA	53:h:18:GLN:NE2	1.92	0.84
53:h:77:ILE:CA	59:q:126:THR:OG1	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:659:LEU:HD13	67:w:14:LYS:HG2	1.59	0.84
67:w:16:GLU:OE2	67:w:78:PHE:CD2	2.29	0.84
2:8:267:ASP:OD1	2:8:267:ASP:N	2.08	0.84
11:PB:822:GLY:HA3	11:PB:825:GLN:HB2	1.58	0.84
46:b:78:ALA:HB3	58:o:621:LEU:HD21	1.58	0.84
10:PA:983:LEU:N	10:PA:983:LEU:HD12	1.91	0.84
49:a:462:LEU:CD2	66:x:11:LEU:HD12	2.06	0.84
48:m:102:ILE:HG23	50:d:167:TRP:CH2	2.13	0.84
53:h:22:LEU:HD12	53:h:22:LEU:O	1.77	0.84
5:DP:218:LYS:HB2	69:X:-23:DG:P	2.16	0.84
37:1:187:ASN:CB	37:1:191:ASP:CB	2.51	0.84
44:c:204:MET:SD	44:c:208:PHE:O	2.34	0.84
46:b:176:THR:HA	46:b:179:LEU:HD21	1.60	0.84
1:0:27:GLY:HA3	1:0:69:ASP:HB2	1.58	0.84
4:DO:65:TYR:HE1	5:DP:191:GLU:HG3	1.43	0.84
10:PA:436:SER:CB	62:t:97:LYS:HZ1	1.86	0.84
26:DF:104:LEU:CB	30:DJ:217:PHE:CZ	2.61	0.84
29:DI:23:LEU:HD21	29:DI:39:MET:HE1	1.58	0.84
48:m:116:GLN:HB3	65:z:594:LEU:CD2	2.07	0.84
56:k:21:ILE:HD12	59:q:168:THR:HG1	1.40	0.84
8:FA:44:GLN:HA	9:FB:9:LEU:HD12	1.60	0.84
11:PB:643:LEU:CD2	11:PB:656:LEU:CD1	2.53	0.84
57:n:359:ILE:HA	57:n:372:ILE:HD12	1.60	0.84
44:c:204:MET:HE1	44:c:208:PHE:CA	2.08	0.84
53:h:182:VAL:CG2	60:r:202:ILE:CD1	2.56	0.84
8:FA:102:VAL:HB	8:FA:108:ARG:HB3	1.59	0.83
42:6:472:ARG:CG	42:6:473:GLU:HG3	2.07	0.83
50:d:42:ARG:HH22	54:i:93:LYS:HA	1.39	0.83
59:q:1:MET:H1	65:z:540:LEU:HD13	1.21	0.83
3:9:60:TYR:HB3	3:9:105:MET:HE1	1.59	0.83
47:l:166:LEU:HD12	56:k:103:LYS:HB3	1.60	0.83
49:a:413:HIS:NE2	49:a:471:ASP:CA	2.37	0.83
57:n:254:VAL:HG13	57:n:304:GLN:NE2	1.92	0.83
59:q:212:ALA:CA	59:q:387:LEU:HD11	2.04	0.83
5:DP:218:LYS:CG	69:X:-23:DG:OP1	2.25	0.83
10:PA:1443:ALA:HB2	11:PB:1167:ILE:HG23	1.59	0.83
49:a:417:TYR:CG	49:a:469:VAL:HG21	2.11	0.83
53:h:72:ARG:HH12	59:q:134:ALA:H	1.19	0.83
55:j:114:SER:HB2	55:j:121:MET:HG2	1.59	0.83
59:q:1:MET:HB2	65:z:541:PRO:CG	2.04	0.83
1:0:300:ALA:HB2	3:9:166:PRO:CA	1.99	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:c:110:ALA:HB1	46:b:168:ILE:HG23	0.85	0.83
51:f:184:LEU:HD23	57:n:299:PHE:HD1	1.42	0.83
10:PA:439:HIS:HD1	60:r:92:GLU:CD	1.86	0.83
44:c:113:TRP:CZ2	46:b:175:HIS:CG	2.65	0.83
45:e:140:GLN:NE2	56:k:105:SER:HA	1.93	0.83
53:h:77:ILE:CG1	59:q:126:THR:HG21	2.08	0.83
63:u:25:VAL:HG21	63:u:58:PHE:CE2	2.14	0.83
1:0:295:ARG:NH1	3:9:165:ARG:NH2	2.26	0.83
5:DP:220:VAL:CG2	69:X:-24:DA:C1'	2.56	0.83
49:a:423:SER:OG	49:a:505:PRO:HD3	1.79	0.83
57:n:265:LEU:CD1	57:n:303:LEU:HD21	2.08	0.83
5:DP:313:THR:HG23	69:X:-27:DA:H4'	1.60	0.83
26:DF:104:LEU:HB2	30:DJ:217:PHE:CZ	2.14	0.83
32:Dc:67:GLY:HA3	30:Dj:116:LEU:HD13	1.60	0.83
43:7:20:GLU:OE1	43:7:482:THR:CG2	2.26	0.83
50:d:121:LEU:HD13	63:u:115:LEU:HB2	0.83	0.83
51:f:180:LEU:CD1	57:n:302:SER:OG	2.25	0.83
55:j:102:MET:HG3	63:u:26:LEU:CD1	2.07	0.83
57:n:141:ARG:NH2	63:u:17:ASP:HA	1.93	0.83
10:PA:1177:TYR:HA	10:PA:1210:TRP:HA	1.59	0.83
12:PC:83:GLN:CG	62:t:204:GLN:OE1	2.27	0.83
48:m:124:GLN:OE1	65:z:590:ARG:HB2	1.78	0.83
50:d:38:GLU:OE2	54:i:96:GLU:HG2	1.79	0.83
50:d:115:LYS:HE2	50:d:115:LYS:HA	1.60	0.83
57:n:192:LEU:HD12	57:n:219:ASN:O	1.78	0.83
57:n:587:LEU:HD13	67:w:15:THR:CB	2.08	0.83
59:q:152:SER:HB2	64:v:58:ASN:CA	2.06	0.83
59:q:451:LEU:CD1	59:q:529:MET:CE	2.57	0.83
63:u:81:SER:HB2	63:u:85:LEU:CA	2.09	0.83
7:BA:280:VAL:CA	70:Y:33:DC:OP2	2.24	0.83
53:h:77:ILE:CD1	59:q:126:THR:HG21	2.09	0.83
16:PG:78:ARG:HH12	16:PG:152:VAL:HG11	1.44	0.82
24:DD:890:GLY:CA	31:DL:104:ARG:HH22	1.92	0.82
29:Di:73:LEU:CG	31:Dl:105:HIS:CE1	2.61	0.82
50:d:110:LEU:O	50:d:110:LEU:HD22	1.79	0.82
66:x:956:VAL:CG1	66:x:968:LEU:CD1	2.49	0.82
25:DE:747:LEU:HD22	25:DE:747:LEU:H	1.43	0.82
49:a:462:LEU:CD2	66:x:11:LEU:CG	2.55	0.82
59:q:93:TRP:HA	59:q:93:TRP:HE3	1.41	0.82
59:q:443:ARG:NE	59:q:443:ARG:HA	1.92	0.82
66:x:956:VAL:CG1	66:x:968:LEU:HG	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DP:220:VAL:HG21	69:X:-24:DA:H1'	1.60	0.82
28:DH:105:ASP:HA	30:DJ:116:LEU:HD21	1.60	0.82
57:n:225:ARG:CB	57:n:231:GLU:OE1	2.27	0.82
59:q:437:HIS:HE1	59:q:472:GLU:N	1.77	0.82
10:PA:811:ILE:HG22	11:PB:674:MET:HE1	1.59	0.82
49:a:417:TYR:HE1	49:a:450:PHE:CE1	1.88	0.82
53:h:142:SER:OG	56:k:39:LYS:CE	2.26	0.82
59:q:482:GLN:CB	59:q:634:ASN:ND2	2.42	0.82
48:m:62:GLU:HG3	52:g:38:ILE:CD1	2.08	0.82
49:a:228:PRO:HD2	49:a:502:MET:HE1	1.59	0.82
49:a:417:TYR:HB2	49:a:469:VAL:HG21	1.60	0.82
59:q:149:LYS:HE2	64:v:40:ALA:O	1.79	0.82
10:PA:436:SER:CA	62:t:97:LYS:NZ	2.43	0.82
13:PD:23:PRO:HD3	16:PG:80:PHE:HZ	1.40	0.82
26:Df:447:ALA:HA	26:Df:456:GLY:HA3	1.60	0.82
51:f:15:TRP:CH2	51:f:35:GLU:OE1	2.32	0.82
53:h:77:ILE:CG1	59:q:126:THR:OG1	2.28	0.82
3:9:52:GLU:HB3	3:9:273:LEU:HD11	1.61	0.82
13:PD:137:LYS:CD	53:h:51:LEU:CD1	2.58	0.82
44:c:111:TYR:CE2	46:b:136:HIS:HD2	1.98	0.82
57:n:192:LEU:CD1	57:n:220:GLY:HA2	2.08	0.82
3:9:229:GLU:OE1	3:9:229:GLU:N	2.11	0.82
7:BA:127:ARG:HH21	7:BA:127:ARG:HG3	1.44	0.82
49:a:321:LEU:HD21	49:a:407:ILE:CG2	2.08	0.82
55:j:105:PHE:CE2	55:j:109:LEU:CD1	2.63	0.82
57:n:265:LEU:CD1	57:n:303:LEU:CD2	2.58	0.82
10:PA:983:LEU:N	10:PA:983:LEU:CD1	2.43	0.82
13:PD:137:LYS:HE3	53:h:51:LEU:CA	2.09	0.82
31:DL:111:LEU:O	31:DL:114:LYS:CG	2.26	0.82
55:j:43:PHE:CZ	61:s:147:THR:O	2.32	0.82
59:q:339:LEU:HD22	59:q:439:PHE:CD2	2.15	0.82
63:u:81:SER:HB3	63:u:85:LEU:CG	2.08	0.82
1:0:287:TYR:CE1	2:8:189:MET:SD	2.73	0.82
39:3:237:GLN:O	39:3:241:LEU:HB3	1.80	0.82
47:l:168:TRP:CE2	59:q:441:ARG:NH1	2.48	0.82
2:8:259:HIS:CD2	10:PA:1669:PRO:CB	2.60	0.81
31:DL:64:GLN:HA	31:DL:67:VAL:HG22	1.60	0.81
38:2:32:ALA:HB3	42:6:72:THR:HB	1.61	0.81
40:4:412:PHE:CD2	40:4:418:PHE:CE1	2.68	0.81
51:f:32:TYR:CD1	51:f:35:GLU:OE2	2.33	0.81
53:h:139:GLN:HE22	56:k:37:LYS:HB2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:462:ALA:O	64:v:131:GLU:HG2	1.79	0.81
10:PA:981:CYS:O	10:PA:983:LEU:CD1	2.28	0.81
10:PA:1242:ASP:HA	10:PA:1262:MET:HB2	1.61	0.81
42:6:309:ASP:O	42:6:310:LEU:HG	1.80	0.81
43:7:519:ASN:HA	43:7:522:ASN:HD22	1.44	0.81
48:m:124:GLN:OE1	65:z:590:ARG:CB	2.28	0.81
50:d:41:SER:CB	54:i:69:VAL:CG1	2.57	0.81
53:h:74:GLN:CD	59:q:129:PRO:HB3	2.05	0.81
63:u:8:LEU:HD12	63:u:72:LEU:CD2	2.10	0.81
69:X:-5:DG:N1	70:Y:4:DA:N6	2.28	0.81
11:PB:59:VAL:HG21	11:PB:91:ILE:HG13	1.60	0.81
45:e:93:CYS:SG	59:q:647:SER:HB3	2.20	0.81
46:b:176:THR:O	46:b:179:LEU:HG	1.80	0.81
51:f:32:TYR:HD1	51:f:35:GLU:OE2	1.62	0.81
57:n:73:LEU:O	57:n:77:SER:CA	2.28	0.81
59:q:437:HIS:HE1	59:q:472:GLU:CA	1.92	0.81
10:PA:436:SER:HB2	62:t:97:LYS:HZ2	1.44	0.81
10:PA:581:LYS:NZ	17:PH:86:ASP:HA	1.95	0.81
49:a:380:ALA:CB	49:a:444:PRO:HD2	2.09	0.81
54:i:68:LEU:HD13	54:i:95:GLN:CG	2.05	0.81
9:FB:147:LYS:HG3	9:FB:148:VAL:N	1.95	0.81
11:PB:628:VAL:HG12	11:PB:629:GLU:O	1.80	0.81
44:c:111:TYR:CZ	46:b:136:HIS:CD2	2.69	0.81
52:g:166:ASN:OD1	52:g:166:ASN:C	2.24	0.81
57:n:274:ILE:HD13	57:n:299:PHE:CG	2.14	0.81
29:DI:132:LEU:HG	30:DJ:121:MET:HE2	1.62	0.81
52:g:161:ILE:CA	54:i:140:MET:CE	1.96	0.81
52:g:161:ILE:CB	54:i:140:MET:HE2	2.00	0.81
57:n:274:ILE:HD12	57:n:299:PHE:CZ	2.15	0.81
26:DF:104:LEU:HD13	30:DJ:217:PHE:HE2	1.44	0.81
28:DH:57:SER:HA	30:DJ:197:MET:SD	2.21	0.81
49:a:364:TYR:O	49:a:428:THR:OG1	1.99	0.81
59:q:186:GLU:CG	59:q:243:LEU:HD21	1.91	0.81
10:PA:436:SER:CA	62:t:97:LYS:HZ1	1.93	0.81
13:PD:137:LYS:HG3	53:h:51:LEU:CD1	2.10	0.81
29:DI:60:HIS:HD2	31:DL:106:ARG:HG3	1.44	0.81
40:4:443:VAL:HB	41:5:6:LYS:HG2	1.62	0.81
55:j:89:LEU:CD1	61:s:93:TYR:CE1	2.63	0.81
10:PA:811:ILE:HG23	11:PB:689:TYR:CZ	2.15	0.81
29:DI:60:HIS:CD2	31:DL:106:ARG:HG3	2.16	0.81
54:i:75:CYS:HB3	54:i:88:ASN:ND2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:274:ILE:HD13	57:n:299:PHE:CD2	2.16	0.81
57:n:870:GLN:HG2	58:o:655:THR:HG22	1.61	0.81
1:0:298:GLN:NE2	2:8:132:TRP:CD1	2.49	0.80
2:8:143:LEU:HD22	2:8:143:LEU:C	2.07	0.80
7:BA:178:LYS:HB3	9:FB:154:LYS:HB3	1.62	0.80
13:PD:137:LYS:HG3	53:h:51:LEU:HD12	1.61	0.80
24:DD:890:GLY:C	31:DL:104:ARG:NH2	2.25	0.80
49:a:364:TYR:CB	49:a:430:LEU:HD12	2.11	0.80
56:k:28:ALA:HB3	59:q:161:LEU:HD21	1.55	0.80
58:o:693:LEU:CD2	59:q:608:ASP:HB2	2.06	0.80
1:0:300:ALA:CB	3:9:166:PRO:CA	2.53	0.80
5:DP:313:THR:CG2	69:X:-27:DA:C4'	2.55	0.80
31:Dl:101:GLN:C	31:Dl:105:HIS:CD2	2.59	0.80
36:EB:148:LYS:HD3	36:EB:174:ALA:HB3	1.61	0.80
46:b:174:ILE:HG12	47:l:75:LEU:CG	2.11	0.80
52:g:161:ILE:HG23	54:i:140:MET:SD	2.21	0.80
55:j:75:ARG:HB3	55:j:80:TYR:CD2	2.15	0.80
55:j:89:LEU:CD2	61:s:93:TYR:CE1	2.63	0.80
56:k:16:ASP:OD2	64:v:79:VAL:HG21	1.80	0.80
64:v:16:GLN:HE22	64:v:20:LYS:HE2	1.41	0.80
4:DO:62:LEU:HA	4:DO:76:LEU:HD13	1.62	0.80
23:DB:621:ALA:N	41:5:36:GLN:HE21	1.80	0.80
57:n:545:LEU:HD11	57:n:653:PRO:CD	2.10	0.80
2:8:207:LEU:HD22	51:f:52:MET:HE2	1.61	0.80
8:FA:44:GLN:C	9:FB:9:LEU:CD1	2.53	0.80
12:PC:87:ASP:O	62:t:201:ARG:NH2	2.14	0.80
22:DA:564:PRO:HG2	23:DB:744:PHE:CD2	2.16	0.80
50:d:45:ILE:C	54:i:76:MET:HG2	2.07	0.80
67:w:394:PRO:CA	68:p:171:PHE:HZ	1.81	0.80
43:7:616:ARG:NH2	43:7:674:TYR:CD2	2.49	0.80
48:m:104:HIS:NE2	57:n:168:ARG:CG	2.44	0.80
53:h:77:ILE:C	59:q:126:THR:OG1	2.20	0.80
57:n:359:ILE:HG12	57:n:372:ILE:HD13	1.64	0.80
58:o:762:GLN:CA	67:w:74:LYS:HE3	2.11	0.80
59:q:451:LEU:HD12	59:q:529:MET:CE	2.11	0.80
12:PC:265:HIS:HD2	62:t:113:ARG:HB2	1.39	0.80
49:a:514:LYS:NZ	49:a:514:LYS:HB3	1.96	0.80
54:i:140:MET:CG	54:i:141:PHE:HD1	1.93	0.80
57:n:230:PHE:CZ	57:n:296:LEU:CB	2.65	0.80
3:9:165:ARG:HB2	3:9:165:ARG:NH1	1.96	0.80
45:e:97:GLN:HE22	59:q:649:CYS:N	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:d:42:ARG:NH2	54:i:96:GLU:OE2	2.14	0.80
56:k:12:ARG:HB3	56:k:66:GLN:HE22	0.63	0.80
57:n:259:THR:OG1	57:n:311:GLN:NE2	2.13	0.80
12:PC:19:VAL:HG23	12:PC:241:PRO:HB2	1.62	0.80
24:Dd:1082:ALA:HB2	31:Dl:83:MET:HE2	1.63	0.80
40:4:314:ARG:O	40:4:316:TYR:HD2	1.63	0.80
44:c:204:MET:CE	44:c:208:PHE:C	2.54	0.80
59:q:149:LYS:HG3	64:v:42:ILE:HG13	1.64	0.80
63:u:83:ALA:HA	63:u:86:GLN:HB2	1.61	0.80
29:DI:23:LEU:HD11	29:DI:39:MET:CE	2.11	0.80
29:DI:23:LEU:CD1	29:DI:39:MET:HE1	2.11	0.80
32:Dc:77:LEU:HD13	30:Dj:116:LEU:HD23	1.62	0.80
50:d:42:ARG:NH2	54:i:93:LYS:HA	1.97	0.80
53:h:29:PHE:HE2	59:q:102:LEU:CD1	1.93	0.80
49:a:462:LEU:HD21	66:x:11:LEU:HG	1.63	0.80
50:d:45:ILE:HG12	54:i:73:ILE:CA	2.10	0.80
63:u:4:ARG:CG	65:z:594:LEU:O	2.29	0.80
3:9:177:ARG:NH1	3:9:177:ARG:HB2	1.97	0.79
5:DP:218:LYS:HG3	69:X:-23:DG:P	2.22	0.79
5:DP:294:ARG:NH2	7:BA:196:LYS:HE2	1.97	0.79
59:q:92:LEU:CD1	59:q:99:ARG:HH22	1.92	0.79
63:u:14:SER:O	63:u:18:GLN:HG3	1.81	0.79
52:g:37:PRO:HG2	52:g:39:LYS:HE3	1.64	0.79
13:PD:137:LYS:CG	53:h:51:LEU:HD12	2.10	0.79
49:a:417:TYR:CD1	49:a:469:VAL:HG23	2.03	0.79
50:d:108:GLN:NE2	57:n:204:VAL:O	2.16	0.79
55:j:70:TYR:HD1	55:j:80:TYR:CD1	1.99	0.79
67:w:5:LEU:HA	67:w:8:ILE:HD12	1.64	0.79
3:9:28:ARG:CZ	3:9:28:ARG:HB2	2.11	0.79
23:DB:621:ALA:HB3	41:5:36:GLN:CG	2.11	0.79
60:r:19:MET:HG3	60:r:21:TYR:CE1	2.18	0.79
63:u:18:GLN:NE2	63:u:65:THR:HG21	1.97	0.79
63:u:83:ALA:N	63:u:86:GLN:CG	2.46	0.79
9:FB:173:GLY:HA3	69:X:-20:DG:H5"	1.65	0.79
10:PA:981:CYS:O	10:PA:983:LEU:HD12	1.82	0.79
26:DF:273:GLN:NE2	26:DF:273:GLN:H	1.81	0.79
55:j:120:ASP:O	55:j:124:TYR:CD2	2.34	0.79
57:n:172:CYS:SG	59:q:21:GLU:HB2	2.22	0.79
57:n:203:LEU:CD1	57:n:215:LEU:HD12	2.11	0.79
59:q:633:ARG:CZ	59:q:633:ARG:HB3	2.11	0.79
67:w:357:HIS:HE1	67:w:397:LYS:CE	1.90	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:146:MET:CE	56:k:45:LEU:HD12	2.12	0.79
59:q:1:MET:HE3	65:z:541:PRO:HG2	0.81	0.79
61:s:92:ALA:HB1	61:s:96:PHE:HE2	1.46	0.79
63:u:61:LEU:HD11	65:z:496:LEU:CD1	2.12	0.79
9:FB:16:THR:O	9:FB:109:ILE:HD12	1.83	0.79
10:PA:439:HIS:CB	60:r:92:GLU:OE1	2.31	0.79
31:Dl:102:LEU:CA	31:Dl:105:HIS:HD2	1.96	0.79
37:1:200:TYR:HB3	37:1:203:VAL:HB	1.65	0.79
48:m:14:ASN:HB3	52:g:39:LYS:HZ1	1.48	0.79
66:x:956:VAL:HG11	66:x:968:LEU:HG	1.62	0.79
70:Y:33:DC:O2	70:Y:34:DG:C5	2.34	0.79
3:9:239:LYS:H	3:9:239:LYS:NZ	1.80	0.79
48:m:106:GLN:NE2	50:d:167:TRP:HZ3	1.81	0.79
49:a:417:TYR:CE1	49:a:450:PHE:HE1	2.00	0.79
49:a:441:GLU:CD	66:x:17:ARG:NH2	2.41	0.79
50:d:46:GLU:HA	54:i:76:MET:HE3	1.65	0.79
1:0:295:ARG:HH11	3:9:165:ARG:HH21	1.25	0.79
56:k:37:LYS:H	56:k:37:LYS:CE	1.96	0.79
2:8:207:LEU:HD22	51:f:52:MET:CE	2.13	0.79
24:DD:1063:LEU:HD12	31:DL:80:VAL:HG13	1.64	0.79
31:DL:101:GLN:O	31:DL:105:HIS:HD2	1.63	0.79
40:4:442:VAL:HB	41:5:44:PHE:CE1	2.17	0.79
48:m:104:HIS:CD2	57:n:169:LEU:N	2.50	0.79
59:q:152:SER:CB	64:v:58:ASN:HA	2.09	0.79
67:w:6:GLN:HB2	67:w:62:TRP:CH2	2.18	0.79
3:9:198:ILE:HD12	3:9:255:MET:HE2	1.62	0.78
52:g:168:LEU:O	52:g:172:PRO:HD2	1.83	0.78
54:i:135:TYR:HH	63:u:125:ILE:CA	1.79	0.78
58:o:715:LEU:CG	66:x:21:TYR:HB2	2.12	0.78
25:De:747:LEU:HD23	25:De:747:LEU:H	1.47	0.78
46:b:174:ILE:HD13	47:l:75:LEU:CD2	2.02	0.78
49:a:413:HIS:NE2	49:a:471:ASP:CB	2.46	0.78
49:a:493:PHE:HE2	49:a:514:LYS:HG3	1.00	0.78
20:PK:38:GLU:HB3	20:PK:71:ILE:HD11	1.66	0.78
25:DE:605:HIS:NE2	26:DF:77:LEU:HD21	1.98	0.78
40:4:407:VAL:O	41:5:6:LYS:HB2	1.83	0.78
51:f:181:LEU:HD11	57:n:270:GLN:HB3	1.65	0.78
53:h:139:GLN:NE2	56:k:37:LYS:HB2	1.97	0.78
55:j:34:GLN:OE1	55:j:37:LEU:HD11	1.82	0.78
11:PB:577:HIS:CE1	11:PB:579:ASP:O	2.37	0.78
45:e:93:CYS:SG	59:q:647:SER:CB	2.72	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:m:104:HIS:HE1	57:n:168:ARG:HG3	0.96	0.78
49:a:321:LEU:HD21	49:a:407:ILE:HD12	1.63	0.78
23:DB:621:ALA:HB3	41:5:36:GLN:HG3	1.63	0.78
46:b:178:LEU:HD23	47:l:82:LEU:HD11	1.64	0.78
53:h:19:VAL:HG11	59:q:113:TYR:HB2	1.65	0.78
65:z:543:LEU:HD23	65:z:545:ARG:HD3	1.65	0.78
70:Y:33:DC:H4'	70:Y:34:DG:OP1	1.83	0.78
12:PC:5:ASN:C	12:PC:6:GLN:NE2	2.41	0.78
50:d:42:ARG:NH2	54:i:96:GLU:CD	2.42	0.78
50:d:45:ILE:CG2	54:i:76:MET:HE2	2.12	0.78
50:d:115:LYS:HE2	50:d:115:LYS:CA	2.13	0.78
51:f:174:ARG:HG3	57:n:270:GLN:HE22	1.29	0.78
57:n:274:ILE:CD1	57:n:299:PHE:CD1	2.66	0.78
63:u:79:GLU:OE1	63:u:82:THR:HG21	1.83	0.78
24:DD:1063:LEU:CD1	31:DL:80:VAL:HG13	2.14	0.78
45:e:97:GLN:OE1	59:q:649:CYS:HA	1.83	0.78
52:g:28:GLU:CD	52:g:30:LEU:HB3	2.06	0.78
58:o:674:ILE:HD13	59:q:609:VAL:HG23	1.63	0.78
7:BA:111:ASP:HB3	7:BA:114:MET:HB2	1.66	0.78
10:PA:538:VAL:HG13	10:PA:539:GLN:H	1.49	0.78
22:DA:638:PRO:HB3	27:DG:39:LEU:HD23	1.63	0.78
50:d:45:ILE:HD11	54:i:73:ILE:CG1	2.13	0.78
51:f:78:LEU:HD11	53:h:81:LEU:HD23	1.65	0.78
52:g:175:LEU:HD21	54:i:132:LEU:HD12	1.64	0.78
56:k:21:ILE:CD1	59:q:168:THR:OG1	2.30	0.78
57:n:199:LEU:HD22	57:n:222:VAL:CG1	2.13	0.78
35:EA:72:ILE:HB	35:EA:96:TYR:HB3	1.65	0.78
52:g:90:LEU:CD1	55:j:124:TYR:CZ	2.66	0.78
53:h:29:PHE:CD2	59:q:102:LEU:HD11	2.19	0.78
56:k:17:ILE:HG23	59:q:171:VAL:CG2	2.06	0.78
56:k:21:ILE:CG2	59:q:168:THR:OG1	2.32	0.78
57:n:359:ILE:CG2	57:n:372:ILE:CD1	2.62	0.78
58:o:715:LEU:N	66:x:25:ILE:HG12	1.99	0.78
59:q:138:LYS:CB	59:q:140:ASN:OD1	2.28	0.78
62:t:98:LEU:HB3	62:t:102:PHE:CD1	2.18	0.78
62:t:144:TYR:HD2	62:t:147:CYS:HB2	1.46	0.78
12:PC:264:SER:HA	12:PC:267:ILE:HG12	1.65	0.78
59:q:644:SER:HA	59:q:647:SER:OG	1.83	0.78
70:Y:4:DA:H2"	70:Y:5:DC:OP2	1.83	0.78
13:PD:137:LYS:HZ1	53:h:51:LEU:HG	1.46	0.77
26:DF:105:TYR:O	30:DJ:217:PHE:CB	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1:163:ASP:OD2	38:2:179:PRO:CD	2.32	0.77
46:b:178:LEU:HD11	47:l:78:LEU:HD13	1.65	0.77
49:a:228:PRO:HD2	49:a:502:MET:SD	2.24	0.77
55:j:82:LYS:HG2	61:s:96:PHE:HD1	1.49	0.77
63:u:71:VAL:HG21	65:z:582:LEU:HD11	1.65	0.77
4:DO:65:TYR:CE1	5:DP:191:GLU:HG3	2.15	0.77
10:PA:436:SER:C	62:t:97:LYS:HZ3	1.90	0.77
34:Dm:31:LEU:H	34:Dm:31:LEU:HD23	1.48	0.77
59:q:149:LYS:HE3	64:v:40:ALA:HA	1.64	0.77
67:w:394:PRO:HA	68:p:171:PHE:HZ	0.98	0.77
1:0:300:ALA:HA	3:9:166:PRO:HG3	1.66	0.77
20:PK:14:GLU:OE2	60:r:8:MET:HB3	1.83	0.77
55:j:75:ARG:HA	55:j:79:LEU:HD12	1.65	0.77
26:DF:418:ILE:H	26:DF:418:ILE:HD12	1.49	0.77
28:DH:56:ALA:CB	30:DJ:214:PRO:CG	2.61	0.77
29:DI:73:LEU:CD2	31:DL:105:HIS:NE2	2.46	0.77
49:a:382:LEU:HD22	49:a:446:SER:CA	2.13	0.77
55:j:71:ILE:HD11	57:n:106:ALA:HB2	1.66	0.77
55:j:78:GLN:HA	55:j:82:LYS:HE3	1.64	0.77
56:k:87:ARG:HA	64:v:105:LEU:HD13	1.62	0.77
12:PC:46:ALA:HA	12:PC:73:LEU:HD12	1.65	0.77
24:DD:1060:LEU:HD13	31:DL:79:ASP:HB3	1.65	0.77
37:1:166:ILE:HD11	37:1:170:PHE:H	1.49	0.77
39:3:224:LEU:O	39:3:228:LEU:HG	1.84	0.77
49:a:229:SER:H	49:a:502:MET:CG	1.87	0.77
53:h:146:MET:CB	56:k:39:LYS:HZ3	1.86	0.77
53:h:153:LYS:HE3	56:k:46:ASP:OD2	1.85	0.77
44:c:111:TYR:CG	46:b:136:HIS:CD2	2.73	0.77
53:h:150:LEU:CD2	56:k:45:LEU:HD11	2.09	0.77
57:n:231:GLU:HB2	57:n:253:LEU:HD21	1.67	0.77
67:w:9:PHE:CG	67:w:66:PHE:CE2	2.73	0.77
2:8:171:HIS:CE1	2:8:188:ARG:HA	2.20	0.77
11:PB:577:HIS:HE1	11:PB:579:ASP:O	1.67	0.77
14:PE:117:SER:HA	14:PE:120:ASP:HB3	1.66	0.77
24:DD:947:PHE:HB3	29:DI:113:PRO:HG3	1.65	0.77
55:j:54:CYS:HA	55:j:57:GLN:CD	2.10	0.77
57:n:587:LEU:HD22	67:w:15:THR:CG2	2.13	0.77
70:Y:33:DC:O2	70:Y:34:DG:C8	2.36	0.77
55:j:96:LYS:HZ3	61:s:81:THR:N	1.83	0.77
57:n:229:GLU:HG3	57:n:300:CYS:SG	2.25	0.77
69:X:-32:DC:N3	70:Y:32:DG:N1	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:X:-19:DG:C2	70:Y:19:DC:N3	2.52	0.77
11:PB:607:ILE:HG21	18:PI:72:VAL:HA	1.67	0.77
13:PD:79:THR:CA	53:h:51:LEU:CD2	2.62	0.77
22:DA:854:ARG:HH21	70:Y:-25:DT:P	2.08	0.77
49:a:514:LYS:HB3	49:a:514:LYS:HZ3	1.49	0.77
31:Dl:93:GLU:O	31:Dl:97:THR:HG23	1.83	0.77
48:m:106:GLN:NE2	50:d:167:TRP:CZ3	2.53	0.77
50:d:76:PHE:HZ	54:i:65:PHE:HE2	1.26	0.77
56:k:24:ILE:HG22	59:q:164:ALA:HB2	1.36	0.77
57:n:73:LEU:C	57:n:77:SER:CB	2.57	0.77
7:BA:27:TYR:HB3	7:BA:28:ARG:NH1	2.00	0.76
55:j:9:GLU:HG2	55:j:56:GLN:CD	2.09	0.76
55:j:109:LEU:CD2	63:u:59:ALA:HA	2.14	0.76
5:DP:220:VAL:HG22	69:X:-24:DA:H2"	1.65	0.76
11:PB:93:LEU:CD1	11:PB:152:ILE:HD12	2.14	0.76
11:PB:657:VAL:CG1	11:PB:658:ALA:N	2.49	0.76
50:d:45:ILE:CD1	54:i:72:ILE:C	2.56	0.76
54:i:131:LEU:CD2	63:u:128:SER:CB	2.63	0.76
57:n:250:LEU:HD23	57:n:275:HIS:CD2	2.00	0.76
58:o:715:LEU:CD1	66:x:21:TYR:CA	2.51	0.76
62:t:131:MET:HB2	62:t:136:ARG:HD2	1.67	0.76
66:x:955:LEU:CD2	66:x:967:VAL:HG22	1.85	0.76
40:4:262:LEU:CD2	40:4:265:LEU:HD12	2.16	0.76
48:m:23:GLU:OE2	52:g:46:GLY:N	2.18	0.76
59:q:288:SER:CB	59:q:289:PRO:HD3	2.13	0.76
3:9:28:ARG:HB2	3:9:28:ARG:NH1	1.99	0.76
26:DF:71:ILE:CD1	29:DI:38:GLN:HE21	1.91	0.76
38:2:32:ALA:HB3	42:6:72:THR:CB	2.16	0.76
1:0:298:GLN:HE22	2:8:132:TRP:CD1	2.04	0.76
7:BA:189:LYS:HG3	69:X:-29:DA:OP2	1.85	0.76
10:PA:436:SER:C	62:t:97:LYS:HZ2	1.93	0.76
13:PD:137:LYS:HE3	53:h:51:LEU:CG	2.13	0.76
22:DA:353:LEU:HD23	26:Df:269:VAL:HG22	1.67	0.76
24:DD:913:LEU:CD2	31:DL:87:ILE:HD13	2.14	0.76
29:DI:132:LEU:CD2	30:DJ:121:MET:CE	2.64	0.76
42:6:472:ARG:HG3	42:6:473:GLU:CG	2.14	0.76
49:a:412:ARG:C	49:a:472:SER:CB	2.58	0.76
62:t:172:ALA:HB1	62:t:173:PRO:CD	2.16	0.76
16:PG:91:GLN:HB2	16:PG:98:PHE:HD2	1.49	0.76
28:DH:56:ALA:CB	30:DJ:214:PRO:HG3	2.15	0.76
31:Dl:76:LEU:HD13	31:Dl:84:LEU:HD12	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DD:1071:ARG:HB2	26:DF:91:PHE:CG	2.20	0.76
37:1:172:ALA:HB1	43:7:563:ARG:HA	1.67	0.76
46:b:174:ILE:HD11	47:l:75:LEU:HD23	1.66	0.76
53:h:182:VAL:HG21	60:r:202:ILE:HD11	1.63	0.76
69:X:-36:DG:H1	70:Y:36:DC:N4	1.81	0.76
8:FA:50:ASP:HB3	8:FA:97:PRO:HG2	1.66	0.76
18:PI:35:LEU:HB3	18:PI:48:ALA:HB3	1.68	0.76
50:d:114:LEU:HD21	63:u:122:LEU:CB	2.16	0.76
56:k:88:LYS:HD2	56:k:88:LYS:O	1.86	0.76
59:q:458:PRO:HG3	59:q:533:GLN:HE21	1.50	0.76
5:DP:314:GLY:CA	69:X:-26:DA:H5'	2.11	0.76
8:FA:44:GLN:CA	9:FB:9:LEU:HD12	2.15	0.76
29:DI:16:ALA:CA	29:DI:40:LEU:HD11	2.13	0.76
42:6:359:LYS:NZ	42:6:436:GLY:CA	2.40	0.76
50:d:45:ILE:HD11	54:i:73:ILE:CA	2.14	0.76
52:g:90:LEU:HD12	55:j:124:TYR:OH	1.86	0.76
60:r:108:ILE:HD13	62:t:91:PHE:HA	1.66	0.76
10:PA:26:LEU:HB3	11:PB:1168:ALA:HB2	1.68	0.76
40:4:245:LEU:HG	40:4:280:ARG:HE	1.50	0.76
49:a:504:ILE:HA	49:a:507:THR:HG23	1.67	0.76
51:f:174:ARG:HD2	57:n:270:GLN:HE22	1.50	0.76
55:j:20:ARG:HD3	57:n:94:GLN:HA	1.66	0.76
56:k:24:ILE:HG21	59:q:164:ALA:CA	2.16	0.76
59:q:92:LEU:HD11	59:q:99:ARG:NH1	1.99	0.76
65:z:540:LEU:HB3	65:z:541:PRO:HD3	1.68	0.76
3:9:181:LEU:HD13	3:9:181:LEU:N	2.01	0.75
26:DF:68:THR:O	26:DF:68:THR:HG22	1.86	0.75
49:a:224:TYR:CE2	49:a:253:MET:HB3	2.21	0.75
50:d:110:LEU:HG	52:g:171:LEU:HD21	1.68	0.75
56:k:33:LEU:HA	56:k:36:SER:OG	1.85	0.75
57:n:274:ILE:HD13	57:n:299:PHE:CD1	2.21	0.75
45:e:129:VAL:CG2	56:k:114:MET:HE2	2.17	0.75
58:o:787:ALA:HB3	66:x:21:TYR:OH	1.86	0.75
67:w:357:HIS:CE1	67:w:397:LYS:CE	2.66	0.75
7:BA:146:TYR:O	7:BA:149:LYS:HG3	1.86	0.75
11:PB:489:ILE:CG2	11:PB:490:GLY:O	2.33	0.75
25:DE:429:LEU:HB3	25:DE:430:PRO:CD	2.16	0.75
38:2:291:CYS:O	38:2:295:ARG:HA	1.87	0.75
49:a:337:ALA:HB1	49:a:338:PRO:CD	2.16	0.75
56:k:70:LEU:HD23	64:v:85:PHE:CD1	2.21	0.75
63:u:18:GLN:NE2	63:u:65:THR:OG1	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:408:ARG:NE	60:r:7:THR:HG21	2.01	0.75
63:u:4:ARG:HG2	65:z:594:LEU:O	1.86	0.75
70:Y:8:DA:H2'	70:Y:9:DC:H5	1.52	0.75
9:FB:47:LYS:HG2	9:FB:52:THR:HG23	1.68	0.75
11:PB:91:ILE:HD13	11:PB:124:LEU:HD11	1.69	0.75
28:DH:56:ALA:HB1	30:DJ:214:PRO:HG3	1.68	0.75
53:h:102:HIS:CD2	53:h:102:HIS:H	2.03	0.75
56:k:87:ARG:HG3	56:k:87:ARG:NH1	2.01	0.75
57:n:680:HIS:HE2	59:q:557:LEU:HD11	1.52	0.75
49:a:109:TYR:OH	49:a:154:LEU:HD21	1.84	0.75
53:h:8:LEU:HA	53:h:69:PRO:HG3	1.68	0.75
57:n:669:GLN:NE2	58:o:681:GLU:HG3	2.00	0.75
67:w:14:LYS:HA	67:w:17:VAL:HG23	1.67	0.75
4:DO:7:ARG:CZ	4:DO:37:LEU:HB3	2.16	0.75
10:PA:606:HIS:HB3	10:PA:626:THR:HG23	1.68	0.75
49:a:413:HIS:HD2	49:a:472:SER:H	0.76	0.75
50:d:164:PRO:HD2	50:d:167:TRP:CB	2.16	0.75
55:j:9:GLU:CG	55:j:56:GLN:HE22	1.96	0.75
56:k:16:ASP:OD2	64:v:79:VAL:CG2	2.34	0.75
11:PB:1056:ASP:OD1	20:PK:1:MET:N	2.19	0.75
24:Dd:906:THR:HG22	31:Dl:91:PHE:HD2	1.52	0.75
29:Di:73:LEU:HD22	31:Dl:105:HIS:CG	2.21	0.75
48:m:116:GLN:HG2	65:z:595:PRO:HD2	1.68	0.75
49:a:227:SER:OG	49:a:502:MET:HE1	1.85	0.75
53:h:85:ARG:HA	53:h:99:VAL:HG12	1.67	0.75
57:n:222:VAL:HG22	57:n:234:LEU:O	1.86	0.75
63:u:83:ALA:N	63:u:86:GLN:HB2	2.02	0.75
3:9:288:ASN:C	3:9:288:ASN:HD22	1.94	0.75
10:PA:439:HIS:CE1	60:r:19:MET:CB	2.69	0.75
10:PA:548:PHE:HE1	10:PA:555:LEU:HD11	1.50	0.75
11:PB:1142:ASN:HD21	11:PB:1145:GLN:HB2	1.52	0.75
13:PD:95:PHE:HA	16:PG:1:MET:HE1	1.69	0.75
22:DA:567:LEU:CD1	23:DB:745:GLN:HG2	2.11	0.75
40:4:442:VAL:HB	41:5:44:PHE:HE1	1.52	0.75
62:t:172:ALA:HB1	62:t:173:PRO:HD2	1.69	0.75
1:0:71:GLU:HA	1:0:74:ILE:HD12	1.69	0.74
36:EB:148:LYS:HD2	36:EB:175:LEU:HD22	1.67	0.74
48:m:104:HIS:NE2	57:n:168:ARG:HG3	1.99	0.74
11:PB:986:GLN:OE1	11:PB:1011:ILE:CG2	2.34	0.74
43:7:147:GLN:O	43:7:148:HIS:HB2	1.86	0.74
44:c:111:TYR:CZ	46:b:136:HIS:CB	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:m:22:LEU:CD2	52:g:45:PHE:HB2	2.18	0.74
49:a:413:HIS:CE1	49:a:471:ASP:OD1	2.40	0.74
54:i:65:PHE:CD1	54:i:99:LYS:CE	2.70	0.74
54:i:65:PHE:CE1	54:i:99:LYS:CB	2.53	0.74
56:k:101:ARG:HB3	56:k:101:ARG:NH1	2.02	0.74
67:w:6:GLN:HB2	67:w:62:TRP:CZ2	2.21	0.74
70:Y:8:DA:C2'	70:Y:9:DC:C6	2.68	0.74
4:DO:82:ARG:HE	4:DO:87:LEU:HB2	1.52	0.74
25:DE:359:LEU:O	25:DE:359:LEU:HD12	1.87	0.74
45:e:60:VAL:CG1	46:b:179:LEU:HB3	2.05	0.74
48:m:124:GLN:HB2	65:z:590:ARG:HD2	1.69	0.74
2:8:169:TYR:HB3	2:8:190:TYR:CE2	2.22	0.74
29:DI:132:LEU:CD2	30:DJ:121:MET:HE1	2.18	0.74
48:m:104:HIS:NE2	57:n:169:LEU:N	2.33	0.74
56:k:104:LEU:CD2	64:v:123:ILE:HD11	2.15	0.74
59:q:34:LEU:N	59:q:34:LEU:HD23	2.01	0.74
59:q:120:ARG:HG2	59:q:120:ARG:NH1	1.98	0.74
59:q:437:HIS:CE1	59:q:472:GLU:CA	2.71	0.74
4:DO:5:LEU:HD22	4:DO:98:CYS:SG	2.27	0.74
37:1:267:LEU:HG	43:7:113:LYS:HE3	1.69	0.74
59:q:647:SER:CB	59:q:648:PRO:HD2	2.17	0.74
63:u:81:SER:OG	63:u:85:LEU:HB2	1.87	0.74
69:X:-13:DG:H1	70:Y:13:DC:H42	1.34	0.74
10:PA:734:ARG:HH22	18:PI:107:ALA:HB3	1.51	0.74
37:1:475:PHE:HE1	37:1:484:PRO:O	1.70	0.74
54:i:75:CYS:CB	54:i:88:ASN:ND2	2.50	0.74
57:n:229:GLU:CG	57:n:300:CYS:SG	2.75	0.74
57:n:281:ARG:NH1	57:n:295:CYS:SG	2.60	0.74
64:v:21:ARG:NH2	64:v:78:LEU:HD22	1.98	0.74
3:9:102:ARG:HG2	3:9:102:ARG:HH11	1.53	0.74
13:PD:137:LYS:CD	53:h:51:LEU:HD12	2.17	0.74
57:n:545:LEU:CD1	57:n:653:PRO:HD3	2.17	0.74
58:o:761:LEU:O	67:w:74:LYS:CD	2.34	0.74
59:q:9:ILE:HD11	63:u:90:LEU:HD22	0.75	0.74
63:u:28:GLN:HG3	65:z:483:ASN:CG	2.13	0.74
1:0:287:TYR:CG	1:0:287:TYR:O	2.40	0.74
7:BA:128:ILE:CG2	9:FB:152:ASN:ND2	2.51	0.74
8:FA:124:TYR:HE1	9:FB:22:LYS:CG	2.01	0.74
13:PD:137:LYS:NZ	53:h:52:LEU:CA	2.50	0.74
37:1:483:THR:HG1	37:1:484:PRO:HD3	1.53	0.74
52:g:93:LEU:CD1	55:j:106:LYS:HG2	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:183:ALA:C	53:h:187:PHE:CE2	2.60	0.74
56:k:101:ARG:HB3	56:k:101:ARG:CZ	2.16	0.74
58:o:787:ALA:CB	66:x:21:TYR:OH	2.36	0.74
59:q:135:LEU:HD12	59:q:135:LEU:O	1.86	0.74
8:FA:156:THR:HG21	11:PB:310:VAL:HG13	1.68	0.74
10:PA:977:VAL:HB	10:PA:979:LEU:HG	1.68	0.74
13:PD:133:ASP:CG	53:h:59:LEU:HD21	2.12	0.74
49:a:509:ARG:CZ	49:a:509:ARG:HB2	2.14	0.74
63:u:18:GLN:HE22	63:u:65:THR:CB	2.01	0.74
66:x:956:VAL:CG1	66:x:968:LEU:HD11	2.15	0.74
10:PA:1486:ILE:H	10:PA:1487:PRO:HD2	1.53	0.74
29:DI:73:LEU:HD22	31:DL:105:HIS:CD2	2.21	0.74
42:6:174:ARG:HG2	42:6:269:SER:HB2	1.70	0.74
49:a:337:ALA:HB1	49:a:338:PRO:HD2	1.70	0.74
52:g:93:LEU:HB3	55:j:106:LYS:NZ	2.03	0.74
67:w:101:LEU:HD11	67:w:121:LEU:HD23	1.70	0.74
1:0:145:GLU:CG	53:h:3:ARG:HH12	2.01	0.73
24:Dd:906:THR:HG22	31:Dl:91:PHE:CD2	2.23	0.73
53:h:85:ARG:HA	53:h:99:VAL:CG1	2.18	0.73
66:x:956:VAL:HG21	66:x:968:LEU:HD11	1.68	0.73
10:PA:118:LEU:HD21	10:PA:188:GLN:HE21	1.51	0.73
11:PB:1115:GLN:HB3	11:PB:1148:LEU:HD21	1.70	0.73
25:DE:605:HIS:CE1	26:DF:77:LEU:HD21	2.23	0.73
29:DI:132:LEU:CG	30:DJ:121:MET:CE	2.65	0.73
44:c:294:PRO:CB	44:c:304:ALA:HB1	2.18	0.73
48:m:26:GLN:CD	52:g:45:PHE:CD2	2.57	0.73
50:d:45:ILE:C	54:i:76:MET:HE3	2.13	0.73
51:f:95:LEU:O	59:q:130:VAL:CG1	2.37	0.73
51:f:101:ILE:HD11	53:h:105:VAL:HG11	1.70	0.73
52:g:90:LEU:HD12	55:j:124:TYR:CZ	2.23	0.73
55:j:109:LEU:CD2	63:u:59:ALA:CA	2.62	0.73
57:n:154:ILE:HB	57:n:155:PRO:HD3	1.69	0.73
57:n:301:LEU:HD13	57:n:361:ILE:HD12	1.68	0.73
57:n:707:ASP:HB2	58:o:684:ARG:NH2	2.03	0.73
62:t:8:GLN:HE22	62:t:200:ILE:HG23	1.52	0.73
67:w:9:PHE:CE2	67:w:66:PHE:CD2	2.72	0.73
10:PA:322:LEU:HG	10:PA:323:PRO:HD2	1.70	0.73
16:PG:117:MET:HA	16:PG:130:THR:HA	1.68	0.73
25:DE:605:HIS:CE1	26:DF:77:LEU:HD11	2.22	0.73
31:DL:61:LYS:O	31:DL:61:LYS:NZ	2.21	0.73
44:c:111:TYR:CG	46:b:136:HIS:HD2	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:228:PRO:CD	49:a:502:MET:SD	2.76	0.73
53:h:72:ARG:NH1	59:q:134:ALA:N	2.33	0.73
66:x:955:LEU:CD1	66:x:967:VAL:HG21	2.17	0.73
11:PB:924:ARG:NH1	12:PC:60:HIS:HB2	2.03	0.73
12:PC:265:HIS:HE1	62:t:113:ARG:HD2	0.96	0.73
48:m:104:HIS:CE1	57:n:169:LEU:H	2.05	0.73
48:m:116:GLN:HG2	65:z:594:LEU:HG	1.69	0.73
50:d:42:ARG:NH2	54:i:93:LYS:HG2	2.04	0.73
10:PA:1248:ASN:HB2	10:PA:1256:VAL:H	1.53	0.73
15:PF:66:LEU:HD11	15:PF:94:MET:HG3	1.70	0.73
22:DA:564:PRO:HG2	23:DB:744:PHE:CE2	2.23	0.73
32:Dc:77:LEU:HD12	30:Dj:116:LEU:HD23	1.69	0.73
56:k:24:ILE:CG2	59:q:164:ALA:HB1	2.11	0.73
57:n:937:ARG:NE	57:n:943:LEU:HD21	2.03	0.73
59:q:290:HIS:HE1	59:q:294:LYS:CE	1.91	0.73
43:7:69:LYS:HD2	43:7:229:ALA:HA	1.71	0.73
49:a:228:PRO:HD2	49:a:502:MET:CE	2.17	0.73
50:d:45:ILE:CG1	54:i:73:ILE:CG1	2.66	0.73
51:f:177:VAL:CG1	57:n:266:VAL:HG22	2.19	0.73
52:g:161:ILE:N	54:i:140:MET:HE1	2.01	0.73
54:i:72:ILE:HD13	54:i:92:SER:HB2	1.65	0.73
55:j:71:ILE:HD11	57:n:106:ALA:CB	2.18	0.73
59:q:595:GLN:HG2	59:q:619:ARG:HB2	1.70	0.73
37:1:483:THR:H	37:1:484:PRO:HD2	1.52	0.73
40:4:262:LEU:HD22	40:4:265:LEU:HD12	1.70	0.73
42:6:472:ARG:HH11	42:6:473:GLU:H	1.36	0.73
55:j:9:GLU:CB	55:j:56:GLN:NE2	2.51	0.73
3:9:175:LYS:N	3:9:175:LYS:HZ2	1.86	0.73
5:DP:218:LYS:HB3	69:X:-23:DG:P	2.26	0.73
11:PB:93:LEU:HD12	11:PB:152:ILE:HD12	1.71	0.73
22:DA:353:LEU:HD21	26:Df:272:VAL:CG2	2.13	0.73
56:k:86:SER:C	64:v:105:LEU:HD13	2.14	0.73
57:n:141:ARG:CZ	63:u:17:ASP:HA	2.19	0.73
1:0:192:LEU:CD1	1:0:196:LEU:HD12	2.19	0.73
8:FA:124:TYR:OH	9:FB:22:LYS:HE2	1.88	0.73
43:7:486:ALA:O	43:7:487:ARG:HB2	1.87	0.73
48:m:106:GLN:OE1	50:d:167:TRP:O	2.06	0.73
50:d:126:TYR:CD2	59:q:36:MET:SD	2.82	0.73
56:k:21:ILE:HG21	59:q:168:THR:HG1	1.54	0.73
58:o:762:GLN:CA	67:w:74:LYS:CE	2.66	0.73
40:4:412:PHE:CE2	41:5:3:ASN:HB2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:229:SER:CA	49:a:502:MET:CB	2.66	0.73
51:f:95:LEU:C	59:q:130:VAL:HG11	2.14	0.73
53:h:29:PHE:CD2	59:q:102:LEU:CD1	2.72	0.73
54:i:122:ARG:C	54:i:122:ARG:HD3	2.14	0.73
57:n:250:LEU:HG	57:n:275:HIS:HB2	1.71	0.73
5:DP:218:LYS:CG	69:X:-23:DG:P	2.77	0.72
8:FA:126:ILE:HB	8:FA:138:PHE:HB2	1.70	0.72
12:PC:265:HIS:NE2	62:t:113:ARG:HB3	1.98	0.72
41:5:8:VAL:HG13	41:5:45:VAL:HB	1.71	0.72
48:m:22:LEU:CD1	52:g:43:MET:HE1	2.18	0.72
49:a:364:TYR:CB	49:a:430:LEU:CG	2.65	0.72
57:n:169:LEU:CB	57:n:170:PRO:CD	2.59	0.72
57:n:265:LEU:HD11	57:n:307:VAL:HG21	1.71	0.72
57:n:482:VAL:HG22	57:n:489:ILE:HG12	1.69	0.72
59:q:109:MET:CA	59:q:109:MET:HE3	2.19	0.72
55:j:7:HIS:O	55:j:11:HIS:CD2	2.42	0.72
57:n:359:ILE:HG13	57:n:372:ILE:HD11	1.64	0.72
69:X:-36:DG:N2	70:Y:36:DC:N3	2.36	0.72
3:9:167:PHE:O	3:9:167:PHE:HD1	1.72	0.72
10:PA:734:ARG:NH1	18:PI:107:ALA:H	1.87	0.72
26:DF:428:LEU:CD1	26:DF:455:LEU:CB	2.64	0.72
62:t:8:GLN:NE2	62:t:200:ILE:HG23	2.04	0.72
65:z:567:GLN:O	65:z:567:GLN:NE2	2.23	0.72
2:8:47:HIS:HA	2:8:52:LYS:HG2	1.70	0.72
26:DF:22:VAL:HG13	29:DI:44:PHE:CE1	2.25	0.72
26:DF:429:LYS:O	26:DF:433:PRO:HD2	1.89	0.72
59:q:633:ARG:HB3	59:q:633:ARG:NH2	2.02	0.72
62:t:122:PHE:CZ	62:t:156:LEU:HD11	2.24	0.72
2:8:86:ASN:HD22	2:8:86:ASN:C	1.97	0.72
9:FB:16:THR:CG2	9:FB:107:GLU:O	2.37	0.72
48:m:104:HIS:NE2	57:n:168:ARG:HD2	2.04	0.72
50:d:110:LEU:HD22	50:d:110:LEU:C	2.13	0.72
57:n:359:ILE:HA	57:n:372:ILE:CD1	2.19	0.72
1:0:300:ALA:HB1	3:9:166:PRO:HA	1.67	0.72
2:8:207:LEU:HA	51:f:52:MET:HE1	1.71	0.72
53:h:72:ARG:HH12	59:q:134:ALA:N	1.87	0.72
2:8:95:GLU:H	2:8:146:ASP:HA	1.54	0.72
23:DB:539:ARG:HE	41:5:32:LYS:HA	1.53	0.72
44:c:111:TYR:CZ	46:b:136:HIS:HB2	2.25	0.72
49:a:417:TYR:CZ	49:a:450:PHE:CD1	2.77	0.72
50:d:31:LEU:CD2	54:i:103:THR:CB	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:149:LYS:HE2	64:v:40:ALA:CA	2.20	0.72
67:w:510:PRO:HD3	67:w:922:MET:HE1	1.71	0.72
6:DQ:55:ALA:O	6:DQ:56:VAL:CG2	2.38	0.72
44:c:111:TYR:OH	46:b:136:HIS:HB2	1.88	0.72
48:m:23:GLU:CD	52:g:46:GLY:H	1.97	0.72
49:a:160:LEU:CD1	49:a:214:ARG:HH21	2.03	0.72
52:g:83:MET:O	52:g:83:MET:HE3	1.89	0.72
7:BA:27:TYR:CB	7:BA:28:ARG:HH11	2.03	0.72
10:PA:734:ARG:NH2	18:PI:107:ALA:HB3	2.04	0.72
17:PH:130:ASN:CB	49:a:46:LYS:HA	2.18	0.72
24:DD:1078:LEU:HD21	31:DL:83:MET:CE	2.14	0.72
31:Dl:106:ARG:HH11	31:Dl:114:LYS:HE2	0.91	0.72
42:6:314:ALA:HB2	42:6:381:TRP:CD1	2.22	0.72
45:e:100:LEU:HB2	59:q:641:LEU:HD22	1.72	0.72
51:f:181:LEU:HD11	57:n:270:GLN:CA	2.20	0.72
56:k:24:ILE:HG23	59:q:164:ALA:HB2	1.59	0.72
57:n:237:MET:HE1	59:q:45:GLN:CA	2.19	0.72
59:q:9:ILE:HG12	63:u:90:LEU:CB	2.19	0.72
10:PA:479:TRP:HD1	20:PK:67:LEU:HD21	1.55	0.72
11:PB:133:ILE:HB	11:PB:139:GLN:HE22	1.55	0.72
13:PD:17:ALA:HB3	16:PG:82:GLY:O	1.90	0.72
13:PD:79:THR:HA	53:h:51:LEU:CD2	2.13	0.72
40:4:307:ILE:HG22	40:4:316:TYR:CB	2.20	0.72
50:d:46:GLU:CA	54:i:76:MET:HE3	2.20	0.72
53:h:88:ASP:OD2	59:q:123:LYS:NZ	2.23	0.72
63:u:83:ALA:N	63:u:86:GLN:HG2	2.04	0.72
3:9:236:LEU:O	3:9:238:LEU:N	2.22	0.71
22:DA:349:TRP:CE2	26:Df:266:GLY:HA3	2.25	0.71
49:a:417:TYR:HD1	49:a:469:VAL:HG21	1.15	0.71
49:a:462:LEU:HD21	66:x:11:LEU:HD12	1.69	0.71
50:d:123:THR:CG2	59:q:37:SER:HB3	2.18	0.71
53:h:22:LEU:HD12	53:h:22:LEU:C	2.13	0.71
55:j:82:LYS:NZ	61:s:99:LYS:CB	2.53	0.71
57:n:659:LEU:CD1	67:w:14:LYS:CG	2.66	0.71
10:PA:1793:THR:H	53:h:102:HIS:HE1	1.35	0.71
11:PB:67:LEU:HD11	11:PB:420:GLN:HG2	1.71	0.71
22:DA:996:ARG:NH1	69:X:2:DG:OP1	2.23	0.71
35:EA:114:ILE:HG12	35:EA:181:ASN:HB3	1.71	0.71
48:m:66:TYR:O	50:d:154:ARG:NH2	2.23	0.71
50:d:126:TYR:CZ	59:q:36:MET:HB2	2.23	0.71
57:n:686:LYS:CE	58:o:730:PRO:HG3	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:581:LYS:HZ3	17:PH:86:ASP:HA	1.53	0.71
46:b:103:ASP:OD1	46:b:103:ASP:N	2.23	0.71
2:8:109:LEU:HD11	51:f:59:HIS:HB3	1.72	0.71
12:PC:265:HIS:HE1	62:t:113:ARG:CD	1.58	0.71
53:h:19:VAL:HG21	59:q:112:LEU:CD2	2.20	0.71
54:i:110:SER:HB2	54:i:111:PRO:HD2	1.72	0.71
69:X:-39:DA:H2'	69:X:-39:DA:N3	2.03	0.71
8:FA:122:THR:HG22	9:FB:24:PRO:CA	2.11	0.71
50:d:121:LEU:HD12	63:u:115:LEU:CA	2.20	0.71
57:n:172:CYS:SG	59:q:21:GLU:CA	2.78	0.71
1:0:145:GLU:CB	53:h:3:ARG:NH1	2.53	0.71
1:0:254:GLU:H	1:0:254:GLU:CD	1.99	0.71
12:PC:7:PRO:HG3	20:PK:97:GLU:HG3	1.71	0.71
16:PG:85:VAL:HG11	16:PG:101:ILE:HD12	1.71	0.71
38:2:12:GLU:OE2	42:6:131:LEU:HD23	1.91	0.71
40:4:317:ALA:CA	40:4:340:ASN:O	2.38	0.71
59:q:428:LEU:HD12	59:q:428:LEU:O	1.89	0.71
63:u:18:GLN:NE2	63:u:65:THR:CG2	2.52	0.71
1:0:289:SER:O	1:0:292:ALA:HB3	1.89	0.71
3:9:64:LEU:HD13	3:9:105:MET:HB3	1.73	0.71
22:DA:564:PRO:CB	23:DB:744:PHE:CE2	2.73	0.71
56:k:70:LEU:HD22	56:k:70:LEU:C	2.14	0.71
58:o:715:LEU:HB3	66:x:25:ILE:CD1	2.21	0.71
10:PA:1315:ASP:HA	10:PA:1318:LYS:HD2	1.73	0.71
40:4:208:THR:HG23	40:4:210:ALA:H	1.56	0.71
45:e:49:GLU:CD	46:b:186:THR:HG21	2.15	0.71
51:f:176:ARG:CZ	57:n:306:GLU:OE2	2.39	0.71
52:g:93:LEU:O	55:j:106:LYS:NZ	2.24	0.71
57:n:192:LEU:CB	57:n:219:ASN:O	2.39	0.71
58:o:696:SER:CB	66:x:111:HIS:CE1	2.64	0.71
59:q:288:SER:CB	59:q:289:PRO:HD2	2.20	0.71
62:t:6:VAL:HG22	62:t:141:GLU:HB2	1.71	0.71
37:1:181:CYS:SG	37:1:182:ASN:N	2.63	0.71
64:v:119:LEU:HD12	64:v:119:LEU:O	1.91	0.71
7:BA:146:TYR:O	7:BA:149:LYS:CG	2.39	0.71
9:FB:221:GLY:HA2	9:FB:236:LYS:HG3	1.72	0.71
14:PE:110:MET:HE3	14:PE:115:LYS:HG2	1.73	0.71
25:DE:489:PHE:CE1	26:DF:129:VAL:HG21	2.26	0.71
31:DL:60:LYS:O	31:DL:60:LYS:NZ	2.19	0.71
52:g:161:ILE:HG12	54:i:140:MET:HE2	0.72	0.71
57:n:274:ILE:HD13	57:n:299:PHE:CE2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:o:690:LEU:CD2	59:q:605:PRO:HG2	2.20	0.71
59:q:106:LEU:HD23	59:q:106:LEU:C	2.15	0.71
67:w:6:GLN:HA	67:w:62:TRP:HH2	1.55	0.71
70:Y:33:DC:H1'	70:Y:34:DG:H8	1.55	0.71
12:PC:89:THR:HG21	62:t:108:SER:OG	1.91	0.70
23:DB:241:PRO:HG2	23:DB:496:MET:HE1	1.72	0.70
49:a:388:LEU:HD21	49:a:447:GLU:HG3	1.72	0.70
51:f:176:ARG:HD3	57:n:306:GLU:OE2	1.91	0.70
52:g:89:PHE:CG	63:u:19:PHE:HE1	2.09	0.70
54:i:72:ILE:HD13	54:i:92:SER:HB3	1.72	0.70
56:k:84:TYR:OH	59:q:206:ASP:O	2.08	0.70
64:v:120:ARG:HG2	64:v:120:ARG:HH11	1.56	0.70
10:PA:1428:MET:HE1	10:PA:1455:SER:HB3	1.73	0.70
11:PB:654:GLN:O	11:PB:657:VAL:HG12	1.90	0.70
52:g:164:ILE:HG21	54:i:140:MET:HB3	1.72	0.70
57:n:254:VAL:HG11	57:n:304:GLN:HG2	1.73	0.70
59:q:212:ALA:O	59:q:383:HIS:HB3	1.91	0.70
2:8:207:LEU:CD2	51:f:52:MET:HE1	2.13	0.70
3:9:207:TYR:HB3	3:9:211:GLN:HE22	1.56	0.70
10:PA:318:VAL:O	10:PA:340:LYS:HB2	1.90	0.70
13:PD:133:ASP:OD1	53:h:59:LEU:HD22	1.88	0.70
51:f:188:PHE:HD2	57:n:295:CYS:HG	1.25	0.70
10:PA:1139:LEU:HD23	10:PA:1341:VAL:HA	1.72	0.70
20:PK:14:GLU:OE1	60:r:8:MET:SD	2.50	0.70
53:h:124:LEU:HD22	59:q:147:ILE:HG21	1.72	0.70
54:i:86:ASP:N	54:i:86:ASP:OD1	2.24	0.70
11:PB:203:ASN:HB3	11:PB:571:GLY:HA3	1.72	0.70
26:DF:14:LEU:HD22	26:DF:15:PRO:HD2	1.73	0.70
26:DF:104:LEU:HB3	30:DJ:217:PHE:HE2	1.51	0.70
29:DI:20:ALA:HB2	29:DI:36:ILE:HD13	1.73	0.70
33:Dk:191:VAL:HG13	33:Dk:200:ILE:HD13	1.74	0.70
42:6:35:GLN:HB3	42:6:159:CYS:SG	2.31	0.70
43:7:738:LEU:O	43:7:738:LEU:HD12	1.90	0.70
50:d:42:ARG:HH22	54:i:93:LYS:CA	2.03	0.70
64:v:120:ARG:HG2	64:v:120:ARG:NH1	2.05	0.70
69:X:-5:DG:C6	70:Y:4:DA:N6	2.60	0.70
1:0:287:TYR:CG	2:8:189:MET:SD	2.84	0.70
5:DP:269:ARG:HB2	5:DP:337:LYS:HE2	1.73	0.70
26:DF:104:LEU:CD1	30:DJ:217:PHE:HE2	2.04	0.70
49:a:336:TYR:CZ	49:a:391:THR:OG1	2.45	0.70
55:j:41:LEU:O	55:j:45:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:j:89:LEU:CD1	61:s:93:TYR:CD1	2.63	0.70
63:u:4:ARG:HD2	65:z:596:TYR:CA	2.22	0.70
63:u:61:LEU:CD1	65:z:496:LEU:CD1	2.70	0.70
1:0:287:TYR:HB3	2:8:189:MET:HG2	1.73	0.70
3:9:174:LEU:HD13	3:9:231:TYR:HE2	1.56	0.70
11:PB:783:ALA:HB2	11:PB:1041:ILE:HG23	1.73	0.70
14:PE:82:VAL:HG21	14:PE:106:VAL:HG22	1.72	0.70
25:DE:506:SER:HB2	25:DE:537:LYS:NZ	2.06	0.70
53:h:12:LEU:C	53:h:12:LEU:HD13	2.17	0.70
54:i:140:MET:CG	54:i:141:PHE:CD1	2.72	0.70
57:n:685:LEU:HD22	58:o:729:TYR:HE2	1.56	0.70
59:q:190:LEU:HD12	59:q:196:LEU:HD11	1.73	0.70
62:t:122:PHE:HZ	62:t:156:LEU:HD11	1.57	0.70
63:u:61:LEU:CD1	65:z:496:LEU:HD11	2.22	0.70
7:BA:281:ALA:HB2	70:Y:33:DC:C6	2.27	0.70
17:PH:130:ASN:HB3	49:a:46:LYS:CA	2.19	0.70
42:6:312:PRO:HG3	42:6:383:THR:HG23	1.74	0.70
49:a:109:TYR:CZ	49:a:154:LEU:CD2	2.72	0.70
57:n:686:LYS:HZ3	58:o:730:PRO:HB3	1.56	0.70
5:DP:300:ILE:HD11	5:DP:320:GLU:HB3	1.73	0.70
7:BA:297:PRO:HB3	7:BA:310:VAL:HG21	1.73	0.70
10:PA:1005:HIS:HB3	10:PA:1008:LYS:HG2	1.74	0.70
43:7:739:LEU:C	43:7:741:LEU:H	1.99	0.70
50:d:42:ARG:NH2	54:i:93:LYS:CA	2.55	0.70
57:n:676:ASP:OD1	59:q:593:MET:HE2	1.92	0.70
64:v:119:LEU:HD12	64:v:119:LEU:C	2.15	0.70
1:0:287:TYR:CD1	1:0:287:TYR:O	2.45	0.70
18:PI:36:LEU:HA	18:PI:47:GLU:HA	1.74	0.70
29:DI:60:HIS:CG	31:DL:106:ARG:HE	2.09	0.70
51:f:15:TRP:HH2	51:f:35:GLU:OE1	1.72	0.70
57:n:237:MET:CE	59:q:45:GLN:HB2	2.21	0.70
2:8:52:LYS:HA	2:8:52:LYS:CE	2.14	0.69
40:4:433:PHE:CZ	41:5:42:HIS:HB3	2.27	0.69
46:b:174:ILE:CG1	47:l:75:LEU:HD11	2.14	0.69
49:a:109:TYR:OH	49:a:154:LEU:CD2	2.40	0.69
49:a:214:ARG:CZ	49:a:214:ARG:HB2	2.20	0.69
54:i:68:LEU:CD1	54:i:95:GLN:HG2	2.09	0.69
59:q:630:MET:HE3	59:q:631:GLU:H	1.55	0.69
67:w:397:LYS:HB3	68:p:171:PHE:HE2	1.57	0.69
2:8:241:CYS:HA	2:8:246:TYR:CD2	2.28	0.69
13:PD:133:ASP:CB	53:h:59:LEU:HD21	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:205:LEU:HD21	40:4:367:PHE:HE2	1.55	0.69
50:d:168:VAL:HB	50:d:169:PRO:CD	2.20	0.69
55:j:102:MET:HA	63:u:26:LEU:HD21	1.74	0.69
59:q:1:MET:H2	65:z:540:LEU:HD12	1.55	0.69
10:PA:1796:SER:HB3	59:q:24:LEU:HD22	1.74	0.69
13:PD:137:LYS:HZ1	53:h:51:LEU:C	1.99	0.69
50:d:38:GLU:CD	54:i:96:GLU:CG	2.61	0.69
59:q:187:LEU:O	59:q:187:LEU:HD12	1.93	0.69
67:w:397:LYS:CB	68:p:171:PHE:HE2	2.05	0.69
11:PB:82:PRO:HB3	11:PB:134:LYS:HB3	1.74	0.69
11:PB:128:ILE:HD11	11:PB:435:ILE:HD11	1.74	0.69
40:4:314:ARG:O	40:4:316:TYR:CD2	2.45	0.69
48:m:22:LEU:HD21	52:g:45:PHE:HB2	1.74	0.69
49:a:131:ASN:ND2	49:a:131:ASN:H	1.90	0.69
52:g:89:PHE:CB	63:u:19:PHE:CE1	2.76	0.69
60:r:19:MET:HE3	60:r:177:ALA:N	2.07	0.69
10:PA:983:LEU:CD1	10:PA:983:LEU:H	2.04	0.69
11:PB:594:MET:SD	11:PB:658:ALA:CA	2.80	0.69
11:PB:801:VAL:HG23	11:PB:801:VAL:O	1.93	0.69
42:6:633:ARG:HD2	42:6:679:PHE:CD1	2.28	0.69
44:c:113:TRP:HH2	46:b:175:HIS:HB2	1.48	0.69
48:m:101:GLN:HA	57:n:169:LEU:HD22	1.71	0.69
52:g:89:PHE:CE1	63:u:19:PHE:CD1	2.80	0.69
55:j:110:ILE:HG21	55:j:128:ARG:NH2	2.07	0.69
57:n:234:LEU:HD21	57:n:282:LEU:HD22	1.73	0.69
8:FA:125:TYR:HD2	9:FB:31:TRP:HZ3	1.40	0.69
13:PD:137:LYS:NZ	53:h:51:LEU:O	2.19	0.69
31:DL:101:GLN:C	31:DL:105:HIS:HD2	1.97	0.69
48:m:14:ASN:C	52:g:39:LYS:HZ3	1.95	0.69
49:a:259:ILE:HD12	49:a:259:ILE:H	1.56	0.69
63:u:57:LEU:HD11	65:z:492:ARG:CZ	2.23	0.69
63:u:81:SER:HB2	63:u:85:LEU:N	2.07	0.69
7:BA:27:TYR:CZ	11:PB:1078:ARG:HB3	2.27	0.69
22:DA:564:PRO:HG2	23:DB:744:PHE:CG	2.28	0.69
49:a:223:LYS:HZ1	49:a:251:LEU:C	2.01	0.69
57:n:937:ARG:HE	57:n:943:LEU:HD21	1.57	0.69
59:q:109:MET:HE3	59:q:109:MET:HA	1.74	0.69
59:q:188:LEU:HD22	64:v:87:ILE:HG13	1.74	0.69
7:BA:18:HIS:CD2	7:BA:18:HIS:N	2.58	0.69
8:FA:45:ALA:N	9:FB:9:LEU:HD11	2.07	0.69
9:FB:16:THR:O	9:FB:109:ILE:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:111:CYS:SG	10:PA:114:CYS:HB3	2.33	0.69
10:PA:811:ILE:HG22	11:PB:674:MET:CE	2.22	0.69
13:PD:137:LYS:HZ2	53:h:52:LEU:CA	2.04	0.69
24:DD:960:GLU:HA	24:DD:963:ARG:HD3	1.74	0.69
40:4:407:VAL:HG12	41:5:6:LYS:HD2	1.73	0.69
47:l:156:LEU:HD22	64:v:134:TYR:HB2	1.75	0.69
49:a:145:LYS:HA	49:a:145:LYS:HE3	1.74	0.69
52:g:127:ARG:HG2	63:u:5:LEU:HD13	1.75	0.69
63:u:15:LEU:HD22	63:u:69:ILE:HD12	1.75	0.69
63:u:28:GLN:CD	65:z:483:ASN:ND2	2.50	0.69
67:w:164:ARG:HH21	67:w:204:LEU:HB2	1.57	0.69
3:9:82:THR:HG23	3:9:160:VAL:HG11	1.73	0.69
43:7:132:GLY:HA2	43:7:391:LEU:HD12	1.73	0.69
53:h:16:LEU:CD2	59:q:116:LEU:HB3	2.22	0.69
54:i:135:TYR:CE2	63:u:125:ILE:CB	2.76	0.69
55:j:43:PHE:CE1	61:s:147:THR:CB	2.76	0.69
57:n:359:ILE:HG23	57:n:372:ILE:HD13	1.74	0.69
67:w:6:GLN:CA	67:w:62:TRP:CH2	2.73	0.69
70:Y:34:DG:H2"	70:Y:35:DC:H5"	1.73	0.69
5:DP:218:LYS:HG3	69:X:-23:DG:OP2	1.93	0.69
11:PB:1030:ASN:HD22	11:PB:1033:THR:H	1.37	0.69
15:PF:100:ARG:HH21	15:PF:124:ILE:HA	1.57	0.69
27:DG:129:LYS:O	27:DG:129:LYS:NZ	2.23	0.69
38:2:32:ALA:HB3	42:6:72:THR:CG2	2.23	0.69
45:e:97:GLN:NE2	59:q:649:CYS:H	1.88	0.69
53:h:19:VAL:HG21	59:q:112:LEU:HD23	1.73	0.69
57:n:815:THR:HG21	57:n:841:ASN:HB3	1.75	0.69
59:q:149:LYS:HD2	64:v:40:ALA:O	1.93	0.69
59:q:633:ARG:HG2	59:q:637:TYR:CD2	2.28	0.69
2:8:266:ASP:O	2:8:269:LEU:HB3	1.93	0.68
15:PF:126:SER:O	15:PF:127:ASP:C	2.35	0.68
26:Df:447:ALA:CA	26:Df:456:GLY:HA3	2.23	0.68
42:6:435:TRP:HB3	42:6:461:HIS:ND1	2.07	0.68
49:a:219:LEU:HD13	49:a:258:THR:HB	1.75	0.68
51:f:115:ILE:HG23	59:q:112:LEU:HD11	1.74	0.68
52:g:159:ARG:O	52:g:159:ARG:HD3	1.92	0.68
53:h:8:LEU:C	53:h:8:LEU:HD23	2.18	0.68
59:q:35:SER:HB3	59:q:42:ARG:HH22	1.58	0.68
59:q:428:LEU:HD12	59:q:428:LEU:C	2.18	0.68
59:q:633:ARG:HG2	59:q:637:TYR:HD2	1.58	0.68
64:v:130:LEU:N	64:v:130:LEU:HD23	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:262:GLU:HA	1:0:294:HIS:CE1	2.28	0.68
5:DP:313:THR:HG21	69:X:-27:DA:O4'	1.91	0.68
10:PA:548:PHE:CE1	10:PA:555:LEU:HD11	2.28	0.68
11:PB:407:MET:HE1	11:PB:444:LEU:HG	1.74	0.68
11:PB:594:MET:SD	11:PB:658:ALA:HB1	2.31	0.68
42:6:35:GLN:OE1	42:6:159:CYS:HB3	1.92	0.68
43:7:102:LEU:HB3	43:7:103:PRO:HD2	1.75	0.68
44:c:183:PRO:HD2	44:c:189:MET:HE2	1.76	0.68
48:m:66:TYR:CE1	52:g:52:ASP:OD2	2.45	0.68
50:d:164:PRO:HD2	50:d:167:TRP:HB2	1.74	0.68
69:X:-22:DG:H2"	69:X:-21:DG:C8	2.28	0.68
10:PA:1206:ARG:HB3	10:PA:1266:GLU:HB2	1.76	0.68
22:DA:567:LEU:HD22	23:DB:745:GLN:HE21	1.57	0.68
47:l:168:TRP:CZ3	59:q:441:ARG:NH1	2.58	0.68
50:d:103:ARG:HG2	50:d:103:ARG:NH1	2.05	0.68
55:j:19:ILE:HG21	55:j:45:VAL:HG23	1.72	0.68
55:j:34:GLN:HB2	55:j:37:LEU:CD1	2.23	0.68
69:X:-10:DC:H2"	69:X:-9:DG:H2'	1.74	0.68
16:PG:13:LEU:HD11	16:PG:26:VAL:HG22	1.74	0.68
25:DE:605:HIS:ND1	26:DF:77:LEU:HD11	2.08	0.68
40:4:422:LEU:HD13	40:4:434:GLU:HB2	1.74	0.68
51:f:180:LEU:CD1	57:n:302:SER:CB	2.72	0.68
55:j:43:PHE:HE1	61:s:147:THR:CA	2.06	0.68
55:j:102:MET:CG	63:u:26:LEU:CD1	2.71	0.68
59:q:482:GLN:CB	59:q:634:ASN:HD22	2.06	0.68
1:0:148:GLU:HB3	53:h:3:ARG:HD3	1.75	0.68
8:FA:49:ARG:NH1	8:FA:96:GLN:O	2.26	0.68
10:PA:121:SER:HA	10:PA:126:ILE:HG21	1.76	0.68
22:DA:481:GLU:HA	22:DA:484:ILE:HD12	1.75	0.68
28:DH:56:ALA:HB2	30:DJ:214:PRO:HG2	1.76	0.68
47:l:164:ARG:NH2	64:v:131:GLU:OE2	2.26	0.68
47:l:167:ILE:HD11	64:v:123:ILE:HG22	1.75	0.68
48:m:70:PRO:CB	57:n:166:TYR:OH	2.36	0.68
50:d:41:SER:HB3	54:i:69:VAL:CG1	2.23	0.68
51:f:184:LEU:HD21	57:n:299:PHE:CD1	2.25	0.68
54:i:65:PHE:CA	54:i:99:LYS:HE2	2.23	0.68
29:DI:28:ILE:CG2	29:DI:31:TYR:CD1	2.76	0.68
44:c:111:TYR:CE2	46:b:136:HIS:CD2	2.81	0.68
48:m:116:GLN:HB3	65:z:594:LEU:HD21	1.75	0.68
49:a:211:LEU:HD13	49:a:222:LEU:HD23	1.76	0.68
53:h:14:ALA:HB1	53:h:63:LEU:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:147:CYS:SG	64:v:41:LYS:CD	2.81	0.68
54:i:72:ILE:HD11	54:i:92:SER:CB	2.18	0.68
55:j:11:HIS:HB3	55:j:15:PHE:HE2	1.58	0.68
57:n:226:VAL:CG1	57:n:230:PHE:O	2.42	0.68
57:n:659:LEU:HD21	67:w:17:VAL:CB	2.22	0.68
10:PA:275:ASP:HB2	10:PA:336:LEU:HD12	1.75	0.68
14:PE:27:LEU:HB2	14:PE:65:ASN:HA	1.74	0.68
16:PG:149:GLY:HA3	16:PG:160:ILE:HB	1.74	0.68
25:De:645:GLY:H	25:De:675:LEU:HD11	1.59	0.68
37:1:187:ASN:HD22	37:1:191:ASP:HB2	1.59	0.68
40:4:316:TYR:CE2	40:4:371:ARG:HD3	2.28	0.68
57:n:305:LEU:HD11	57:n:361:ILE:HG12	1.75	0.68
59:q:375:LEU:CD2	59:q:431:ILE:HG13	2.24	0.68
7:BA:18:HIS:CE1	7:BA:37:CYS:HB3	2.29	0.68
10:PA:18:ILE:HD12	11:PB:1171:MET:HB3	1.76	0.68
23:DB:539:ARG:HD2	40:4:408:LEU:CD1	2.22	0.68
58:o:762:GLN:CA	67:w:74:LYS:HZ1	2.05	0.68
70:Y:7:DA:H2"	70:Y:8:DA:C8	2.28	0.68
13:PD:103:LEU:HD11	16:PG:84:VAL:HG13	1.76	0.68
55:j:102:MET:HG3	63:u:26:LEU:CG	2.23	0.68
55:j:102:MET:CA	63:u:26:LEU:HD21	2.23	0.68
57:n:245:TRP:CB	57:n:282:LEU:CD1	2.57	0.68
58:o:707:ILE:HG23	58:o:720:PRO:HA	1.73	0.68
59:q:31:LEU:N	59:q:32:PRO:HD2	2.09	0.68
62:t:8:GLN:HA	62:t:138:ILE:O	1.94	0.68
63:u:7:GLN:HE21	65:z:594:LEU:HD22	1.59	0.68
24:DD:1078:LEU:CD2	31:DL:83:MET:HE1	2.23	0.68
29:DI:23:LEU:CD2	29:DI:39:MET:HE1	2.23	0.68
49:a:229:SER:HA	49:a:502:MET:CB	2.24	0.68
51:f:95:LEU:C	59:q:130:VAL:CG1	2.67	0.68
57:n:254:VAL:HG11	57:n:304:GLN:CG	2.24	0.68
2:8:191:GLY:C	2:8:193:GLY:H	2.02	0.67
2:8:207:LEU:O	51:f:52:MET:SD	2.52	0.67
10:PA:1192:TRP:HA	10:PA:1195:VAL:HG13	1.75	0.67
10:PA:1309:MET:HG3	10:PA:1336:LEU:HD23	1.76	0.67
11:PB:805:PHE:O	11:PB:806:PHE:HB2	1.93	0.67
13:PD:142:TYR:HD1	64:v:70:ARG:HH11	1.43	0.67
26:Df:381:ALA:HA	26:Df:388:ILE:HG22	1.76	0.67
38:2:250:ILE:HD13	39:3:297:LEU:HB2	1.76	0.67
39:3:257:CYS:HB2	39:3:275:PHE:HB3	1.74	0.67
45:e:132:HIS:HD2	64:v:126:ASP:OD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:i:65:PHE:HD1	54:i:99:LYS:CE	2.05	0.67
58:o:715:LEU:HD13	66:x:21:TYR:C	2.18	0.67
59:q:1:MET:CE	65:z:541:PRO:CB	2.68	0.67
59:q:186:GLU:CB	59:q:243:LEU:HD22	2.25	0.67
1:0:295:ARG:HA	2:8:132:TRP:NE1	2.08	0.67
2:8:98:LEU:HB3	2:8:143:LEU:HD21	1.76	0.67
11:PB:592:ARG:NH1	11:PB:592:ARG:HB3	2.00	0.67
14:PE:171:PRO:HB2	14:PE:207:ARG:HG2	1.75	0.67
37:1:458:GLN:HA	37:1:461:LEU:HB3	1.75	0.67
42:6:472:ARG:NH1	42:6:473:GLU:HA	2.09	0.67
48:m:23:GLU:CD	52:g:46:GLY:N	2.53	0.67
50:d:64:GLN:HE21	50:d:68:LEU:HD12	1.58	0.67
51:f:174:ARG:CD	57:n:270:GLN:NE2	2.53	0.67
54:i:136:LYS:HE2	54:i:136:LYS:O	1.95	0.67
55:j:34:GLN:HB2	55:j:37:LEU:HD12	1.74	0.67
55:j:70:TYR:CD1	55:j:80:TYR:CG	2.74	0.67
56:k:45:LEU:HD22	56:k:45:LEU:C	2.19	0.67
57:n:937:ARG:HE	57:n:943:LEU:CD2	2.06	0.67
63:u:82:THR:HA	63:u:86:GLN:CD	2.18	0.67
67:w:9:PHE:CE2	67:w:66:PHE:HD2	2.11	0.67
29:DI:23:LEU:HD21	29:DI:39:MET:CE	2.23	0.67
43:7:487:ARG:HG3	43:7:487:ARG:NH1	2.08	0.67
49:a:382:LEU:CD2	49:a:446:SER:HA	2.23	0.67
51:f:184:LEU:HD22	57:n:299:PHE:HD1	1.38	0.67
59:q:437:HIS:CE1	59:q:472:GLU:C	2.69	0.67
60:r:19:MET:CE	60:r:177:ALA:HB2	2.13	0.67
61:s:92:ALA:C	61:s:96:PHE:CD2	2.71	0.67
67:w:41:LEU:HD21	67:w:85:MET:HG3	1.76	0.67
55:j:114:SER:CB	55:j:121:MET:HG2	2.24	0.67
62:t:78:LEU:HD12	62:t:84:CYS:HB3	1.76	0.67
13:PD:137:LYS:CE	53:h:51:LEU:O	2.42	0.67
31:DL:101:GLN:O	31:DL:105:HIS:CG	2.42	0.67
38:2:54:ARG:HG2	38:2:55:LEU:HD12	1.76	0.67
44:c:111:TYR:OH	46:b:136:HIS:CB	2.41	0.67
49:a:364:TYR:HB2	49:a:430:LEU:HG	1.76	0.67
57:n:237:MET:HE1	59:q:45:GLN:HA	1.76	0.67
59:q:184:ASN:OD1	64:v:83:LYS:CD	2.43	0.67
59:q:578:TYR:CD1	59:q:646:LEU:HD12	2.29	0.67
63:u:85:LEU:HD11	65:z:551:ASP:HB2	1.76	0.67
70:Y:18:DA:C6	70:Y:19:DC:N4	2.62	0.67
10:PA:381:PRO:HB3	10:PA:480:SER:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:83:ARG:HG3	11:PB:133:ILE:HG23	1.75	0.67
25:DE:426:ARG:HH11	25:DE:640:ASN:HD22	1.41	0.67
25:DE:509:GLN:O	25:DE:513:LEU:N	2.27	0.67
38:2:272:SER:HB3	38:2:285:THR:HG22	1.75	0.67
50:d:41:SER:HB3	54:i:69:VAL:HG11	1.76	0.67
66:x:912:LEU:HD22	66:x:958:VAL:HG21	1.76	0.67
67:w:1291:MET:SD	67:w:1328:ARG:NH2	2.67	0.67
2:8:207:LEU:CA	51:f:52:MET:HE1	2.25	0.67
29:DI:28:ILE:CG2	29:DI:31:TYR:HD1	2.07	0.67
43:7:739:LEU:O	43:7:741:LEU:N	2.22	0.67
46:b:65:PRO:HA	46:b:68:LYS:HE2	1.76	0.67
46:b:101:ARG:HH22	57:n:944:PHE:HE2	1.43	0.67
50:d:71:HIS:CE1	50:d:72:ARG:HD3	2.30	0.67
51:f:174:ARG:HD2	57:n:270:GLN:NE2	2.09	0.67
56:k:28:ALA:HB2	59:q:161:LEU:CD2	2.05	0.67
62:t:112:THR:HG22	62:t:129:VAL:HG22	1.77	0.67
62:t:129:VAL:HG21	62:t:200:ILE:CD1	2.17	0.67
66:x:955:LEU:HD22	66:x:967:VAL:HG21	0.67	0.67
50:d:46:GLU:N	54:i:76:MET:HE3	2.09	0.67
52:g:88:ASN:HB3	61:s:69:ARG:NH1	2.10	0.67
52:g:172:PRO:HA	52:g:175:LEU:HG	1.75	0.67
55:j:26:VAL:HG21	55:j:38:ASN:OD1	1.95	0.67
56:k:56:VAL:HG13	64:v:26:ILE:HD12	1.77	0.67
58:o:765:ASP:OD1	58:o:766:LYS:N	2.27	0.67
64:v:21:ARG:NH1	64:v:78:LEU:HD23	2.03	0.67
10:PA:672:ILE:O	10:PA:676:ILE:HG12	1.95	0.67
18:PI:87:GLN:HE22	18:PI:123:TRP:CD1	2.13	0.67
22:DA:970:ASN:OD1	22:DA:970:ASN:N	2.20	0.67
31:Dl:82:GLU:O	31:Dl:86:GLN:HG3	1.95	0.67
53:h:74:GLN:NE2	59:q:129:PRO:CB	2.54	0.67
59:q:184:ASN:OD1	64:v:83:LYS:HD2	1.94	0.67
62:t:130:THR:HA	62:t:135:ALA:HA	1.77	0.67
10:PA:1190:GLN:HA	10:PA:1193:VAL:HB	1.77	0.67
10:PA:1794:SER:HB2	10:PA:1795:PRO:HD3	1.76	0.67
11:PB:628:VAL:HG22	11:PB:633:LEU:HD23	1.75	0.67
28:DH:56:ALA:HB2	30:DJ:214:PRO:CG	2.24	0.67
29:DI:132:LEU:CG	30:DJ:121:MET:SD	2.83	0.67
24:Dd:1082:ALA:HB2	31:Dl:83:MET:CE	2.24	0.67
48:m:104:HIS:CG	57:n:169:LEU:CA	2.68	0.67
16:PG:78:ARG:NH1	16:PG:152:VAL:HG11	2.09	0.66
18:PI:36:LEU:HD23	18:PI:47:GLU:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DI:60:HIS:NE2	31:DL:106:ARG:CZ	2.58	0.66
42:6:158:LEU:HD11	42:6:161:VAL:HG22	1.75	0.66
42:6:330:ASN:HD21	42:6:334:ARG:HB2	1.60	0.66
49:a:367:LEU:HD13	49:a:509:ARG:NH1	2.08	0.66
51:f:177:VAL:HG12	57:n:270:GLN:HG2	1.77	0.66
54:i:131:LEU:HD21	63:u:128:SER:CB	2.25	0.66
55:j:89:LEU:CG	61:s:93:TYR:CE1	2.78	0.66
58:o:715:LEU:CD1	66:x:21:TYR:HA	2.18	0.66
1:0:148:GLU:OE1	53:h:3:ARG:CB	2.44	0.66
12:PC:259:LEU:HD11	20:PK:35:ILE:HD13	1.76	0.66
16:PG:51:ILE:HG12	16:PG:72:TYR:CE2	2.30	0.66
25:DE:359:LEU:HD13	25:DE:627:LEU:HD12	1.76	0.66
25:DE:773:TYR:OH	26:DF:140:GLY:HA2	1.95	0.66
26:DF:104:LEU:HB3	30:DJ:217:PHE:CZ	2.21	0.66
40:4:304:PRO:CG	40:4:372:ALA:HA	2.24	0.66
49:a:160:LEU:HD11	49:a:219:LEU:HD21	1.77	0.66
51:f:181:LEU:HD11	57:n:270:GLN:HA	1.78	0.66
56:k:17:ILE:HD13	59:q:171:VAL:HG22	1.75	0.66
56:k:86:SER:O	64:v:105:LEU:HD13	1.95	0.66
10:PA:886:VAL:HG11	10:PA:889:LEU:HD13	1.77	0.66
31:Dl:106:ARG:HH11	31:Dl:114:LYS:NZ	1.93	0.66
37:1:187:ASN:HB2	37:1:191:ASP:HB2	1.72	0.66
48:m:67:LEU:HD13	48:m:73:LEU:HD11	1.76	0.66
49:a:364:TYR:HB3	49:a:430:LEU:HD11	1.71	0.66
59:q:647:SER:HB3	59:q:648:PRO:HD2	1.76	0.66
64:v:61:MET:HE2	64:v:64:ARG:NH1	2.10	0.66
7:BA:129:ASN:HD22	11:PB:99:TRP:HE1	1.41	0.66
10:PA:811:ILE:N	11:PB:689:TYR:OH	2.29	0.66
10:PA:1176:TYR:CD1	18:PI:52:CYS:HB2	2.30	0.66
13:PD:140:PHE:CE1	64:v:64:ARG:HD3	2.30	0.66
25:DE:489:PHE:CZ	26:DF:129:VAL:HG21	2.31	0.66
43:7:84:ILE:HG12	43:7:174:ILE:HD11	1.78	0.66
53:h:16:LEU:HD23	59:q:116:LEU:HB3	1.77	0.66
59:q:89:GLN:HB3	59:q:90:PRO:HD2	1.78	0.66
64:v:131:GLU:O	64:v:135:TYR:HD2	1.79	0.66
4:DO:57:ASN:O	4:DO:57:ASN:ND2	2.28	0.66
10:PA:811:ILE:CG2	11:PB:674:MET:HE1	2.25	0.66
10:PA:1102:MET:HB2	10:PA:1120:GLY:HA2	1.76	0.66
12:PC:154:ARG:HD3	19:PJ:64:PRO:HD3	1.77	0.66
29:DI:132:LEU:CD1	30:DJ:121:MET:SD	2.84	0.66
31:Dl:101:GLN:O	31:Dl:105:HIS:CG	2.47	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:262:LEU:HD13	40:4:271:VAL:HG11	1.78	0.66
55:j:102:MET:HG2	63:u:26:LEU:CD2	2.25	0.66
57:n:192:LEU:HD12	57:n:219:ASN:C	2.19	0.66
59:q:15:CYS:SG	59:q:15:CYS:O	2.53	0.66
59:q:162:LYS:O	59:q:166:ARG:HG2	1.96	0.66
59:q:457:ASP:HB2	59:q:458:PRO:HD3	1.77	0.66
63:u:4:ARG:HD2	65:z:596:TYR:HA	1.78	0.66
1:0:82:TYR:HA	1:0:85:ARG:HB2	1.78	0.66
26:DF:138:ILE:HG13	28:DH:159:TYR:HE2	1.59	0.66
52:g:123:ILE:O	52:g:127:ARG:HG3	1.96	0.66
55:j:9:GLU:CD	55:j:56:GLN:OE1	2.39	0.66
66:x:956:VAL:CG1	66:x:968:LEU:CG	2.70	0.66
69:X:-5:DG:N1	70:Y:4:DA:C6	2.64	0.66
10:PA:457:ILE:HD11	10:PA:515:ILE:HD12	1.78	0.66
42:6:285:ILE:O	42:6:290:PRO:HG2	1.96	0.66
44:c:30:ARG:NE	57:n:861:LYS:HE3	2.10	0.66
53:h:33:LEU:HD21	59:q:95:TRP:HZ3	1.59	0.66
53:h:147:CYS:SG	64:v:41:LYS:HG3	2.35	0.66
59:q:307:ILE:HG12	59:q:379:ILE:CG1	2.15	0.66
64:v:50:ARG:HD2	64:v:51:ALA:H	1.61	0.66
7:BA:281:ALA:HB2	70:Y:33:DC:H6	1.59	0.66
8:FA:121:ASN:C	9:FB:25:LYS:HG3	2.21	0.66
10:PA:791:GLN:HG2	10:PA:839:HIS:HA	1.78	0.66
13:PD:137:LYS:HE3	53:h:51:LEU:O	1.95	0.66
40:4:300:THR:HG23	40:4:373:HIS:HB3	1.77	0.66
44:c:281:CYS:HB3	44:c:284:CYS:H	1.61	0.66
53:h:19:VAL:HG12	59:q:113:TYR:HB2	1.75	0.66
59:q:28:GLU:HA	59:q:28:GLU:OE2	1.94	0.66
67:w:318:GLU:HG2	67:w:320:LYS:H	1.59	0.66
28:DH:57:SER:OG	30:DJ:200:LEU:CD1	2.43	0.66
29:DI:31:TYR:HD2	29:DI:35:VAL:HB	1.60	0.66
31:DL:99:ALA:HB1	31:DL:115:ASP:HB3	1.76	0.66
37:1:274:ASP:O	43:7:128:LYS:HD2	1.96	0.66
40:4:405:GLU:HA	41:5:47:ALA:CB	2.26	0.66
48:m:104:HIS:HB3	57:n:169:LEU:HD23	1.77	0.66
50:d:156:SER:CB	50:d:161:VAL:HG11	2.26	0.66
53:h:146:MET:HG3	56:k:39:LYS:CD	2.24	0.66
53:h:147:CYS:SG	64:v:41:LYS:HD2	2.36	0.66
57:n:250:LEU:HG	57:n:275:HIS:CB	2.26	0.66
57:n:359:ILE:HG23	57:n:372:ILE:HD12	1.78	0.66
11:PB:289:ILE:HG21	11:PB:297:MET:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DF:106:PHE:CE1	29:DI:13:PRO:HD3	2.30	0.66
50:d:97:GLU:HA	50:d:97:GLU:OE2	1.95	0.66
57:n:127:ILE:O	63:u:27:GLN:NE2	2.28	0.66
61:s:92:ALA:C	61:s:96:PHE:HD2	2.04	0.66
62:t:165:LEU:HD23	62:t:169:THR:HA	1.77	0.66
2:8:207:LEU:HD23	51:f:52:MET:HE2	1.65	0.65
22:DA:567:LEU:HB3	23:DB:745:GLN:NE2	2.11	0.65
30:DJ:128:PRO:HB2	30:DJ:160:GLN:HE22	1.62	0.65
49:a:413:HIS:HA	49:a:472:SER:HA	1.76	0.65
51:f:95:LEU:O	59:q:130:VAL:HG11	1.96	0.65
57:n:237:MET:HE1	59:q:45:GLN:HB2	1.77	0.65
1:0:208:LEU:HD12	1:0:209:GLU:N	2.10	0.65
5:DP:169:VAL:CB	69:X:-25:DA:C2	2.74	0.65
7:BA:128:ILE:HG22	9:FB:152:ASN:ND2	2.11	0.65
9:FB:31:TRP:HD1	9:FB:62:LEU:HD21	1.62	0.65
37:1:444:GLY:HA2	38:2:269:PRO:HB3	1.77	0.65
44:c:203:VAL:HG11	59:q:467:ILE:HD11	1.78	0.65
54:i:68:LEU:O	54:i:72:ILE:HG13	1.96	0.65
58:o:723:LEU:HD11	58:o:734:PRO:HB2	1.78	0.65
59:q:647:SER:CB	59:q:648:PRO:CD	2.73	0.65
3:9:175:LYS:HZ2	3:9:175:LYS:CA	2.08	0.65
22:DA:569:ASN:HD22	23:DB:689:GLN:HA	1.61	0.65
26:Df:239:ARG:HD3	26:Df:284:ARG:HH11	1.60	0.65
42:6:504:LYS:HB2	42:6:655:TYR:HA	1.76	0.65
57:n:282:LEU:HB2	57:n:288:PRO:HB3	1.78	0.65
64:v:42:ILE:H	64:v:42:ILE:HD12	1.62	0.65
67:w:1183:TRP:CZ2	67:w:1185:GLY:HA3	2.32	0.65
5:DP:292:ILE:HG23	5:DP:301:VAL:HG13	1.79	0.65
11:PB:594:MET:SD	11:PB:658:ALA:HA	2.35	0.65
23:DB:402:ILE:HD12	23:DB:455:LEU:HD12	1.77	0.65
29:DI:60:HIS:CD2	31:DL:106:ARG:CG	2.79	0.65
39:3:15:VAL:HA	39:3:164:ILE:HB	1.79	0.65
39:3:165:LYS:HE2	39:3:200:SER:HB2	1.78	0.65
48:m:121:GLU:O	48:m:124:GLN:HG2	1.96	0.65
49:a:502:MET:HG3	49:a:503:SER:N	2.11	0.65
55:j:35:ALA:O	55:j:39:GLN:HG2	1.96	0.65
55:j:70:TYR:CD1	55:j:80:TYR:CD1	2.84	0.65
57:n:141:ARG:NH1	63:u:17:ASP:HB2	2.11	0.65
58:o:761:LEU:O	67:w:74:LYS:HD2	1.96	0.65
59:q:92:LEU:HD11	59:q:99:ARG:HH22	1.43	0.65
1:0:68:VAL:HG22	1:0:71:GLU:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:148:GLU:OE1	53:h:3:ARG:CD	2.44	0.65
20:PK:15:GLY:HA3	60:r:10:PRO:CD	2.27	0.65
23:DB:490:SER:HA	23:DB:493:TRP:HB2	1.78	0.65
26:Df:320:ARG:HB3	26:Df:320:ARG:NH1	2.12	0.65
49:a:413:HIS:NE2	49:a:471:ASP:HB3	2.10	0.65
51:f:111:LEU:CD1	53:h:76:ILE:HD11	2.24	0.65
53:h:146:MET:CG	56:k:39:LYS:CE	2.75	0.65
57:n:937:ARG:HH21	57:n:943:LEU:HD23	1.61	0.65
58:o:715:LEU:CB	66:x:25:ILE:CG1	2.60	0.65
63:u:8:LEU:HD12	63:u:72:LEU:HD22	1.77	0.65
2:8:33:ASN:N	2:8:33:ASN:OD1	2.29	0.65
3:9:60:TYR:CB	3:9:105:MET:HE1	2.24	0.65
3:9:111:LEU:HD12	3:9:111:LEU:O	1.96	0.65
3:9:268:GLU:CD	3:9:268:GLU:H	2.04	0.65
10:PA:1200:PRO:HB2	10:PA:1203:ASP:HB3	1.78	0.65
26:DF:19:MET:SD	29:DI:47:VAL:HG11	2.37	0.65
40:4:58:ARG:NH1	40:4:59:MET:SD	2.70	0.65
44:c:296:TRP:CD1	44:c:311:GLN:HG3	2.32	0.65
52:g:93:LEU:CD1	55:j:106:LYS:HE2	2.26	0.65
55:j:75:ARG:CG	55:j:80:TYR:CZ	2.74	0.65
56:k:43:ARG:HB2	56:k:43:ARG:HH11	1.61	0.65
59:q:109:MET:HA	59:q:109:MET:CE	2.23	0.65
63:u:64:ARG:HH22	65:z:589:GLY:HA3	1.61	0.65
3:9:28:ARG:O	3:9:28:ARG:HG3	1.94	0.65
7:BA:128:ILE:HG22	9:FB:152:ASN:HD22	1.62	0.65
10:PA:155:GLU:HB2	10:PA:182:GLY:H	1.60	0.65
10:PA:589:LYS:HG2	10:PA:635:LEU:HD23	1.79	0.65
14:PE:208:LEU:HG	14:PE:209:VAL:N	2.12	0.65
39:3:248:HIS:ND1	39:3:248:HIS:O	2.29	0.65
50:d:45:ILE:HD13	54:i:73:ILE:N	2.00	0.65
56:k:21:ILE:HD12	59:q:168:THR:CA	2.26	0.65
63:u:83:ALA:N	63:u:86:GLN:CB	2.60	0.65
3:9:200:LEU:O	3:9:200:LEU:HD22	1.96	0.65
10:PA:1318:LYS:HD3	10:PA:1330:ALA:HB1	1.79	0.65
22:DA:355:VAL:O	22:DA:355:VAL:HG23	1.97	0.65
50:d:45:ILE:HG23	54:i:76:MET:CG	2.22	0.65
55:j:34:GLN:OE1	55:j:37:LEU:CD1	2.44	0.65
56:k:70:LEU:HG	64:v:82:LEU:CD2	2.27	0.65
58:o:690:LEU:HD22	59:q:605:PRO:HG2	1.77	0.65
42:6:361:CYS:SG	42:6:362:LEU:N	2.70	0.65
43:7:88:ARG:HH11	43:7:174:ILE:HG23	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:u:68:ASP:OD1	65:z:585:HIS:CE1	2.50	0.65
67:w:29:THR:HA	67:w:33:GLU:OE2	1.95	0.65
2:8:47:HIS:CG	2:8:47:HIS:O	2.50	0.65
8:FA:15:VAL:HA	9:FB:42:LYS:HA	1.79	0.65
38:2:182:ILE:HG13	38:2:185:LEU:HD12	1.77	0.65
42:6:79:ALA:H	42:6:84:ILE:HG22	1.62	0.65
43:7:487:ARG:HG3	43:7:487:ARG:HH11	1.60	0.65
45:e:133:LEU:HG	56:k:111:CYS:SG	2.37	0.65
48:m:116:GLN:CB	65:z:594:LEU:HG	2.27	0.65
51:f:71:LEU:HD12	51:f:82:ARG:HE	1.61	0.65
52:g:74:HIS:HB2	52:g:126:TYR:CG	2.32	0.65
57:n:170:PRO:HB3	59:q:22:VAL:HG23	1.78	0.65
2:8:178:TYR:CD1	2:8:178:TYR:N	2.64	0.64
11:PB:744:MET:HE2	11:PB:906:GLN:HE21	1.61	0.64
22:DA:996:ARG:HA	22:DA:1026:ILE:HD13	1.79	0.64
38:2:250:ILE:HG12	39:3:266:TYR:HB2	1.80	0.64
42:6:326:LYS:HD2	42:6:489:TYR:HB2	1.79	0.64
52:g:94:ASP:HA	52:g:97:ILE:HG13	1.79	0.64
67:w:6:GLN:CB	67:w:62:TRP:HH2	2.10	0.64
68:p:50:ASP:HA	68:p:59:THR:HG22	1.79	0.64
1:0:255:THR:HA	3:9:4:ASN:HB2	1.79	0.64
2:8:37:ILE:N	2:8:37:ILE:HD12	2.12	0.64
7:BA:134:ILE:HG12	7:BA:171:GLU:HG3	1.77	0.64
37:1:497:LEU:HD11	37:1:536:LEU:HD22	1.79	0.64
40:4:44:VAL:O	40:4:53:LYS:NZ	2.30	0.64
44:c:21:ILE:HD13	46:b:116:LEU:HB3	1.79	0.64
44:c:166:ILE:HD13	44:c:190:LEU:HD21	1.80	0.64
50:d:38:GLU:OE2	54:i:96:GLU:CB	2.46	0.64
2:8:191:GLY:O	2:8:193:GLY:N	2.31	0.64
2:8:215:GLY:HA3	2:8:221:GLN:HB2	1.79	0.64
22:DA:464:TRP:CG	22:DA:464:TRP:O	2.48	0.64
31:DL:111:LEU:HA	31:DL:114:LYS:HZ2	0.65	0.64
40:4:368:LEU:HD11	40:4:387:ILE:HG21	1.80	0.64
45:e:129:VAL:CG2	56:k:114:MET:CE	2.64	0.64
50:d:27:ARG:HG2	54:i:107:ILE:HG22	1.79	0.64
50:d:121:LEU:CD1	63:u:115:LEU:CA	2.74	0.64
51:f:181:LEU:O	51:f:185:ARG:HG3	1.96	0.64
55:j:9:GLU:CG	55:j:56:GLN:CD	2.69	0.64
56:k:70:LEU:HD23	64:v:85:PHE:HD1	1.57	0.64
57:n:587:LEU:HD22	67:w:15:THR:HG21	1.79	0.64
5:DP:204:ILE:HG13	5:DP:207:PRO:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DD:940:VAL:HA	24:DD:943:GLN:HB2	1.79	0.64
48:m:104:HIS:ND1	57:n:169:LEU:HG	2.13	0.64
49:a:109:TYR:CE2	49:a:154:LEU:CD2	2.80	0.64
49:a:232:LEU:C	49:a:232:LEU:HD13	2.22	0.64
51:f:180:LEU:HD13	57:n:302:SER:CB	2.25	0.64
53:h:142:SER:HG	56:k:39:LYS:HE3	1.60	0.64
56:k:44:LEU:HD22	56:k:47:ARG:HH22	1.62	0.64
59:q:489:LYS:O	59:q:507:ARG:NH2	2.30	0.64
63:u:81:SER:HB2	63:u:85:LEU:H	1.63	0.64
65:z:529:HIS:HA	65:z:568:ASP:HA	1.80	0.64
3:9:229:GLU:H	3:9:229:GLU:CD	2.04	0.64
7:BA:179:GLU:HG2	9:FB:154:LYS:HZ3	1.61	0.64
23:DB:361:ARG:HD2	23:DB:367:GLU:HB2	1.80	0.64
25:DE:507:VAL:HG22	25:DE:574:THR:HA	1.80	0.64
38:2:32:ALA:CB	42:6:72:THR:HG22	2.27	0.64
52:g:89:PHE:CG	63:u:19:PHE:HD1	2.09	0.64
55:j:19:ILE:CG2	55:j:45:VAL:CG2	2.54	0.64
56:k:21:ILE:HD12	59:q:168:THR:CB	2.27	0.64
56:k:77:GLN:HG3	60:r:192:GLN:HG2	1.79	0.64
57:n:359:ILE:CA	57:n:372:ILE:CD1	2.75	0.64
59:q:149:LYS:HD2	64:v:40:ALA:HA	1.77	0.64
11:PB:657:VAL:HG13	11:PB:658:ALA:N	2.12	0.64
38:2:343:ARG:HG3	38:2:351:GLU:HG3	1.79	0.64
43:7:415:THR:HG1	43:7:436:SER:HG	1.41	0.64
51:f:70:LEU:HD21	51:f:73:ALA:HB2	1.79	0.64
54:i:65:PHE:CD1	54:i:99:LYS:HE2	2.32	0.64
63:u:4:ARG:NE	65:z:596:TYR:N	2.44	0.64
37:1:417:LYS:HG2	39:3:224:LEU:HD21	1.80	0.64
38:2:195:ARG:HE	38:2:217:GLY:HA2	1.62	0.64
38:2:304:GLU:HA	38:2:312:LEU:H	1.63	0.64
55:j:34:GLN:HB2	55:j:37:LEU:CG	2.27	0.64
64:v:108:LEU:C	64:v:108:LEU:HD12	2.23	0.64
66:x:780:THR:HG22	66:x:816:CYS:HB3	1.80	0.64
22:DA:353:LEU:HD11	26:Df:272:VAL:HG11	1.80	0.64
25:DE:745:GLU:OE1	25:DE:745:GLU:HA	1.97	0.64
42:6:309:ASP:O	42:6:310:LEU:CG	2.46	0.64
43:7:487:ARG:HH22	43:7:728:PHE:HB3	1.62	0.64
48:m:22:LEU:HD11	52:g:43:MET:HE1	1.80	0.64
51:f:188:PHE:CG	57:n:295:CYS:SG	2.83	0.64
56:k:39:LYS:HG3	56:k:39:LYS:O	1.97	0.64
57:n:359:ILE:CA	57:n:372:ILE:HD11	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:o:765:ASP:CB	67:w:72:SER:OG	2.46	0.64
59:q:631:GLU:HA	59:q:631:GLU:OE2	1.97	0.64
2:8:241:CYS:HA	2:8:246:TYR:CG	2.32	0.64
21:PL:57:ALA:O	21:PL:58:ARG:C	2.40	0.64
40:4:338:PHE:HB2	40:4:339:PRO:HD2	1.79	0.64
49:a:364:TYR:HB3	49:a:430:LEU:HG	1.67	0.64
49:a:417:TYR:CD1	49:a:450:PHE:HE1	2.15	0.64
50:d:156:SER:HA	50:d:161:VAL:CG1	2.27	0.64
54:i:65:PHE:HZ	54:i:102:SER:HG	1.46	0.64
55:j:34:GLN:HB2	55:j:37:LEU:HG	1.78	0.64
57:n:237:MET:CE	59:q:45:GLN:CB	2.73	0.64
57:n:790:ILE:HG22	57:n:792:ALA:H	1.62	0.64
63:u:61:LEU:HD21	65:z:495:SER:OG	1.98	0.64
10:PA:1210:TRP:CH2	18:PI:28:GLU:HG2	2.32	0.64
14:PE:45:GLY:HA3	14:PE:53:PRO:HD3	1.80	0.64
22:DA:564:PRO:CG	23:DB:744:PHE:CD2	2.80	0.64
48:m:54:TYR:OH	52:g:36:PRO:HD3	1.96	0.64
50:d:42:ARG:CZ	54:i:96:GLU:OE2	2.45	0.64
55:j:43:PHE:HZ	61:s:147:THR:O	1.79	0.64
55:j:96:LYS:NZ	61:s:80:SER:C	2.56	0.64
63:u:7:GLN:HE22	65:z:594:LEU:HD22	1.60	0.64
67:w:361:ALA:CB	68:p:251:GLU:HB3	2.27	0.64
69:X:-33:DG:C2	70:Y:34:DG:N1	2.65	0.64
1:0:298:GLN:NE2	2:8:132:TRP:NE1	2.45	0.63
7:BA:173:VAL:HB	7:BA:175:ARG:HH12	1.64	0.63
26:DF:68:THR:HA	29:DI:32:GLU:CD	2.23	0.63
45:e:129:VAL:HG13	56:k:111:CYS:HG	1.63	0.63
49:a:364:TYR:O	49:a:428:THR:HG21	1.98	0.63
53:h:146:MET:HG2	56:k:39:LYS:CE	2.26	0.63
57:n:658:ARG:HH22	67:w:21:ALA:HA	1.63	0.63
62:t:31:LEU:HD11	62:t:164:PHE:HB3	1.79	0.63
64:v:21:ARG:NE	64:v:78:LEU:HD22	2.05	0.63
66:x:143:ARG:HH22	66:x:205:ASN:HB2	1.62	0.63
1:0:78:VAL:HA	1:0:82:TYR:HD2	1.62	0.63
2:8:24:ALA:HA	2:8:44:LYS:HB2	1.80	0.63
7:BA:128:ILE:HG23	9:FB:152:ASN:ND2	2.12	0.63
11:PB:256:ILE:HB	11:PB:269:ILE:HG12	1.80	0.63
24:DD:940:VAL:HA	24:DD:943:GLN:CB	2.28	0.63
26:DF:106:PHE:CD1	29:DI:13:PRO:HD3	2.33	0.63
32:Dc:67:GLY:CA	30:Dj:116:LEU:HD11	2.25	0.63
35:EA:141:ALA:HB1	35:EA:152:PHE:HE2	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1:461:LEU:HD21	37:1:504:LYS:CD	2.28	0.63
43:7:497:ARG:HH11	43:7:710:VAL:HB	1.64	0.63
63:u:25:VAL:HG21	63:u:58:PHE:HE2	1.62	0.63
67:w:13:VAL:HG11	67:w:75:ARG:CG	2.27	0.63
13:PD:137:LYS:CD	53:h:55:GLN:CD	2.69	0.63
38:2:224:ASP:H	38:2:227:HIS:HB3	1.63	0.63
47:l:108:PRO:HD2	47:l:109:ILE:HD12	1.81	0.63
48:m:14:ASN:HB3	52:g:39:LYS:NZ	2.12	0.63
49:a:160:LEU:HD11	49:a:214:ARG:HH21	1.61	0.63
49:a:441:GLU:CD	66:x:17:ARG:HH22	2.04	0.63
52:g:89:PHE:HB2	63:u:19:PHE:CE1	2.32	0.63
53:h:142:SER:C	56:k:39:LYS:HZ1	2.03	0.63
59:q:166:ARG:CZ	59:q:166:ARG:HB3	2.27	0.63
14:PE:100:THR:HG23	14:PE:126:ILE:H	1.63	0.63
16:PG:77:PHE:O	16:PG:78:ARG:C	2.42	0.63
31:DL:78:GLU:O	31:DL:82:GLU:HG3	1.99	0.63
42:6:514:MET:HG2	42:6:665:GLN:HE21	1.63	0.63
49:a:321:LEU:HA	49:a:410:LEU:HD12	1.81	0.63
52:g:81:LEU:HB3	52:g:119:VAL:HG23	1.80	0.63
53:h:77:ILE:HG13	59:q:126:THR:HB	1.77	0.63
57:n:74:PRO:HA	57:n:82:LYS:CB	2.28	0.63
57:n:192:LEU:CD1	57:n:219:ASN:O	2.46	0.63
58:o:715:LEU:H	66:x:25:ILE:HD11	1.64	0.63
1:0:28:HIS:HE1	1:0:49:CYS:SG	2.21	0.63
4:DO:3:TYR:C	4:DO:5:LEU:H	2.04	0.63
11:PB:205:VAL:HG13	11:PB:368:MET:HG3	1.80	0.63
35:EA:131:VAL:HG21	35:EA:159:THR:HG21	1.80	0.63
42:6:62:ARG:HD3	42:6:75:PRO:HD3	1.80	0.63
45:e:146:ILE:C	45:e:148:VAL:H	2.07	0.63
55:j:53:LYS:O	55:j:57:GLN:HG3	1.99	0.63
55:j:85:LEU:CD1	61:s:96:PHE:CZ	2.82	0.63
14:PE:48:PRO:HA	14:PE:53:PRO:O	1.99	0.63
16:PG:114:PRO:O	16:PG:117:MET:HG3	1.98	0.63
36:EB:120:MET:HA	36:EB:124:LEU:HD12	1.79	0.63
46:b:103:ASP:HB3	58:o:645:ALA:HB2	1.81	0.63
49:a:220:MET:HB2	49:a:257:VAL:HG12	1.80	0.63
51:f:181:LEU:HD11	57:n:270:GLN:CG	2.29	0.63
55:j:82:LYS:HZ3	61:s:99:LYS:CB	2.10	0.63
62:t:25:THR:HB	62:t:117:TYR:OH	1.97	0.63
67:w:18:ILE:HA	67:w:21:ALA:HB2	1.79	0.63
10:PA:37:THR:HA	10:PA:61:ARG:HH12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:72:GLN:HG2	35:EA:156:PHE:CZ	2.34	0.63
37:1:478:CYS:CB	37:1:484:PRO:HG3	2.29	0.63
51:f:180:LEU:CD1	57:n:302:SER:HB2	2.28	0.63
55:j:76:ASN:H	55:j:79:LEU:HD12	1.62	0.63
56:k:37:LYS:HB3	59:q:150:LYS:HE3	1.80	0.63
57:n:172:CYS:SG	59:q:21:GLU:CB	2.86	0.63
62:t:120:CYS:O	62:t:120:CYS:SG	2.56	0.63
63:u:28:GLN:OE1	65:z:483:ASN:ND2	2.32	0.63
14:PE:45:GLY:HA3	14:PE:52:ARG:HB2	1.81	0.63
40:4:304:PRO:HG2	40:4:372:ALA:HA	1.80	0.63
43:7:203:ASN:O	43:7:204:VAL:CG2	2.43	0.63
49:a:109:TYR:CE2	49:a:154:LEU:HD21	2.34	0.63
49:a:364:TYR:HB2	49:a:428:THR:OG1	1.98	0.63
57:n:196:ASN:OD1	57:n:219:ASN:HA	1.99	0.63
59:q:93:TRP:N	59:q:94:PRO:CD	2.62	0.63
63:u:80:GLU:HB2	65:z:563:VAL:HG22	1.80	0.63
66:x:637:GLU:O	66:x:641:GLN:NE2	2.31	0.63
69:X:-24:DA:C5'	69:X:-24:DA:H8	2.11	0.63
11:PB:82:PRO:HB3	11:PB:134:LYS:HA	1.81	0.63
11:PB:625:LEU:HD12	11:PB:665:ILE:HB	1.81	0.63
25:DE:359:LEU:HD11	25:DE:648:ASP:HB2	1.80	0.63
26:DF:71:ILE:HD11	29:DI:35:VAL:HG22	1.81	0.63
29:DI:15:ASP:O	29:DI:40:LEU:HD21	1.99	0.63
29:Di:73:LEU:HD13	31:Dl:105:HIS:CE1	2.33	0.63
43:7:523:LEU:C	43:7:523:LEU:HD12	2.23	0.63
63:u:82:THR:C	63:u:86:GLN:CB	2.71	0.63
67:w:1184:VAL:O	67:w:1184:VAL:HG22	1.98	0.63
70:Y:38:DT:H2"	70:Y:39:DT:H5'	1.80	0.63
10:PA:626:THR:HG22	10:PA:627:LYS:H	1.64	0.62
16:PG:18:PHE:HA	16:PG:22:LEU:HD13	1.80	0.62
24:DD:913:LEU:HD23	31:DL:87:ILE:CD1	2.27	0.62
30:DJ:171:LEU:CD1	30:DJ:193:TYR:CE1	2.59	0.62
31:Dl:106:ARG:O	31:Dl:106:ARG:HG2	1.99	0.62
49:a:424:CYS:HA	49:a:505:PRO:HG3	1.79	0.62
22:DA:567:LEU:HB3	23:DB:745:GLN:CD	2.24	0.62
22:DA:854:ARG:HH22	70:Y:-25:DT:C5'	2.12	0.62
29:DI:73:LEU:CD2	31:DL:105:HIS:CD2	2.81	0.62
49:a:374:TYR:CE2	49:a:440:PHE:HD2	2.17	0.62
50:d:38:GLU:OE2	54:i:96:GLU:CG	2.47	0.62
50:d:100:VAL:HG13	54:i:128:LYS:NZ	2.14	0.62
59:q:93:TRP:H	59:q:94:PRO:HD2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:255:ALA:HB3	59:q:301:VAL:HG22	1.80	0.62
63:u:82:THR:HA	63:u:86:GLN:HG3	1.56	0.62
67:w:107:LEU:HD11	67:w:115:TRP:HA	1.81	0.62
5:DP:301:VAL:HB	69:X:-27:DA:C5'	2.16	0.62
26:DF:392:ILE:O	26:DF:392:ILE:HG22	1.99	0.62
57:n:229:GLU:HG2	57:n:300:CYS:SG	2.39	0.62
59:q:92:LEU:HD21	59:q:99:ARG:NE	2.13	0.62
59:q:327:VAL:HG23	59:q:328:LYS:H	1.65	0.62
68:p:47:PHE:HE2	68:p:49:MET:HE2	1.64	0.62
25:DE:451:VAL:O	25:DE:453:LEU:N	2.31	0.62
37:1:339:SER:HA	43:7:16:TYR:OH	1.99	0.62
37:1:454:PRO:HB2	38:2:274:ALA:HB3	1.80	0.62
39:3:12:VAL:HB	39:3:161:ILE:HA	1.80	0.62
40:4:15:GLN:OE1	40:4:46:ARG:NH1	2.32	0.62
42:6:372:GLU:HA	42:6:375:LYS:HE3	1.81	0.62
42:6:472:ARG:HH11	42:6:473:GLU:N	1.97	0.62
48:m:66:TYR:HE1	52:g:52:ASP:OD2	1.82	0.62
48:m:74:HIS:HB2	57:n:166:TYR:HB2	1.79	0.62
50:d:165:LEU:HD11	63:u:6:THR:HG22	1.79	0.62
57:n:634:MET:N	57:n:634:MET:SD	2.73	0.62
59:q:149:LYS:CE	64:v:40:ALA:O	2.47	0.62
63:u:79:GLU:OE2	63:u:82:THR:CG2	2.47	0.62
10:PA:1171:ALA:HB3	10:PA:1215:GLU:HG3	1.80	0.62
10:PA:1263:ASN:HA	10:PA:1266:GLU:OE1	2.00	0.62
22:DA:567:LEU:HA	23:DB:745:GLN:NE2	2.14	0.62
37:1:415:THR:N	37:1:416:PRO:HD3	2.14	0.62
42:6:325:ARG:NH1	43:7:499:ASN:OD1	2.27	0.62
42:6:507:CYS:HA	42:6:659:PHE:HB3	1.81	0.62
50:d:109:GLN:HA	50:d:112:LYS:HZ1	1.63	0.62
51:f:39:PRO:HG3	52:g:11:LEU:HG	1.80	0.62
9:FB:149:VAL:HG21	11:PB:146:LYS:HB3	1.81	0.62
10:PA:1221:MET:HE1	10:PA:1231:ILE:HD11	1.80	0.62
18:PI:22:ASN:HD22	18:PI:41:ASN:HB2	1.65	0.62
22:DA:567:LEU:CA	23:DB:745:GLN:NE2	2.62	0.62
31:DL:62:LYS:O	31:DL:62:LYS:NZ	2.21	0.62
36:EB:171:ILE:HG12	36:EB:177:ASN:HB2	1.81	0.62
38:2:320:ARG:NH2	39:3:174:TYR:OH	2.31	0.62
38:2:348:CYS:O	39:3:146:ARG:NH2	2.32	0.62
40:4:304:PRO:HG2	40:4:373:HIS:H	1.64	0.62
46:b:176:THR:HA	46:b:179:LEU:CG	2.29	0.62
52:g:81:LEU:HD12	52:g:122:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:r:121:MET:HE2	62:t:102:PHE:CZ	2.34	0.62
67:w:6:GLN:N	67:w:62:TRP:CH2	2.68	0.62
67:w:1181:THR:O	67:w:1184:VAL:HB	2.00	0.62
1:0:300:ALA:O	3:9:210:SER:HB3	1.99	0.62
10:PA:721:HIS:HE1	18:PI:98:GLN:HE21	1.47	0.62
11:PB:675:LEU:HA	11:PB:695:HIS:O	1.99	0.62
26:DF:106:PHE:CD1	29:DI:13:PRO:HG3	2.35	0.62
24:Dd:884:GLU:HA	24:Dd:887:LYS:HE3	1.82	0.62
35:EA:22:ILE:HB	35:EA:34:LEU:HD13	1.81	0.62
44:c:110:ALA:HB3	46:b:168:ILE:CG2	2.00	0.62
45:e:71:GLU:OE1	45:e:74:ARG:NH2	2.33	0.62
48:m:106:GLN:CD	50:d:167:TRP:HE3	2.07	0.62
52:g:74:HIS:CE1	52:g:125:GLU:HB3	2.35	0.62
59:q:7:VAL:HG23	63:u:90:LEU:HD21	1.82	0.62
59:q:149:LYS:CD	64:v:40:ALA:O	2.48	0.62
64:v:21:ARG:CD	64:v:78:LEU:HD21	2.28	0.62
10:PA:1208:SER:HB2	10:PA:1260:ARG:HB2	1.80	0.62
12:PC:6:GLN:NE2	12:PC:6:GLN:H	1.77	0.62
29:DI:32:GLU:HB2	29:DI:35:VAL:HG23	1.82	0.62
29:Di:73:LEU:HD21	31:Dl:105:HIS:CD2	2.33	0.62
37:1:264:ASN:OD1	43:7:581:LEU:HD23	2.00	0.62
40:4:49:PRO:O	40:4:53:LYS:CG	2.41	0.62
43:7:705:ASN:HA	43:7:708:LEU:HD21	1.82	0.62
46:b:176:THR:C	46:b:179:LEU:HG	2.24	0.62
49:a:127:HIS:CE1	49:a:171:THR:HG22	2.35	0.62
52:g:164:ILE:HB	54:i:140:MET:SD	2.40	0.62
57:n:226:VAL:CG1	57:n:230:PHE:H	2.12	0.62
67:w:101:LEU:HD22	67:w:118:THR:HG23	1.82	0.62
69:X:-5:DG:H1	70:Y:5:DC:N4	1.98	0.62
1:0:295:ARG:HA	2:8:132:TRP:HE1	1.62	0.62
10:PA:1245:CYS:HB2	10:PA:1259:ILE:HG23	1.80	0.62
13:PD:78:GLU:OE1	53:h:51:LEU:CG	2.45	0.62
14:PE:121:MET:HB3	14:PE:124:LYS:HB2	1.81	0.62
39:3:48:HIS:O	39:3:55:ASN:ND2	2.32	0.62
43:7:705:ASN:CB	43:7:708:LEU:HD11	2.27	0.62
50:d:41:SER:HB2	54:i:69:VAL:CG1	2.19	0.62
56:k:109:ARG:HH11	56:k:109:ARG:HG3	1.65	0.62
57:n:226:VAL:HG13	57:n:230:PHE:H	1.64	0.62
57:n:587:LEU:HD22	67:w:15:THR:HG22	1.82	0.62
62:t:8:GLN:HE21	62:t:200:ILE:HD13	1.63	0.62
62:t:98:LEU:HD13	62:t:102:PHE:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:w:40:CYS:HB3	67:w:82:CYS:SG	2.40	0.62
69:X:-5:DG:H1	70:Y:5:DC:H42	1.46	0.62
22:DA:349:TRP:CZ2	26:Df:266:GLY:HA3	2.35	0.62
39:3:196:LEU:HD21	39:3:223:LEU:HD22	1.82	0.62
39:3:237:GLN:O	39:3:241:LEU:CB	2.48	0.62
48:m:66:TYR:OH	52:g:40:ASP:OD1	2.18	0.62
68:p:148:GLU:HB3	68:p:370:VAL:HG21	1.82	0.62
69:X:-26:DA:H3'	69:X:-26:DA:OP2	2.00	0.62
5:DP:173:ASN:CB	5:DP:218:LYS:HZ3	2.13	0.61
8:FA:125:TYR:HE2	9:FB:31:TRP:CZ3	2.03	0.61
16:PG:30:LEU:HD13	16:PG:70:VAL:HG11	1.80	0.61
26:Df:301:VAL:HG22	26:Df:340:ILE:HD11	1.82	0.61
43:7:489:CYS:SG	43:7:490:LEU:N	2.73	0.61
43:7:566:LEU:H	43:7:594:ALA:HA	1.65	0.61
57:n:354:VAL:HG12	57:n:355:HIS:H	1.64	0.61
59:q:93:TRP:H	59:q:94:PRO:CD	2.11	0.61
62:t:96:VAL:O	62:t:99:LYS:HB2	2.00	0.61
64:v:120:ARG:HH11	64:v:120:ARG:CG	2.13	0.61
70:Y:35:DC:H1'	70:Y:36:DC:C5	2.35	0.61
3:9:33:LYS:O	3:9:33:LYS:HD3	2.00	0.61
3:9:277:LEU:O	3:9:277:LEU:HD12	1.99	0.61
12:PC:148:ILE:HD11	19:PJ:13:ILE:HG21	1.81	0.61
24:DD:890:GLY:HA3	31:DL:104:ARG:HH22	1.64	0.61
39:3:190:LEU:HB2	39:3:235:GLN:HE21	1.66	0.61
42:6:62:ARG:HB2	42:6:75:PRO:HD3	1.81	0.61
43:7:315:LEU:HD23	43:7:373:ARG:HH21	1.65	0.61
48:m:101:GLN:HA	57:n:169:LEU:HD23	1.80	0.61
48:m:124:GLN:OE1	65:z:590:ARG:HB3	1.98	0.61
49:a:316:ALA:HB2	49:a:447:GLU:HG2	1.82	0.61
56:k:12:ARG:CD	56:k:66:GLN:NE2	2.61	0.61
67:w:6:GLN:CB	67:w:62:TRP:CH2	2.83	0.61
67:w:19:GLU:HA	67:w:25:MET:CG	2.30	0.61
10:PA:191:ILE:HG23	10:PA:200:ALA:HB2	1.80	0.61
12:PC:44:ILE:HG23	12:PC:176:TRP:HB3	1.82	0.61
13:PD:137:LYS:HZ2	53:h:52:LEU:HA	1.56	0.61
29:DI:23:LEU:HD21	29:DI:39:MET:SD	2.40	0.61
48:m:59:LYS:HZ3	48:m:77:GLU:CD	1.99	0.61
50:d:121:LEU:HD11	63:u:111:GLY:O	2.00	0.61
57:n:229:GLU:HB2	57:n:254:VAL:HG22	1.82	0.61
58:o:690:LEU:HD22	59:q:605:PRO:CG	2.30	0.61
59:q:34:LEU:HD23	59:q:34:LEU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:p:225:ASN:ND2	68:p:245:CYS:SG	2.74	0.61
2:8:237:TRP:CG	2:8:237:TRP:O	2.53	0.61
13:PD:137:LYS:NZ	53:h:52:LEU:N	2.47	0.61
37:1:187:ASN:CA	37:1:191:ASP:HB3	2.30	0.61
52:g:24:GLU:HB2	52:g:33:LYS:HE2	1.80	0.61
54:i:72:ILE:CD1	54:i:92:SER:HB3	2.24	0.61
58:o:718:VAL:HG12	58:o:720:PRO:HD2	1.82	0.61
5:DP:220:VAL:HG22	69:X:-24:DA:C1'	2.29	0.61
11:PB:625:LEU:HD13	11:PB:675:LEU:HD21	1.83	0.61
48:m:68:LYS:CE	52:g:50:GLN:HE22	2.13	0.61
56:k:42:GLU:HA	56:k:42:GLU:OE2	2.00	0.61
57:n:659:LEU:HD12	67:w:14:LYS:HG2	1.77	0.61
59:q:213:GLY:HA3	59:q:386:THR:OG1	1.99	0.61
7:BA:297:PRO:HA	7:BA:310:VAL:HG11	1.82	0.61
8:FA:121:ASN:O	9:FB:25:LYS:HE2	2.01	0.61
25:DE:613:ALA:HB2	25:DE:620:LEU:HD11	1.81	0.61
29:DI:16:ALA:HA	29:DI:40:LEU:CD1	2.22	0.61
35:EA:136:PHE:HB3	35:EA:144:LEU:HD11	1.82	0.61
37:1:161:LYS:O	37:1:162:GLN:HB2	1.99	0.61
37:1:369:VAL:HA	37:1:374:LEU:HB2	1.81	0.61
40:4:364:ILE:O	40:4:368:LEU:N	2.33	0.61
40:4:441:MET:N	41:5:5:LEU:HD23	2.11	0.61
42:6:425:ARG:HA	42:6:428:GLU:HG2	1.81	0.61
43:7:460:THR:HG23	43:7:661:ALA:HB3	1.81	0.61
54:i:109:LEU:CD2	54:i:117:GLN:HE22	2.13	0.61
57:n:706:LEU:O	58:o:684:ARG:NH2	2.29	0.61
69:X:5:DG:H21	70:Y:-5:DC:H5	1.47	0.61
3:9:164:TYR:O	3:9:167:PHE:N	2.33	0.61
14:PE:194:ILE:HG12	14:PE:204:ILE:HG23	1.81	0.61
26:DF:28:ILE:CG1	29:DI:55:LYS:HD3	2.29	0.61
40:4:443:VAL:HG21	40:4:451:VAL:HG11	1.81	0.61
42:6:76:LEU:HD23	42:6:87:GLU:HG2	1.81	0.61
52:g:89:PHE:HE1	63:u:23:ILE:HD11	1.66	0.61
52:g:111:ASP:HB3	61:s:69:ARG:HH21	1.64	0.61
52:g:159:ARG:HD3	52:g:159:ARG:C	2.26	0.61
59:q:142:GLN:H	59:q:142:GLN:CD	2.08	0.61
59:q:149:LYS:CE	64:v:40:ALA:C	2.68	0.61
1:0:288:THR:C	1:0:290:SER:N	2.57	0.61
8:FA:47:LEU:HB3	9:FB:7:LEU:HB2	1.82	0.61
10:PA:72:GLN:HG2	35:EA:156:PHE:CE2	2.35	0.61
13:PD:15:GLU:HA	13:PD:21:ILE:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DI:32:GLU:CB	29:DI:35:VAL:HG23	2.31	0.61
35:EA:34:LEU:HA	35:EA:37:LEU:HB2	1.83	0.61
39:3:289:PHE:HB2	39:3:294:PRO:HG2	1.82	0.61
42:6:359:LYS:HZ2	42:6:436:GLY:HA2	1.63	0.61
50:d:45:ILE:CD1	54:i:73:ILE:CG1	2.78	0.61
55:j:61:ILE:HG22	55:j:61:ILE:O	2.01	0.61
58:o:762:GLN:C	67:w:74:LYS:HZ2	2.08	0.61
60:r:19:MET:CG	60:r:21:TYR:CE1	2.84	0.61
2:8:276:PHE:O	2:8:277:LEU:C	2.42	0.61
3:9:175:LYS:HA	3:9:175:LYS:NZ	2.15	0.61
10:PA:193:ARG:HA	10:PA:198:LEU:HA	1.83	0.61
10:PA:1374:VAL:HG11	10:PA:1411:LEU:HD11	1.83	0.61
11:PB:223:SER:HB2	11:PB:233:SER:H	1.64	0.61
13:PD:140:PHE:HE1	64:v:64:ARG:HD3	1.64	0.61
35:EA:55:ASP:HB3	35:EA:58:GLN:HB2	1.82	0.61
40:4:339:PRO:HG2	42:6:55:GLU:HG2	1.83	0.61
42:6:538:PRO:HA	42:6:541:PHE:HB3	1.83	0.61
48:m:66:TYR:HE1	52:g:52:ASP:CG	2.09	0.61
48:m:108:TYR:CZ	57:n:168:ARG:NH1	2.69	0.61
50:d:47:MET:HA	50:d:47:MET:HE3	1.83	0.61
52:g:88:ASN:HD22	61:s:69:ARG:NH2	1.99	0.61
56:k:87:ARG:CA	64:v:105:LEU:HD13	2.21	0.61
57:n:199:LEU:HD22	57:n:222:VAL:HG13	1.83	0.61
57:n:417:LYS:HG3	57:n:421:ARG:HE	1.65	0.61
66:x:650:LEU:HB2	66:x:659:TYR:HE2	1.64	0.61
1:0:199:ALA:HA	1:0:202:LYS:HB2	1.83	0.61
4:DO:5:LEU:HA	24:DD:1007:THR:HG21	1.83	0.61
5:DP:313:THR:CG2	69:X:-27:DA:C5'	2.78	0.61
22:DA:349:TRP:NE1	26:Df:262:PHE:O	2.33	0.61
24:DD:965:ILE:HG23	24:DD:983:ARG:HD3	1.81	0.61
26:DF:28:ILE:HG12	29:DI:55:LYS:HD3	1.83	0.61
29:DI:132:LEU:CG	30:DJ:121:MET:HE2	2.30	0.61
36:EB:158:HIS:O	36:EB:161:ARG:HG3	2.01	0.61
48:m:56:LEU:CD2	48:m:80:GLN:HE22	2.12	0.61
49:a:224:TYR:CZ	49:a:253:MET:HB3	2.36	0.61
50:d:121:LEU:CB	63:u:115:LEU:HD12	2.24	0.61
52:g:89:PHE:CD2	63:u:19:PHE:CE1	2.89	0.61
67:w:19:GLU:HA	67:w:25:MET:HG2	1.82	0.61
5:DP:287:LEU:HG	69:X:-29:DA:H5"	1.82	0.60
9:FB:20:LEU:O	9:FB:113:ARG:HA	2.01	0.60
31:Dl:76:LEU:HD13	31:Dl:84:LEU:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1:513:ARG:HG3	37:1:514:ARG:HG3	1.81	0.60
40:4:377:LEU:HD23	40:4:378:LYS:HG3	1.82	0.60
51:f:177:VAL:HG11	57:n:266:VAL:HG22	1.82	0.60
56:k:101:ARG:HH11	56:k:101:ARG:CG	2.14	0.60
56:k:109:ARG:HH11	56:k:109:ARG:CG	2.14	0.60
63:u:57:LEU:HD13	65:z:492:ARG:CG	2.31	0.60
23:DB:203:LYS:HD3	23:DB:237:MET:HE3	1.83	0.60
38:2:12:GLU:CD	42:6:130:GLY:HA3	2.25	0.60
38:2:363:CYS:SG	38:2:365:ASN:ND2	2.74	0.60
43:7:67:VAL:HB	43:7:228:LYS:HD2	1.82	0.60
53:h:99:VAL:O	53:h:99:VAL:HG23	2.01	0.60
59:q:1:MET:H3	65:z:540:LEU:HD13	1.31	0.60
10:PA:983:LEU:H	10:PA:983:LEU:HD13	1.66	0.60
32:Dc:67:GLY:CA	30:Dj:116:LEU:CD1	2.71	0.60
29:Di:73:LEU:HB2	31:Dl:105:HIS:HE1	1.66	0.60
40:4:205:LEU:HD22	40:4:367:PHE:CE2	2.30	0.60
59:q:109:MET:HE3	59:q:109:MET:O	2.00	0.60
62:t:136:ARG:HG3	62:t:136:ARG:O	2.00	0.60
16:PG:108:ILE:HD13	16:PG:163:LEU:HD13	1.83	0.60
23:DB:400:ASP:HA	23:DB:403:VAL:HG22	1.83	0.60
28:DH:192:ARG:NH1	28:DH:209:SER:O	2.34	0.60
31:DL:56:GLN:NE2	31:DL:85:LEU:HD22	2.17	0.60
38:2:63:VAL:HB	38:2:106:ILE:HA	1.82	0.60
42:6:343:GLY:H	42:6:346:LYS:HZ2	1.48	0.60
42:6:625:GLN:NE2	42:6:627:SER:O	2.35	0.60
48:m:56:LEU:HG	48:m:80:GLN:HE22	1.66	0.60
4:DO:58:PHE:CD2	6:DQ:370:ALA:HB1	2.37	0.60
5:DP:301:VAL:CB	69:X:-27:DA:H5"	2.15	0.60
8:FA:121:ASN:O	9:FB:25:LYS:CG	2.47	0.60
9:FB:131:GLN:HA	9:FB:134:GLU:HB3	1.84	0.60
11:PB:1068:GLN:HG2	11:PB:1075:MET:HB2	1.82	0.60
37:1:234:ARG:HG2	37:1:240:LYS:HD3	1.83	0.60
43:7:482:THR:OG1	43:7:695:ARG:NE	2.35	0.60
48:m:22:LEU:HD13	52:g:43:MET:CE	2.30	0.60
56:k:29:GLY:O	56:k:33:LEU:CG	2.42	0.60
58:o:715:LEU:H	66:x:25:ILE:CD1	2.15	0.60
63:u:57:LEU:HD11	65:z:492:ARG:NE	2.17	0.60
64:v:48:VAL:CG2	64:v:52:THR:OG1	2.49	0.60
64:v:127:LEU:HD12	64:v:127:LEU:O	2.02	0.60
67:w:25:MET:SD	67:w:28:ASP:HB3	2.40	0.60
67:w:113:GLN:HE22	67:w:159:GLN:HE22	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:FB:137:LYS:O	9:FB:137:LYS:HD3	2.01	0.60
10:PA:406:VAL:HG23	10:PA:429:LEU:HD13	1.84	0.60
11:PB:636:LYS:H	11:PB:639:HIS:HD2	1.50	0.60
23:DB:583:GLU:CD	23:DB:583:GLU:H	2.06	0.60
29:DI:23:LEU:CD1	29:DI:31:TYR:CZ	2.85	0.60
30:DJ:170:ALA:HB2	30:DJ:203:ALA:HB2	1.83	0.60
44:c:214:VAL:H	44:c:243:THR:HG22	1.65	0.60
45:e:136:LEU:CD1	56:k:107:VAL:HG12	2.32	0.60
45:e:140:GLN:HE22	56:k:105:SER:HA	1.65	0.60
49:a:229:SER:HB3	49:a:502:MET:CB	2.23	0.60
50:d:27:ARG:HD2	54:i:108:HIS:CA	2.25	0.60
50:d:46:GLU:HA	54:i:76:MET:CE	2.30	0.60
51:f:181:LEU:CD2	57:n:274:ILE:CG1	2.79	0.60
53:h:19:VAL:HG11	59:q:113:TYR:CB	2.30	0.60
59:q:36:MET:HE2	59:q:40:LEU:HD23	1.84	0.60
67:w:33:GLU:HB3	67:w:36:LYS:HB3	1.82	0.60
3:9:239:LYS:NZ	3:9:239:LYS:HB2	2.17	0.60
15:PF:64:ARG:HH21	16:PG:61:PRO:HB3	1.66	0.60
17:PH:123:MET:HE3	17:PH:125:LEU:HB2	1.83	0.60
18:PI:24:LEU:HD23	18:PI:39:CYS:N	2.16	0.60
32:Dc:18:CYS:O	32:Dc:23:TRP:HB2	2.01	0.60
32:Dc:99:PHE:HB2	32:Dc:100:PRO:HD3	1.83	0.60
34:Dm:31:LEU:HD23	34:Dm:31:LEU:N	2.16	0.60
46:b:59:ARG:HH21	46:b:63:LEU:HD11	1.66	0.60
54:i:65:PHE:HE1	54:i:99:LYS:CA	2.15	0.60
54:i:119:GLN:OE1	54:i:119:GLN:HA	2.01	0.60
55:j:34:GLN:OE1	55:j:37:LEU:CG	2.50	0.60
55:j:43:PHE:CE1	61:s:147:THR:O	2.54	0.60
57:n:141:ARG:HH22	63:u:16:ALA:C	2.09	0.60
11:PB:584:MET:HE1	11:PB:612:ILE:HG12	1.82	0.60
35:EA:73:LYS:HG2	35:EA:100:VAL:HG13	1.83	0.60
37:1:175:ARG:HH21	37:1:310:HIS:HB2	1.65	0.60
40:4:307:ILE:HG22	40:4:316:TYR:HB3	1.83	0.60
43:7:70:LEU:HD23	43:7:204:VAL:HG13	1.84	0.60
50:d:121:LEU:HD13	63:u:115:LEU:CD1	2.30	0.60
52:g:89:PHE:CD2	63:u:19:PHE:CD1	2.89	0.60
56:k:21:ILE:CD1	59:q:168:THR:CA	2.80	0.60
7:BA:189:LYS:CE	69:X:-29:DA:OP2	2.46	0.60
14:PE:84:ILE:HG23	14:PE:114:ALA:HA	1.84	0.60
18:PI:86:CYS:HB3	18:PI:90:GLY:H	1.66	0.60
24:DD:895:HIS:CE1	24:DD:896:PRO:HD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1:257:MET:SD	43:7:582:GLU:HB2	2.42	0.60
37:1:478:CYS:HB3	37:1:484:PRO:HG3	1.84	0.60
43:7:229:ALA:HB3	43:7:451:PHE:HA	1.83	0.60
48:m:17:ARG:HH22	52:g:33:LYS:HB3	1.65	0.60
52:g:93:LEU:HD13	55:j:106:LYS:HE2	1.84	0.60
56:k:21:ILE:HD12	59:q:168:THR:HA	1.83	0.60
57:n:651:ASN:OD1	57:n:680:HIS:NE2	2.34	0.60
58:o:691:VAL:HA	58:o:708:CYS:HA	1.84	0.60
59:q:19:VAL:O	59:q:19:VAL:HG22	2.01	0.60
60:r:17:ASN:OD1	60:r:17:ASN:N	2.35	0.60
62:t:175:VAL:HG21	62:t:192:GLN:HG3	1.82	0.60
1:0:200:GLN:O	1:0:204:ARG:NH1	2.34	0.60
4:DO:5:LEU:HD13	4:DO:98:CYS:SG	2.42	0.60
10:PA:871:VAL:HG12	10:PA:879:VAL:HG12	1.83	0.60
35:EA:141:ALA:HA	35:EA:144:LEU:HB2	1.84	0.60
57:n:685:LEU:CD2	58:o:729:TYR:HE2	2.14	0.60
63:u:28:GLN:CG	65:z:483:ASN:ND2	2.65	0.60
64:v:48:VAL:HG22	64:v:52:THR:OG1	2.02	0.60
66:x:251:GLU:HG3	66:x:263:LEU:HD13	1.82	0.60
1:0:68:VAL:HG13	1:0:71:GLU:HB3	1.83	0.59
1:0:287:TYR:CB	2:8:189:MET:HG2	2.32	0.59
3:9:167:PHE:C	3:9:167:PHE:CD1	2.78	0.59
8:FA:121:ASN:C	9:FB:25:LYS:HE2	2.26	0.59
8:FA:126:ILE:N	8:FA:138:PHE:O	2.22	0.59
13:PD:137:LYS:CD	53:h:55:GLN:HB3	2.15	0.59
16:PG:49:THR:HG23	16:PG:50:THR:H	1.67	0.59
23:DB:431:LEU:O	23:DB:431:LEU:HD23	2.02	0.59
31:DL:111:LEU:O	31:DL:114:LYS:HE3	2.01	0.59
29:Di:73:LEU:CD1	31:Dl:105:HIS:CE1	2.84	0.59
42:6:164:GLY:HA2	42:6:293:ALA:HB3	1.83	0.59
49:a:417:TYR:CD1	49:a:450:PHE:CE1	2.89	0.59
49:a:509:ARG:CZ	49:a:509:ARG:CB	2.79	0.59
51:f:101:ILE:CD1	53:h:105:VAL:CG1	2.79	0.59
57:n:821:SER:O	57:n:833:ILE:HA	2.02	0.59
59:q:130:VAL:O	59:q:130:VAL:HG12	2.01	0.59
63:u:4:ARG:CD	65:z:594:LEU:O	2.50	0.59
67:w:13:VAL:CG1	67:w:75:ARG:CG	2.79	0.59
67:w:281:ASP:OD1	67:w:281:ASP:N	2.31	0.59
67:w:765:ARG:HA	67:w:768:LYS:HE2	1.84	0.59
2:8:239:ASP:CA	2:8:242:SER:HB3	2.28	0.59
10:PA:811:ILE:HG12	11:PB:689:TYR:OH	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:PE:59:THR:HG22	14:PE:76:PHE:H	1.66	0.59
29:DI:23:LEU:CG	29:DI:39:MET:HE1	2.31	0.59
57:n:203:LEU:HD21	57:n:224:PHE:HZ	1.67	0.59
57:n:685:LEU:HD22	58:o:729:TYR:CE2	2.36	0.59
63:u:79:GLU:CD	63:u:82:THR:HG21	2.28	0.59
10:PA:630:VAL:HG22	10:PA:635:LEU:HD12	1.84	0.59
11:PB:629:GLU:O	11:PB:630:LYS:C	2.44	0.59
11:PB:677:MET:HE2	11:PB:700:PRO:HB3	1.83	0.59
13:PD:23:PRO:HD3	16:PG:80:PHE:CE2	2.36	0.59
28:DH:94:VAL:HG12	28:DH:104:VAL:HG21	1.84	0.59
44:c:111:TYR:CZ	46:b:136:HIS:CG	2.90	0.59
49:a:131:ASN:H	49:a:131:ASN:HD22	1.50	0.59
49:a:367:LEU:HD22	49:a:509:ARG:HH11	1.67	0.59
49:a:380:ALA:HB3	49:a:444:PRO:CG	2.32	0.59
53:h:61:LYS:HG2	53:h:65:HIS:CE1	2.37	0.59
53:h:77:ILE:CG1	59:q:126:THR:CG2	2.69	0.59
56:k:88:LYS:HD2	56:k:88:LYS:C	2.27	0.59
57:n:315:LEU:HD22	57:n:319:ARG:HD2	1.83	0.59
66:x:414:GLU:OE2	66:x:460:LYS:NZ	2.34	0.59
69:X:-33:DG:C6	70:Y:34:DG:C6	2.88	0.59
3:9:181:LEU:O	3:9:181:LEU:HD22	2.03	0.59
8:FA:102:VAL:O	8:FA:108:ARG:N	2.35	0.59
10:PA:397:PHE:HB3	15:PF:87:THR:HG23	1.83	0.59
11:PB:112:GLU:HG3	21:PL:43:ILE:HD11	1.84	0.59
37:1:188:LEU:H	37:1:191:ASP:HB3	1.67	0.59
39:3:213:LEU:HD11	39:3:245:PRO:HG2	1.84	0.59
40:4:346:VAL:HG12	40:4:348:ARG:H	1.68	0.59
43:7:495:ILE:O	43:7:708:LEU:N	2.35	0.59
43:7:599:VAL:HG12	43:7:602:GLY:H	1.67	0.59
45:e:129:VAL:HG11	56:k:114:MET:HE2	1.84	0.59
52:g:89:PHE:CB	63:u:19:PHE:HE1	2.14	0.59
57:n:237:MET:HE1	59:q:45:GLN:CG	2.32	0.59
57:n:371:GLN:HG3	57:n:390:MET:HE1	1.84	0.59
57:n:937:ARG:NE	57:n:943:LEU:CD2	2.64	0.59
59:q:9:ILE:CG1	63:u:90:LEU:HB2	2.31	0.59
63:u:16:ALA:HA	63:u:19:PHE:HD2	1.67	0.59
67:w:394:PRO:HG3	68:p:171:PHE:CE1	2.36	0.59
1:0:78:VAL:HG11	43:7:334:ARG:HH22	1.68	0.59
1:0:145:GLU:HG3	53:h:3:ARG:HH12	1.54	0.59
7:BA:27:TYR:CB	7:BA:28:ARG:NH1	2.64	0.59
11:PB:156:LEU:HD22	11:PB:184:TYR:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:274:ARG:O	11:PB:277:GLY:N	2.36	0.59
11:PB:592:ARG:CB	11:PB:592:ARG:CZ	2.77	0.59
11:PB:929:PRO:HB3	11:PB:935:PHE:HZ	1.68	0.59
11:PB:1062:ARG:CZ	11:PB:1074:PRO:HB3	2.32	0.59
25:DE:518:LYS:HA	25:DE:523:VAL:HG11	1.83	0.59
29:DI:23:LEU:HD12	29:DI:31:TYR:CZ	2.37	0.59
26:Df:330:ARG:HH22	26:Df:371:THR:HB	1.66	0.59
50:d:38:GLU:OE2	54:i:96:GLU:HB3	2.03	0.59
52:g:56:ILE:HD12	52:g:56:ILE:N	2.18	0.59
55:j:19:ILE:HD12	55:j:45:VAL:HG22	1.82	0.59
55:j:75:ARG:HA	55:j:79:LEU:CD1	2.33	0.59
57:n:659:LEU:HD13	67:w:14:LYS:CG	2.29	0.59
59:q:162:LYS:O	59:q:166:ARG:CG	2.50	0.59
10:PA:1167:ARG:HG2	10:PA:1293:LEU:HG	1.84	0.59
22:DA:475:LEU:HD21	26:Df:301:VAL:HG12	1.85	0.59
42:6:497:GLN:HE21	42:6:504:LYS:HA	1.68	0.59
42:6:688:LYS:NZ	42:6:689:VAL:O	2.33	0.59
49:a:232:LEU:HD13	49:a:232:LEU:O	2.02	0.59
51:f:106:TYR:CE2	53:h:106:PRO:HG3	2.38	0.59
52:g:88:ASN:HD22	61:s:69:ARG:CZ	2.15	0.59
53:h:19:VAL:HG12	59:q:113:TYR:HD2	1.67	0.59
53:h:26:LEU:HD22	59:q:102:LEU:HD22	1.84	0.59
54:i:85:GLN:HG2	54:i:86:ASP:OD1	1.98	0.59
55:j:42:ASN:O	55:j:46:THR:HG23	2.01	0.59
57:n:192:LEU:HD11	57:n:220:GLY:HA3	1.84	0.59
57:n:587:LEU:CD1	67:w:15:THR:HB	2.29	0.59
58:o:765:ASP:HB3	67:w:72:SER:OG	2.02	0.59
59:q:451:LEU:HD11	59:q:529:MET:CE	2.32	0.59
67:w:895:ASP:O	67:w:899:ARG:NH1	2.35	0.59
1:0:288:THR:O	1:0:290:SER:N	2.36	0.59
10:PA:189:PRO:HA	10:PA:202:TRP:HA	1.83	0.59
10:PA:419:ILE:HD12	10:PA:438:LEU:HD22	1.83	0.59
10:PA:544:ALA:HB1	10:PA:676:ILE:HG22	1.83	0.59
13:PD:133:ASP:OD2	53:h:59:LEU:HD22	2.03	0.59
16:PG:30:LEU:HD22	16:PG:72:TYR:CZ	2.37	0.59
22:DA:349:TRP:CE2	26:Df:266:GLY:CA	2.85	0.59
22:DA:567:LEU:CB	23:DB:745:GLN:NE2	2.66	0.59
49:a:160:LEU:CD1	49:a:219:LEU:HD21	2.33	0.59
52:g:171:LEU:HG	54:i:132:LEU:HD22	1.83	0.59
53:h:151:LEU:HD21	64:v:37:ILE:HB	1.83	0.59
57:n:266:VAL:HG23	57:n:303:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:t:131:MET:O	62:t:131:MET:HE3	2.02	0.59
63:u:79:GLU:OE2	63:u:82:THR:HG23	2.02	0.59
69:X:-33:DG:N1	70:Y:34:DG:O6	2.31	0.59
1:0:198:LEU:HD23	1:0:199:ALA:N	2.17	0.59
7:BA:127:ARG:HG3	7:BA:127:ARG:NH2	2.16	0.59
11:PB:47:PHE:C	11:PB:49:GLU:H	2.10	0.59
11:PB:128:ILE:HD12	11:PB:431:LEU:HD13	1.83	0.59
11:PB:274:ARG:HG2	11:PB:279:VAL:HA	1.82	0.59
22:DA:353:LEU:HD11	22:DA:495:LEU:HG	1.84	0.59
37:1:481:VAL:HG12	37:1:483:THR:HG23	1.85	0.59
37:1:491:VAL:HG23	37:1:494:LYS:HD2	1.84	0.59
42:6:158:LEU:HD11	42:6:161:VAL:HA	1.83	0.59
56:k:101:ARG:HH11	56:k:101:ARG:HG2	1.67	0.59
62:t:6:VAL:HA	62:t:140:VAL:O	2.03	0.59
68:p:61:MET:HE2	68:p:75:SER:HB3	1.85	0.59
4:DO:58:PHE:HB2	6:DQ:371:ILE:O	2.02	0.59
38:2:335:PRO:O	38:2:353:LYS:NZ	2.35	0.59
48:m:116:GLN:CG	65:z:594:LEU:CG	2.61	0.59
52:g:89:PHE:CZ	63:u:19:PHE:HD1	2.21	0.59
57:n:918:PHE:HB2	57:n:922:TYR:HB2	1.85	0.59
59:q:138:LYS:CD	59:q:140:ASN:OD1	2.41	0.59
68:p:166:PRO:HG2	68:p:169:THR:HG22	1.84	0.59
68:p:232:ASP:OD1	68:p:232:ASP:N	2.31	0.59
10:PA:40:GLY:HA2	10:PA:87:HIS:O	2.02	0.59
11:PB:128:ILE:CD1	11:PB:435:ILE:HD11	2.33	0.59
23:DB:158:GLY:HA2	23:DB:188:PHE:HB3	1.84	0.59
37:1:166:ILE:HG23	37:1:166:ILE:O	2.03	0.59
37:1:387:THR:HG23	37:1:388:PRO:HD3	1.85	0.59
40:4:200:GLY:O	40:4:204:LEU:N	2.33	0.59
42:6:728:VAL:HG13	70:Y:-14:DG:OP1	2.03	0.59
43:7:53:LEU:HA	43:7:56:ILE:HB	1.84	0.59
46:b:78:ALA:CB	58:o:621:LEU:HD21	2.31	0.59
49:a:364:TYR:O	49:a:428:THR:CG2	2.51	0.59
59:q:290:HIS:HE1	59:q:294:LYS:NZ	2.01	0.59
59:q:534:VAL:HG11	59:q:567:SER:HB3	1.83	0.59
59:q:597:PRO:HA	59:q:619:ARG:HA	1.84	0.59
1:0:274:HIS:H	1:0:277:ALA:HA	1.66	0.58
2:8:191:GLY:C	2:8:193:GLY:N	2.59	0.58
3:9:177:ARG:HB2	3:9:177:ARG:CZ	2.32	0.58
5:DP:218:LYS:HG3	69:X:-23:DG:OP1	2.00	0.58
10:PA:395:THR:HG22	10:PA:396:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:491:PRO:HG2	10:PA:535:MET:HE2	1.86	0.58
10:PA:1424:THR:HB	10:PA:1428:MET:HB3	1.84	0.58
18:PI:24:LEU:HD13	18:PI:46:GLN:HE22	1.66	0.58
24:DD:937:ALA:HB3	29:DI:126:ASN:HB3	1.85	0.58
53:h:74:GLN:HE21	59:q:129:PRO:HB3	1.61	0.58
53:h:86:ASP:H	53:h:99:VAL:HG12	1.67	0.58
55:j:96:LYS:NZ	61:s:81:THR:N	2.50	0.58
57:n:250:LEU:HG	57:n:275:HIS:CA	2.33	0.58
67:w:433:ASN:ND2	67:w:445:ILE:O	2.35	0.58
1:0:282:ASP:O	1:0:285:GLY:N	2.36	0.58
4:DO:75:VAL:HG21	6:DQ:327:GLU:HG3	1.84	0.58
12:PC:261:THR:HG21	62:t:135:ALA:HB2	1.84	0.58
24:DD:940:VAL:O	24:DD:944:LEU:HB2	2.02	0.58
37:1:360:TYR:O	37:1:364:GLY:N	2.36	0.58
37:1:516:TYR:HA	37:1:519:THR:HG22	1.86	0.58
42:6:52:LYS:O	42:6:56:TYR:N	2.33	0.58
43:7:84:ILE:HG23	43:7:174:ILE:HG12	1.84	0.58
44:c:111:TYR:CE1	46:b:136:HIS:CG	2.91	0.58
56:k:24:ILE:HG21	59:q:164:ALA:HB2	0.59	0.58
57:n:192:LEU:HD12	57:n:220:GLY:N	2.16	0.58
59:q:186:GLU:HG2	59:q:243:LEU:HD22	1.58	0.58
59:q:647:SER:HB3	59:q:648:PRO:CD	2.32	0.58
62:t:9:MET:H	62:t:138:ILE:HG22	1.69	0.58
3:9:114:LYS:HA	3:9:114:LYS:CE	2.33	0.58
8:FA:45:ALA:HB2	9:FB:9:LEU:HD21	1.83	0.58
11:PB:220:GLU:HG2	11:PB:236:TRP:CD1	2.38	0.58
21:PL:16:ILE:HD11	21:PL:25:GLU:HB2	1.85	0.58
25:DE:586:TYR:HB3	25:DE:605:HIS:HB3	1.85	0.58
32:Dc:12:VAL:HG23	26:Df:118:ILE:HA	1.86	0.58
37:1:387:THR:OG1	37:1:393:GLN:NE2	2.37	0.58
38:2:111:SER:HA	38:2:141:GLY:HA3	1.86	0.58
48:m:116:GLN:HG3	65:z:594:LEU:CG	2.13	0.58
51:f:101:ILE:CD1	53:h:105:VAL:HG11	2.33	0.58
53:h:8:LEU:HD23	53:h:8:LEU:O	2.03	0.58
55:j:96:LYS:HE2	61:s:81:THR:HA	1.86	0.58
55:j:97:GLY:O	55:j:101:THR:HG23	2.03	0.58
57:n:155:PRO:HA	57:n:158:ILE:HD12	1.83	0.58
62:t:8:GLN:HG3	62:t:196:LEU:HD21	1.84	0.58
3:9:114:LYS:HA	3:9:114:LYS:HE2	1.84	0.58
3:9:229:GLU:N	3:9:229:GLU:CD	2.61	0.58
35:EA:127:PHE:HE2	35:EA:138:ASP:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:15:GLN:OE1	40:4:18:ASN:ND2	2.36	0.58
41:5:18:GLN:HE21	42:6:520:ARG:HE	1.52	0.58
43:7:114:ASN:HB3	43:7:181:LYS:HE3	1.84	0.58
49:a:94:LEU:HD23	49:a:94:LEU:H	1.69	0.58
51:f:181:LEU:CD2	57:n:274:ILE:HG13	2.32	0.58
52:g:48:GLN:OE1	52:g:48:GLN:N	2.22	0.58
53:h:77:ILE:CG1	59:q:126:THR:HB	2.33	0.58
53:h:85:ARG:HD2	53:h:99:VAL:HG11	1.85	0.58
57:n:265:LEU:O	57:n:265:LEU:HD22	2.02	0.58
60:r:19:MET:HE1	60:r:177:ALA:CA	2.07	0.58
64:v:86:LEU:O	64:v:90:ASP:HB2	2.04	0.58
67:w:9:PHE:CB	67:w:66:PHE:HE2	1.93	0.58
67:w:764:TYR:OH	67:w:799:GLU:OE2	2.22	0.58
2:8:132:TRP:HA	2:8:132:TRP:CE3	2.38	0.58
10:PA:541:THR:HG21	10:PA:673:GLN:HA	1.84	0.58
23:DB:489:GLN:OE1	23:DB:489:GLN:N	2.34	0.58
26:DF:324:ASP:HA	26:DF:327:TRP:HD1	1.67	0.58
53:h:142:SER:OG	56:k:39:LYS:HE2	2.00	0.58
57:n:234:LEU:HD21	57:n:282:LEU:CD2	2.33	0.58
57:n:375:ASP:HB3	57:n:376:PRO:HD3	1.85	0.58
57:n:377:PRO:HG2	57:n:408:ARG:HH21	1.66	0.58
10:PA:1210:TRP:CH2	18:PI:28:GLU:HB3	2.38	0.58
22:DA:564:PRO:HG2	23:DB:744:PHE:CZ	2.39	0.58
40:4:71:VAL:HA	40:4:74:TRP:HB2	1.84	0.58
42:6:625:GLN:OE1	42:6:676:ARG:NH2	2.37	0.58
42:6:665:GLN:O	42:6:667:THR:OG1	2.22	0.58
47:l:156:LEU:CD2	64:v:134:TYR:HB2	2.34	0.58
48:m:23:GLU:OE1	52:g:46:GLY:N	2.37	0.58
49:a:160:LEU:CD1	49:a:214:ARG:NH2	2.67	0.58
52:g:93:LEU:HB3	55:j:106:LYS:CD	2.33	0.58
53:h:97:VAL:HG23	53:h:104:VAL:HG21	1.85	0.58
56:k:32:ILE:HG13	59:q:157:ALA:HB1	1.85	0.58
57:n:587:LEU:CD1	67:w:15:THR:CG2	2.80	0.58
61:s:80:SER:O	61:s:83:LEU:HD23	2.04	0.58
63:u:81:SER:C	63:u:83:ALA:H	2.12	0.58
69:X:-33:DG:C2	70:Y:34:DG:C6	2.90	0.58
7:BA:189:LYS:CD	69:X:-30:DT:H5'	2.25	0.58
8:FA:46:ARG:NH2	9:FB:3:GLU:OE1	2.36	0.58
9:FB:199:LEU:HB2	9:FB:233:TRP:HE1	1.69	0.58
11:PB:34:PHE:HZ	11:PB:528:LEU:HB3	1.67	0.58
11:PB:289:ILE:HD13	11:PB:297:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:941:GLN:HE21	11:PB:977:THR:HG21	1.68	0.58
23:DB:629:ARG:NH1	23:DB:658:ASP:OD2	2.37	0.58
23:DB:732:CYS:SG	28:DH:173:GLN:HB2	2.44	0.58
26:Df:297:LEU:O	26:Df:301:VAL:HB	2.04	0.58
38:2:305:CYS:SG	38:2:306:LYS:N	2.76	0.58
42:6:415:HIS:NE2	70:Y:-12:DT:C5'	2.50	0.58
57:n:250:LEU:HG	57:n:275:HIS:HA	1.86	0.58
57:n:820:ILE:HD11	57:n:833:ILE:HB	1.86	0.58
64:v:108:LEU:HD12	64:v:108:LEU:O	2.04	0.58
67:w:726:ASN:ND2	67:w:726:ASN:H	2.01	0.58
10:PA:581:LYS:HZ1	17:PH:86:ASP:HA	1.69	0.58
11:PB:729:GLY:C	11:PB:731:GLN:H	2.11	0.58
24:Dd:1082:ALA:CB	31:Dl:83:MET:HE2	2.31	0.58
37:1:496:ASN:HA	37:1:499:ARG:HB2	1.84	0.58
48:m:14:ASN:CA	52:g:39:LYS:HZ1	2.17	0.58
49:a:316:ALA:CB	49:a:447:GLU:HG2	2.34	0.58
50:d:42:ARG:NH2	54:i:96:GLU:OE1	2.35	0.58
53:h:33:LEU:HD23	53:h:40:LEU:HD23	1.86	0.58
55:j:89:LEU:CG	61:s:93:TYR:HE1	2.17	0.58
62:t:124:VAL:HG13	62:t:142:VAL:HG22	1.86	0.58
67:w:855:TRP:O	67:w:858:ASN:ND2	2.37	0.58
3:9:239:LYS:HB2	3:9:239:LYS:HZ3	1.69	0.58
5:DP:220:VAL:HG22	69:X:-24:DA:H1'	1.81	0.58
8:FA:125:TYR:HD2	9:FB:23:VAL:HG21	1.69	0.58
13:PD:79:THR:HG23	53:h:51:LEU:HD11	1.86	0.58
13:PD:137:LYS:CD	53:h:51:LEU:HD11	2.30	0.58
14:PE:47:LYS:O	14:PE:53:PRO:HD2	2.03	0.58
24:DD:962:GLU:HA	24:DD:965:ILE:HB	1.85	0.58
39:3:78:LEU:HA	39:3:81:PHE:HB3	1.86	0.58
42:6:62:ARG:CA	42:6:73:SER:HB2	2.22	0.58
43:7:535:ILE:HG12	43:7:617:ALA:HB3	1.86	0.58
44:c:238:VAL:HG23	62:t:121:ASP:OD2	2.02	0.58
49:a:416:ALA:HB1	49:a:472:SER:O	2.04	0.58
59:q:190:LEU:CD2	59:q:291:TRP:CE3	2.87	0.58
1:0:283:LEU:HD23	1:0:283:LEU:C	2.29	0.58
10:PA:346:LYS:HA	10:PA:351:ARG:HD3	1.85	0.58
10:PA:1174:ALA:O	10:PA:1212:LEU:HA	2.04	0.58
11:PB:1108:PHE:CE1	11:PB:1113:PRO:HA	2.39	0.58
16:PG:60:GLN:HG2	16:PG:63:ARG:HH21	1.68	0.58
22:DA:564:PRO:CG	23:DB:744:PHE:CE2	2.87	0.58
26:DF:319:LEU:HD12	26:DF:322:ASP:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:278:SER:OG	40:4:279:ARG:N	2.37	0.58
43:7:616:ARG:CZ	43:7:674:TYR:HD2	2.17	0.58
46:b:118:LEU:HB2	57:n:907:LEU:HD11	1.86	0.58
52:g:97:ILE:HG23	55:j:103:LYS:HE2	1.86	0.58
57:n:589:GLN:HE21	57:n:591:PHE:HE1	1.52	0.58
62:t:78:LEU:HD22	62:t:78:LEU:N	2.18	0.58
66:x:355:CYS:SG	66:x:359:CYS:HB3	2.44	0.58
26:Df:349:ASN:HB3	26:Df:351:ILE:HG13	1.84	0.57
37:1:417:LYS:NZ	39:3:43:VAL:HG21	2.18	0.57
42:6:153:MET:O	42:6:156:ILE:HG22	2.03	0.57
42:6:481:ASN:OD1	42:6:487:LYS:NZ	2.37	0.57
48:m:106:GLN:CD	50:d:167:TRP:CE3	2.81	0.57
53:h:22:LEU:HG	59:q:109:MET:HG3	1.86	0.57
55:j:39:GLN:CD	61:s:151:GLY:HA2	2.28	0.57
57:n:545:LEU:HD11	57:n:653:PRO:HD3	1.80	0.57
59:q:548:VAL:HA	59:q:571:VAL:HG12	1.85	0.57
67:w:425:MET:N	67:w:425:MET:SD	2.72	0.57
2:8:135:HIS:HD2	2:8:137:ASP:H	1.51	0.57
2:8:140:PRO:CA	2:8:202:ILE:HD11	2.30	0.57
3:9:87:PHE:CD1	3:9:87:PHE:C	2.82	0.57
37:1:163:ASP:OD2	38:2:179:PRO:HD3	2.04	0.57
37:1:410:GLU:HA	37:1:413:ALA:HB3	1.86	0.57
38:2:166:GLU:HG2	38:2:195:ARG:HB3	1.86	0.57
42:6:91:PRO:HB2	42:6:96:ALA:CB	2.33	0.57
44:c:162:VAL:HG13	44:c:207:LEU:HD13	1.86	0.57
46:b:178:LEU:CD2	47:l:82:LEU:HD11	2.33	0.57
49:a:336:TYR:CE1	49:a:391:THR:OG1	2.52	0.57
52:g:93:LEU:CB	55:j:106:LYS:CE	2.58	0.57
53:h:23:LYS:HB3	53:h:23:LYS:HZ3	1.66	0.57
53:h:89:LEU:HD11	59:q:124:PHE:CD2	2.38	0.57
66:x:439:LEU:HB3	66:x:495:ILE:HG21	1.86	0.57
2:8:136:ARG:HB2	2:8:159:ALA:HA	1.85	0.57
8:FA:126:ILE:O	8:FA:138:PHE:N	2.35	0.57
10:PA:1134:PRO:HG2	10:PA:1137:PRO:HB3	1.86	0.57
10:PA:1789:SER:O	51:f:76:PRO:HB3	2.04	0.57
18:PI:28:GLU:HA	18:PI:36:LEU:HD12	1.86	0.57
18:PI:35:LEU:HD12	18:PI:51:SER:HA	1.85	0.57
23:DB:769:LYS:O	23:DB:769:LYS:HG3	2.03	0.57
25:DE:742:LYS:HA	25:DE:745:GLU:HG2	1.86	0.57
32:Dc:21:LEU:C	32:Dc:21:LEU:HD12	2.29	0.57
40:4:359:ILE:HG21	40:4:395:GLU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:412:PHE:CD2	40:4:418:PHE:HD1	2.20	0.57
50:d:44:LEU:HD22	50:d:48:LEU:HD11	1.84	0.57
60:r:38:ARG:NH1	60:r:192:GLN:HG3	2.18	0.57
66:x:404:GLN:NE2	66:x:408:GLN:OE1	2.37	0.57
67:w:9:PHE:HZ	67:w:63:ILE:HG12	1.68	0.57
67:w:122:VAL:O	67:w:126:ILE:HB	2.03	0.57
1:0:204:ARG:HD2	42:6:266:GLN:NE2	2.19	0.57
2:8:15:LEU:H	2:8:29:ALA:HB2	1.69	0.57
11:PB:764:MET:O	11:PB:765:GLU:C	2.46	0.57
22:DA:929:THR:HG22	22:DA:954:ALA:HA	1.86	0.57
39:3:104:LEU:O	39:3:108:ASN:N	2.36	0.57
40:4:224:GLN:OE1	40:4:226:ARG:NH2	2.35	0.57
49:a:267:LYS:H	49:a:267:LYS:HD2	1.70	0.57
49:a:382:LEU:CD2	49:a:446:SER:CA	2.82	0.57
49:a:504:ILE:N	49:a:505:PRO:CD	2.67	0.57
50:d:45:ILE:CD1	54:i:73:ILE:HG13	2.31	0.57
53:h:150:LEU:HD21	56:k:45:LEU:HD13	1.81	0.57
56:k:21:ILE:CD1	59:q:168:THR:HA	2.35	0.57
57:n:507:GLN:NE2	57:n:636:ALA:O	2.37	0.57
70:Y:-8:DT:H2"	70:Y:-7:DC:C5	2.38	0.57
10:PA:1793:THR:H	53:h:102:HIS:CE1	2.20	0.57
11:PB:124:LEU:HD13	11:PB:152:ILE:HD11	1.86	0.57
13:PD:140:PHE:HZ	64:v:64:ARG:HH21	1.50	0.57
25:De:484:LEU:HD21	25:De:504:LEU:HD21	1.85	0.57
40:4:342:VAL:O	40:4:342:VAL:HG13	2.02	0.57
50:d:126:TYR:CD2	59:q:36:MET:CB	2.77	0.57
52:g:60:GLU:HG3	52:g:60:GLU:O	2.03	0.57
53:h:139:GLN:HE22	56:k:37:LYS:CB	2.16	0.57
57:n:229:GLU:HG3	57:n:300:CYS:HB2	1.85	0.57
57:n:528:HIS:HB3	57:n:530:ILE:HG22	1.84	0.57
1:0:70:LYS:O	1:0:74:ILE:HG13	2.04	0.57
6:DQ:55:ALA:C	6:DQ:56:VAL:HG23	2.30	0.57
10:PA:706:ILE:HD11	10:PA:787:VAL:HG22	1.87	0.57
11:PB:131:THR:HA	11:PB:141:GLN:HA	1.87	0.57
36:EB:86:LYS:HA	36:EB:139:PHE:HE1	1.70	0.57
37:1:408:ARG:HD3	39:3:116:LYS:HB2	1.87	0.57
47:l:160:MET:HE1	64:v:134:TYR:CD2	2.40	0.57
53:h:23:LYS:HD3	59:q:110:CYS:SG	2.45	0.57
57:n:707:ASP:CB	58:o:684:ARG:NH2	2.68	0.57
59:q:315:ALA:HB2	59:q:428:LEU:HD23	1.87	0.57
59:q:562:SER:HB2	59:q:587:GLU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:s:92:ALA:HB1	61:s:96:PHE:CE2	2.34	0.57
66:x:956:VAL:CG2	66:x:968:LEU:HD11	2.34	0.57
10:PA:1248:ASN:CB	10:PA:1256:VAL:H	2.18	0.57
13:PD:137:LYS:HE3	53:h:51:LEU:HA	1.87	0.57
16:PG:163:LEU:HB3	16:PG:168:LEU:HD13	1.87	0.57
38:2:32:ALA:HB3	42:6:72:THR:HG22	1.86	0.57
43:7:487:ARG:HH11	43:7:487:ARG:CG	2.18	0.57
49:a:401:PRO:O	49:a:405:PRO:HD3	2.04	0.57
51:f:180:LEU:HD11	57:n:302:SER:HG	1.68	0.57
51:f:181:LEU:CD2	57:n:274:ILE:HD11	2.34	0.57
52:g:127:ARG:N	52:g:128:PRO:HD2	2.20	0.57
54:i:103:THR:O	54:i:107:ILE:HB	2.05	0.57
54:i:131:LEU:HD22	63:u:128:SER:CB	2.34	0.57
55:j:105:PHE:HD1	63:u:55:ALA:HB1	1.68	0.57
57:n:234:LEU:HD22	57:n:245:TRP:HB3	1.86	0.57
57:n:706:LEU:HB2	57:n:725:VAL:HG23	1.87	0.57
59:q:314:GLU:OE1	59:q:427:LEU:N	2.38	0.57
67:w:397:LYS:CB	68:p:171:PHE:CE2	2.88	0.57
3:9:201:THR:C	3:9:203:ALA:H	2.11	0.57
3:9:275:GLN:C	3:9:275:GLN:CD	2.73	0.57
4:DO:96:VAL:HG21	24:DD:1010:ALA:HB1	1.87	0.57
7:BA:43:ASP:HB3	10:PA:79:THR:HG21	1.85	0.57
10:PA:346:LYS:O	10:PA:347:GLU:HB2	2.04	0.57
10:PA:388:MET:HE1	10:PA:503:LEU:HD23	1.86	0.57
10:PA:583:ARG:HG3	10:PA:585:LEU:HD13	1.87	0.57
11:PB:854:ILE:HD13	11:PB:858:VAL:HG21	1.86	0.57
11:PB:1003:ASN:HB3	11:PB:1006:VAL:HG22	1.86	0.57
23:DB:539:ARG:NE	41:5:32:LYS:HA	2.19	0.57
25:DE:645:GLY:H	25:DE:675:LEU:HD11	1.70	0.57
29:DI:132:LEU:CD2	30:DJ:121:MET:HE2	2.34	0.57
25:De:562:SER:OG	25:De:564:ASP:OD1	2.21	0.57
37:1:483:THR:N	37:1:484:PRO:HD2	2.16	0.57
38:2:334:ILE:HG12	38:2:336:LEU:H	1.69	0.57
39:3:255:CYS:HB2	39:3:260:ASN:HD21	1.70	0.57
41:5:33:PHE:HA	41:5:45:VAL:HG13	1.86	0.57
48:m:104:HIS:CB	57:n:169:LEU:HA	2.31	0.57
50:d:164:PRO:HD2	50:d:167:TRP:CG	2.40	0.57
52:g:129:HIS:NE2	63:u:79:GLU:HA	2.20	0.57
59:q:93:TRP:N	59:q:94:PRO:HD2	2.19	0.57
59:q:184:ASN:CG	64:v:83:LYS:CD	2.78	0.57
1:0:209:GLU:O	1:0:209:GLU:CD	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:281:GLN:HA	1:0:281:GLN:NE2	2.20	0.57
4:DO:22:LEU:HB2	4:DO:28:ILE:HG12	1.87	0.57
8:FA:112:GLY:HA2	8:FA:145:ASN:O	2.05	0.57
11:PB:800:ALA:C	11:PB:802:ASP:H	2.10	0.57
13:PD:137:LYS:HD3	53:h:55:GLN:CD	2.27	0.57
19:PJ:1:MET:HA	19:PJ:55:LEU:HB2	1.86	0.57
43:7:273:ILE:HG22	43:7:278:GLU:HG2	1.85	0.57
44:c:110:ALA:HB2	46:b:168:ILE:HG22	1.84	0.57
49:a:423:SER:HB2	49:a:503:SER:CB	2.32	0.57
49:a:454:PHE:HA	66:x:14:TRP:HH2	1.70	0.57
51:f:176:ARG:CD	57:n:306:GLU:OE2	2.52	0.57
57:n:224:PHE:HE2	57:n:289:LEU:HD21	1.69	0.57
57:n:237:MET:CE	59:q:45:GLN:CG	2.83	0.57
69:X:-21:DG:H1	70:Y:21:DC:H42	1.51	0.57
5:DP:192:TYR:HB2	5:DP:200:VAL:HG22	1.87	0.57
7:BA:295:ARG:HG2	7:BA:299:LEU:HG	1.86	0.57
26:DF:125:VAL:HG22	28:DH:32:ALA:HB1	1.86	0.57
24:Dd:917:ILE:HD11	24:Dd:1063:LEU:HD13	1.87	0.57
37:1:497:LEU:C	37:1:497:LEU:HD23	2.30	0.57
40:4:63:GLU:OE1	40:4:64:GLN:NE2	2.38	0.57
42:6:76:LEU:HD22	42:6:86:LEU:HA	1.85	0.57
58:o:756:MET:O	58:o:760:LEU:HG	2.05	0.57
59:q:38:GLN:HB2	59:q:42:ARG:HH21	1.70	0.57
7:BA:18:HIS:N	7:BA:18:HIS:HD2	2.03	0.56
7:BA:214:PHE:HB3	7:BA:218:PHE:CE2	2.40	0.56
9:FB:18:VAL:N	9:FB:109:ILE:O	2.32	0.56
11:PB:93:LEU:HD11	11:PB:152:ILE:HD12	1.87	0.56
18:PI:27:LYS:HG3	18:PI:36:LEU:HB2	1.87	0.56
23:DB:560:TYR:CD2	23:DB:581:ILE:HD11	2.40	0.56
26:Df:320:ARG:CB	26:Df:320:ARG:HH11	2.18	0.56
37:1:165:GLY:O	38:2:179:PRO:HB2	2.05	0.56
38:2:123:ASN:O	38:2:127:HIS:ND1	2.37	0.56
53:h:151:LEU:CD2	64:v:37:ILE:HB	2.34	0.56
54:i:118:LEU:HD23	54:i:118:LEU:C	2.30	0.56
66:x:376:ALA:O	66:x:380:ASN:ND2	2.38	0.56
67:w:169:TYR:CZ	67:w:177:LEU:HD11	2.40	0.56
67:w:397:LYS:HB3	68:p:171:PHE:CE2	2.39	0.56
67:w:1034:LEU:HD22	67:w:1038:ARG:HD2	1.87	0.56
2:8:207:LEU:O	51:f:52:MET:CE	2.53	0.56
8:FA:24:LYS:HA	9:FB:99:SER:HA	1.87	0.56
9:FB:31:TRP:CD1	9:FB:62:LEU:HD21	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:581:LYS:O	10:PA:582:PRO:C	2.48	0.56
10:PA:693:ILE:HG21	11:PB:1023:ARG:HH12	1.69	0.56
12:PC:93:PHE:H	12:PC:166:LYS:NZ	2.03	0.56
14:PE:122:ALA:HB3	14:PE:123:PRO:HD3	1.87	0.56
26:DF:359:PHE:HB3	26:DF:380:LEU:HD21	1.87	0.56
37:1:165:GLY:O	38:2:179:PRO:CB	2.52	0.56
42:6:633:ARG:HD2	42:6:679:PHE:CG	2.38	0.56
43:7:24:TYR:OH	43:7:41:GLU:O	2.20	0.56
48:m:22:LEU:HD13	52:g:43:MET:HE1	1.87	0.56
50:d:45:ILE:CG2	54:i:76:MET:CG	2.81	0.56
51:f:176:ARG:NH1	57:n:306:GLU:OE2	2.38	0.56
54:i:65:PHE:HA	54:i:99:LYS:CE	2.28	0.56
55:j:17:GLU:C	55:j:20:ARG:HG2	2.30	0.56
57:n:199:LEU:HD13	57:n:222:VAL:HG13	1.87	0.56
63:u:15:LEU:HD12	63:u:18:GLN:OE1	2.04	0.56
63:u:57:LEU:CD1	65:z:492:ARG:NE	2.68	0.56
8:FA:47:LEU:CB	9:FB:7:LEU:HB2	2.35	0.56
9:FB:175:ARG:HB2	9:FB:208:GLN:HA	1.86	0.56
10:PA:154:CYS:HB2	10:PA:186:ARG:O	2.06	0.56
16:PG:110:ARG:HA	16:PG:113:ILE:HD11	1.86	0.56
25:DE:507:VAL:HB	25:DE:513:LEU:CD2	2.29	0.56
28:DH:194:MET:HE1	26:Df:226:GLU:HG3	1.87	0.56
25:De:636:HIS:HD2	25:De:638:ASN:H	1.53	0.56
26:Df:280:ILE:O	26:Df:284:ARG:HG3	2.05	0.56
37:1:229:TYR:O	43:7:553:TYR:OH	2.23	0.56
38:2:116:LYS:HE2	38:2:119:GLU:HA	1.86	0.56
39:3:263:GLU:HG3	39:3:264:ILE:HG12	1.86	0.56
42:6:337:VAL:H	42:6:488:LEU:HD13	1.69	0.56
43:7:273:ILE:HG21	43:7:277:ASP:HB2	1.87	0.56
44:c:281:CYS:HB3	44:c:284:CYS:N	2.20	0.56
48:m:100:GLN:HE22	57:n:172:CYS:HB2	1.70	0.56
49:a:127:HIS:HE1	49:a:171:THR:CG2	2.19	0.56
50:d:128:ALA:HB1	63:u:108:VAL:HG22	1.86	0.56
53:h:182:VAL:CG2	60:r:202:ILE:HD11	2.32	0.56
55:j:20:ARG:CZ	57:n:94:GLN:CB	2.79	0.56
57:n:523:SER:OG	57:n:584:MET:SD	2.63	0.56
58:o:690:LEU:HD22	59:q:605:PRO:HB2	1.88	0.56
64:v:16:GLN:HE21	64:v:20:LYS:HE2	0.76	0.56
8:FA:18:VAL:HG22	8:FA:137:ALA:HB3	1.86	0.56
10:PA:1486:ILE:O	10:PA:1487:PRO:C	2.49	0.56
13:PD:79:THR:CB	53:h:51:LEU:CD2	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:259:ILE:HG13	38:2:261:SER:H	1.69	0.56
40:4:358:GLY:C	40:4:394:TRP:HE1	2.13	0.56
43:7:74:SER:O	43:7:209:TYR:N	2.35	0.56
53:h:12:LEU:HD13	53:h:12:LEU:O	2.05	0.56
57:n:199:LEU:HD22	57:n:222:VAL:HG11	1.87	0.56
57:n:250:LEU:CG	57:n:275:HIS:HB2	2.35	0.56
63:u:16:ALA:HA	63:u:19:PHE:CD2	2.41	0.56
65:z:551:ASP:OD1	65:z:551:ASP:N	2.37	0.56
69:X:-24:DA:H8	69:X:-24:DA:O5'	1.88	0.56
3:9:167:PHE:HD1	3:9:167:PHE:C	2.12	0.56
10:PA:408:ARG:NH2	60:r:7:THR:HG23	2.21	0.56
20:PK:15:GLY:HA3	60:r:10:PRO:HD2	1.87	0.56
25:DE:773:TYR:HA	26:DF:142:GLN:OE1	2.06	0.56
26:DF:15:PRO:HD3	29:DI:18:MET:CG	2.23	0.56
42:6:91:PRO:O	42:6:94:LYS:HG2	2.04	0.56
56:k:60:GLU:HG2	64:v:22:LEU:HD11	1.86	0.56
56:k:63:LEU:HD23	64:v:22:LEU:HD13	1.87	0.56
56:k:70:LEU:O	56:k:73:VAL:HG22	2.05	0.56
68:p:243:LYS:NZ	68:p:245:CYS:SG	2.79	0.56
2:8:207:LEU:C	51:f:52:MET:SD	2.88	0.56
4:DO:58:PHE:HD2	6:DQ:370:ALA:HB1	1.70	0.56
11:PB:856:PRO:HG2	21:PL:48:ARG:HA	1.87	0.56
14:PE:84:ILE:HB	22:DA:1038:ARG:HD2	1.88	0.56
26:DF:86:PHE:HA	30:DJ:212:LYS:NZ	2.21	0.56
31:DL:119:HIS:NE2	31:DL:123:GLN:OE1	2.38	0.56
44:c:176:MET:HE1	44:c:267:MET:HB3	1.86	0.56
49:a:430:LEU:N	49:a:430:LEU:HD23	2.21	0.56
50:d:42:ARG:NH2	54:i:93:LYS:CG	2.69	0.56
52:g:45:PHE:CD1	52:g:45:PHE:C	2.83	0.56
53:h:19:VAL:CG2	59:q:112:LEU:CD2	2.84	0.56
55:j:43:PHE:HE1	61:s:147:THR:HA	1.68	0.56
55:j:106:LYS:O	55:j:110:ILE:HG13	2.05	0.56
64:v:122:GLU:OE1	64:v:122:GLU:HA	2.05	0.56
67:w:68:HIS:NE2	67:w:114:LEU:HD11	2.21	0.56
2:8:135:HIS:C	2:8:135:HIS:CD2	2.84	0.56
10:PA:1210:TRP:CD1	10:PA:1210:TRP:H	2.24	0.56
23:DB:259:ASP:HB3	23:DB:262:MET:O	2.06	0.56
23:DB:539:ARG:HE	41:5:32:LYS:CA	2.19	0.56
43:7:262:ASN:C	43:7:262:ASN:OD1	2.49	0.56
43:7:343:ARG:NH2	43:7:431:PRO:O	2.38	0.56
57:n:250:LEU:CD2	57:n:275:HIS:CB	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:319:ARG:HG3	57:n:320:TRP:HD1	1.70	0.56
59:q:9:ILE:CG1	63:u:90:LEU:CD2	2.78	0.56
64:v:35:GLU:OE2	64:v:64:ARG:CZ	2.54	0.56
67:w:8:ILE:O	67:w:12:VAL:HG12	2.04	0.56
2:8:84:LYS:HA	2:8:84:LYS:HZ2	1.70	0.56
3:9:288:ASN:C	3:9:288:ASN:ND2	2.57	0.56
7:BA:173:VAL:O	7:BA:175:ARG:NH1	2.38	0.56
10:PA:437:ASP:N	62:t:97:LYS:HZ3	1.99	0.56
11:PB:924:ARG:CZ	12:PC:60:HIS:CB	2.84	0.56
13:PD:137:LYS:HZ1	53:h:52:LEU:N	2.02	0.56
16:PG:91:GLN:HB2	16:PG:98:PHE:CD2	2.36	0.56
23:DB:621:ALA:N	41:5:36:GLN:NE2	2.36	0.56
29:DI:132:LEU:HD11	30:DJ:121:MET:SD	2.46	0.56
31:DL:80:VAL:O	31:DL:84:LEU:HG	2.06	0.56
31:DL:113:VAL:HG13	31:DL:113:VAL:O	2.06	0.56
37:1:187:ASN:HB2	37:1:191:ASP:CA	2.35	0.56
38:2:250:ILE:HD12	39:3:293:LEU:HG	1.87	0.56
55:j:76:ASN:OD1	55:j:77:PRO:HD2	2.05	0.56
58:o:715:LEU:HD21	66:x:21:TYR:HB2	1.86	0.56
10:PA:18:ILE:HG12	11:PB:1149:VAL:HG21	1.88	0.56
10:PA:189:PRO:HB2	10:PA:200:ALA:HB1	1.87	0.56
22:DA:355:VAL:O	22:DA:355:VAL:CG2	2.54	0.56
22:DA:851:ASP:OD1	22:DA:851:ASP:N	2.38	0.56
24:DD:940:VAL:HB	24:DD:943:GLN:HB3	1.88	0.56
26:DF:265:GLU:OE2	26:DF:265:GLU:HA	2.06	0.56
37:1:314:VAL:O	37:1:318:GLY:N	2.38	0.56
39:3:21:TRP:O	39:3:25:GLN:N	2.38	0.56
43:7:517:ILE:HA	43:7:520:TYR:HD2	1.71	0.56
43:7:542:TYR:HB3	43:7:572:GLN:HE21	1.71	0.56
44:c:113:TRP:CZ2	46:b:175:HIS:HB2	2.34	0.56
48:m:68:LYS:HD3	52:g:45:PHE:CE1	2.40	0.56
49:a:107:MET:O	49:a:107:MET:HE2	2.06	0.56
50:d:45:ILE:HD13	54:i:72:ILE:O	2.05	0.56
55:j:17:GLU:O	55:j:20:ARG:CG	2.50	0.56
58:o:765:ASP:OD2	67:w:73:PRO:CD	2.50	0.56
2:8:171:HIS:NE2	2:8:188:ARG:HA	2.21	0.56
3:9:98:GLU:HA	3:9:98:GLU:OE2	2.05	0.56
7:BA:284:THR:HG21	70:Y:32:DG:H5"	1.88	0.56
10:PA:283:ILE:HG12	10:PA:313:HIS:HB3	1.88	0.56
10:PA:784:VAL:HG13	11:PB:978:ILE:HG13	1.88	0.56
29:Di:73:LEU:CD1	31:Dl:105:HIS:NE2	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:412:PHE:HD2	40:4:418:PHE:HD1	1.54	0.56
41:5:8:VAL:HG11	41:5:50:VAL:HG21	1.88	0.56
44:c:281:CYS:HB3	44:c:284:CYS:CA	2.36	0.56
46:b:176:THR:HA	46:b:179:LEU:HG	1.87	0.56
55:j:9:GLU:HB2	55:j:56:GLN:NE2	2.21	0.56
55:j:102:MET:HA	63:u:26:LEU:CD2	2.36	0.56
57:n:231:GLU:CB	57:n:253:LEU:HD21	2.34	0.56
59:q:477:VAL:HB	59:q:493:LEU:HB2	1.88	0.56
62:t:131:MET:C	62:t:131:MET:SD	2.89	0.56
3:9:171:LEU:O	3:9:171:LEU:HD13	2.06	0.55
4:DO:43:ALA:CB	6:DQ:21:VAL:HG22	2.37	0.55
10:PA:1130:ILE:HG12	10:PA:1411:LEU:HD23	1.87	0.55
10:PA:1375:ARG:HD2	10:PA:1402:CYS:SG	2.46	0.55
24:DD:940:VAL:HG23	24:DD:944:LEU:HB2	1.87	0.55
25:DE:431:GLU:HG3	29:DI:109:PRO:HA	1.87	0.55
25:DE:509:GLN:O	25:DE:513:LEU:HG	2.06	0.55
25:DE:561:SER:HB2	25:DE:588:VAL:HB	1.88	0.55
40:4:254:MET:HA	40:4:258:LEU:HD22	1.87	0.55
45:e:146:ILE:CG2	45:e:147:ASN:N	2.52	0.55
49:a:259:ILE:HD12	49:a:259:ILE:N	2.20	0.55
49:a:413:HIS:ND1	49:a:471:ASP:HA	2.21	0.55
51:f:118:ARG:HB3	59:q:108:GLU:OE2	2.06	0.55
51:f:177:VAL:HG13	57:n:266:VAL:HG22	1.88	0.55
52:g:75:LYS:HG3	52:g:126:TYR:CE2	2.41	0.55
55:j:102:MET:CG	63:u:26:LEU:CD2	2.83	0.55
57:n:545:LEU:CD1	57:n:653:PRO:CD	2.77	0.55
59:q:149:LYS:HE3	64:v:40:ALA:CA	2.30	0.55
59:q:437:HIS:ND1	59:q:472:GLU:N	2.53	0.55
59:q:591:LYS:NZ	59:q:593:MET:SD	2.75	0.55
59:q:633:ARG:CG	59:q:637:TYR:CD2	2.88	0.55
61:s:85:THR:HB	61:s:90:GLU:OE2	2.06	0.55
65:z:540:LEU:C	65:z:540:LEU:CD2	2.78	0.55
67:w:18:ILE:O	67:w:18:ILE:HD13	2.07	0.55
67:w:41:LEU:CD1	67:w:85:MET:HB3	2.33	0.55
8:FA:47:LEU:HB2	9:FB:7:LEU:HD22	1.87	0.55
10:PA:403:GLN:NE2	60:r:17:ASN:HD21	2.04	0.55
11:PB:856:PRO:HA	11:PB:904:VAL:HG22	1.88	0.55
40:4:338:PHE:CE1	42:6:79:ALA:HB2	2.41	0.55
4:DO:57:ASN:HD22	4:DO:57:ASN:H	1.54	0.55
7:BA:29:ALA:O	11:PB:1066:PRO:HA	2.05	0.55
11:PB:297:MET:HE2	11:PB:298:MET:SD	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:PC:246:LEU:HD21	20:PK:105:PHE:CD1	2.42	0.55
14:PE:26:TYR:HA	14:PE:64:HIS:HA	1.88	0.55
22:DA:639:LEU:HD12	22:DA:639:LEU:O	2.07	0.55
26:Df:352:GLN:O	26:Df:356:THR:OG1	2.24	0.55
36:EB:158:HIS:O	36:EB:161:ARG:CG	2.53	0.55
40:4:59:MET:HA	40:4:62:LEU:HB2	1.89	0.55
40:4:245:LEU:HD23	40:4:246:GLY:O	2.05	0.55
42:6:556:ASP:OD2	42:6:647:LYS:NZ	2.34	0.55
43:7:255:THR:HG23	43:7:396:PRO:HB3	1.87	0.55
43:7:506:SER:HB3	43:7:509:GLU:HA	1.88	0.55
49:a:199:PRO:HG2	49:a:244:GLU:O	2.06	0.55
51:f:82:ARG:HD2	51:f:84:GLN:HE21	1.71	0.55
51:f:185:ARG:NE	57:n:273:PHE:HZ	2.03	0.55
52:g:161:ILE:CA	54:i:140:MET:SD	2.86	0.55
57:n:154:ILE:HB	57:n:155:PRO:CD	2.35	0.55
57:n:777:TYR:HA	57:n:780:VAL:HG22	1.89	0.55
59:q:9:ILE:HD11	63:u:90:LEU:HD21	1.70	0.55
62:t:66:MET:HG2	62:t:78:LEU:HD21	1.87	0.55
7:BA:18:HIS:HD2	7:BA:18:HIS:H	1.55	0.55
9:FB:30:GLN:HG2	9:FB:62:LEU:HG	1.87	0.55
11:PB:99:TRP:CZ3	11:PB:105:PRO:HB3	2.34	0.55
11:PB:640:ILE:O	11:PB:644:LYS:HG3	2.07	0.55
31:DL:102:LEU:HA	31:DL:105:HIS:HD2	1.69	0.55
38:2:196:VAL:H	38:2:215:THR:HG21	1.71	0.55
40:4:60:LEU:HA	40:4:119:ARG:HE	1.71	0.55
40:4:130:SER:O	40:4:131:ASP:OD1	2.24	0.55
42:6:59:LYS:HG3	42:6:62:ARG:NH2	2.21	0.55
42:6:582:GLY:O	42:6:589:ARG:NH2	2.39	0.55
53:h:139:GLN:NE2	56:k:37:LYS:CB	2.68	0.55
53:h:159:ARG:HG2	53:h:159:ARG:O	2.05	0.55
55:j:102:MET:N	63:u:26:LEU:HD21	2.22	0.55
56:k:92:MET:HE3	59:q:376:HIS:CB	2.36	0.55
58:o:757:THR:O	58:o:761:LEU:HG	2.07	0.55
67:w:627:LEU:HD22	67:w:645:VAL:HG23	1.89	0.55
5:DP:253:PHE:CD2	5:DP:253:PHE:O	2.59	0.55
8:FA:45:ALA:HB3	9:FB:9:LEU:CD2	2.29	0.55
11:PB:68:GLN:HA	11:PB:83:ARG:HA	1.89	0.55
12:PC:169:PHE:O	12:PC:176:TRP:HB2	2.07	0.55
18:PI:96:PHE:CD2	18:PI:110:LEU:HD21	2.41	0.55
26:DF:71:ILE:CD1	29:DI:35:VAL:HG22	2.36	0.55
26:Df:219:GLU:OE1	26:Df:219:GLU:N	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:156:LEU:HD11	38:2:165:ARG:HG2	1.88	0.55
42:6:565:VAL:O	42:6:569:LYS:N	2.37	0.55
45:e:139:TRP:HE1	64:v:122:GLU:HG3	1.71	0.55
50:d:31:LEU:CD2	54:i:103:THR:OG1	2.45	0.55
52:g:48:GLN:H	52:g:48:GLN:CD	2.13	0.55
55:j:26:VAL:HG11	55:j:38:ASN:CG	2.18	0.55
56:k:16:ASP:CG	64:v:79:VAL:HG21	2.31	0.55
59:q:259:VAL:HG22	59:q:343:ILE:HG23	1.88	0.55
62:t:4:THR:HG22	62:t:143:GLU:HB2	1.89	0.55
64:v:47:GLN:OE1	64:v:47:GLN:HA	2.05	0.55
66:x:581:ILE:HD11	66:x:616:LEU:HD22	1.87	0.55
69:X:-36:DG:C2	70:Y:36:DC:N4	2.75	0.55
2:8:178:TYR:N	2:8:178:TYR:HD1	2.04	0.55
2:8:239:ASP:C	2:8:239:ASP:OD1	2.48	0.55
3:9:212:ILE:HG12	3:9:255:MET:HE1	1.89	0.55
7:BA:18:HIS:CD2	7:BA:18:HIS:H	2.23	0.55
7:BA:46:ILE:HG13	7:BA:47:ASP:H	1.72	0.55
10:PA:364:ARG:HD3	11:PB:1060:HIS:HD2	1.72	0.55
10:PA:1040:LEU:HD22	14:PE:200:ALA:O	2.06	0.55
11:PB:796:MET:HB3	11:PB:948:GLN:HG2	1.87	0.55
26:DF:104:LEU:HD13	30:DJ:217:PHE:CE2	2.33	0.55
26:Df:223:TYR:HD2	26:Df:255:MET:HE1	1.71	0.55
38:2:77:LYS:HE3	38:2:78:PRO:HD2	1.87	0.55
42:6:625:GLN:N	42:6:660:TYR:O	2.39	0.55
51:f:188:PHE:CE1	57:n:298:SER:OG	2.57	0.55
52:g:90:LEU:CD1	55:j:124:TYR:OH	2.53	0.55
55:j:77:PRO:O	55:j:81:THR:HB	2.07	0.55
58:o:765:ASP:HB2	67:w:72:SER:OG	2.06	0.55
63:u:11:ALA:O	63:u:69:ILE:HD11	2.07	0.55
70:Y:35:DC:H1'	70:Y:36:DC:C6	2.41	0.55
10:PA:537:ILE:HG22	10:PA:541:THR:HB	1.88	0.55
10:PA:634:GLU:O	10:PA:635:LEU:C	2.50	0.55
18:PI:80:ARG:HA	18:PI:94:ALA:O	2.07	0.55
23:DB:61:ASN:O	23:DB:130:VAL:HG23	2.06	0.55
35:EA:184:ILE:HG23	36:EB:212:VAL:HG11	1.88	0.55
37:1:274:ASP:O	43:7:128:LYS:CD	2.55	0.55
40:4:304:PRO:CG	40:4:373:HIS:H	2.20	0.55
42:6:444:HIS:HD2	42:6:467:THR:HG23	1.71	0.55
42:6:557:LYS:HA	42:6:603:ASN:HB2	1.89	0.55
50:d:42:ARG:HH22	54:i:93:LYS:HG2	1.71	0.55
55:j:96:LYS:HZ2	61:s:80:SER:CA	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:j:109:LEU:HD21	63:u:59:ALA:HB2	1.83	0.55
56:k:86:SER:HB2	64:v:105:LEU:HD12	1.87	0.55
57:n:274:ILE:HD12	57:n:299:PHE:CE2	2.34	0.55
58:o:697:HIS:C	66:x:957:LYS:HD3	2.31	0.55
58:o:722:GLU:HG3	58:o:737:ILE:HB	1.88	0.55
59:q:482:GLN:HB2	59:q:634:ASN:ND2	2.21	0.55
66:x:955:LEU:HD13	66:x:967:VAL:HG21	1.88	0.55
67:w:369:ARG:NH1	67:w:402:LEU:O	2.37	0.55
2:8:98:LEU:CB	2:8:143:LEU:HD21	2.36	0.55
3:9:228:MET:HB3	3:9:231:TYR:HB2	1.88	0.55
10:PA:1474:LEU:HD23	16:PG:58:VAL:HA	1.88	0.55
11:PB:68:GLN:HB3	11:PB:83:ARG:HB3	1.88	0.55
11:PB:643:LEU:CD2	11:PB:656:LEU:HD11	2.31	0.55
11:PB:924:ARG:NH1	12:PC:62:GLU:HG3	2.22	0.55
12:PC:131:THR:HB	12:PC:146:ASP:O	2.07	0.55
20:PK:34:THR:HG23	20:PK:72:ILE:HG12	1.89	0.55
26:DF:22:VAL:HG13	29:DI:44:PHE:HE1	1.67	0.55
26:DF:106:PHE:CD1	29:DI:13:PRO:CG	2.90	0.55
25:De:610:ARG:HD3	25:De:619:PRO:HG3	1.89	0.55
37:1:359:GLU:O	37:1:363:LEU:N	2.36	0.55
38:2:254:PHE:N	39:3:263:GLU:O	2.39	0.55
41:5:15:ALA:HA	42:6:516:PRO:HB3	1.89	0.55
44:c:292:LEU:O	44:c:293:PRO:C	2.50	0.55
49:a:417:TYR:HH	49:a:450:PHE:HB3	1.72	0.55
49:a:420:LEU:CD1	49:a:475:VAL:HG21	2.37	0.55
51:f:82:ARG:HH11	51:f:94:PRO:HB3	1.72	0.55
57:n:230:PHE:CD2	57:n:296:LEU:CB	2.89	0.55
57:n:301:LEU:HB3	57:n:361:ILE:HG13	1.89	0.55
57:n:693:ILE:HD11	57:n:775:ARG:HG2	1.88	0.55
59:q:633:ARG:CG	59:q:637:TYR:HD2	2.19	0.55
67:w:1072:ILE:HD11	67:w:1126:LEU:HD22	1.89	0.55
69:X:-33:DG:O6	70:Y:34:DG:O6	2.24	0.55
1:0:199:ALA:HA	1:0:202:LYS:CB	2.36	0.55
10:PA:734:ARG:NH1	18:PI:107:ALA:N	2.55	0.55
11:PB:657:VAL:O	11:PB:660:GLY:N	2.32	0.55
13:PD:137:LYS:HE3	53:h:51:LEU:CD1	1.98	0.55
25:DE:345:MET:HE3	25:DE:346:PRO:HD2	1.88	0.55
31:DL:58:LEU:HA	31:DL:62:LYS:HD2	1.89	0.55
37:1:257:MET:SD	43:7:582:GLU:HG3	2.47	0.55
41:5:5:LEU:HD11	41:5:35:ILE:HD13	1.89	0.55
42:6:472:ARG:HG3	42:6:473:GLU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:c:204:MET:HE3	44:c:208:PHE:O	2.04	0.55
47:l:107:ASP:N	47:l:108:PRO:HD3	2.22	0.55
48:m:66:TYR:C	50:d:154:ARG:NH2	2.65	0.55
59:q:166:ARG:CZ	59:q:166:ARG:CB	2.85	0.55
64:v:25:ASP:HB3	64:v:75:LEU:HD21	1.88	0.55
1:0:28:HIS:CE1	1:0:49:CYS:SG	3.00	0.55
4:DO:90:VAL:HG21	4:DO:93:VAL:HB	1.89	0.55
11:PB:65:ILE:HB	11:PB:86:LEU:HB2	1.88	0.55
11:PB:592:ARG:HE	11:PB:627:ILE:HD13	1.71	0.55
12:PC:130:VAL:O	12:PC:131:THR:C	2.46	0.55
22:DA:484:ILE:HD11	26:Df:306:PRO:HA	1.89	0.55
25:DE:278:ASP:OD2	25:DE:649:ARG:NH2	2.41	0.55
25:DE:295:GLU:HA	25:DE:298:LEU:HB2	1.89	0.55
42:6:693:LEU:HD12	42:6:696:MET:HG2	1.88	0.55
45:e:136:LEU:HD22	56:k:104:LEU:HD22	1.89	0.55
48:m:56:LEU:CG	48:m:80:GLN:HE22	2.20	0.55
49:a:128:HIS:CG	49:a:128:HIS:O	2.60	0.55
50:d:47:MET:HE3	50:d:47:MET:CA	2.35	0.55
54:i:105:PRO:CD	54:i:107:ILE:HG13	2.34	0.55
57:n:707:ASP:HA	58:o:684:ARG:NH2	2.22	0.55
59:q:633:ARG:CG	59:q:633:ARG:HH21	2.20	0.55
64:v:21:ARG:NH2	64:v:78:LEU:HD23	2.17	0.55
2:8:30:ARG:HB3	2:8:30:ARG:CZ	2.34	0.54
2:8:241:CYS:O	2:8:241:CYS:SG	2.64	0.54
7:BA:45:VAL:HG12	10:PA:78:MET:HG2	1.89	0.54
10:PA:1186:VAL:HG12	10:PA:1188:GLU:HG2	1.89	0.54
11:PB:223:SER:HB3	11:PB:349:PRO:HD2	1.87	0.54
16:PG:11:ILE:HD11	16:PG:30:LEU:HB2	1.88	0.54
18:PI:85:PRO:HA	18:PI:92:LYS:HA	1.89	0.54
22:DA:1052:ARG:HD2	22:DA:1052:ARG:O	2.07	0.54
40:4:295:SER:OG	40:4:369:ARG:NH1	2.39	0.54
42:6:309:ASP:HA	42:6:384:ILE:HD11	1.88	0.54
43:7:741:LEU:HD12	43:7:741:LEU:O	2.06	0.54
48:m:68:LYS:HD2	52:g:50:GLN:CD	2.30	0.54
53:h:81:LEU:HD12	53:h:101:SER:O	2.06	0.54
54:i:110:SER:CB	54:i:111:PRO:HD2	2.37	0.54
57:n:169:LEU:O	59:q:19:VAL:HG13	2.07	0.54
58:o:767:HIS:CD2	58:o:772:LEU:HD21	2.42	0.54
59:q:194:TRP:CZ2	59:q:295:LEU:HB3	2.42	0.54
59:q:437:HIS:HD2	59:q:437:HIS:O	1.89	0.54
64:v:39:THR:C	64:v:41:LYS:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:143:LEU:HD23	2:8:151:LEU:HD11	1.87	0.54
20:PK:42:LEU:HA	20:PK:45:ILE:HG22	1.90	0.54
22:DA:401:ASN:H	22:DA:401:ASN:HD22	1.53	0.54
25:De:646:SER:OG	25:De:647:ALA:N	2.41	0.54
37:1:355:GLN:NE2	39:3:285:CYS:SG	2.80	0.54
38:2:199:ILE:HG12	38:2:220:HIS:HB2	1.89	0.54
52:g:89:PHE:CE1	63:u:23:ILE:HD11	2.42	0.54
53:h:124:LEU:HD22	59:q:147:ILE:CG2	2.37	0.54
59:q:578:TYR:CE1	59:q:646:LEU:HD13	2.41	0.54
67:w:625:SER:HB2	67:w:674:THR:HG22	1.89	0.54
67:w:781:SER:O	67:w:783:GLN:NE2	2.41	0.54
2:8:86:ASN:ND2	2:8:86:ASN:C	2.58	0.54
5:DP:313:THR:HG23	69:X:-27:DA:C5'	2.33	0.54
6:DQ:333:ASN:HD22	6:DQ:360:LEU:HB3	1.71	0.54
11:PB:110:PRO:HG2	11:PB:163:LEU:CD1	2.22	0.54
22:DA:505:ASN:HB2	26:DF:209:LYS:HD2	1.88	0.54
32:Dc:67:GLY:CA	30:Dj:116:LEU:HD13	2.33	0.54
37:1:257:MET:SD	43:7:582:GLU:CB	2.96	0.54
56:k:43:ARG:HH11	56:k:43:ARG:CB	2.19	0.54
59:q:9:ILE:CG1	63:u:90:LEU:CD1	2.68	0.54
59:q:247:ILE:HD11	59:q:294:LYS:HB3	1.88	0.54
63:u:8:LEU:HD12	63:u:72:LEU:HD23	1.85	0.54
64:v:37:ILE:C	64:v:39:THR:N	2.64	0.54
67:w:10:GLU:OE1	67:w:66:PHE:HZ	1.91	0.54
7:BA:225:PRO:HG2	7:BA:228:VAL:HG23	1.90	0.54
8:FA:16:VAL:HG23	9:FB:43:LEU:HB2	1.90	0.54
8:FA:135:PHE:HE2	9:FB:43:LEU:HD22	1.70	0.54
11:PB:647:GLU:CD	11:PB:647:GLU:H	2.15	0.54
12:PC:30:VAL:HA	20:PK:45:ILE:HD12	1.89	0.54
13:PD:90:LYS:HB3	13:PD:122:PHE:CZ	2.42	0.54
14:PE:10:LEU:HD23	14:PE:13:ILE:HD12	1.89	0.54
17:PH:27:ARG:HD2	17:PH:40:ILE:HG22	1.89	0.54
18:PI:78:LEU:HB3	18:PI:95:VAL:HG23	1.90	0.54
29:DI:31:TYR:CD2	29:DI:35:VAL:HB	2.41	0.54
25:De:368:ASN:ND2	25:De:701:GLY:HA3	2.22	0.54
40:4:155:ARG:HA	40:4:158:VAL:HG12	1.89	0.54
42:6:390:CYS:HB2	42:6:406:ALA:HA	1.89	0.54
43:7:203:ASN:C	43:7:204:VAL:HG23	2.33	0.54
49:a:229:SER:CB	49:a:502:MET:CB	2.82	0.54
49:a:248:SER:HB3	49:a:251:LEU:HB2	1.90	0.54
55:j:58:LEU:O	55:j:59:HIS:CG	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:678:PHE:CZ	59:q:583:ARG:HB2	2.43	0.54
57:n:870:GLN:CG	58:o:655:THR:HG22	2.36	0.54
2:8:241:CYS:HB2	2:8:246:TYR:CE1	2.43	0.54
5:DP:218:LYS:CG	69:X:-23:DG:OP2	2.56	0.54
19:PJ:3:ILE:HD11	19:PJ:49:LEU:HD12	1.89	0.54
23:DB:248:SER:OG	23:DB:322:MET:SD	2.65	0.54
31:DL:106:ARG:HH12	31:DL:114:LYS:HD2	1.72	0.54
35:EA:145:PHE:HB2	35:EA:152:PHE:CE1	2.43	0.54
37:1:132:VAL:O	37:1:135:GLN:NE2	2.41	0.54
44:c:296:TRP:NE1	44:c:311:GLN:HG3	2.23	0.54
46:b:160:TYR:O	46:b:164:ILE:HG12	2.07	0.54
49:a:336:TYR:CD1	49:a:391:THR:HG23	2.43	0.54
57:n:175:ASP:OD2	59:q:20:HIS:CE1	2.61	0.54
65:z:480:LEU:HD23	65:z:480:LEU:O	2.08	0.54
67:w:339:ILE:O	67:w:343:LEU:HB2	2.08	0.54
67:w:1185:GLY:O	67:w:1186:TYR:C	2.50	0.54
69:X:-19:DG:N2	70:Y:19:DC:C2	2.52	0.54
2:8:133:ILE:O	2:8:133:ILE:HG22	2.07	0.54
5:DP:304:ILE:HD11	5:DP:328:ILE:HD11	1.89	0.54
7:BA:214:PHE:O	7:BA:218:PHE:HD2	1.89	0.54
23:DB:571:LEU:HD21	23:DB:619:MET:HE1	1.89	0.54
25:DE:563:GLU:HG2	25:DE:587:PRO:HG3	1.90	0.54
31:DL:91:PHE:O	31:DL:95:VAL:HG23	2.07	0.54
37:1:130:ASP:HA	37:1:133:VAL:HB	1.90	0.54
40:4:17:ARG:HA	40:4:20:GLN:HB3	1.90	0.54
40:4:328:ILE:HA	40:4:331:PHE:HB3	1.89	0.54
42:6:337:VAL:O	42:6:488:LEU:N	2.35	0.54
43:7:224:GLU:HG2	43:7:450:ARG:HG3	1.89	0.54
43:7:242:VAL:O	43:7:246:SER:N	2.41	0.54
48:m:70:PRO:CB	57:n:166:TYR:HH	2.16	0.54
59:q:109:MET:HE3	59:q:109:MET:C	2.32	0.54
67:w:169:TYR:CE2	67:w:177:LEU:HD11	2.43	0.54
2:8:132:TRP:HA	2:8:132:TRP:HE3	1.73	0.54
11:PB:517:GLY:H	11:PB:520:VAL:HG23	1.72	0.54
14:PE:55:ARG:HB3	14:PE:78:GLU:HA	1.88	0.54
24:DD:1068:GLU:OE2	25:DE:582:LYS:NZ	2.40	0.54
28:DH:159:TYR:N	28:DH:159:TYR:CD1	2.75	0.54
43:7:503:ALA:HA	43:7:682:LYS:HD2	1.90	0.54
48:m:70:PRO:C	57:n:166:TYR:HH	2.16	0.54
37:1:368:SER:HB3	37:1:373:ALA:HB1	1.89	0.54
37:1:408:ARG:HG2	39:3:112:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:110:LYS:HE3	38:2:140:HIS:H	1.73	0.54
49:a:109:TYR:HE1	49:a:150:PHE:HZ	1.56	0.54
50:d:166:THR:HG23	50:d:166:THR:O	2.08	0.54
55:j:77:PRO:C	55:j:79:LEU:H	2.15	0.54
57:n:780:VAL:HG12	57:n:808:LEU:HD11	1.90	0.54
58:o:715:LEU:N	66:x:25:ILE:CG1	2.68	0.54
58:o:776:TRP:O	58:o:780:VAL:HG23	2.08	0.54
59:q:184:ASN:CG	64:v:83:LYS:HD2	2.32	0.54
67:w:1:MET:H2	67:w:4:GLN:HG3	1.72	0.54
10:PA:436:SER:HB2	62:t:97:LYS:HD2	1.90	0.54
18:PI:73:SER:HA	18:PI:95:VAL:HG11	1.90	0.54
23:DB:66:ASN:HD21	23:DB:119:PRO:HB3	1.73	0.54
24:DD:1003:ASP:O	24:DD:1007:THR:HG23	2.07	0.54
31:DL:111:LEU:HB2	31:DL:115:ASP:OD2	2.07	0.54
38:2:87:LEU:HD13	38:2:229:LYS:HD3	1.90	0.54
40:4:245:LEU:CG	40:4:280:ARG:HE	2.21	0.54
40:4:360:THR:O	40:4:364:ILE:N	2.37	0.54
42:6:192:PRO:HA	42:6:196:GLU:HA	1.90	0.54
42:6:363:VAL:HA	42:6:439:ILE:HB	1.89	0.54
43:7:275:GLU:HA	43:7:278:GLU:HB2	1.90	0.54
49:a:270:ILE:O	49:a:270:ILE:HG22	2.08	0.54
53:h:72:ARG:HH11	59:q:134:ALA:H	1.48	0.54
57:n:172:CYS:SG	59:q:20:HIS:O	2.52	0.54
67:w:261:ASP:OD1	67:w:261:ASP:N	2.38	0.54
67:w:958:ASN:N	67:w:958:ASN:OD1	2.40	0.54
67:w:1036:ASP:OD1	67:w:1036:ASP:N	2.38	0.54
11:PB:773:PRO:HG2	19:PJ:53:VAL:HG11	1.90	0.54
12:PC:93:PHE:HB2	12:PC:164:TYR:CD2	2.42	0.54
22:DA:564:PRO:HG2	23:DB:744:PHE:CD1	2.43	0.54
23:DB:539:ARG:HB2	40:4:408:LEU:HD11	1.89	0.54
24:Dd:911:GLN:NE2	31:Dl:69:GLU:OE2	2.40	0.54
25:De:251:LEU:O	25:De:256:HIS:HB2	2.08	0.54
26:Df:253:TYR:O	26:Df:254:GLN:HB3	2.06	0.54
36:EB:175:LEU:HD21	36:EB:180:LYS:HE3	1.90	0.54
43:7:538:PHE:HB3	43:7:600:ALA:HB2	1.89	0.54
49:a:383:PRO:HD3	49:a:445:LEU:O	2.07	0.54
51:f:39:PRO:HD3	52:g:11:LEU:HD11	1.90	0.54
53:h:110:ARG:C	53:h:110:ARG:HD3	2.33	0.54
56:k:70:LEU:CD2	64:v:85:PHE:HD1	2.02	0.54
57:n:879:LEU:HA	57:n:882:ILE:HG22	1.90	0.54
58:o:759:ARG:HE	58:o:762:GLN:HG2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:123:LYS:HG2	59:q:124:PHE:CE2	2.43	0.54
59:q:647:SER:HB2	59:q:648:PRO:HD2	1.90	0.54
63:u:68:ASP:OD1	65:z:585:HIS:NE2	2.41	0.54
2:8:22:GLN:H	2:8:22:GLN:CD	2.16	0.53
3:9:227:THR:HB	3:9:229:GLU:OE1	2.07	0.53
7:BA:46:ILE:HB	10:PA:67:ARG:NH2	2.23	0.53
28:DH:60:THR:CG2	30:DJ:211:VAL:HG23	2.34	0.53
35:EA:122:THR:O	35:EA:124:ARG:N	2.41	0.53
37:1:199:THR:HG23	37:1:317:ALA:HB2	1.90	0.53
39:3:250:ASP:N	39:3:250:ASP:OD1	2.39	0.53
40:4:231:VAL:O	40:4:235:SER:N	2.41	0.53
43:7:464:LEU:HD13	43:7:477:THR:HG22	1.91	0.53
43:7:523:LEU:HB2	43:7:710:VAL:HG21	1.90	0.53
43:7:684:PHE:O	43:7:689:LYS:NZ	2.41	0.53
50:d:111:GLN:NE2	57:n:201:HIS:CE1	2.75	0.53
55:j:9:GLU:HG2	55:j:56:GLN:OE1	2.07	0.53
66:x:956:VAL:HG13	66:x:968:LEU:HG	1.90	0.53
67:w:16:GLU:OE1	67:w:75:ARG:HA	2.06	0.53
8:FA:119:THR:HG22	8:FA:123:SER:HA	1.89	0.53
9:FB:147:LYS:CG	9:FB:148:VAL:N	2.65	0.53
10:PA:153:ILE:HA	10:PA:187:TYR:HB3	1.90	0.53
10:PA:406:VAL:HG21	10:PA:419:ILE:HD11	1.88	0.53
11:PB:224:CYS:O	11:PB:224:CYS:SG	2.66	0.53
15:PF:75:MET:O	15:PF:76:CYS:HB2	2.08	0.53
15:PF:79:VAL:HG21	15:PF:83:LEU:HD11	1.90	0.53
22:DA:349:TRP:CD2	26:Df:266:GLY:HA2	2.44	0.53
39:3:191:ILE:HB	39:3:210:THR:HG21	1.89	0.53
42:6:65:MET:HB2	42:6:73:SER:HB3	1.91	0.53
42:6:177:VAL:HG11	42:6:184:VAL:HG22	1.90	0.53
43:7:277:ASP:HA	43:7:280:ARG:HD2	1.90	0.53
48:m:106:GLN:HA	50:d:163:ALA:CB	2.38	0.53
49:a:367:LEU:HD22	49:a:509:ARG:NH1	2.23	0.53
52:g:93:LEU:C	55:j:106:LYS:HZ3	2.17	0.53
52:g:120:HIS:O	52:g:123:ILE:HG12	2.07	0.53
52:g:161:ILE:O	54:i:140:MET:SD	2.66	0.53
53:h:147:CYS:SG	53:h:148:SER:N	2.81	0.53
57:n:549:TYR:HB2	57:n:571:MET:HE2	1.90	0.53
58:o:748:PHE:O	58:o:752:VAL:HG13	2.09	0.53
59:q:166:ARG:CG	59:q:166:ARG:HH11	2.21	0.53
59:q:223:GLU:HB2	59:q:246:GLN:HB3	1.90	0.53
59:q:482:GLN:H	59:q:634:ASN:ND2	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:288:THR:C	1:0:290:SER:H	2.15	0.53
10:PA:286:ILE:HG12	10:PA:289:GLN:HE21	1.73	0.53
22:DA:349:TRP:HZ2	26:Df:282:LEU:HD21	1.74	0.53
23:DB:544:LEU:HD23	23:DB:590:ILE:HD11	1.89	0.53
23:DB:808:PRO:HA	23:DB:864:ASN:HB3	1.91	0.53
25:DE:304:LYS:NZ	25:DE:335:GLU:O	2.42	0.53
32:Dc:33:LEU:HD13	30:Dj:197:MET:HE1	1.90	0.53
43:7:705:ASN:CA	43:7:708:LEU:HD21	2.38	0.53
43:7:739:LEU:C	43:7:741:LEU:N	2.65	0.53
49:a:412:ARG:HB3	49:a:472:SER:OG	2.06	0.53
50:d:45:ILE:HD13	54:i:73:ILE:CA	2.38	0.53
53:h:25:SER:OG	53:h:52:LEU:HB2	2.09	0.53
54:i:140:MET:O	63:u:114:LEU:HD23	2.08	0.53
57:n:587:LEU:CD2	67:w:15:THR:HG22	2.38	0.53
65:z:560:TRP:CD1	65:z:561:PRO:HD2	2.44	0.53
66:x:358:ASP:OD1	66:x:389:ARG:NE	2.41	0.53
66:x:628:VAL:HG13	66:x:636:ARG:HG2	1.91	0.53
67:w:1302:LYS:NZ	67:w:1308:ASP:OD1	2.41	0.53
1:0:75:ARG:HG3	1:0:76:LYS:N	2.23	0.53
1:0:295:ARG:NE	3:9:165:ARG:HE	2.07	0.53
4:DO:56:VAL:HG22	6:DQ:369:LYS:O	2.08	0.53
13:PD:110:GLU:HA	16:PG:167:TYR:CE2	2.43	0.53
20:PK:40:HIS:CE1	20:PK:63:VAL:HG21	2.43	0.53
23:DB:152:LEU:HD23	23:DB:155:PRO:HB3	1.91	0.53
25:DE:461:ILE:O	26:DF:135:TRP:HA	2.08	0.53
29:DI:60:HIS:CD2	31:DL:106:ARG:CD	2.92	0.53
37:1:372:ILE:HG21	39:3:201:GLY:HA3	1.91	0.53
42:6:62:ARG:HG3	42:6:74:ARG:HA	1.89	0.53
44:c:167:SER:OG	44:c:171:ARG:NH1	2.41	0.53
49:a:106:ASP:N	49:a:106:ASP:OD1	2.40	0.53
49:a:412:ARG:CA	49:a:472:SER:HB3	2.38	0.53
57:n:208:LEU:HD12	57:n:208:LEU:O	2.08	0.53
57:n:229:GLU:HG3	57:n:300:CYS:CB	2.38	0.53
57:n:864:ASN:ND2	57:n:867:GLN:OE1	2.41	0.53
59:q:326:VAL:HG12	59:q:331:ILE:HG12	1.90	0.53
62:t:128:THR:O	62:t:128:THR:OG1	2.27	0.53
67:w:999:ASP:N	67:w:999:ASP:OD1	2.40	0.53
7:BA:193:ARG:NH1	70:Y:22:DC:OP2	2.42	0.53
10:PA:1106:THR:CG2	10:PA:1119:LEU:HB2	2.37	0.53
12:PC:220:TYR:CE2	12:PC:222:PRO:HB3	2.43	0.53
14:PE:72:MET:HA	14:PE:101:ARG:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:PL:16:ILE:HG23	21:PL:47:LYS:HB2	1.91	0.53
23:DB:345:CYS:HA	23:DB:348:GLN:HE21	1.73	0.53
29:DI:23:LEU:HD12	29:DI:31:TYR:OH	2.09	0.53
24:Dd:963:ARG:NH2	24:Dd:964:GLU:OE2	2.42	0.53
29:Di:73:LEU:HB2	31:Dl:105:HIS:CE1	2.41	0.53
35:EA:136:PHE:CB	35:EA:144:LEU:HD11	2.37	0.53
37:1:321:LYS:HG2	38:2:180:SER:H	1.73	0.53
37:1:533:TYR:O	37:1:537:HIS:N	2.36	0.53
39:3:25:GLN:NE2	39:3:32:PHE:O	2.38	0.53
40:4:26:LEU:O	40:4:94:ARG:NH1	2.38	0.53
40:4:339:PRO:CG	42:6:55:GLU:HG2	2.38	0.53
43:7:49:THR:O	43:7:53:LEU:N	2.41	0.53
49:a:160:LEU:CG	49:a:219:LEU:HD21	2.38	0.53
52:g:93:LEU:HD22	55:j:106:LYS:HE3	1.88	0.53
53:h:187:PHE:CE2	53:h:189:LYS:HB2	2.44	0.53
55:j:75:ARG:CA	55:j:79:LEU:HD12	2.37	0.53
55:j:82:LYS:HZ1	61:s:99:LYS:CB	2.19	0.53
57:n:250:LEU:HD23	57:n:275:HIS:CB	2.36	0.53
59:q:451:LEU:HD12	59:q:460:ILE:HD12	1.89	0.53
61:s:152:PHE:C	61:s:154:LEU:H	2.17	0.53
64:v:21:ARG:HD2	64:v:78:LEU:HD21	1.90	0.53
2:8:259:HIS:CE1	10:PA:1669:PRO:HB3	2.27	0.53
10:PA:18:ILE:HD11	11:PB:1149:VAL:HG21	1.89	0.53
10:PA:437:ASP:CA	62:t:97:LYS:HZ3	2.22	0.53
14:PE:63:ALA:HB2	14:PE:71:GLN:HG2	1.89	0.53
22:DA:567:LEU:CD2	23:DB:745:GLN:HE21	2.21	0.53
25:DE:774:MET:HG3	26:DF:149:PRO:HG3	1.91	0.53
36:EB:103:LEU:HB3	36:EB:109:LEU:HA	1.90	0.53
39:3:14:VAL:O	39:3:164:ILE:N	2.38	0.53
39:3:145:HIS:HA	39:3:148:ASN:HD22	1.72	0.53
40:4:307:ILE:HD13	40:4:371:ARG:HB3	1.91	0.53
42:6:35:GLN:OE1	42:6:159:CYS:CB	2.55	0.53
42:6:197:CYS:SG	42:6:198:ARG:N	2.82	0.53
42:6:299:ASN:HB3	42:6:332:ARG:HD3	1.90	0.53
48:m:26:GLN:NE2	52:g:45:PHE:CD2	2.76	0.53
51:f:188:PHE:HD2	57:n:295:CYS:SG	2.18	0.53
58:o:693:LEU:CD2	59:q:608:ASP:CB	2.77	0.53
3:9:33:LYS:HD3	3:9:33:LYS:C	2.34	0.53
7:BA:267:GLU:OE1	7:BA:269:ARG:NH2	2.41	0.53
8:FA:135:PHE:CE2	9:FB:43:LEU:HD22	2.43	0.53
10:PA:678:ASN:O	10:PA:682:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:916:PHE:HE2	10:PA:960:ARG:HA	1.73	0.53
11:PB:924:ARG:CZ	12:PC:60:HIS:HB3	2.39	0.53
13:PD:137:LYS:CE	53:h:51:LEU:CB	2.81	0.53
22:DA:569:ASN:HB3	22:DA:572:TYR:HD2	1.73	0.53
37:1:266:LEU:HD22	43:7:575:ALA:HA	1.90	0.53
38:2:59:ARG:HA	38:2:164:SER:HB2	1.91	0.53
40:4:447:GLY:O	40:4:451:VAL:HG23	2.09	0.53
42:6:153:MET:HA	42:6:156:ILE:HG22	1.91	0.53
47:l:30:THR:OG1	47:l:102:ASN:ND2	2.40	0.53
51:f:32:TYR:CD1	51:f:35:GLU:CD	2.87	0.53
51:f:32:TYR:HD1	51:f:35:GLU:CD	2.16	0.53
55:j:43:PHE:CE1	61:s:147:THR:CA	2.91	0.53
57:n:254:VAL:HG11	57:n:304:GLN:NE2	2.11	0.53
57:n:327:GLU:HG3	57:n:356:LYS:HG2	1.91	0.53
57:n:449:SER:OG	57:n:450:GLU:N	2.41	0.53
58:o:690:LEU:O	58:o:692:ASN:ND2	2.42	0.53
2:8:146:ASP:OD1	2:8:149:GLY:N	2.33	0.53
10:PA:1661:SER:CB	50:d:183:ARG:HD3	2.39	0.53
12:PC:83:GLN:CD	62:t:204:GLN:OE1	2.52	0.53
12:PC:181:GLY:HA3	19:PJ:42:ARG:NH1	2.23	0.53
23:DB:539:ARG:NH1	41:5:35:ILE:HG23	2.24	0.53
24:DD:1069:ASN:O	26:DF:95:ARG:HD3	2.08	0.53
26:Df:447:ALA:O	26:Df:453:GLY:HA2	2.09	0.53
37:1:461:LEU:HD21	37:1:504:LYS:HD2	1.90	0.53
40:4:50:SER:O	40:4:54:ASN:ND2	2.41	0.53
40:4:418:PHE:CE2	40:4:439:ARG:HA	2.43	0.53
50:d:47:MET:HA	50:d:47:MET:CE	2.37	0.53
55:j:43:PHE:HE1	61:s:147:THR:CB	2.19	0.53
57:n:686:LYS:NZ	58:o:730:PRO:CB	2.62	0.53
62:t:78:LEU:HD22	62:t:78:LEU:H	1.74	0.53
65:z:540:LEU:C	65:z:540:LEU:HD22	2.34	0.53
65:z:582:LEU:HD23	65:z:591:LEU:HB3	1.91	0.53
67:w:522:PRO:HG3	67:w:565:GLU:HG2	1.90	0.53
1:0:275:VAL:HG13	1:0:276:ARG:HE	1.73	0.53
2:8:171:HIS:HB3	2:8:172:GLN:NE2	2.24	0.53
6:DQ:333:ASN:HB3	6:DQ:360:LEU:HD23	1.91	0.53
7:BA:129:ASN:ND2	11:PB:99:TRP:HE1	2.07	0.53
10:PA:439:HIS:ND1	60:r:92:GLU:CD	2.55	0.53
18:PI:15:ARG:HB3	18:PI:24:LEU:CD1	2.39	0.53
24:DD:1078:LEU:HD11	31:DL:86:GLN:HB3	1.91	0.53
25:De:423:PRO:HG2	25:De:426:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3:112:VAL:HA	39:3:115:ILE:HG22	1.91	0.53
49:a:445:LEU:HD11	49:a:451:SER:HB3	1.90	0.53
51:f:176:ARG:NE	57:n:306:GLU:OE2	2.42	0.53
51:f:188:PHE:HB3	57:n:295:CYS:SG	2.49	0.53
52:g:93:LEU:C	55:j:106:LYS:NZ	2.67	0.53
57:n:362:ASP:O	57:n:363:GLU:C	2.52	0.53
69:X:-26:DA:H3'	69:X:-26:DA:P	2.47	0.53
1:0:191:ASP:OD2	1:0:193:PRO:HG3	2.09	0.53
3:9:268:GLU:OE1	3:9:268:GLU:N	2.29	0.53
8:FA:46:ARG:HB2	8:FA:101:ARG:HB2	1.91	0.53
9:FB:145:LEU:HG	11:PB:92:TYR:HB3	1.91	0.53
10:PA:405:LEU:HD13	10:PA:448:ARG:HG3	1.91	0.53
10:PA:909:LEU:HD21	10:PA:975:SER:HA	1.91	0.53
10:PA:1148:ALA:O	10:PA:1334:TRP:HD1	1.92	0.53
10:PA:1352:VAL:O	10:PA:1353:ASP:C	2.51	0.53
11:PB:404:PHE:HA	11:PB:407:MET:HE2	1.91	0.53
22:DA:999:SER:O	22:DA:1001:LYS:N	2.41	0.53
23:DB:529:VAL:HG11	23:DB:560:TYR:HB2	1.91	0.53
25:DE:653:LEU:HB2	25:DE:663:ARG:HB2	1.90	0.53
26:DF:209:LYS:HB2	26:DF:210:PRO:HD2	1.91	0.53
40:4:409:TYR:HD2	41:5:3:ASN:CB	2.22	0.53
42:6:497:GLN:HG2	42:6:504:LYS:HG2	1.91	0.53
49:a:226:VAL:HG12	49:a:226:VAL:O	2.08	0.53
49:a:321:LEU:C	49:a:321:LEU:HD13	2.34	0.53
50:d:86:GLN:OE1	54:i:107:ILE:HA	2.09	0.53
50:d:153:HIS:HB2	52:g:56:ILE:HG23	1.91	0.53
56:k:9:GLU:CG	64:v:86:LEU:HG	2.20	0.53
56:k:17:ILE:CG2	59:q:171:VAL:HG22	2.10	0.53
57:n:141:ARG:HH22	63:u:17:ASP:HA	1.74	0.53
59:q:140:ASN:N	59:q:141:PRO:HD2	2.24	0.53
60:r:19:MET:HE2	60:r:177:ALA:HB1	1.88	0.53
66:x:472:ASN:ND2	66:x:496:SER:OG	2.42	0.53
70:Y:32:DG:H2'	70:Y:33:DC:C5	2.44	0.53
3:9:192:ASP:C	3:9:192:ASP:OD1	2.53	0.52
10:PA:593:SER:HB3	10:PA:634:GLU:HA	1.90	0.52
10:PA:1211:LEU:HB2	10:PA:1260:ARG:HB3	1.91	0.52
11:PB:311:ILE:HD11	11:PB:320:PHE:HB2	1.90	0.52
13:PD:60:VAL:HG21	16:PG:36:GLY:HA2	1.91	0.52
22:DA:484:ILE:HD13	26:Df:309:MET:HB3	1.90	0.52
22:DA:854:ARG:NH2	70:Y:-25:DT:C5'	2.71	0.52
23:DB:628:ILE:O	23:DB:644:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Df:283:MET:HG3	26:Df:329:LEU:HD11	1.90	0.52
37:1:257:MET:SD	43:7:582:GLU:CG	2.97	0.52
51:f:181:LEU:CD1	57:n:270:GLN:HG3	2.39	0.52
55:j:70:TYR:CE1	55:j:80:TYR:HB3	2.39	0.52
59:q:155:GLY:CA	64:v:62:HIS:CE1	2.63	0.52
59:q:437:HIS:ND1	59:q:471:TYR:C	2.67	0.52
63:u:82:THR:HA	63:u:86:GLN:NE2	2.24	0.52
66:x:175:ARG:HH21	66:x:221:LEU:HD22	1.73	0.52
66:x:976:PRO:HA	66:x:979:ARG:HE	1.73	0.52
10:PA:436:SER:CB	62:t:97:LYS:CE	2.76	0.52
17:PH:60:ILE:HG21	17:PH:135:PHE:HE1	1.74	0.52
23:DB:937:THR:HG23	23:DB:939:ASN:H	1.73	0.52
25:DE:516:ILE:HD12	25:DE:527:ILE:HA	1.91	0.52
37:1:163:ASP:OD2	38:2:179:PRO:HD2	2.07	0.52
38:2:172:SER:HA	38:2:201:LEU:HB3	1.91	0.52
42:6:435:TRP:CB	42:6:461:HIS:ND1	2.71	0.52
49:a:228:PRO:CA	49:a:502:MET:SD	2.97	0.52
51:f:15:TRP:CH2	51:f:35:GLU:HB2	2.44	0.52
54:i:75:CYS:HB3	54:i:88:ASN:HD21	1.70	0.52
57:n:278:VAL:HG11	57:n:292:MET:HG2	1.92	0.52
64:v:133:GLU:OE1	64:v:133:GLU:HA	2.09	0.52
69:X:3:DT:H2"	69:X:4:DC:C6	2.44	0.52
2:8:98:LEU:HD12	2:8:98:LEU:O	2.10	0.52
7:BA:146:TYR:O	7:BA:149:LYS:HG2	2.09	0.52
10:PA:437:ASP:HA	62:t:97:LYS:HZ3	1.75	0.52
10:PA:823:VAL:HG22	10:PA:835:GLU:HB3	1.91	0.52
11:PB:785:TYR:H	11:PB:789:ASN:HD21	1.57	0.52
13:PD:95:PHE:O	13:PD:99:CYS:HB2	2.10	0.52
13:PD:116:PRO:O	13:PD:119:GLU:HB2	2.09	0.52
23:DB:217:ASN:ND2	23:DB:320:ALA:O	2.35	0.52
25:DE:423:PRO:HG2	25:DE:426:ARG:HB2	1.91	0.52
25:DE:507:VAL:CG2	25:DE:513:LEU:HD11	2.40	0.52
26:Df:318:CYS:SG	26:Df:326:HIS:HB3	2.49	0.52
37:1:257:MET:HG3	43:7:579:VAL:HG22	1.91	0.52
37:1:417:LYS:HZ1	39:3:43:VAL:HG21	1.73	0.52
40:4:304:PRO:HG2	40:4:372:ALA:CA	2.39	0.52
42:6:472:ARG:NH1	42:6:473:GLU:CA	2.71	0.52
47:l:51:ILE:O	47:l:55:LEU:HG	2.09	0.52
49:a:348:LEU:HD13	49:a:425:VAL:HG12	1.89	0.52
51:f:181:LEU:HD23	51:f:184:LEU:HD21	1.91	0.52
52:g:126:TYR:C	52:g:128:PRO:HD2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:n:836:GLY:O	57:n:846:ASN:ND2	2.37	0.52
57:n:923:CYS:SG	57:n:924:ILE:N	2.82	0.52
3:9:41:LEU:HG	3:9:41:LEU:O	2.07	0.52
3:9:165:ARG:HB3	3:9:166:PRO:HD3	1.92	0.52
11:PB:924:ARG:CZ	12:PC:60:HIS:HB2	2.40	0.52
14:PE:100:THR:HA	14:PE:125:TYR:HA	1.92	0.52
24:DD:910:LEU:HD11	31:DL:88:ALA:HB2	1.92	0.52
24:Dd:943:GLN:NE2	25:De:509:GLN:O	2.41	0.52
37:1:483:THR:C	37:1:485:PHE:H	2.16	0.52
38:2:167:VAL:HB	38:2:196:VAL:HA	1.91	0.52
39:3:14:VAL:N	39:3:162:LEU:O	2.40	0.52
39:3:236:ASP:O	39:3:240:GLN:HB2	2.09	0.52
40:4:328:ILE:O	40:4:332:SER:N	2.32	0.52
43:7:81:GLU:HA	43:7:84:ILE:HD12	1.92	0.52
43:7:262:ASN:HA	43:7:265:THR:HB	1.92	0.52
43:7:519:ASN:HD22	43:7:522:ASN:ND2	2.07	0.52
45:e:97:GLN:NE2	59:q:647:SER:HB2	2.25	0.52
51:f:181:LEU:CD1	57:n:270:GLN:CG	2.87	0.52
52:g:96:LEU:HD13	55:j:102:MET:HE1	1.91	0.52
58:o:775:THR:HA	58:o:778:GLN:HG2	1.91	0.52
59:q:190:LEU:HD23	59:q:291:TRP:CE3	2.44	0.52
62:t:8:GLN:NE2	62:t:200:ILE:HD13	2.24	0.52
7:BA:218:PHE:HD1	7:BA:277:ILE:HG22	1.74	0.52
10:PA:480:SER:HB3	20:PK:2:ASN:ND2	2.24	0.52
11:PB:588:ARG:O	11:PB:589:LYS:C	2.48	0.52
11:PB:1060:HIS:ND1	11:PB:1080:ARG:HG2	2.25	0.52
13:PD:57:LEU:HB2	13:PD:62:MET:HE2	1.91	0.52
14:PE:59:THR:HB	14:PE:73:PHE:HE1	1.74	0.52
25:DE:601:VAL:HG21	25:DE:642:VAL:HG11	1.92	0.52
26:DF:76:LYS:HG3	26:DF:96:PHE:HB3	1.91	0.52
26:DF:86:PHE:HA	30:DJ:212:LYS:HZ3	1.75	0.52
25:De:607:ARG:NH1	29:Di:87:PRO:O	2.43	0.52
38:2:87:LEU:HB2	38:2:228:TYR:HE2	1.74	0.52
40:4:322:GLU:HA	40:4:325:ILE:HD12	1.92	0.52
42:6:266:GLN:O	42:6:268:VAL:N	2.41	0.52
43:7:672:THR:OG1	43:7:731:GLU:OE1	2.27	0.52
43:7:697:ILE:HG22	43:7:701:LEU:HD22	1.92	0.52
44:c:46:GLU:H	44:c:46:GLU:CD	2.17	0.52
49:a:127:HIS:HE1	49:a:171:THR:HG22	1.73	0.52
53:h:102:HIS:CD2	53:h:102:HIS:N	2.73	0.52
55:j:12:LEU:O	55:j:16:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:577:ASP:HB2	59:q:597:PRO:HG3	1.91	0.52
64:v:110:GLU:OE1	64:v:110:GLU:HA	2.09	0.52
67:w:378:GLN:HE22	67:w:532:THR:HA	1.75	0.52
9:FB:173:GLY:HA3	69:X:-20:DG:C5'	2.38	0.52
13:PD:79:THR:CB	53:h:51:LEU:HD21	2.39	0.52
13:PD:100:LEU:O	13:PD:105:PRO:HD3	2.10	0.52
25:DE:294:ASN:C	25:DE:296:THR:H	2.18	0.52
26:DF:418:ILE:HD12	26:DF:418:ILE:N	2.20	0.52
30:DJ:137:TYR:OH	30:DJ:141:ARG:NH2	2.43	0.52
25:De:595:PRO:HD2	25:De:639:SER:HB3	1.91	0.52
38:2:11:TRP:O	38:2:15:TYR:N	2.38	0.52
42:6:132:GLN:HG3	42:6:134:SER:H	1.74	0.52
45:e:96:LEU:HD13	59:q:640:GLU:HG2	1.92	0.52
50:d:64:GLN:HE21	50:d:68:LEU:CD1	2.23	0.52
52:g:90:LEU:HD12	55:j:124:TYR:HE1	1.53	0.52
53:h:82:SER:C	53:h:84:ASP:H	2.18	0.52
55:j:39:GLN:HB3	55:j:43:PHE:HE2	1.75	0.52
55:j:75:ARG:HB2	55:j:80:TYR:HE2	0.74	0.52
55:j:82:LYS:HG2	61:s:96:PHE:CD1	2.38	0.52
57:n:160:VAL:HG22	57:n:166:TYR:HE1	1.74	0.52
57:n:231:GLU:HB2	57:n:253:LEU:CD2	2.38	0.52
59:q:9:ILE:CG1	63:u:90:LEU:CG	2.88	0.52
62:t:131:MET:SD	62:t:132:GLY:N	2.83	0.52
66:x:86:ASP:O	66:x:88:PHE:N	2.43	0.52
2:8:140:PRO:O	2:8:143:LEU:HD12	2.10	0.52
3:9:73:PRO:HB2	3:9:118:PHE:HZ	1.75	0.52
3:9:190:THR:HB	3:9:223:ARG:HH21	1.73	0.52
3:9:252:MET:O	3:9:256:ARG:HG2	2.10	0.52
10:PA:431:PHE:O	10:PA:432:HIS:C	2.50	0.52
10:PA:436:SER:CB	62:t:97:LYS:HD2	2.40	0.52
11:PB:313:GLU:HG3	11:PB:316:VAL:H	1.74	0.52
14:PE:84:ILE:HB	22:DA:1038:ARG:CD	2.38	0.52
19:PJ:16:ASN:OD1	19:PJ:17:LYS:HG3	2.08	0.52
40:4:264:HIS:ND1	40:4:267:GLU:OE1	2.42	0.52
42:6:324:LEU:HD12	42:6:327:MET:HB3	1.92	0.52
43:7:266:LEU:O	43:7:269:THR:OG1	2.25	0.52
44:c:200:VAL:HG13	44:c:214:VAL:HG12	1.91	0.52
44:c:311:GLN:HE22	57:n:715:ARG:HH22	1.58	0.52
45:e:104:VAL:HG11	47:l:114:LEU:HD12	1.90	0.52
48:m:66:TYR:HE2	52:g:38:ILE:HG23	1.75	0.52
49:a:127:HIS:CE1	49:a:171:THR:CG2	2.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:g:158:GLU:OE2	52:g:158:GLU:HA	2.10	0.52
55:j:34:GLN:CB	55:j:37:LEU:HG	2.39	0.52
56:k:14:LEU:N	56:k:14:LEU:HD23	2.25	0.52
56:k:109:ARG:CB	56:k:109:ARG:CZ	2.86	0.52
57:n:203:LEU:HD13	57:n:215:LEU:HD11	1.88	0.52
67:w:767:TRP:HE1	67:w:804:ASN:HD21	1.58	0.52
70:Y:18:DA:C2	70:Y:19:DC:C4	2.98	0.52
2:8:304:GLY:HA2	2:8:307:LEU:HB2	1.90	0.52
5:DP:169:VAL:HG23	5:DP:256:GLN:HB2	1.92	0.52
7:BA:21:ALA:HB1	7:BA:36:GLU:CD	2.34	0.52
7:BA:263:GLN:HA	7:BA:268:LYS:HG2	1.91	0.52
8:FA:48:GLU:O	8:FA:99:LEU:N	2.38	0.52
10:PA:18:ILE:CD1	11:PB:1149:VAL:HG21	2.40	0.52
10:PA:635:LEU:HD11	10:PA:640:LEU:HD21	1.92	0.52
10:PA:1048:THR:HA	10:PA:1053:ARG:HH11	1.74	0.52
24:DD:935:GLU:H	29:DI:127:TYR:HD2	1.57	0.52
25:DE:562:SER:OG	25:DE:564:ASP:OD1	2.28	0.52
26:DF:418:ILE:H	26:DF:418:ILE:CD1	2.22	0.52
31:DL:60:LYS:HE3	31:DL:60:LYS:H	1.75	0.52
37:1:509:GLN:HG2	37:1:512:ILE:HD11	1.91	0.52
43:7:140:SER:HA	43:7:387:GLU:OE2	2.10	0.52
43:7:277:ASP:OD1	43:7:280:ARG:NH1	2.42	0.52
43:7:420:PRO:HB2	43:7:428:ILE:HD11	1.92	0.52
44:c:178:ILE:HG23	44:c:192:VAL:HG22	1.92	0.52
45:e:132:HIS:HD2	64:v:126:ASP:CG	2.16	0.52
46:b:181:CYS:SG	47:l:82:LEU:HD22	2.50	0.52
49:a:321:LEU:HD21	49:a:407:ILE:CD1	2.35	0.52
49:a:466:VAL:O	49:a:466:VAL:HG13	2.08	0.52
51:f:142:SER:O	51:f:143:LYS:HB2	2.10	0.52
56:k:24:ILE:HG22	59:q:164:ALA:HB1	1.80	0.52
67:w:13:VAL:HG11	67:w:75:ARG:HG3	1.84	0.52
67:w:231:VAL:O	67:w:1099:ASN:ND2	2.39	0.52
67:w:418:GLN:HA	67:w:421:HIS:HD2	1.75	0.52
68:p:91:GLN:NE2	68:p:137:LEU:O	2.43	0.52
2:8:49:SER:HB2	2:8:52:LYS:HD2	1.92	0.52
7:BA:193:ARG:CZ	70:Y:22:DC:OP2	2.57	0.52
9:FB:51:ARG:HG2	9:FB:52:THR:N	2.24	0.52
10:PA:16:ARG:HD2	11:PB:1147:SER:OG	2.09	0.52
10:PA:1177:TYR:CE1	10:PA:1179:PRO:HD3	2.45	0.52
14:PE:9:ARG:HG3	14:PE:136:LEU:HD21	1.92	0.52
17:PH:98:ARG:HG2	17:PH:115:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:PI:79:PRO:O	18:PI:95:VAL:HA	2.09	0.52
24:DD:1063:LEU:HD13	31:DL:80:VAL:HG13	1.90	0.52
24:DD:1078:LEU:HD23	31:DL:83:MET:HE1	1.84	0.52
25:DE:324:LYS:HG2	25:DE:327:ASN:HD22	1.74	0.52
25:DE:676:THR:HG22	25:DE:685:ALA:HB3	1.92	0.52
34:Dm:28:ARG:HH21	34:Dm:31:LEU:HD21	1.75	0.52
37:1:260:LEU:HG	37:1:328:GLN:HB3	1.92	0.52
37:1:360:TYR:HA	37:1:363:LEU:HB3	1.91	0.52
38:2:12:GLU:OE1	42:6:130:GLY:CA	2.46	0.52
42:6:360:ARG:NH2	42:6:403:CYS:SG	2.83	0.52
42:6:703:PHE:O	42:6:709:GLN:NE2	2.40	0.52
44:c:111:TYR:CD2	46:b:136:HIS:CD2	2.82	0.52
44:c:204:MET:SD	44:c:208:PHE:C	2.92	0.52
52:g:63:GLY:C	52:g:64:ILE:HG12	2.34	0.52
55:j:74:GLY:O	55:j:75:ARG:HG3	2.10	0.52
57:n:141:ARG:HH21	63:u:20:CYS:HB3	1.75	0.52
58:o:725:VAL:HA	58:o:734:PRO:HB3	1.92	0.52
63:u:20:CYS:SG	63:u:21:ASN:N	2.83	0.52
10:PA:228:ILE:HG21	10:PA:245:PRO:HG2	1.91	0.52
10:PA:402:LEU:O	10:PA:406:VAL:HG12	2.10	0.52
11:PB:565:THR:HG21	11:PB:580:PRO:HB3	1.92	0.52
11:PB:566:LYS:HB3	11:PB:573:TRP:NE1	2.24	0.52
16:PG:168:LEU:O	16:PG:168:LEU:HG	2.04	0.52
20:PK:32:LEU:HD13	20:PK:74:ARG:HB2	1.92	0.52
38:2:229:LYS:HA	38:2:232:LEU:HD12	1.92	0.52
38:2:350:GLY:HA3	39:3:146:ARG:HH12	1.75	0.52
40:4:304:PRO:HG3	40:4:372:ALA:HA	1.91	0.52
41:5:32:LYS:HB3	41:5:46:ILE:HB	1.92	0.52
45:e:93:CYS:SG	59:q:647:SER:OG	2.66	0.52
49:a:480:TYR:HB3	66:x:52:ILE:O	2.10	0.52
49:a:504:ILE:H	49:a:505:PRO:HD3	1.75	0.52
55:j:72:ASP:OD2	61:s:132:GLU:CB	2.58	0.52
56:k:38:GLU:HG3	56:k:38:GLU:O	2.10	0.52
57:n:678:PHE:HB2	59:q:555:VAL:HG21	1.92	0.52
58:o:674:ILE:HD12	59:q:611:GLN:OE1	2.09	0.52
65:z:572:ASN:N	65:z:572:ASN:OD1	2.42	0.52
67:w:1:MET:N	67:w:1:MET:CE	2.73	0.52
67:w:115:TRP:HE1	67:w:163:ALA:HB2	1.74	0.52
67:w:633:VAL:O	67:w:817:ARG:NH2	2.43	0.52
2:8:43:ILE:HG23	2:8:43:ILE:O	2.09	0.51
2:8:229:LEU:HD11	2:8:276:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:239:ASP:C	2:8:242:SER:H	2.17	0.51
22:DA:1166:LYS:HE3	27:DG:182:GLU:HG3	1.92	0.51
37:1:334:ASN:ND2	43:7:85:GLU:OE2	2.43	0.51
37:1:396:THR:O	37:1:400:ILE:N	2.39	0.51
40:4:209:PRO:HA	40:4:212:LEU:HD13	1.92	0.51
43:7:571:THR:HG22	43:7:573:ASP:H	1.76	0.51
50:d:90:HIS:C	50:d:90:HIS:CD2	2.88	0.51
51:f:29:VAL:HG11	51:f:79:PHE:HB3	1.92	0.51
53:h:19:VAL:HG11	59:q:113:TYR:CA	2.39	0.51
56:k:41:ASN:O	56:k:45:LEU:HB2	2.10	0.51
56:k:43:ARG:CB	56:k:43:ARG:NH1	2.73	0.51
56:k:44:LEU:HD22	56:k:47:ARG:HH12	1.76	0.51
57:n:446:CYS:SG	57:n:447:GLY:N	2.84	0.51
62:t:144:TYR:CD2	62:t:147:CYS:HB2	2.36	0.51
67:w:681:GLU:OE2	67:w:685:ARG:NH1	2.41	0.51
68:p:304:SER:OG	68:p:349:ASP:O	2.28	0.51
1:0:200:GLN:HE22	42:6:181:HIS:HB2	1.75	0.51
7:BA:46:ILE:HB	10:PA:67:ARG:CZ	2.41	0.51
10:PA:436:SER:OG	62:t:97:LYS:CD	2.57	0.51
11:PB:309:PHE:C	11:PB:311:ILE:H	2.17	0.51
11:PB:561:ILE:HA	11:PB:576:ILE:HD13	1.92	0.51
23:DB:781:TYR:O	28:DH:176:ARG:NH2	2.44	0.51
26:DF:273:GLN:H	26:DF:273:GLN:CD	2.17	0.51
25:De:747:LEU:H	25:De:747:LEU:CD2	2.22	0.51
39:3:31:GLN:O	39:3:36:LYS:NZ	2.33	0.51
40:4:308:VAL:HG11	42:6:115:GLU:HG3	1.91	0.51
40:4:424:HIS:CE1	40:4:454:PHE:HB2	2.45	0.51
42:6:105:GLU:HA	42:6:124:TYR:HB2	1.92	0.51
42:6:316:LEU:HB3	42:6:320:GLN:HE21	1.75	0.51
42:6:672:TYR:HE2	42:6:676:ARG:HH11	1.58	0.51
43:7:343:ARG:HG2	43:7:347:GLN:HE21	1.75	0.51
43:7:601:ARG:HH12	43:7:626:VAL:HG22	1.73	0.51
44:c:110:ALA:HB2	46:b:168:ILE:HG21	1.56	0.51
46:b:67:LEU:HD22	46:b:116:LEU:HD12	1.91	0.51
52:g:28:GLU:OE1	52:g:30:LEU:C	2.52	0.51
52:g:134:THR:HG22	65:z:597:VAL:HG22	1.91	0.51
54:i:66:LEU:HD13	54:i:66:LEU:C	2.35	0.51
55:j:22:LEU:O	55:j:26:VAL:HG23	2.10	0.51
57:n:587:LEU:HD13	67:w:15:THR:HG21	1.86	0.51
59:q:523:ASP:HB3	59:q:563:ILE:HD12	1.93	0.51
60:r:206:ARG:HE	60:r:206:ARG:C	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:v:61:MET:HE2	64:v:64:ARG:HH12	1.74	0.51
66:x:968:LEU:HD13	66:x:985:ALA:HB3	1.92	0.51
67:w:19:GLU:HG2	67:w:25:MET:HE3	1.93	0.51
3:9:100:HIS:CG	3:9:101:PRO:HD2	2.46	0.51
7:BA:36:GLU:CD	7:BA:36:GLU:H	2.15	0.51
11:PB:29:VAL:HG23	11:PB:653:TRP:HZ3	1.75	0.51
12:PC:83:GLN:HG2	62:t:204:GLN:CD	2.33	0.51
12:PC:103:LEU:HD23	12:PC:104:ASP:N	2.25	0.51
15:PF:66:LEU:HD21	15:PF:94:MET:HA	1.92	0.51
23:DB:202:TRP:HB2	23:DB:238:LEU:HB3	1.91	0.51
24:DD:951:ASP:HB2	29:DI:112:GLY:HA2	1.92	0.51
25:DE:468:ASN:ND2	26:DF:127:LEU:HB3	2.25	0.51
26:DF:104:LEU:CD1	30:DJ:217:PHE:CE2	2.91	0.51
31:DL:111:LEU:O	31:DL:114:LYS:CE	2.59	0.51
25:De:269:GLY:O	29:Di:97:ARG:NH2	2.43	0.51
35:EA:126:SER:HB2	35:EA:164:ASP:CG	2.35	0.51
38:2:292:PRO:HB3	39:3:263:GLU:HB2	1.91	0.51
39:3:101:TYR:OH	40:4:125:GLY:O	2.27	0.51
39:3:165:LYS:NZ	39:3:169:ASP:OD1	2.43	0.51
39:3:219:GLN:HG2	39:3:221:PRO:HD2	1.92	0.51
39:3:229:TRP:HZ2	40:4:58:ARG:HD3	1.76	0.51
40:4:308:VAL:HG13	40:4:310:GLU:H	1.75	0.51
48:m:64:ALA:HA	48:m:67:LEU:HD12	1.92	0.51
49:a:69:LEU:HB3	54:i:70:HIS:HE1	1.75	0.51
52:g:93:LEU:CB	55:j:106:LYS:NZ	2.72	0.51
53:h:19:VAL:CG1	59:q:113:TYR:CB	2.75	0.51
57:n:203:LEU:HD21	57:n:224:PHE:CZ	2.46	0.51
59:q:166:ARG:CB	59:q:166:ARG:NH1	2.73	0.51
64:v:86:LEU:O	64:v:86:LEU:HD12	2.11	0.51
64:v:130:LEU:N	64:v:130:LEU:CD2	2.73	0.51
67:w:1:MET:HE3	67:w:1:MET:H1	1.75	0.51
1:0:134:GLN:O	1:0:138:LEU:N	2.42	0.51
4:DO:5:LEU:HD23	4:DO:6:TYR:CZ	2.45	0.51
10:PA:1165:THR:HG23	10:PA:1167:ARG:HG3	1.92	0.51
24:DD:1071:ARG:HB2	26:DF:91:PHE:CE2	2.45	0.51
26:DF:47:ILE:HD11	29:DI:43:ALA:CB	2.28	0.51
31:Dl:76:LEU:CD1	31:Dl:84:LEU:HD12	2.39	0.51
38:2:19:TRP:NE1	38:2:23:LYS:HB2	2.26	0.51
43:7:391:LEU:O	43:7:395:SER:N	2.43	0.51
43:7:524:LEU:O	43:7:528:SER:N	2.40	0.51
47:l:44:ILE:O	47:l:48:THR:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:l:166:LEU:HD22	64:v:123:ILE:CD1	2.41	0.51
50:d:128:ALA:CB	63:u:108:VAL:HG22	2.40	0.51
53:h:19:VAL:HG12	59:q:113:TYR:CD2	2.44	0.51
55:j:37:LEU:O	55:j:41:LEU:HG	2.09	0.51
58:o:682:VAL:HG22	58:o:691:VAL:HG11	1.93	0.51
10:PA:262:PRO:O	10:PA:274:ASP:HB3	2.10	0.51
10:PA:360:ASP:HB3	11:PB:1062:ARG:HE	1.75	0.51
10:PA:782:SER:O	10:PA:786:ALA:HB3	2.10	0.51
10:PA:1016:LEU:HD23	10:PA:1045:LEU:HD21	1.93	0.51
11:PB:357:CYS:C	11:PB:359:THR:H	2.19	0.51
21:PL:15:MET:SD	21:PL:15:MET:N	2.84	0.51
23:DB:621:ALA:HB3	41:5:36:GLN:HG2	1.93	0.51
32:Dc:21:LEU:HD12	32:Dc:21:LEU:O	2.11	0.51
35:EA:120:ASP:HB2	35:EA:174:ARG:HB2	1.92	0.51
43:7:487:ARG:HD2	43:7:724:MET:SD	2.50	0.51
43:7:697:ILE:HA	43:7:701:LEU:HB3	1.92	0.51
49:a:364:TYR:CB	49:a:430:LEU:CD1	2.54	0.51
49:a:429:ILE:O	49:a:429:ILE:HG13	2.11	0.51
53:h:77:ILE:O	59:q:126:THR:CB	2.57	0.51
65:z:560:TRP:HD1	65:z:561:PRO:HD2	1.75	0.51
67:w:1118:SER:OG	67:w:1119:GLY:N	2.43	0.51
69:X:-26:DA:OP2	69:X:-26:DA:C3'	2.58	0.51
2:8:15:LEU:HD23	2:8:15:LEU:C	2.35	0.51
2:8:232:PRO:HB2	2:8:240:MET:SD	2.51	0.51
3:9:17:GLU:OE2	3:9:17:GLU:HA	2.08	0.51
4:DO:79:VAL:HG21	4:DO:93:VAL:HG12	1.92	0.51
9:FB:17:GLY:HA2	9:FB:109:ILE:O	2.10	0.51
11:PB:665:ILE:HD11	11:PB:695:HIS:NE2	2.26	0.51
14:PE:45:GLY:CA	14:PE:53:PRO:HD3	2.40	0.51
14:PE:193:ILE:HB	14:PE:205:THR:HG23	1.92	0.51
26:DF:219:GLU:CD	28:DH:156:PRO:HB2	2.36	0.51
29:DI:60:HIS:CE1	31:DL:106:ARG:NE	2.70	0.51
26:Df:320:ARG:NH1	26:Df:320:ARG:CB	2.73	0.51
42:6:113:VAL:O	42:6:115:GLU:N	2.43	0.51
42:6:532:LEU:HD12	42:6:724:ALA:HB2	1.93	0.51
45:e:95:PHE:HB3	47:l:38:GLN:HG2	1.92	0.51
49:a:94:LEU:O	49:a:94:LEU:HG	2.10	0.51
49:a:340:TYR:O	49:a:344:THR:HG23	2.11	0.51
49:a:364:TYR:CD1	49:a:430:LEU:HB2	2.44	0.51
50:d:42:ARG:CZ	54:i:93:LYS:HG2	2.41	0.51
50:d:183:ARG:HH12	51:f:17:ASP:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:143:LEU:HD21	56:k:34:GLU:O	2.11	0.51
55:j:34:GLN:OE1	55:j:37:LEU:HG	2.10	0.51
59:q:184:ASN:CG	64:v:83:LYS:HD3	2.36	0.51
67:w:872:ARG:HB3	67:w:874:HIS:HD2	1.76	0.51
2:8:261:PHE:CZ	2:8:272:ILE:HD12	2.46	0.51
4:DO:32:LEU:O	4:DO:36:VAL:HG23	2.11	0.51
5:DP:207:PRO:HD2	5:DP:207:PRO:O	2.11	0.51
8:FA:127:PHE:O	9:FB:19:TRP:HB2	2.11	0.51
10:PA:1106:THR:HG21	10:PA:1119:LEU:HB2	1.93	0.51
10:PA:1218:ARG:HA	10:PA:1221:MET:HB2	1.92	0.51
14:PE:111:THR:HG23	14:PE:114:ALA:HB2	1.92	0.51
23:DB:90:THR:O	23:DB:968:ARG:NH2	2.43	0.51
25:DE:466:PHE:HB2	25:DE:796:ALA:HA	1.93	0.51
24:Dd:1080:TYR:OH	25:De:606:ASP:OD2	2.26	0.51
25:De:474:THR:OG1	25:De:546:VAL:O	2.28	0.51
25:De:650:THR:HG22	25:De:666:THR:HG22	1.93	0.51
33:Dk:191:VAL:HG13	33:Dk:200:ILE:CD1	2.41	0.51
37:1:169:ALA:HA	38:2:177:CYS:HB3	1.92	0.51
37:1:262:VAL:HG11	37:1:330:SER:HB2	1.93	0.51
38:2:319:ALA:HA	39:3:272:LEU:HD11	1.93	0.51
44:c:297:ARG:HA	44:c:303:GLU:O	2.11	0.51
49:a:246:ASN:N	49:a:246:ASN:OD1	2.44	0.51
54:i:118:LEU:HD23	54:i:118:LEU:O	2.11	0.51
56:k:77:GLN:HE21	60:r:192:GLN:HB2	1.75	0.51
58:o:634:PHE:O	58:o:637:SER:OG	2.25	0.51
61:s:84:ILE:HB	61:s:90:GLU:HG2	1.92	0.51
62:t:3:VAL:HG22	62:t:150:ALA:HB2	1.93	0.51
67:w:31:GLU:O	67:w:32:ASP:HB2	2.11	0.51
67:w:113:GLN:HE22	67:w:159:GLN:NE2	2.08	0.51
68:p:437:SER:OG	68:p:438:TRP:N	2.44	0.51
2:8:283:ARG:HB2	2:8:283:ARG:CZ	2.41	0.51
10:PA:1051:SER:O	10:PA:1052:ARG:C	2.51	0.51
10:PA:1139:LEU:HD13	10:PA:1346:VAL:HG11	1.93	0.51
10:PA:1179:PRO:HA	10:PA:1209:PRO:HA	1.91	0.51
10:PA:1484:MET:O	10:PA:1485:GLU:C	2.53	0.51
11:PB:239:MET:HB2	11:PB:372:LEU:HD21	1.93	0.51
12:PC:179:THR:OG1	12:PC:180:ALA:N	2.43	0.51
18:PI:17:CYS:SG	18:PI:44:TYR:HB3	2.51	0.51
24:DD:1071:ARG:HG3	26:DF:91:PHE:CE1	2.46	0.51
31:Dl:106:ARG:HH12	31:Dl:114:LYS:CE	1.95	0.51
36:EB:73:TYR:HB2	36:EB:115:GLN:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1:447:GLN:HB3	38:2:269:PRO:HB2	1.93	0.51
38:2:76:LEU:HD22	38:2:225:GLU:HG3	1.92	0.51
40:4:48:LEU:HG	40:4:48:LEU:O	2.11	0.51
40:4:310:GLU:HB3	40:4:315:LEU:HD22	1.91	0.51
42:6:359:LYS:HZ1	42:6:436:GLY:N	2.09	0.51
43:7:646:ILE:O	43:7:647:ARG:NH1	2.42	0.51
49:a:223:LYS:NZ	49:a:251:LEU:C	2.68	0.51
50:d:44:LEU:CD2	50:d:48:LEU:HD11	2.40	0.51
52:g:69:PRO:HD2	52:g:77:GLU:OE2	2.11	0.51
55:j:19:ILE:HD13	55:j:45:VAL:HG23	1.89	0.51
56:k:16:ASP:OD2	64:v:79:VAL:HG22	2.11	0.51
56:k:109:ARG:CZ	56:k:109:ARG:HB3	2.41	0.51
57:n:259:THR:CG2	57:n:311:GLN:HE21	2.24	0.51
58:o:717:SER:HB2	58:o:752:VAL:HG21	1.93	0.51
59:q:17:LYS:HE2	59:q:30:TYR:CD2	2.43	0.51
59:q:92:LEU:HD13	59:q:99:ARG:NH2	2.10	0.51
59:q:186:GLU:HG3	59:q:243:LEU:HD22	1.41	0.51
59:q:330:GLN:HG3	59:q:344:SER:HB3	1.93	0.51
59:q:437:HIS:C	59:q:437:HIS:CD2	2.86	0.51
69:X:-16:DG:H2"	69:X:-15:DG:C8	2.46	0.51
70:Y:7:DA:H2"	70:Y:8:DA:H8	1.73	0.51
3:9:102:ARG:HG2	3:9:102:ARG:NH1	2.22	0.51
3:9:181:LEU:H	3:9:181:LEU:CD1	2.03	0.51
10:PA:392:GLU:OE1	10:PA:402:LEU:HD21	2.11	0.51
10:PA:868:MET:HG2	10:PA:1404:THR:HG21	1.93	0.51
22:DA:639:LEU:HD11	22:DA:774:ARG:HG2	1.93	0.51
25:DE:461:ILE:O	26:DF:135:TRP:HE3	1.93	0.51
25:DE:507:VAL:HB	25:DE:513:LEU:HD11	1.93	0.51
28:DH:56:ALA:CB	30:DJ:214:PRO:HG2	2.35	0.51
25:De:747:LEU:O	25:De:747:LEU:HG	2.10	0.51
40:4:412:PHE:CZ	41:5:3:ASN:HB2	2.45	0.51
40:4:426:ARG:NH2	40:4:434:GLU:HB3	2.25	0.51
41:5:17:LYS:NZ	41:5:40:ASP:O	2.44	0.51
42:6:62:ARG:NH2	42:6:77:TRP:CZ3	2.79	0.51
45:e:125:LYS:NZ	47:l:153:ASN:OD1	2.43	0.51
48:m:116:GLN:HE21	65:z:595:PRO:HD3	1.76	0.51
49:a:107:MET:HE2	49:a:107:MET:C	2.35	0.51
49:a:160:LEU:HD12	49:a:214:ARG:NH2	2.26	0.51
49:a:461:SER:HA	66:x:49:GLN:NE2	2.25	0.51
54:i:109:LEU:CD2	54:i:117:GLN:NE2	2.73	0.51
67:w:337:GLN:HE21	67:w:341:PHE:HE2	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:w:1193:PHE:C	67:w:1195:ALA:H	2.19	0.51
70:Y:36:DC:H3'	70:Y:36:DC:OP2	2.09	0.51
5:DP:294:ARG:HG2	5:DP:301:VAL:HG22	1.93	0.51
6:DQ:312:GLU:HB2	6:DQ:313:PRO:HD3	1.93	0.51
10:PA:916:PHE:CE2	10:PA:960:ARG:HA	2.46	0.51
10:PA:1129:ASN:HB3	10:PA:1415:THR:HB	1.93	0.51
10:PA:1243:LEU:HD12	10:PA:1259:ILE:HG22	1.93	0.51
13:PD:90:LYS:HE3	13:PD:130:ILE:HG13	1.92	0.51
19:PJ:27:ALA:O	19:PJ:28:GLU:HB3	2.10	0.51
23:DB:66:ASN:OD1	23:DB:187:ARG:NH1	2.43	0.51
32:Dc:77:LEU:O	32:Dc:77:LEU:HD23	2.11	0.51
38:2:320:ARG:HE	39:3:178:MET:HE2	1.75	0.51
39:3:8:LEU:HD11	39:3:157:MET:HG3	1.93	0.51
40:4:145:VAL:HG13	40:4:146:PRO:HD3	1.92	0.51
40:4:433:PHE:CE1	41:5:9:LEU:HD13	2.46	0.51
43:7:195:ALA:HA	43:7:198:SER:OG	2.10	0.51
43:7:311:PRO:HD2	43:7:410:TYR:HE2	1.75	0.51
49:a:67:LYS:HB3	49:a:83:SER:HB2	1.93	0.51
57:n:683:ARG:NE	58:o:684:ARG:HD2	2.26	0.51
67:w:1241:THR:OG1	67:w:1242:GLU:N	2.44	0.51
68:p:398:SER:OG	68:p:400:GLN:NE2	2.43	0.51
70:Y:37:DC:C2'	70:Y:38:DT:H71	2.41	0.51
3:9:279:ARG:NE	3:9:279:ARG:O	2.44	0.50
10:PA:18:ILE:HB	10:PA:1462:GLN:HE22	1.76	0.50
10:PA:521:VAL:N	10:PA:522:PRO:HD2	2.26	0.50
10:PA:811:ILE:HD12	18:PI:79:PRO:HB3	1.93	0.50
10:PA:837:PHE:CD2	10:PA:841:MET:HE2	2.46	0.50
10:PA:988:TRP:O	10:PA:989:ASN:C	2.54	0.50
11:PB:26:CYS:HA	11:PB:29:VAL:HG13	1.94	0.50
11:PB:310:VAL:C	11:PB:312:GLN:H	2.18	0.50
12:PC:89:THR:CG2	62:t:108:SER:OG	2.57	0.50
23:DB:274:LEU:HG	23:DB:278:LYS:HE2	1.92	0.50
24:DD:890:GLY:CA	31:DL:104:ARG:NH2	2.68	0.50
25:De:439:ASP:OD1	25:De:555:ARG:NH2	2.44	0.50
26:Df:24:GLU:HG2	31:Dl:145:THR:HG21	1.93	0.50
38:2:223:LEU:HA	43:7:722:ARG:HD3	1.92	0.50
42:6:151:GLY:HA2	42:6:154:GLN:HB2	1.93	0.50
62:t:41:VAL:HG22	62:t:68:ASN:HA	1.93	0.50
63:u:104:LEU:O	63:u:108:VAL:HG23	2.10	0.50
2:8:37:ILE:HD12	2:8:37:ILE:H	1.75	0.50
2:8:83:HIS:HD2	2:8:84:LYS:HG2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:174:VAL:HG23	2:8:179:ARG:HD2	1.93	0.50
2:8:272:ILE:O	2:8:273:GLN:C	2.50	0.50
7:BA:131:PRO:HG2	11:PB:101:ARG:HG3	1.91	0.50
10:PA:505:LEU:O	10:PA:506:PRO:C	2.54	0.50
10:PA:721:HIS:CE1	18:PI:98:GLN:HE21	2.28	0.50
11:PB:272:VAL:HG13	11:PB:365:LEU:HD21	1.94	0.50
20:PK:59:ALA:HA	20:PK:74:ARG:O	2.11	0.50
39:3:13:ILE:HA	39:3:162:LEU:HB3	1.92	0.50
42:6:438:MET:HB2	42:6:463:LYS:HA	1.94	0.50
43:7:523:LEU:HA	43:7:710:VAL:HG11	1.92	0.50
43:7:673:ASP:O	43:7:674:TYR:HB2	2.09	0.50
57:n:915:ARG:NE	57:n:923:CYS:SG	2.85	0.50
63:u:28:GLN:CD	65:z:483:ASN:HD22	2.19	0.50
2:8:22:GLN:CD	2:8:22:GLN:N	2.69	0.50
2:8:213:LEU:HD22	2:8:225:ILE:HG12	1.92	0.50
5:DP:220:VAL:HG21	69:X:-24:DA:H2'	1.87	0.50
7:BA:35:PRO:C	7:BA:37:CYS:H	2.19	0.50
9:FB:225:VAL:HG11	69:X:-11:DG:OP1	2.11	0.50
10:PA:18:ILE:CG1	11:PB:1149:VAL:HG21	2.41	0.50
10:PA:403:GLN:NE2	60:r:17:ASN:ND2	2.60	0.50
11:PB:202:THR:HA	11:PB:222:ARG:HB2	1.92	0.50
11:PB:274:ARG:O	11:PB:277:GLY:CA	2.59	0.50
22:DA:854:ARG:HH22	70:Y:-25:DT:H5'	1.76	0.50
22:DA:927:VAL:O	22:DA:933:ASN:ND2	2.44	0.50
26:DF:22:VAL:CG1	29:DI:44:PHE:CE1	2.94	0.50
30:DJ:139:LEU:HB3	30:DJ:144:PHE:HB3	1.92	0.50
37:1:398:GLN:O	37:1:402:ASN:N	2.44	0.50
39:3:219:GLN:HB3	39:3:222:SER:HB3	1.93	0.50
40:4:312:ASN:HB3	40:4:386:THR:HG21	1.93	0.50
46:b:132:ASP:C	46:b:132:ASP:OD1	2.54	0.50
49:a:197:ALA:HB1	49:a:201:ASP:HB2	1.94	0.50
51:f:36:ARG:HA	51:f:41:TYR:HE1	1.76	0.50
52:g:74:HIS:H	52:g:74:HIS:CD2	2.27	0.50
59:q:523:ASP:CB	59:q:563:ILE:HD12	2.41	0.50
59:q:561:GLU:OE2	59:q:588:SER:OG	2.29	0.50
59:q:576:GLY:O	59:q:619:ARG:NH2	2.43	0.50
67:w:150:ASN:O	67:w:199:TRP:CE2	2.64	0.50
67:w:726:ASN:ND2	67:w:726:ASN:N	2.60	0.50
70:Y:37:DC:H2'	70:Y:38:DT:H71	1.92	0.50
2:8:151:LEU:HD23	2:8:151:LEU:C	2.36	0.50
3:9:46:VAL:HG22	3:9:279:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DP:312:LEU:H	5:DP:312:LEU:HD12	1.75	0.50
10:PA:891:TYR:CE1	10:PA:1087:VAL:HG11	2.47	0.50
11:PB:42:GLN:O	11:PB:42:GLN:CG	2.59	0.50
12:PC:75:SER:HB3	12:PC:79:VAL:HG13	1.94	0.50
26:DF:273:GLN:CD	26:DF:273:GLN:N	2.70	0.50
29:Di:73:LEU:CB	31:Dl:105:HIS:CE1	2.94	0.50
37:1:187:ASN:N	37:1:191:ASP:CB	2.75	0.50
37:1:390:GLN:O	37:1:394:TYR:N	2.37	0.50
37:1:463:HIS:HA	37:1:466:VAL:HG22	1.93	0.50
40:4:409:TYR:H	41:5:5:LEU:CD1	2.24	0.50
42:6:634:ARG:O	42:6:638:GLN:N	2.44	0.50
43:7:89:LYS:O	43:7:93:PHE:N	2.45	0.50
44:c:281:CYS:O	44:c:282:GLN:C	2.53	0.50
50:d:111:GLN:NE2	57:n:201:HIS:ND1	2.60	0.50
51:f:139:TYR:CD2	64:v:73:GLU:OE1	2.64	0.50
56:k:41:ASN:O	56:k:45:LEU:CB	2.59	0.50
56:k:77:GLN:CG	60:r:192:GLN:HG2	2.40	0.50
57:n:256:ASP:HB2	57:n:395:LEU:HB2	1.92	0.50
59:q:117:SER:O	59:q:120:ARG:HB3	2.11	0.50
64:v:16:GLN:O	64:v:20:LYS:HG2	2.11	0.50
1:0:284:ALA:HB1	2:8:243:LEU:HD22	1.94	0.50
10:PA:1020:LEU:HB3	10:PA:1076:PHE:CD1	2.47	0.50
11:PB:605:ARG:HG3	11:PB:612:ILE:HG12	1.94	0.50
12:PC:83:GLN:CD	62:t:204:GLN:CD	2.79	0.50
16:PG:15:PRO:O	16:PG:16:ARG:HB2	2.11	0.50
22:DA:564:PRO:HD2	23:DB:744:PHE:HB3	1.94	0.50
26:DF:257:PRO:O	26:DF:261:THR:OG1	2.26	0.50
40:4:114:PHE:O	40:4:118:LEU:N	2.41	0.50
40:4:443:VAL:N	41:5:6:LYS:HA	2.16	0.50
42:6:578:PRO:O	42:6:606:PHE:N	2.45	0.50
43:7:101:LYS:HG3	43:7:101:LYS:O	2.11	0.50
47:l:36:ILE:O	47:l:39:GLU:HG2	2.11	0.50
50:d:100:VAL:HG13	54:i:128:LYS:HZ3	1.76	0.50
55:j:96:LYS:NZ	61:s:80:SER:HA	2.27	0.50
67:w:394:PRO:CG	68:p:171:PHE:CE1	2.95	0.50
3:9:25:ASP:OD1	3:9:26:ALA:N	2.45	0.50
5:DP:273:LEU:HB2	5:DP:335:PHE:HZ	1.77	0.50
10:PA:365:THR:HG22	10:PA:482:PHE:CD2	2.47	0.50
10:PA:1064:ALA:O	10:PA:1065:PHE:C	2.49	0.50
11:PB:82:PRO:HB3	11:PB:134:LYS:CB	2.42	0.50
11:PB:131:THR:HB	11:PB:141:GLN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:994:GLY:HA2	19:PJ:50:LEU:HD22	1.93	0.50
23:DB:656:GLU:HG2	23:DB:661:ALA:HB3	1.92	0.50
25:DE:507:VAL:HG21	25:DE:513:LEU:HD11	1.93	0.50
26:DF:43:VAL:HA	29:DI:46:TYR:HD2	1.76	0.50
25:De:500:THR:HG22	25:De:502:LYS:H	1.76	0.50
48:m:107:HIS:O	48:m:111:LYS:HB3	2.12	0.50
48:m:116:GLN:NE2	65:z:595:PRO:HD3	2.26	0.50
49:a:423:SER:CB	49:a:503:SER:CB	2.85	0.50
53:h:20:ALA:HB2	59:q:113:TYR:HE2	1.77	0.50
56:k:109:ARG:CG	56:k:109:ARG:NH1	2.73	0.50
56:k:109:ARG:CB	56:k:109:ARG:NH1	2.74	0.50
58:o:759:ARG:HD3	67:w:26:PHE:HD2	1.76	0.50
59:q:437:HIS:CE1	59:q:472:GLU:H	2.21	0.50
2:8:111:PRO:HG3	51:f:49:VAL:HG11	1.92	0.50
3:9:207:TYR:HB3	3:9:211:GLN:NE2	2.27	0.50
8:FA:125:TYR:CD2	9:FB:23:VAL:HG21	2.46	0.50
9:FB:18:VAL:O	9:FB:110:VAL:HA	2.12	0.50
11:PB:566:LYS:HB3	11:PB:573:TRP:HE1	1.77	0.50
13:PD:137:LYS:CE	53:h:51:LEU:CA	2.81	0.50
16:PG:5:ILE:HG12	16:PG:76:VAL:HG21	1.94	0.50
16:PG:54:ILE:HG13	16:PG:70:VAL:HG23	1.94	0.50
25:DE:324:LYS:O	25:DE:327:ASN:ND2	2.44	0.50
28:DH:40:VAL:HG11	30:DJ:130:ILE:HG12	1.94	0.50
32:Dc:1:MET:HG3	26:Df:126:PRO:HB3	1.94	0.50
26:Df:393:LEU:O	26:Df:396:LEU:HB2	2.12	0.50
34:Dm:69:THR:HG23	34:Dm:80:ARG:HE	1.77	0.50
37:1:478:CYS:HB2	37:1:484:PRO:HG3	1.93	0.50
42:6:471:VAL:O	42:6:634:ARG:NH1	2.39	0.50
42:6:570:GLU:OE2	42:6:715:LYS:NZ	2.39	0.50
49:a:462:LEU:HD11	66:x:14:TRP:CG	2.47	0.50
50:d:125:VAL:HG12	52:g:153:PHE:CZ	2.46	0.50
52:g:157:LEU:HD23	52:g:157:LEU:C	2.36	0.50
57:n:234:LEU:HD23	57:n:247:LEU:HA	1.92	0.50
66:x:618:VAL:HG13	66:x:673:MET:HE1	1.92	0.50
67:w:571:LEU:HB2	67:w:612:MET:HE1	1.93	0.50
67:w:671:ASP:OD1	67:w:671:ASP:N	2.44	0.50
67:w:1200:TYR:CD2	67:w:1200:TYR:O	2.64	0.50
3:9:15:SER:N	3:9:18:GLN:OE1	2.42	0.50
4:DO:57:ASN:HD22	4:DO:57:ASN:N	2.07	0.50
6:DQ:310:GLU:HB3	6:DQ:313:PRO:HD2	1.93	0.50
7:BA:295:ARG:NH2	7:BA:298:ASP:OD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:435:PRO:HA	10:PA:438:LEU:HD12	1.93	0.50
11:PB:411:LEU:HD11	11:PB:435:ILE:HG23	1.94	0.50
11:PB:584:MET:SD	11:PB:605:ARG:HB2	2.52	0.50
11:PB:597:ILE:HB	11:PB:601:VAL:HG21	1.93	0.50
11:PB:829:PHE:CE1	11:PB:869:LYS:HG2	2.47	0.50
29:DI:132:LEU:HD21	30:DJ:121:MET:CE	2.22	0.50
37:1:423:SER:O	37:1:427:ALA:N	2.41	0.50
38:2:32:ALA:HB1	42:6:72:THR:HG22	1.93	0.50
40:4:449:SER:HA	40:4:452:LYS:HE3	1.93	0.50
42:6:296:ASP:N	42:6:296:ASP:OD1	2.44	0.50
43:7:516:VAL:HG12	43:7:520:TYR:HE2	1.77	0.50
43:7:616:ARG:CZ	43:7:674:TYR:CD2	2.94	0.50
45:e:60:VAL:HG11	46:b:179:LEU:CA	2.41	0.50
51:f:101:ILE:HD13	53:h:105:VAL:HB	1.92	0.50
52:g:109:LEU:HD13	57:n:136:LEU:HD13	1.94	0.50
54:i:85:GLN:CG	54:i:86:ASP:N	2.32	0.50
54:i:121:LEU:O	54:i:125:VAL:HG23	2.11	0.50
55:j:65:LEU:C	55:j:67:VAL:H	2.19	0.50
58:o:696:SER:HB2	66:x:111:HIS:HE1	1.71	0.50
60:r:112:GLU:C	60:r:114:LEU:H	2.20	0.50
62:t:98:LEU:O	62:t:101:PHE:N	2.43	0.50
3:9:59:TYR:HB2	3:9:265:PRO:HG2	1.94	0.50
3:9:212:ILE:HA	3:9:255:MET:HE1	1.93	0.50
10:PA:240:PRO:HA	10:PA:243:ALA:O	2.11	0.50
10:PA:357:LYS:HD2	11:PB:1107:LEU:O	2.12	0.50
10:PA:892:GLY:O	10:PA:893:GLU:HB2	2.10	0.50
11:PB:88:PHE:HD2	11:PB:126:VAL:HG21	1.77	0.50
11:PB:564:ALA:HB3	11:PB:576:ILE:HD11	1.94	0.50
25:DE:232:HIS:HD1	25:DE:313:SER:HG	1.56	0.50
35:EA:153:ARG:HA	35:EA:161:VAL:H	1.77	0.50
42:6:313:THR:HG23	42:6:313:THR:O	2.12	0.50
42:6:377:GLN:HB3	42:6:381:TRP:CZ3	2.46	0.50
43:7:148:HIS:CE1	43:7:151:SER:H	2.30	0.50
43:7:640:LEU:HD12	43:7:643:GLN:HB2	1.94	0.50
45:e:77:VAL:HA	45:e:80:CYS:SG	2.51	0.50
52:g:88:ASN:HB3	61:s:69:ARG:CZ	2.42	0.50
57:n:545:LEU:HD12	57:n:653:PRO:HD3	1.92	0.50
57:n:937:ARG:NH2	57:n:943:LEU:HD23	2.27	0.50
59:q:95:TRP:N	59:q:95:TRP:CD1	2.79	0.50
69:X:-24:DA:C5'	69:X:-24:DA:C8	2.94	0.50
1:0:116:ASP:O	1:0:120:LYS:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DO:59:ARG:HG2	4:DO:59:ARG:O	2.12	0.49
9:FB:229:HIS:HE1	70:Y:13:DC:H1'	1.77	0.49
10:PA:1790:TYR:CG	53:h:83:PRO:HD3	2.47	0.49
11:PB:657:VAL:HG12	11:PB:658:ALA:N	2.25	0.49
12:PC:67:ARG:NH1	19:PJ:2:ILE:HG23	2.26	0.49
13:PD:32:LEU:HD12	13:PD:37:VAL:HG22	1.94	0.49
20:PK:77:THR:HB	20:PK:81:TYR:HB3	1.93	0.49
26:Df:39:LEU:HD22	29:Di:47:VAL:HG13	1.94	0.49
42:6:75:PRO:HA	42:6:144:SER:HA	1.94	0.49
42:6:664:SER:N	42:6:669:GLU:OE1	2.43	0.49
43:7:240:ASP:OD2	43:7:636:ARG:NH2	2.31	0.49
43:7:565:LYS:HE3	43:7:593:GLY:HA3	1.94	0.49
49:a:467:MET:HE1	49:a:504:ILE:CG1	2.40	0.49
50:d:76:PHE:CZ	54:i:65:PHE:CZ	2.88	0.49
56:k:101:ARG:NH1	56:k:101:ARG:CB	2.72	0.49
57:n:808:LEU:HB2	57:n:822:ILE:HB	1.93	0.49
59:q:120:ARG:HH11	59:q:120:ARG:CG	2.14	0.49
59:q:255:ALA:CB	59:q:301:VAL:HG22	2.41	0.49
64:v:49:SER:HB3	64:v:50:ARG:CZ	2.42	0.49
66:x:20:ASP:OD1	66:x:20:ASP:N	2.44	0.49
2:8:279:ASN:O	2:8:282:ALA:N	2.45	0.49
5:DP:297:LYS:HB3	5:DP:298:PRO:HD3	1.94	0.49
8:FA:124:TYR:CE1	9:FB:22:LYS:HE2	2.47	0.49
9:FB:16:THR:HB	9:FB:108:GLY:HA2	1.93	0.49
10:PA:990:ALA:HB2	10:PA:1067:TRP:CZ3	2.47	0.49
10:PA:1143:LEU:HB2	10:PA:1148:ALA:HB2	1.94	0.49
10:PA:1301:ILE:HG12	10:PA:1345:ARG:HB2	1.93	0.49
10:PA:1662:PRO:HD3	51:f:16:VAL:O	2.11	0.49
13:PD:142:TYR:CE2	64:v:24:ASP:OD2	2.65	0.49
22:DA:507:GLU:C	22:DA:509:LEU:H	2.20	0.49
24:DD:940:VAL:HG22	29:DI:123:THR:CG2	2.29	0.49
25:DE:470:TYR:CD2	26:DF:126:PRO:HB2	2.47	0.49
25:DE:693:VAL:HB	25:DE:707:LEU:HB2	1.94	0.49
25:De:234:ALA:HB2	25:De:648:ASP:HB2	1.94	0.49
37:1:372:ILE:HD13	39:3:201:GLY:H	1.77	0.49
40:4:96:TRP:HD1	40:4:110:LEU:HA	1.77	0.49
42:6:62:ARG:HH11	42:6:75:PRO:HG3	1.76	0.49
43:7:309:VAL:HG11	43:7:409:THR:HB	1.93	0.49
49:a:417:TYR:HB2	49:a:469:VAL:CG2	2.36	0.49
50:d:121:LEU:CD1	63:u:115:LEU:CD1	2.88	0.49
50:d:161:VAL:HG21	57:n:153:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:g:134:THR:HB	65:z:597:VAL:HG13	1.94	0.49
54:i:66:LEU:N	54:i:67:PRO:HD2	2.25	0.49
56:k:96:ARG:CD	64:v:116:LEU:HD12	2.42	0.49
57:n:136:LEU:HD23	57:n:139:LEU:HD21	1.94	0.49
58:o:692:ASN:OD1	59:q:607:SER:HA	2.11	0.49
59:q:379:ILE:HD11	59:q:427:LEU:HD22	1.94	0.49
64:v:131:GLU:HG3	64:v:135:TYR:HE2	1.77	0.49
67:w:1195:ALA:C	67:w:1197:HIS:H	2.21	0.49
2:8:155:ASP:C	2:8:155:ASP:OD1	2.55	0.49
2:8:259:HIS:HE2	10:PA:1669:PRO:CB	2.04	0.49
3:9:177:ARG:HB2	3:9:177:ARG:HH11	1.77	0.49
7:BA:248:ARG:HH11	7:BA:284:THR:HG23	1.76	0.49
8:FA:45:ALA:N	9:FB:9:LEU:CD1	2.75	0.49
11:PB:677:MET:HA	11:PB:677:MET:HE3	1.95	0.49
11:PB:789:ASN:HB3	11:PB:795:ILE:HG13	1.94	0.49
38:2:290:PHE:CE1	38:2:295:ARG:HB3	2.47	0.49
39:3:241:LEU:HA	40:4:75:VAL:HG22	1.94	0.49
43:7:705:ASN:HB2	43:7:708:LEU:CD1	2.33	0.49
52:g:73:ASP:O	52:g:74:HIS:C	2.55	0.49
54:i:133:GLN:O	54:i:133:GLN:CD	2.56	0.49
57:n:776:LEU:O	57:n:780:VAL:HG13	2.12	0.49
57:n:845:SER:OG	57:n:846:ASN:N	2.43	0.49
59:q:1:MET:H3	65:z:540:LEU:HD11	1.66	0.49
62:t:138:ILE:O	62:t:138:ILE:HG22	2.11	0.49
64:v:90:ASP:O	64:v:91:PHE:HB2	2.11	0.49
67:w:10:GLU:HB3	67:w:14:LYS:HE3	1.95	0.49
67:w:113:GLN:NE2	67:w:159:GLN:HE22	2.10	0.49
11:PB:309:PHE:HZ	18:PI:40:ARG:HB2	1.77	0.49
11:PB:679:PRO:HA	11:PB:683:GLN:HG3	1.94	0.49
17:PH:64:LEU:O	17:PH:84:ARG:HB3	2.12	0.49
39:3:115:ILE:O	39:3:119:MET:N	2.41	0.49
40:4:310:GLU:HG3	40:4:311:THR:HG23	1.94	0.49
43:7:354:PRO:HG3	43:7:415:THR:HA	1.94	0.49
49:a:223:LYS:NZ	49:a:251:LEU:O	2.46	0.49
49:a:420:LEU:HB3	49:a:504:ILE:HD12	1.94	0.49
50:d:34:LEU:HD21	54:i:65:PHE:CD1	2.47	0.49
50:d:103:ARG:NH1	50:d:103:ARG:CG	2.73	0.49
50:d:115:LYS:CA	50:d:115:LYS:CE	2.86	0.49
51:f:123:VAL:HB	64:v:55:GLU:OE1	2.12	0.49
57:n:707:ASP:CG	58:o:684:ARG:HD3	2.37	0.49
59:q:482:GLN:H	59:q:634:ASN:HD22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:s:92:ALA:O	61:s:96:PHE:CE2	2.58	0.49
1:0:27:GLY:HA3	1:0:69:ASP:CB	2.36	0.49
2:8:57:ARG:HH22	2:8:158:LEU:HD23	1.78	0.49
3:9:228:MET:O	3:9:229:GLU:C	2.54	0.49
12:PC:47:ILE:HG13	12:PC:73:LEU:HD11	1.94	0.49
18:PI:72:VAL:HG12	18:PI:78:LEU:HD12	1.94	0.49
22:DA:675:ASP:OD1	27:DG:78:LYS:NZ	2.37	0.49
22:DA:828:GLU:HA	22:DA:831:LYS:HB2	1.92	0.49
24:DD:1059:ASN:O	31:DL:80:VAL:CG2	2.60	0.49
26:DF:339:GLN:HA	26:DF:342:LYS:HD3	1.93	0.49
37:1:264:ASN:OD1	43:7:581:LEU:CD2	2.60	0.49
40:4:350:SER:HA	40:4:353:GLN:HB2	1.94	0.49
49:a:417:TYR:HB2	49:a:469:VAL:HG11	1.93	0.49
51:f:169:SER:OG	51:f:170:SER:N	2.44	0.49
51:f:181:LEU:HD22	57:n:274:ILE:HG13	1.93	0.49
59:q:428:LEU:C	59:q:428:LEU:CD1	2.85	0.49
59:q:484:TYR:CD1	59:q:636:VAL:HG11	2.48	0.49
67:w:1172:ILE:O	67:w:1244:GLN:NE2	2.41	0.49
7:BA:169:ARG:HD3	7:BA:207:ASP:H	1.77	0.49
7:BA:169:ARG:HH11	7:BA:206:VAL:HB	1.77	0.49
10:PA:1184:THR:OG1	10:PA:1190:GLN:HB2	2.12	0.49
10:PA:1408:ARG:HD3	14:PE:172:ARG:HH11	1.77	0.49
11:PB:564:ALA:HB1	11:PB:578:LYS:HA	1.95	0.49
11:PB:1114:TYR:CD2	11:PB:1116:VAL:CG1	2.95	0.49
11:PB:1162:LEU:HA	11:PB:1165:MET:HE3	1.95	0.49
12:PC:65:ALA:O	12:PC:66:HIS:C	2.53	0.49
13:PD:108:ALA:HB1	13:PD:127:LEU:HB3	1.95	0.49
16:PG:17:TYR:HB3	16:PG:25:THR:HG21	1.95	0.49
37:1:338:ASN:HD22	43:7:670:GLY:HA3	1.76	0.49
43:7:192:TYR:O	43:7:196:ARG:HG2	2.11	0.49
43:7:552:TRP:HA	43:7:557:ILE:HD13	1.95	0.49
44:c:200:VAL:HA	44:c:214:VAL:HA	1.92	0.49
48:m:59:LYS:NZ	48:m:77:GLU:CD	2.66	0.49
59:q:1:MET:HG2	59:q:2:SER:N	2.28	0.49
62:t:130:THR:O	62:t:130:THR:OG1	2.25	0.49
64:v:16:GLN:HE21	64:v:20:LYS:CD	2.23	0.49
67:w:23:PRO:HA	67:w:26:PHE:CD1	2.48	0.49
67:w:108:GLU:HG3	67:w:111:ARG:H	1.77	0.49
68:p:51:LEU:HB2	68:p:58:LEU:HB3	1.94	0.49
1:0:22:MET:HA	1:0:59:ARG:O	2.12	0.49
1:0:295:ARG:HD2	1:0:295:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DO:7:ARG:NH1	4:DO:37:LEU:HD13	2.28	0.49
7:BA:117:ALA:O	7:BA:121:ILE:N	2.46	0.49
8:FA:44:GLN:CA	9:FB:9:LEU:CD1	2.85	0.49
10:PA:1105:ASN:OD1	10:PA:1107:PHE:HD1	1.96	0.49
11:PB:639:HIS:O	11:PB:642:GLN:HG2	2.13	0.49
13:PD:79:THR:N	53:h:51:LEU:CD2	2.75	0.49
14:PE:84:ILE:HG12	14:PE:114:ALA:HB2	1.93	0.49
16:PG:57:GLY:HA3	16:PG:66:VAL:CG1	2.43	0.49
22:DA:824:ARG:HB3	22:DA:863:VAL:HG12	1.95	0.49
23:DB:570:GLU:HA	23:DB:625:LEU:HA	1.95	0.49
23:DB:598:ARG:HH11	23:DB:619:MET:HE3	1.77	0.49
23:DB:621:ALA:CB	41:5:36:GLN:HE21	2.25	0.49
26:Df:97:ALA:HB2	26:Df:106:PHE:HE1	1.78	0.49
26:Df:257:PRO:O	26:Df:261:THR:OG1	2.31	0.49
37:1:166:ILE:HA	38:2:179:PRO:HG3	1.95	0.49
37:1:461:LEU:CD2	37:1:504:LYS:HE3	2.42	0.49
40:4:300:THR:O	40:4:300:THR:HG22	2.12	0.49
43:7:638:GLU:O	43:7:642:ASP:N	2.46	0.49
46:b:162:ALA:HA	46:b:165:LYS:HD3	1.93	0.49
48:m:66:TYR:CE1	52:g:52:ASP:CG	2.88	0.49
51:f:16:VAL:HG13	51:f:104:VAL:HA	1.94	0.49
53:h:36:GLU:O	53:h:38:GLY:N	2.45	0.49
59:q:149:LYS:HD2	64:v:40:ALA:CA	2.41	0.49
63:u:4:ARG:HG3	65:z:595:PRO:O	2.13	0.49
67:w:366:ILE:HG23	67:w:369:ARG:HD3	1.93	0.49
67:w:397:LYS:HB2	68:p:171:PHE:CE2	2.47	0.49
67:w:980:VAL:O	67:w:983:SER:OG	2.31	0.49
3:9:82:THR:HG23	3:9:160:VAL:CG1	2.42	0.49
14:PE:116:GLN:O	14:PE:119:VAL:HG22	2.12	0.49
22:DA:997:ARG:HH11	70:Y:0:DG:H2"	1.78	0.49
23:DB:27:LYS:HE3	23:DB:490:SER:HB3	1.95	0.49
23:DB:739:ASN:ND2	23:DB:782:ASN:OD1	2.44	0.49
25:DE:651:VAL:HB	25:DE:665:PHE:HB2	1.95	0.49
26:DF:249:ASP:HB3	26:DF:252:LEU:HB2	1.94	0.49
24:Dd:916:LYS:NZ	24:Dd:1070:GLU:OE2	2.42	0.49
25:De:586:TYR:HB3	25:De:605:HIS:HB3	1.94	0.49
35:EA:154:CYS:HB3	35:EA:157:CYS:O	2.12	0.49
38:2:88:LEU:O	38:2:92:VAL:N	2.43	0.49
39:3:75:ASN:O	39:3:79:GLY:N	2.39	0.49
40:4:71:VAL:O	40:4:83:GLN:NE2	2.45	0.49
40:4:144:ASP:O	40:4:147:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:165:LYS:HB2	42:6:294:GLU:HA	1.93	0.49
42:6:570:GLU:HA	42:6:573:ILE:HB	1.95	0.49
42:6:575:LEU:O	42:6:577:LYS:NZ	2.35	0.49
43:7:377:GLU:O	43:7:381:SER:N	2.37	0.49
44:c:111:TYR:OH	46:b:136:HIS:HB3	2.13	0.49
50:d:45:ILE:HG22	54:i:76:MET:HE3	1.86	0.49
52:g:38:ILE:HG22	52:g:38:ILE:O	2.12	0.49
52:g:168:LEU:HD11	54:i:136:LYS:HA	1.94	0.49
53:h:19:VAL:HG11	59:q:113:TYR:HA	1.93	0.49
53:h:85:ARG:HA	53:h:99:VAL:HG11	1.94	0.49
55:j:114:SER:HB2	55:j:121:MET:CG	2.37	0.49
57:n:169:LEU:CB	57:n:170:PRO:HD3	2.26	0.49
59:q:109:MET:HE1	59:q:112:LEU:HD22	1.95	0.49
65:z:528:LEU:HA	65:z:582:LEU:HD12	1.95	0.49
66:x:555:GLU:HA	66:x:558:VAL:HG12	1.94	0.49
67:w:164:ARG:NH2	67:w:204:LEU:HB2	2.25	0.49
2:8:140:PRO:HA	2:8:202:ILE:CD1	2.33	0.49
3:9:102:ARG:HH11	3:9:102:ARG:CG	2.25	0.49
7:BA:222:LEU:HD22	7:BA:269:ARG:HG3	1.95	0.49
10:PA:18:ILE:HB	10:PA:1462:GLN:NE2	2.28	0.49
10:PA:836:PHE:O	10:PA:837:PHE:C	2.52	0.49
10:PA:1478:GLU:O	10:PA:1481:LYS:HG2	2.13	0.49
11:PB:860:VAL:O	11:PB:901:THR:HA	2.13	0.49
12:PC:54:ALA:O	12:PC:159:LEU:HA	2.13	0.49
22:DA:567:LEU:HD22	23:DB:745:GLN:CG	2.43	0.49
22:DA:1055:VAL:HG13	22:DA:1056:ALA:H	1.78	0.49
27:DG:94:MET:HE3	27:DG:96:VAL:HG22	1.94	0.49
28:DH:57:SER:HB2	30:DJ:197:MET:CG	2.42	0.49
25:De:693:VAL:HB	25:De:707:LEU:HB2	1.94	0.49
36:EB:98:THR:O	36:EB:102:ILE:HG13	2.13	0.49
39:3:257:CYS:HB3	39:3:276:CYS:HB2	1.94	0.49
40:4:332:SER:C	40:4:343:VAL:HG11	2.37	0.49
42:6:309:ASP:OD1	42:6:309:ASP:C	2.54	0.49
42:6:360:ARG:NH1	42:6:432:THR:O	2.41	0.49
51:f:15:TRP:HH2	51:f:35:GLU:HB2	1.77	0.49
51:f:181:LEU:HD21	57:n:274:ILE:HD11	1.93	0.49
57:n:711:ARG:HH12	57:n:723:GLU:CD	2.21	0.49
58:o:762:GLN:C	67:w:74:LYS:NZ	2.69	0.49
59:q:19:VAL:CG2	59:q:22:VAL:HG22	2.43	0.49
59:q:155:GLY:C	64:v:62:HIS:CE1	2.91	0.49
63:u:18:GLN:CD	63:u:62:ILE:HA	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:w:726:ASN:N	67:w:726:ASN:HD22	2.10	0.49
67:w:1187:PRO:HA	67:w:1190:LEU:HB3	1.94	0.49
10:PA:520:MET:O	10:PA:521:VAL:C	2.54	0.49
10:PA:686:THR:HG21	11:PB:1041:ILE:HA	1.94	0.49
10:PA:689:ILE:HD11	11:PB:1008:VAL:HG21	1.95	0.49
12:PC:28:LEU:HA	12:PC:229:PHE:CZ	2.48	0.49
12:PC:72:PRO:HG3	19:PJ:13:ILE:HD13	1.95	0.49
12:PC:211:LEU:HD13	12:PC:215:GLU:HB2	1.95	0.49
13:PD:136:THR:O	13:PD:139:SER:HB3	2.13	0.49
18:PI:68:ILE:HG13	18:PI:122:ARG:HD2	1.94	0.49
23:DB:560:TYR:HD2	23:DB:581:ILE:HD11	1.78	0.49
29:DI:32:GLU:HB2	29:DI:35:VAL:CG2	2.43	0.49
40:4:309:VAL:HG22	40:4:312:ASN:HA	1.94	0.49
43:7:485:LEU:HB2	43:7:732:ASP:HB2	1.94	0.49
45:e:132:HIS:CD2	64:v:126:ASP:OD2	2.62	0.49
49:a:335:THR:O	49:a:391:THR:HG22	2.07	0.49
53:h:110:ARG:C	53:h:110:ARG:CD	2.85	0.49
54:i:135:TYR:CE1	63:u:121:ALA:O	2.66	0.49
57:n:266:VAL:HG21	57:n:303:LEU:HD12	1.89	0.49
58:o:720:PRO:O	58:o:721:LEU:C	2.55	0.49
59:q:188:LEU:CD1	59:q:188:LEU:C	2.86	0.49
59:q:633:ARG:HG2	59:q:633:ARG:HH21	1.78	0.49
64:v:108:LEU:C	64:v:108:LEU:CD1	2.86	0.49
68:p:38:ALA:HA	68:p:435:GLN:HE21	1.78	0.49
1:0:75:ARG:HH12	43:7:364:ARG:HD3	1.78	0.48
2:8:66:LEU:HD12	2:8:66:LEU:HA	1.70	0.48
3:9:85:MET:HE2	3:9:160:VAL:HB	1.95	0.48
8:FA:45:ALA:HB2	9:FB:9:LEU:HD11	1.95	0.48
8:FA:176:ILE:O	8:FA:176:ILE:HG22	2.13	0.48
10:PA:1140:THR:O	10:PA:1357:THR:HG23	2.13	0.48
10:PA:1178:ASP:HB3	10:PA:1260:ARG:HH22	1.78	0.48
10:PA:1661:SER:HB3	50:d:183:ARG:HD3	1.93	0.48
16:PG:158:PHE:HB2	35:EA:142:ASN:CG	2.38	0.48
25:DE:747:LEU:HD22	25:DE:747:LEU:N	2.19	0.48
25:De:724:GLU:OE1	25:De:789:ASN:ND2	2.46	0.48
37:1:285:SER:HA	43:7:423:ASP:HB2	1.94	0.48
39:3:242:ILE:HB	40:4:76:LYS:H	1.78	0.48
40:4:412:PHE:HZ	41:5:5:LEU:HB2	1.78	0.48
42:6:55:GLU:OE2	42:6:62:ARG:NH1	2.42	0.48
42:6:62:ARG:NE	42:6:77:TRP:CH2	2.81	0.48
42:6:363:VAL:HG22	42:6:439:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:7:72:TYR:HB3	43:7:206:VAL:HG22	1.94	0.48
43:7:238:ASN:HB3	43:7:241:ASN:HD22	1.78	0.48
46:b:176:THR:CA	46:b:179:LEU:HG	2.43	0.48
47:l:177:ARG:CZ	64:v:113:ASP:OD2	2.61	0.48
49:a:467:MET:HE2	49:a:504:ILE:HD13	1.88	0.48
53:h:12:LEU:C	53:h:12:LEU:CD1	2.85	0.48
54:i:109:LEU:HD22	54:i:117:GLN:NE2	2.28	0.48
55:j:120:ASP:HB3	55:j:124:TYR:HE2	1.77	0.48
57:n:247:LEU:HB3	57:n:275:HIS:CD2	2.48	0.48
59:q:106:LEU:HD23	59:q:106:LEU:O	2.12	0.48
1:0:300:ALA:HB1	3:9:166:PRO:CA	2.37	0.48
5:DP:167:ASN:O	5:DP:258:MET:HA	2.13	0.48
10:PA:781:ILE:O	10:PA:785:ILE:HG13	2.14	0.48
10:PA:966:LEU:HD21	10:PA:1040:LEU:HD11	1.95	0.48
10:PA:1141:VAL:HG13	10:PA:1352:VAL:HG13	1.94	0.48
10:PA:1178:ASP:N	10:PA:1209:PRO:O	2.46	0.48
10:PA:1192:TRP:O	10:PA:1195:VAL:HG22	2.13	0.48
10:PA:1248:ASN:HB2	10:PA:1256:VAL:O	2.12	0.48
11:PB:1114:TYR:HD2	11:PB:1116:VAL:HG13	1.77	0.48
16:PG:30:LEU:HD22	16:PG:72:TYR:CE1	2.48	0.48
24:DD:1085:LYS:NZ	31:DL:83:MET:SD	2.85	0.48
27:DG:48:HIS:HD2	27:DG:54:GLY:HA2	1.78	0.48
32:Dc:119:GLU:HG3	25:De:790:LEU:HD11	1.95	0.48
25:De:720:SER:OG	25:De:721:ARG:N	2.46	0.48
37:1:187:ASN:H	37:1:191:ASP:HB2	1.78	0.48
37:1:419:THR:HG22	37:1:422:LEU:H	1.79	0.48
38:2:277:ASP:OD1	38:2:277:ASP:N	2.43	0.48
39:3:38:ILE:O	39:3:42:MET:N	2.41	0.48
42:6:508:ALA:O	42:6:661:SER:N	2.41	0.48
42:6:532:LEU:HD11	42:6:723:ASP:HB2	1.95	0.48
43:7:338:GLU:HG3	43:7:342:TRP:CD1	2.48	0.48
43:7:482:THR:H	43:7:695:ARG:HG3	1.77	0.48
44:c:111:TYR:CZ	46:b:136:HIS:HD2	2.16	0.48
49:a:274:ILE:HG22	49:a:274:ILE:O	2.11	0.48
50:d:110:LEU:C	50:d:110:LEU:CD2	2.86	0.48
57:n:305:LEU:CD1	57:n:361:ILE:HG12	2.43	0.48
63:u:26:LEU:CD1	63:u:26:LEU:C	2.86	0.48
63:u:81:SER:C	63:u:83:ALA:N	2.71	0.48
66:x:374:SER:O	66:x:377:SER:OG	2.30	0.48
67:w:1195:ALA:C	67:w:1197:HIS:N	2.69	0.48
1:0:78:VAL:HG11	43:7:334:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:3:HIS:N	3:9:3:HIS:ND1	2.59	0.48
7:BA:35:PRO:C	7:BA:37:CYS:N	2.71	0.48
8:FA:125:TYR:CZ	9:FB:31:TRP:HE3	2.28	0.48
9:FB:18:VAL:HG23	9:FB:110:VAL:HG22	1.94	0.48
9:FB:135:SER:O	9:FB:137:LYS:N	2.45	0.48
10:PA:13:CYS:HB3	11:PB:1146:ILE:O	2.13	0.48
10:PA:408:ARG:CZ	60:r:7:THR:CG2	2.90	0.48
13:PD:133:ASP:HB3	53:h:59:LEU:HD21	1.95	0.48
14:PE:121:MET:SD	14:PE:124:LYS:HD2	2.53	0.48
16:PG:120:ASP:HB2	16:PG:122:ASN:OD1	2.13	0.48
22:DA:410:TRP:HB3	26:DF:306:PRO:HD3	1.95	0.48
22:DA:854:ARG:NH2	70:Y:-25:DT:P	2.82	0.48
31:DL:111:LEU:CA	31:DL:114:LYS:CE	2.90	0.48
38:2:28:GLY:O	38:2:31:LYS:NZ	2.42	0.48
38:2:129:THR:O	38:2:133:LYS:N	2.44	0.48
39:3:124:ILE:HD11	39:3:129:THR:H	1.77	0.48
40:4:143:ARG:HD3	40:4:148:LEU:HD21	1.95	0.48
42:6:442:GLU:N	42:6:466:LEU:O	2.45	0.48
42:6:673:SER:HA	42:6:676:ARG:HB3	1.95	0.48
43:7:217:ILE:HG12	43:7:305:LEU:HA	1.95	0.48
45:e:146:ILE:C	45:e:148:VAL:N	2.71	0.48
49:a:462:LEU:CG	66:x:11:LEU:CD1	2.84	0.48
50:d:115:LYS:CD	50:d:115:LYS:C	2.86	0.48
50:d:125:VAL:HG12	52:g:153:PHE:HZ	1.79	0.48
51:f:97:ASP:HB2	53:h:75:VAL:HG11	1.94	0.48
52:g:172:PRO:HA	52:g:175:LEU:CG	2.42	0.48
56:k:17:ILE:HG21	59:q:171:VAL:CG1	2.43	0.48
57:n:196:ASN:HD21	57:n:219:ASN:C	2.22	0.48
63:u:57:LEU:HD13	65:z:492:ARG:HG2	1.95	0.48
7:BA:214:PHE:HB3	7:BA:218:PHE:HE2	1.75	0.48
7:BA:231:ALA:HA	7:BA:301:PRO:HG3	1.93	0.48
10:PA:408:ARG:HH21	60:r:7:THR:HG23	1.78	0.48
10:PA:703:GLN:HE21	10:PA:703:GLN:HB3	1.44	0.48
10:PA:790:GLN:HA	10:PA:822:PHE:HA	1.96	0.48
10:PA:883:ILE:HB	10:PA:885:GLN:HG3	1.95	0.48
11:PB:986:GLN:OE1	11:PB:986:GLN:HA	2.11	0.48
12:PC:93:PHE:H	12:PC:166:LYS:HZ1	1.62	0.48
12:PC:148:ILE:HG12	19:PJ:5:VAL:HG13	1.95	0.48
14:PE:11:TRP:HB2	14:PE:40:PHE:CD2	2.49	0.48
23:DB:818:THR:OG1	23:DB:819:LEU:N	2.45	0.48
25:DE:746:ASP:OD1	25:DE:746:ASP:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Df:254:GLN:O	26:Df:258:ARG:NH2	2.47	0.48
37:1:177:GLN:C	37:1:192:ILE:HD11	2.39	0.48
39:3:180:VAL:O	39:3:184:ALA:N	2.39	0.48
40:4:148:LEU:HA	40:4:151:TYR:HD2	1.78	0.48
40:4:260:ASN:O	40:4:263:GLN:HB2	2.13	0.48
40:4:304:PRO:HG2	40:4:373:HIS:N	2.28	0.48
43:7:484:THR:OG1	43:7:695:ARG:NH2	2.45	0.48
49:a:393:VAL:HG13	49:a:393:VAL:O	2.13	0.48
49:a:489:CYS:HA	49:a:514:LYS:NZ	2.29	0.48
51:f:78:LEU:HD11	53:h:81:LEU:CD2	2.39	0.48
52:g:98:ARG:HH11	61:s:72:PRO:HB2	1.77	0.48
53:h:8:LEU:C	53:h:8:LEU:CD2	2.85	0.48
55:j:78:GLN:CA	55:j:82:LYS:HE3	2.38	0.48
56:k:36:SER:HB3	56:k:37:LYS:HZ2	1.78	0.48
67:w:1193:PHE:C	67:w:1195:ALA:N	2.70	0.48
3:9:40:VAL:HB	3:9:44:ASP:OD2	2.13	0.48
7:BA:244:LEU:HD11	7:BA:295:ARG:HD3	1.95	0.48
8:FA:26:TYR:CD1	8:FA:138:PHE:HB3	2.48	0.48
10:PA:1194:ASN:O	10:PA:1198:GLU:N	2.46	0.48
22:DA:493:ARG:H	22:DA:493:ARG:HG2	1.47	0.48
24:DD:991:MET:HE3	24:DD:991:MET:HB3	1.63	0.48
26:DF:106:PHE:HA	30:DJ:217:PHE:HB3	1.94	0.48
25:De:651:VAL:HG13	25:De:665:PHE:HB2	1.95	0.48
39:3:235:GLN:HA	39:3:238:ARG:HG2	1.95	0.48
43:7:370:LYS:HD3	43:7:374:PHE:HE2	1.78	0.48
48:m:19:GLN:OE1	52:g:44:MET:HB2	2.14	0.48
51:f:32:TYR:CE1	51:f:35:GLU:OE2	2.66	0.48
53:h:26:LEU:HD23	53:h:26:LEU:HA	1.75	0.48
57:n:922:TYR:CE1	57:n:955:PRO:HA	2.47	0.48
63:u:79:GLU:CD	63:u:82:THR:CG2	2.86	0.48
3:9:190:THR:OG1	3:9:220:SER:HB3	2.14	0.48
10:PA:12:ALA:O	10:PA:13:CYS:C	2.56	0.48
10:PA:1157:ILE:HA	10:PA:1160:ARG:HB2	1.96	0.48
11:PB:553:LEU:O	11:PB:556:ILE:HG22	2.13	0.48
12:PC:154:ARG:HG2	12:PC:155:LYS:H	1.78	0.48
18:PI:15:ARG:HB3	18:PI:24:LEU:HD12	1.95	0.48
22:DA:1014:GLU:O	22:DA:1018:LYS:HB2	2.13	0.48
37:1:150:ASN:HA	37:1:153:ASP:HB2	1.94	0.48
40:4:48:LEU:N	40:4:49:PRO:CD	2.77	0.48
40:4:98:THR:HA	40:4:108:LEU:HG	1.95	0.48
42:6:309:ASP:C	42:6:310:LEU:HG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:7:102:LEU:CB	43:7:103:PRO:HD2	2.42	0.48
43:7:541:SER:H	43:7:544:TYR:HB3	1.79	0.48
54:i:85:GLN:HG3	54:i:86:ASP:CG	2.32	0.48
59:q:633:ARG:NH2	59:q:633:ARG:CB	2.74	0.48
62:t:202:LYS:O	62:t:203:GLN:C	2.56	0.48
67:w:315:SER:OG	67:w:319:GLU:OE1	2.31	0.48
67:w:777:ILE:HA	67:w:810:VAL:HG22	1.95	0.48
68:p:367:ASP:HA	68:p:370:VAL:HG22	1.96	0.48
7:BA:118:PHE:HE1	7:BA:142:PHE:HB3	1.79	0.48
7:BA:179:GLU:HG2	9:FB:154:LYS:NZ	2.28	0.48
10:PA:1373:ALA:O	10:PA:1374:VAL:C	2.56	0.48
11:PB:16:GLU:O	11:PB:637:LYS:HB2	2.13	0.48
11:PB:47:PHE:C	11:PB:49:GLU:N	2.71	0.48
11:PB:82:PRO:CB	11:PB:134:LYS:HA	2.43	0.48
11:PB:896:LEU:HG	11:PB:900:GLU:HG2	1.96	0.48
12:PC:173:HIS:CE1	12:PC:175:LYS:HG3	2.49	0.48
23:DB:636:VAL:HG23	23:DB:638:ARG:HB3	1.96	0.48
26:DF:38:LEU:HD23	29:DI:71:VAL:HB	1.96	0.48
29:DI:63:LYS:HE3	29:DI:63:LYS:HB3	1.73	0.48
37:1:493:MET:HE1	37:1:535:LYS:HG3	1.95	0.48
42:6:324:LEU:O	42:6:328:PHE:N	2.41	0.48
42:6:667:THR:H	42:6:670:MET:HB3	1.78	0.48
43:7:539:PHE:N	43:7:598:SER:O	2.43	0.48
43:7:609:ASP:OD1	43:7:666:ARG:NH1	2.46	0.48
43:7:634:LYS:HA	43:7:637:LEU:HD12	1.96	0.48
44:c:209:ILE:HB	44:c:250:LEU:HD13	1.96	0.48
49:a:420:LEU:HD22	49:a:504:ILE:HG13	1.96	0.48
52:g:75:LYS:HG3	52:g:126:TYR:HE2	1.76	0.48
52:g:97:ILE:HB	52:g:98:ARG:HD2	1.95	0.48
54:i:135:TYR:OH	63:u:125:ILE:HA	1.99	0.48
56:k:21:ILE:CD1	59:q:168:THR:N	2.76	0.48
56:k:35:LEU:HD12	56:k:35:LEU:O	2.14	0.48
59:q:484:TYR:O	59:q:488:CYS:HB2	2.14	0.48
59:q:644:SER:CA	59:q:647:SER:OG	2.58	0.48
2:8:143:LEU:O	2:8:143:LEU:HD22	2.13	0.48
3:9:226:ILE:HD13	3:9:226:ILE:N	2.28	0.48
3:9:277:LEU:HA	3:9:280:CYS:SG	2.54	0.48
6:DQ:312:GLU:O	6:DQ:314:LEU:N	2.46	0.48
7:BA:189:LYS:CG	69:X:-29:DA:OP2	2.59	0.48
10:PA:18:ILE:CD1	11:PB:1171:MET:HB3	2.42	0.48
10:PA:881:ASN:CG	10:PA:882:SER:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:917:GLU:HG3	10:PA:956:PHE:CZ	2.49	0.48
10:PA:1102:MET:HE2	10:PA:1386:ILE:HG23	1.94	0.48
10:PA:1176:TYR:HD1	18:PI:53:ILE:H	1.62	0.48
22:DA:564:PRO:HB2	23:DB:744:PHE:CD2	2.44	0.48
22:DA:953:VAL:O	27:DG:149:ARG:NH2	2.47	0.48
38:2:210:VAL:HA	38:2:213:ARG:HG2	1.95	0.48
38:2:360:CYS:SG	38:2:361:ALA:N	2.87	0.48
42:6:562:ALA:HA	42:6:626:ILE:HB	1.96	0.48
43:7:325:THR:HG23	43:7:382:LEU:HD13	1.96	0.48
43:7:335:ARG:O	43:7:339:TYR:N	2.46	0.48
43:7:570:GLU:HB3	43:7:577:THR:HG23	1.95	0.48
52:g:161:ILE:CG2	54:i:140:MET:CE	2.91	0.48
56:k:64:SER:HB2	56:k:68:ARG:CZ	2.43	0.48
59:q:335:PRO:HB3	59:q:436:LYS:HG3	1.95	0.48
65:z:582:LEU:HG	65:z:584:PRO:HD3	1.95	0.48
66:x:544:HIS:HD2	66:x:546:CYS:H	1.62	0.48
67:w:101:LEU:HD11	67:w:121:LEU:CD2	2.41	0.48
68:p:88:GLU:OE2	68:p:288:ARG:NH1	2.47	0.48
1:0:89:PHE:HB2	1:0:90:PRO:HD3	1.96	0.48
1:0:189:SER:HB3	42:6:189:LEU:HD21	1.94	0.48
2:8:136:ARG:HG3	2:8:136:ARG:NH1	2.28	0.48
2:8:139:LYS:HB3	2:8:139:LYS:HZ3	1.78	0.48
5:DP:292:ILE:HG23	5:DP:301:VAL:CG1	2.42	0.48
12:PC:263:LEU:O	12:PC:267:ILE:N	2.45	0.48
19:PJ:3:ILE:HD12	19:PJ:4:PRO:HD2	1.96	0.48
25:DE:461:ILE:O	26:DF:135:TRP:CE3	2.67	0.48
26:DF:39:LEU:HD13	29:DI:51:LEU:HD11	1.96	0.48
32:Dc:26:VAL:HG23	30:Dj:195:LEU:HB3	1.96	0.48
35:EA:38:ILE:HD12	35:EA:38:ILE:HA	1.67	0.48
35:EA:64:ASN:HA	35:EA:67:LYS:HB2	1.96	0.48
41:5:49:LEU:HD13	41:5:56:ARG:HH22	1.78	0.48
42:6:103:ILE:HG23	42:6:106:PRO:HB2	1.95	0.48
42:6:178:GLU:HG3	42:6:180:CYS:H	1.79	0.48
42:6:185:ILE:H	42:6:185:ILE:HG12	1.39	0.48
42:6:288:GLU:HB2	42:6:290:PRO:HD3	1.96	0.48
42:6:433:GLN:O	42:6:434:GLU:HB2	2.13	0.48
45:e:49:GLU:HG2	47:l:89:PHE:CE1	2.49	0.48
49:a:108:PHE:O	49:a:108:PHE:CD1	2.66	0.48
49:a:417:TYR:CZ	49:a:450:PHE:HD1	2.21	0.48
55:j:9:GLU:CD	55:j:56:GLN:CD	2.81	0.48
57:n:208:LEU:HA	57:n:289:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:r:206:ARG:C	60:r:206:ARG:NE	2.72	0.48
63:u:4:ARG:CD	65:z:596:TYR:N	2.76	0.48
66:x:621:VAL:HG11	66:x:670:LEU:HD22	1.96	0.48
69:X:-36:DG:C6	70:Y:36:DC:N4	2.82	0.48
2:8:192:VAL:O	2:8:192:VAL:HG12	2.12	0.48
8:FA:122:THR:HB	9:FB:23:VAL:O	2.14	0.48
10:PA:1372:GLU:HG3	14:PE:193:ILE:HG12	1.95	0.48
10:PA:1413:ALA:HB3	10:PA:1418:GLY:HA3	1.95	0.48
11:PB:721:ARG:NE	11:PB:975:ARG:HB2	2.29	0.48
11:PB:1094:GLN:HB2	11:PB:1103:LEU:HD13	1.95	0.48
23:DB:329:LEU:HB3	23:DB:342:THR:HG23	1.96	0.48
26:DF:68:THR:O	26:DF:69:SER:HB3	2.13	0.48
36:EB:127:ASN:HB2	36:EB:130:ILE:HB	1.95	0.48
39:3:43:VAL:O	39:3:47:SER:N	2.46	0.48
39:3:194:CYS:HA	39:3:215:LEU:HB3	1.96	0.48
44:c:240:GLN:O	44:c:243:THR:OG1	2.26	0.48
44:c:251:LEU:HD11	59:q:494:GLN:HB2	1.95	0.48
48:m:68:LYS:CD	52:g:50:GLN:NE2	2.44	0.48
49:a:229:SER:H	49:a:502:MET:CE	2.25	0.48
50:d:121:LEU:HD13	63:u:115:LEU:CG	2.41	0.48
52:g:159:ARG:C	52:g:159:ARG:CD	2.86	0.48
52:g:161:ILE:HG23	54:i:141:PHE:CE1	2.49	0.48
55:j:96:LYS:HZ2	61:s:80:SER:C	2.20	0.48
56:k:19:ARG:HA	56:k:19:ARG:HD3	1.51	0.48
56:k:60:GLU:HG3	64:v:26:ILE:HG13	1.96	0.48
57:n:229:GLU:HB3	57:n:254:VAL:HG13	1.95	0.48
58:o:690:LEU:HD22	59:q:605:PRO:CB	2.44	0.48
60:r:21:TYR:HE1	60:r:175:ALA:HB3	1.78	0.48
62:t:128:THR:O	62:t:130:THR:N	2.46	0.48
64:v:133:GLU:O	64:v:136:SER:N	2.46	0.48
67:w:94:PRO:O	67:w:129:VAL:HG22	2.14	0.48
67:w:164:ARG:NE	67:w:204:LEU:HD22	2.29	0.48
67:w:863:ASP:OD1	67:w:863:ASP:N	2.45	0.48
69:X:-36:DG:N1	70:Y:36:DC:C4	2.77	0.48
1:0:167:LYS:O	1:0:171:LEU:N	2.46	0.47
2:8:143:LEU:O	2:8:143:LEU:CD1	2.52	0.47
3:9:185:GLU:O	3:9:188:ARG:HB3	2.13	0.47
3:9:215:THR:HG23	3:9:252:MET:HG3	1.96	0.47
5:DP:299:ARG:C	5:DP:300:ILE:HG12	2.39	0.47
26:DF:43:VAL:HG23	29:DI:46:TYR:HB3	1.94	0.47
25:De:554:ASP:OD1	25:De:554:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:307:ILE:HG21	40:4:371:ARG:HD2	1.95	0.47
40:4:349:GLU:O	40:4:353:GLN:N	2.47	0.47
41:5:17:LYS:HE2	41:5:38:ILE:H	1.79	0.47
42:6:105:GLU:HG2	42:6:121:TYR:HE1	1.78	0.47
42:6:136:ILE:HD12	42:6:136:ILE:HA	1.74	0.47
49:a:157:LEU:HD23	49:a:217:GLY:HA2	1.96	0.47
49:a:461:SER:HA	66:x:49:GLN:HE21	1.77	0.47
55:j:89:LEU:CD1	61:s:93:TYR:HE1	2.26	0.47
56:k:70:LEU:HG	64:v:82:LEU:HD21	1.95	0.47
59:q:190:LEU:HD22	59:q:291:TRP:CZ3	2.48	0.47
59:q:214:SER:HB3	59:q:383:HIS:CE1	2.48	0.47
59:q:456:GLU:HG2	64:v:140:SER:HA	1.95	0.47
63:u:18:GLN:CD	63:u:65:THR:OG1	2.56	0.47
6:DQ:17:VAL:O	6:DQ:21:VAL:HG23	2.14	0.47
10:PA:77:ASN:O	10:PA:79:THR:N	2.43	0.47
10:PA:343:LEU:HD11	11:PB:1165:MET:HE1	1.95	0.47
10:PA:688:GLY:C	10:PA:690:GLY:N	2.69	0.47
10:PA:959:MET:HE1	10:PA:1050:CYS:HB2	1.96	0.47
15:PF:84:GLU:HG2	15:PF:84:GLU:O	2.14	0.47
16:PG:77:PHE:O	16:PG:77:PHE:CG	2.67	0.47
18:PI:61:GLU:H	18:PI:61:GLU:HG3	1.38	0.47
22:DA:854:ARG:HH22	70:Y:-25:DT:H5”	1.78	0.47
25:DE:249:LEU:HA	25:DE:252:VAL:HG22	1.95	0.47
26:Df:102:ARG:HD3	31:Dl:151:ARG:HG3	1.96	0.47
33:Dk:173:CYS:SG	33:Dk:179:MET:O	2.72	0.47
35:EA:183:GLN:O	35:EA:186:PRO:HD2	2.13	0.47
37:1:475:PHE:CE1	37:1:484:PRO:O	2.58	0.47
39:3:10:LEU:N	39:3:158:LYS:O	2.48	0.47
40:4:409:TYR:HD2	41:5:3:ASN:HB3	1.78	0.47
40:4:461:SER:O	40:4:462:SER:C	2.57	0.47
41:5:17:LYS:HZ2	41:5:42:HIS:H	1.63	0.47
42:6:128:SER:HB2	42:6:131:LEU:HD21	1.96	0.47
43:7:539:PHE:HB2	43:7:599:VAL:HG22	1.95	0.47
49:a:502:MET:CG	49:a:503:SER:N	2.77	0.47
50:d:31:LEU:CG	54:i:103:THR:HG21	2.39	0.47
50:d:119:GLN:HE21	50:d:119:GLN:HB2	1.48	0.47
58:o:644:PRO:O	58:o:648:ALA:N	2.44	0.47
60:r:8:MET:HB2	60:r:9:MET:H	1.41	0.47
63:u:18:GLN:OE1	63:u:65:THR:OG1	2.32	0.47
65:z:488:SER:HB2	65:z:492:ARG:NH2	2.29	0.47
65:z:582:LEU:CD2	65:z:591:LEU:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:x:431:SER:O	66:x:431:SER:OG	2.31	0.47
67:w:234:SER:HB2	67:w:660:GLU:HG3	1.96	0.47
2:8:280:PRO:HA	2:8:283:ARG:NH1	2.29	0.47
7:BA:45:VAL:HG23	10:PA:67:ARG:NH2	2.29	0.47
8:FA:49:ARG:HB3	8:FA:96:GLN:HB3	1.95	0.47
10:PA:1038:THR:O	10:PA:1039:LEU:C	2.57	0.47
10:PA:1182:GLN:O	10:PA:1184:THR:HG22	2.14	0.47
11:PB:973:PRO:O	11:PB:976:MET:HG3	2.14	0.47
17:PH:57:ARG:HH21	17:PH:148:LEU:HD21	1.79	0.47
23:DB:431:LEU:HD23	23:DB:431:LEU:C	2.38	0.47
26:DF:43:VAL:HA	29:DI:46:TYR:CD2	2.49	0.47
24:Dd:922:GLN:NE2	31:Dl:71:ASP:OD2	2.47	0.47
40:4:38:PRO:HG3	40:4:129:TRP:CD1	2.49	0.47
40:4:339:PRO:HG3	42:6:52:LYS:CB	2.45	0.47
42:6:339:VAL:N	42:6:489:TYR:O	2.42	0.47
43:7:26:ARG:HD3	43:7:29:LYS:HD3	1.95	0.47
46:b:62:MET:HA	46:b:62:MET:CE	2.34	0.47
48:m:107:HIS:O	48:m:111:LYS:CB	2.62	0.47
48:m:117:GLN:HE21	63:u:7:GLN:NE2	2.12	0.47
49:a:187:MET:HE1	49:a:401:PRO:HB2	1.96	0.47
49:a:228:PRO:CG	49:a:502:MET:SD	3.02	0.47
50:d:109:GLN:HA	50:d:112:LYS:HE3	1.95	0.47
54:i:65:PHE:HE1	54:i:99:LYS:HA	1.79	0.47
56:k:94:LEU:HD21	64:v:108:LEU:HD11	1.97	0.47
62:t:8:GLN:HG3	62:t:196:LEU:CD2	2.45	0.47
2:8:99:GLU:CD	2:8:99:GLU:C	2.83	0.47
2:8:116:ALA:HB2	2:8:302:THR:H	1.78	0.47
4:DO:22:LEU:CB	4:DO:28:ILE:HG12	2.43	0.47
8:FA:17:ARG:HA	9:FB:39:GLU:HA	1.96	0.47
10:PA:811:ILE:CD1	18:PI:79:PRO:HB3	2.44	0.47
10:PA:1380:ARG:HH22	14:PE:143:GLU:CD	2.22	0.47
11:PB:36:GLU:OE1	11:PB:652:SER:HB3	2.14	0.47
11:PB:89:GLU:HB2	11:PB:127:ASP:HB2	1.95	0.47
11:PB:393:LEU:HD22	11:PB:485:LEU:HD22	1.97	0.47
12:PC:130:VAL:C	12:PC:132:SER:N	2.69	0.47
13:PD:75:LYS:O	13:PD:76:ASN:C	2.56	0.47
22:DA:564:PRO:HG2	23:DB:744:PHE:CE1	2.49	0.47
23:DB:135:TRP:HA	23:DB:138:VAL:HG12	1.95	0.47
23:DB:559:LYS:HZ3	23:DB:559:LYS:HB2	1.79	0.47
25:DE:299:ASP:OD2	25:DE:607:ARG:NH2	2.38	0.47
25:DE:508:LYS:HB2	25:DE:512:ASP:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DF:75:LEU:HD13	26:DF:82:PRO:HA	1.95	0.47
26:DF:132:LYS:HE3	26:DF:132:LYS:HB3	1.44	0.47
29:Di:73:LEU:CD2	31:Dl:105:HIS:CG	2.92	0.47
37:1:350:LYS:HG3	37:1:353:LYS:HB3	1.96	0.47
38:2:189:LEU:HA	38:2:192:ALA:HB3	1.97	0.47
39:3:14:VAL:HB	39:3:163:VAL:HA	1.96	0.47
39:3:96:SER:OG	40:4:244:THR:HB	2.14	0.47
40:4:145:VAL:O	40:4:149:ASP:N	2.46	0.47
40:4:342:VAL:O	40:4:342:VAL:HG22	2.14	0.47
40:4:354:ALA:O	40:4:358:GLY:N	2.47	0.47
42:6:410:TYR:HB3	42:6:450:MET:HE2	1.96	0.47
43:7:112:ARG:H	43:7:112:ARG:HD2	1.78	0.47
43:7:252:THR:HG23	43:7:430:ASN:HD21	1.79	0.47
45:e:129:VAL:CB	56:k:114:MET:HE2	2.44	0.47
45:e:146:ILE:O	45:e:148:VAL:N	2.46	0.47
46:b:101:ARG:NH2	57:n:944:PHE:CE2	2.74	0.47
47:l:176:MET:HE2	59:q:378:LEU:HG	1.96	0.47
49:a:228:PRO:C	49:a:502:MET:SD	2.96	0.47
49:a:259:ILE:HD12	49:a:259:ILE:O	2.14	0.47
53:h:151:LEU:HD11	64:v:37:ILE:O	2.13	0.47
55:j:17:GLU:HA	55:j:20:ARG:CD	2.45	0.47
57:n:154:ILE:CB	57:n:155:PRO:HD3	2.43	0.47
57:n:669:GLN:HE22	58:o:681:GLU:HG3	1.77	0.47
3:9:175:LYS:HA	3:9:175:LYS:HZ2	1.73	0.47
10:PA:414:PRO:HG2	60:r:7:THR:HG22	1.97	0.47
10:PA:1207:ILE:HG13	10:PA:1260:ARG:CZ	2.44	0.47
11:PB:82:PRO:HA	11:PB:134:LYS:HA	1.97	0.47
11:PB:544:PHE:HB2	11:PB:596:ILE:HD13	1.96	0.47
11:PB:712:PRO:HG2	11:PB:939:HIS:CE1	2.49	0.47
11:PB:1003:ASN:C	11:PB:1005:ALA:H	2.21	0.47
11:PB:1019:GLY:O	12:PC:204:PRO:HG2	2.14	0.47
11:PB:1127:ILE:HD12	11:PB:1127:ILE:H	1.79	0.47
11:PB:1127:ILE:HD13	11:PB:1138:ARG:HG3	1.97	0.47
13:PD:73:ARG:HD2	13:PD:138:ARG:CD	2.44	0.47
15:PF:97:LEU:HD12	15:PF:97:LEU:HA	1.75	0.47
16:PG:83:GLU:O	16:PG:147:ILE:HG22	2.15	0.47
17:PH:102:ASP:C	17:PH:109:ALA:HB2	2.40	0.47
18:PI:91:HIS:CB	18:PI:116:ALA:HB2	2.44	0.47
23:DB:953:LEU:HD12	23:DB:979:PHE:HE2	1.79	0.47
25:De:589:TRP:HB3	26:Df:60:MET:HE3	1.97	0.47
38:2:171:PHE:HE2	38:2:205:VAL:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:316:PRO:HD2	38:2:317:HIS:CE1	2.50	0.47
39:3:266:TYR:H	39:3:274:ILE:HG23	1.78	0.47
40:4:88:GLY:O	40:4:92:GLY:N	2.47	0.47
43:7:236:ALA:HB1	43:7:239:ILE:HD11	1.97	0.47
46:b:107:GLU:HB3	58:o:649:ILE:HD11	1.96	0.47
49:a:160:LEU:HG	49:a:219:LEU:HD21	1.96	0.47
57:n:361:ILE:HA	57:n:370:LEU:HD21	1.95	0.47
67:w:270:LEU:HD23	67:w:303:GLN:HG3	1.96	0.47
69:X:-35:DG:C6	69:X:-34:DC:N4	2.82	0.47
1:0:208:LEU:HD12	1:0:208:LEU:C	2.39	0.47
7:BA:13:VAL:HG11	7:BA:41:VAL:HG23	1.96	0.47
11:PB:750:VAL:HG12	11:PB:751:LEU:N	2.30	0.47
11:PB:977:THR:C	11:PB:979:GLY:H	2.21	0.47
13:PD:46:GLN:O	13:PD:50:SER:HB3	2.15	0.47
14:PE:48:PRO:HA	14:PE:53:PRO:HB2	1.97	0.47
16:PG:30:LEU:O	16:PG:31:PHE:C	2.57	0.47
16:PG:151:ARG:HD2	35:EA:139:LEU:HD13	1.95	0.47
21:PL:51:ARG:HE	21:PL:51:ARG:HB2	1.30	0.47
24:DD:942:ALA:HB3	25:DE:510:ALA:HB1	1.97	0.47
36:EB:86:LYS:O	36:EB:90:GLN:HG2	2.15	0.47
37:1:302:ALA:O	37:1:306:ARG:N	2.46	0.47
42:6:309:ASP:O	42:6:309:ASP:OD1	2.31	0.47
42:6:463:LYS:HD2	42:6:484:ILE:HA	1.96	0.47
42:6:624:ILE:HA	42:6:660:TYR:HB2	1.96	0.47
43:7:692:LYS:HB3	43:7:697:ILE:HG23	1.97	0.47
44:c:176:MET:HG2	44:c:194:LEU:HG	1.96	0.47
44:c:294:PRO:O	44:c:295:THR:C	2.56	0.47
45:e:75:THR:O	45:e:79:GLN:HG2	2.14	0.47
46:b:71:LEU:O	46:b:75:MET:HG2	2.14	0.47
51:f:78:LEU:CD1	53:h:81:LEU:HD23	2.42	0.47
55:j:76:ASN:CG	55:j:77:PRO:HD2	2.40	0.47
57:n:371:GLN:HG3	57:n:390:MET:CE	2.44	0.47
59:q:160:LEU:HD23	64:v:69:VAL:HG23	1.96	0.47
59:q:190:LEU:CD2	59:q:291:TRP:CZ3	2.97	0.47
60:r:8:MET:HB2	60:r:10:PRO:HD2	1.97	0.47
67:w:6:GLN:HA	67:w:62:TRP:CH2	2.44	0.47
1:0:84:LYS:HB2	1:0:84:LYS:HE3	1.49	0.47
1:0:191:ASP:OD2	1:0:193:PRO:HD3	2.15	0.47
2:8:114:ILE:HG23	2:8:206:LEU:HD12	1.97	0.47
5:DP:299:ARG:NH2	69:X:-26:DA:H5"	2.30	0.47
7:BA:268:LYS:O	7:BA:269:ARG:NH1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:397:PHE:CB	15:PF:87:THR:HG23	2.45	0.47
10:PA:460:ARG:HD2	10:PA:462:PRO:HD2	1.96	0.47
10:PA:810:PHE:HA	11:PB:689:TYR:HE2	1.77	0.47
10:PA:910:LYS:N	10:PA:911:PRO:HD2	2.29	0.47
10:PA:1206:ARG:HA	10:PA:1206:ARG:HD3	1.69	0.47
11:PB:121:SER:HB2	11:PB:151:LYS:HB3	1.96	0.47
11:PB:728:MET:O	11:PB:731:GLN:HB2	2.15	0.47
11:PB:851:ASP:HB2	21:PL:15:MET:HE1	1.96	0.47
12:PC:28:LEU:HA	12:PC:229:PHE:CE2	2.50	0.47
12:PC:148:ILE:HD11	19:PJ:13:ILE:CG2	2.43	0.47
14:PE:11:TRP:CD2	14:PE:37:LEU:HB2	2.49	0.47
23:DB:820:ASP:OD1	23:DB:820:ASP:N	2.37	0.47
24:DD:938:SER:O	25:DE:576:THR:HG21	2.15	0.47
25:DE:321:LEU:HB3	25:DE:330:TRP:HB2	1.97	0.47
30:DJ:170:ALA:HB2	30:DJ:203:ALA:CB	2.43	0.47
24:Dd:941:ARG:NH2	29:Di:123:THR:O	2.47	0.47
26:Df:326:HIS:O	26:Df:330:ARG:HG2	2.15	0.47
37:1:264:ASN:HA	43:7:581:LEU:CD2	2.45	0.47
38:2:36:ASP:CG	42:6:70:ASP:OD2	2.58	0.47
38:2:293:GLN:HB2	38:2:308:CYS:HB2	1.97	0.47
39:3:115:ILE:HD12	39:3:118:LEU:HB2	1.96	0.47
40:4:307:ILE:HG22	40:4:316:TYR:HB2	1.96	0.47
40:4:339:PRO:HG3	42:6:52:LYS:HB2	1.96	0.47
40:4:340:ASN:OD1	40:4:340:ASN:N	2.48	0.47
40:4:379:GLN:HB3	40:4:383:LEU:HD21	1.96	0.47
40:4:408:LEU:HA	41:5:5:LEU:HD12	1.97	0.47
44:c:288:LEU:CB	44:c:306:HIS:CD2	2.98	0.47
46:b:178:LEU:HD13	47:l:55:LEU:CD2	2.44	0.47
47:l:149:LEU:CD1	64:v:139:SER:HA	2.45	0.47
47:l:168:TRP:CE3	59:q:441:ARG:CZ	2.90	0.47
49:a:148:ASP:OD1	49:a:148:ASP:N	2.47	0.47
49:a:321:LEU:HA	49:a:410:LEU:CD1	2.44	0.47
49:a:412:ARG:CB	49:a:472:SER:CB	2.64	0.47
49:a:432:GLU:OE1	49:a:432:GLU:HA	2.14	0.47
51:f:74:GLN:HB3	51:f:78:LEU:HB2	1.97	0.47
55:j:9:GLU:CG	55:j:56:GLN:OE1	2.63	0.47
55:j:17:GLU:HA	55:j:20:ARG:HG2	1.97	0.47
55:j:75:ARG:HB3	55:j:79:LEU:HB2	1.97	0.47
57:n:686:LYS:NZ	58:o:730:PRO:HB3	2.27	0.47
59:q:17:LYS:CE	59:q:30:TYR:CD2	2.97	0.47
59:q:190:LEU:O	59:q:190:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:t:5:CYS:O	62:t:141:GLU:HA	2.14	0.47
66:x:968:LEU:CD1	66:x:986:ILE:HG13	2.45	0.47
69:X:-32:DC:N4	70:Y:32:DG:C6	2.66	0.47
8:FA:48:GLU:OE2	9:FB:5:GLY:HA3	2.14	0.47
8:FA:110:PHE:CD1	8:FA:148:PRO:HA	2.50	0.47
10:PA:36:VAL:HG22	10:PA:61:ARG:HH11	1.79	0.47
13:PD:63:LYS:HD2	16:PG:103:PRO:HA	1.97	0.47
13:PD:90:LYS:HB2	13:PD:90:LYS:HE2	1.43	0.47
13:PD:137:LYS:HZ1	53:h:52:LEU:CA	2.28	0.47
16:PG:59:ILE:HA	16:PG:66:VAL:HG22	1.95	0.47
17:PH:4:ILE:HD11	17:PH:7:GLU:HB2	1.96	0.47
26:DF:28:ILE:HD11	29:DI:55:LYS:HE2	1.96	0.47
26:DF:388:ILE:HG22	26:DF:392:ILE:HG13	1.95	0.47
29:DI:119:ARG:NH1	29:DI:120:TYR:OH	2.48	0.47
38:2:205:VAL:O	38:2:209:THR:N	2.47	0.47
38:2:205:VAL:HG12	38:2:208:CYS:H	1.80	0.47
38:2:276:LEU:HD21	38:2:297:LYS:HB2	1.97	0.47
39:3:234:ASP:C	39:3:236:ASP:H	2.22	0.47
39:3:249:VAL:O	39:3:249:VAL:HG13	2.14	0.47
40:4:220:LEU:HD11	40:4:226:ARG:H	1.79	0.47
42:6:104:ALA:H	42:6:106:PRO:HD2	1.79	0.47
43:7:88:ARG:NH1	43:7:174:ILE:HG23	2.28	0.47
45:e:136:LEU:HD11	56:k:107:VAL:HG12	1.96	0.47
50:d:131:LYS:HB2	50:d:131:LYS:HE2	1.35	0.47
51:f:72:HIS:CE1	53:h:79:LEU:O	2.68	0.47
52:g:89:PHE:CD2	63:u:19:PHE:HD1	2.31	0.47
52:g:93:LEU:CA	55:j:106:LYS:NZ	2.78	0.47
52:g:112:LEU:N	61:s:69:ARG:HH22	2.13	0.47
53:h:86:ASP:N	53:h:99:VAL:HG12	2.28	0.47
54:i:75:CYS:CB	54:i:88:ASN:HD21	2.22	0.47
56:k:88:LYS:HG3	59:q:380:ARG:HH11	1.80	0.47
57:n:170:PRO:HG2	57:n:173:ILE:HD11	1.97	0.47
58:o:678:LEU:HD11	58:o:725:VAL:HG11	1.96	0.47
59:q:187:LEU:HD12	59:q:187:LEU:C	2.38	0.47
62:t:11:VAL:HA	62:t:20:THR:HG21	1.95	0.47
67:w:787:PRO:HB3	67:w:822:HIS:CD2	2.50	0.47
2:8:95:GLU:N	2:8:145:LEU:O	2.47	0.47
2:8:258:HIS:C	2:8:258:HIS:ND1	2.73	0.47
10:PA:190:ARG:O	10:PA:200:ALA:HA	2.15	0.47
10:PA:990:ALA:O	10:PA:991:GLN:C	2.56	0.47
11:PB:801:VAL:O	11:PB:801:VAL:CG2	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:PG:79:PRO:HB3	16:PG:104:MET:SD	2.54	0.47
22:DA:1195:VAL:HG22	22:DA:1198:ARG:HH12	1.80	0.47
25:DE:694:LEU:HD22	25:DE:703:MET:HE3	1.96	0.47
31:DL:111:LEU:N	31:DL:114:LYS:NZ	2.63	0.47
24:Dd:1061:ARG:NH1	29:Di:119:ARG:O	2.48	0.47
26:Df:328:ALA:C	26:Df:330:ARG:N	2.71	0.47
26:Df:364:VAL:HG22	26:Df:395:ARG:HD2	1.96	0.47
35:EA:55:ASP:HB2	36:EB:194:ARG:HB3	1.97	0.47
37:1:333:SER:O	37:1:334:ASN:C	2.58	0.47
40:4:79:PHE:HB3	40:4:82:ALA:HB3	1.96	0.47
42:6:154:GLN:C	42:6:156:ILE:H	2.23	0.47
42:6:496:LEU:HB3	42:6:502:ILE:HD12	1.96	0.47
43:7:28:LEU:HG	43:7:32:LEU:HD13	1.97	0.47
43:7:253:ARG:HB2	43:7:343:ARG:HH21	1.80	0.47
45:e:132:HIS:CD2	64:v:126:ASP:HB3	2.50	0.47
49:a:364:TYR:CD1	49:a:430:LEU:HD12	2.49	0.47
49:a:462:LEU:CD2	66:x:11:LEU:HG	2.31	0.47
52:g:175:LEU:HD22	54:i:129:ASN:OD1	2.15	0.47
56:k:58:HIS:C	56:k:58:HIS:ND1	2.73	0.47
56:k:80:GLU:N	56:k:80:GLU:OE1	2.48	0.47
59:q:290:HIS:NE2	59:q:294:LYS:CE	2.71	0.47
59:q:339:LEU:CD2	59:q:439:PHE:CD2	2.93	0.47
59:q:644:SER:HA	59:q:647:SER:HG	1.75	0.47
62:t:6:VAL:HG22	62:t:141:GLU:CB	2.41	0.47
66:x:843:TYR:HD1	66:x:847:PHE:HE2	1.62	0.47
67:w:111:ARG:HB3	67:w:114:LEU:HB3	1.97	0.47
67:w:383:SER:O	67:w:383:SER:OG	2.32	0.47
67:w:1229:LYS:O	67:w:1233:GLU:HB2	2.14	0.47
68:p:191:SER:HA	68:p:200:LEU:O	2.15	0.47
8:FA:42:TRP:CD1	8:FA:102:VAL:HG11	2.50	0.47
8:FA:143:TRP:NE1	8:FA:145:ASN:OD1	2.37	0.47
9:FB:51:ARG:NH1	9:FB:53:GLU:HB2	2.30	0.47
10:PA:625:ASP:O	10:PA:638:GLY:HA2	2.15	0.47
10:PA:693:ILE:CD1	11:PB:1008:VAL:HG11	2.36	0.47
10:PA:1149:ARG:HE	10:PA:1149:ARG:HB2	1.35	0.47
11:PB:912:ASN:HB3	11:PB:914:GLU:HG2	1.97	0.47
12:PC:27:ASP:HB2	12:PC:30:VAL:HG23	1.97	0.47
13:PD:64:THR:O	13:PD:65:LEU:C	2.58	0.47
17:PH:75:TYR:O	17:PH:77:PRO:HD3	2.14	0.47
18:PI:86:CYS:HB3	18:PI:90:GLY:N	2.30	0.47
25:DE:515:LEU:C	25:DE:517:ASP:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DI:31:TYR:OH	29:DI:36:ILE:HD11	2.15	0.47
25:De:556:ASN:HA	25:De:572:LEU:HB2	1.96	0.47
39:3:195:VAL:HG22	39:3:216:LYS:HA	1.96	0.47
40:4:348:ARG:O	40:4:352:GLN:N	2.40	0.47
40:4:357:SER:OG	40:4:358:GLY:O	2.32	0.47
40:4:415:GLN:HB2	40:4:439:ARG:HH21	1.79	0.47
42:6:123:LEU:HD23	42:6:479:ASP:HB3	1.97	0.47
42:6:634:ARG:HA	42:6:637:ALA:HB3	1.97	0.47
42:6:700:ASP:OD1	42:6:700:ASP:N	2.47	0.47
43:7:132:GLY:CA	43:7:391:LEU:HD12	2.42	0.47
44:c:205:ARG:HG3	59:q:466:ASN:ND2	2.30	0.47
46:b:174:ILE:HD13	47:l:58:MET:HE2	1.97	0.47
49:a:228:PRO:N	49:a:502:MET:SD	2.88	0.47
49:a:297:VAL:HG12	49:a:299:LEU:HG	1.97	0.47
50:d:121:LEU:HD22	50:d:125:VAL:HG13	1.96	0.47
50:d:126:TYR:CD2	59:q:36:MET:CG	2.99	0.47
51:f:106:TYR:CZ	53:h:106:PRO:HG3	2.50	0.47
58:o:710:LEU:HG	58:o:776:TRP:CH2	2.50	0.47
58:o:715:LEU:HD22	66:x:21:TYR:HB2	1.92	0.47
66:x:708:LYS:HB2	68:p:128:GLY:HA3	1.97	0.47
67:w:11:GLU:HA	67:w:14:LYS:HD2	1.97	0.47
7:BA:18:HIS:HE1	7:BA:36:GLU:C	2.23	0.46
9:FB:30:GLN:NE2	9:FB:62:LEU:O	2.27	0.46
9:FB:30:GLN:O	9:FB:62:LEU:HD11	2.15	0.46
10:PA:26:LEU:HD11	10:PA:31:LEU:HD21	1.98	0.46
10:PA:618:TYR:CE2	17:PH:29:HIS:HE1	2.33	0.46
11:PB:368:MET:HE3	11:PB:368:MET:HB2	1.75	0.46
12:PC:131:THR:O	12:PC:132:SER:C	2.58	0.46
14:PE:48:PRO:CA	14:PE:53:PRO:HB2	2.44	0.46
18:PI:50:ASN:HB2	18:PI:52:CYS:SG	2.54	0.46
24:DD:886:GLY:HA2	24:DD:891:ILE:H	1.79	0.46
24:DD:913:LEU:CD2	31:DL:87:ILE:CD1	2.90	0.46
26:DF:66:LEU:HD13	29:DI:31:TYR:HA	1.96	0.46
26:Df:327:TRP:O	26:Df:330:ARG:HB2	2.16	0.46
36:EB:210:PHE:HB2	36:EB:212:VAL:HG13	1.97	0.46
39:3:102:GLU:HA	39:3:105:THR:HG22	1.97	0.46
42:6:394:SER:O	42:6:394:SER:OG	2.29	0.46
42:6:472:ARG:HH11	42:6:473:GLU:CA	2.27	0.46
42:6:579:TYR:HA	42:6:606:PHE:HB2	1.97	0.46
43:7:186:ARG:HA	43:7:186:ARG:HD2	1.42	0.46
43:7:311:PRO:O	43:7:410:TYR:OH	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:c:205:ARG:NH2	64:v:128:TYR:HD2	2.14	0.46
49:a:504:ILE:H	49:a:505:PRO:CD	2.26	0.46
51:f:100:ILE:HG12	51:f:105:ILE:HG12	1.96	0.46
52:g:108:LYS:HG3	61:s:69:ARG:HE	1.79	0.46
55:j:26:VAL:HG12	55:j:38:ASN:ND2	2.14	0.46
55:j:63:VAL:N	55:j:64:PRO:HD3	2.30	0.46
57:n:509:ILE:HG21	57:n:540:ILE:HD13	1.97	0.46
59:q:484:TYR:CD1	59:q:636:VAL:CG1	2.99	0.46
67:w:615:ILE:O	67:w:620:ARG:NH2	2.48	0.46
2:8:134:LEU:HG	2:8:162:PHE:CD1	2.50	0.46
2:8:189:MET:HB2	2:8:189:MET:HE3	1.58	0.46
3:9:98:GLU:HG3	3:9:99:TYR:CZ	2.49	0.46
5:DP:192:TYR:CG	5:DP:192:TYR:O	2.65	0.46
9:FB:183:VAL:HA	9:FB:186:MET:HE2	1.97	0.46
10:PA:225:PHE:O	10:PA:228:ILE:HB	2.15	0.46
10:PA:245:PRO:HA	10:PA:248:MET:SD	2.54	0.46
10:PA:299:ALA:HB3	10:PA:302:VAL:HG12	1.97	0.46
10:PA:470:MET:HE3	10:PA:521:VAL:HB	1.95	0.46
11:PB:277:GLY:O	11:PB:278:PHE:HB2	2.14	0.46
11:PB:702:MET:HE3	11:PB:702:MET:HB3	1.67	0.46
11:PB:996:ILE:HD12	11:PB:996:ILE:HA	1.60	0.46
25:DE:520:SER:HB3	25:DE:523:VAL:HG13	1.96	0.46
26:Df:326:HIS:ND1	26:Df:326:HIS:N	2.63	0.46
37:1:187:ASN:ND2	37:1:191:ASP:HB2	2.29	0.46
37:1:519:THR:HA	37:1:522:VAL:HG22	1.97	0.46
40:4:179:LEU:HD22	40:4:184:LEU:HD12	1.98	0.46
40:4:230:LEU:HD21	40:4:258:LEU:HB2	1.96	0.46
40:4:438:LYS:HG3	41:5:37:ASP:O	2.15	0.46
44:c:290:ASP:CB	62:t:120:CYS:HB3	2.44	0.46
48:m:106:GLN:HA	50:d:163:ALA:HB2	1.96	0.46
51:f:185:ARG:HG2	57:n:277:LEU:CD1	2.45	0.46
53:h:23:LYS:CD	59:q:110:CYS:SG	3.03	0.46
55:j:26:VAL:CB	55:j:38:ASN:ND2	2.57	0.46
57:n:207:ASP:OD1	57:n:207:ASP:N	2.44	0.46
57:n:929:ARG:HB2	57:n:933:VAL:HG13	1.97	0.46
58:o:715:LEU:H	66:x:25:ILE:CG1	2.27	0.46
59:q:188:LEU:C	59:q:188:LEU:HD12	2.40	0.46
62:t:204:GLN:NE2	62:t:204:GLN:HA	2.29	0.46
10:PA:542:LEU:HD12	10:PA:542:LEU:HA	1.75	0.46
11:PB:200:MET:HG2	11:PB:222:ARG:NH1	2.30	0.46
11:PB:1070:LEU:H	11:PB:1070:LEU:HG	1.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:PE:17:ILE:HD11	14:PE:135:LEU:HD13	1.98	0.46
14:PE:34:ASP:O	14:PE:35:GLN:C	2.57	0.46
23:DB:27:LYS:CE	23:DB:490:SER:HB3	2.45	0.46
25:DE:470:TYR:CD1	28:DH:26:ALA:HA	2.50	0.46
26:DF:106:PHE:CD1	29:DI:13:PRO:CD	2.98	0.46
26:DF:318:CYS:HB2	26:DF:323:VAL:HG11	1.96	0.46
37:1:206:LYS:HG2	37:1:241:ASP:HB3	1.97	0.46
38:2:271:PHE:N	38:2:285:THR:O	2.48	0.46
39:3:32:PHE:HA	39:3:36:LYS:HD3	1.96	0.46
39:3:92:ASN:HD21	40:4:141:HIS:HD2	1.61	0.46
40:4:90:LEU:HD12	40:4:93:LEU:HD12	1.96	0.46
42:6:62:ARG:CZ	42:6:77:TRP:CZ3	2.99	0.46
43:7:21:GLN:O	43:7:25:MET:N	2.47	0.46
43:7:568:PHE:HB2	43:7:596:LEU:HA	1.98	0.46
43:7:583:LYS:O	43:7:587:ALA:N	2.35	0.46
48:m:110:ARG:NH1	50:d:165:LEU:HA	2.30	0.46
49:a:377:ASN:CB	49:a:442:VAL:O	2.55	0.46
52:g:93:LEU:HD13	55:j:106:LYS:CD	2.45	0.46
56:k:44:LEU:CD1	56:k:44:LEU:C	2.88	0.46
56:k:96:ARG:HD3	64:v:116:LEU:HD12	1.97	0.46
57:n:320:TRP:HA	59:q:316:VAL:HG11	1.97	0.46
57:n:801:ARG:NE	57:n:811:CYS:HB3	2.31	0.46
62:t:150:ALA:HB2	62:t:184:TYR:HB2	1.97	0.46
3:9:234:GLU:C	3:9:234:GLU:CD	2.83	0.46
5:DP:257:ASN:C	5:DP:258:MET:HG3	2.40	0.46
7:BA:126:ASP:C	7:BA:129:ASN:H	2.23	0.46
10:PA:74:CYS:O	10:PA:75:ALA:C	2.55	0.46
10:PA:538:VAL:HG13	10:PA:539:GLN:N	2.26	0.46
10:PA:1196:TYR:CD1	10:PA:1246:ILE:HG13	2.50	0.46
10:PA:1214:VAL:HG23	10:PA:1259:ILE:CD1	2.46	0.46
11:PB:580:PRO:O	11:PB:581:GLU:C	2.58	0.46
16:PG:93:ASN:HB3	16:PG:96:GLY:H	1.80	0.46
22:DA:569:ASN:ND2	23:DB:689:GLN:HA	2.27	0.46
26:DF:68:THR:HA	29:DI:32:GLU:OE1	2.15	0.46
27:DG:180:ARG:HA	27:DG:180:ARG:HD2	1.41	0.46
31:DL:101:GLN:HB3	31:DL:105:HIS:NE2	2.30	0.46
26:Df:311:CYS:HB3	26:Df:329:LEU:HG	1.97	0.46
35:EA:42:CYS:HB3	35:EA:77:ARG:HH22	1.80	0.46
38:2:206:ARG:HH21	43:7:613:HIS:CE1	2.34	0.46
38:2:319:ALA:HB1	39:3:272:LEU:HD21	1.98	0.46
38:2:375:VAL:HA	38:2:379:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:12:VAL:HB	40:4:202:GLN:HE21	1.80	0.46
40:4:238:PHE:CZ	40:4:270:LEU:HB2	2.50	0.46
42:6:286:HIS:HA	42:6:290:PRO:O	2.14	0.46
48:m:112:ARG:HH22	65:z:598:CYS:C	2.22	0.46
49:a:160:LEU:HD12	49:a:214:ARG:HH21	1.79	0.46
50:d:93:MET:HE3	50:d:93:MET:HB3	1.75	0.46
52:g:83:MET:HE3	52:g:83:MET:CA	2.45	0.46
52:g:164:ILE:HD12	54:i:140:MET:HE3	1.97	0.46
52:g:166:ASN:OD1	52:g:167:CYS:CA	2.63	0.46
57:n:922:TYR:HE1	57:n:955:PRO:HA	1.80	0.46
59:q:186:GLU:HB3	59:q:243:LEU:HD22	1.97	0.46
66:x:566:GLU:C	66:x:568:LYS:H	2.24	0.46
70:Y:8:DA:H2"	70:Y:9:DC:C5	2.29	0.46
2:8:135:HIS:HD2	2:8:137:ASP:N	2.14	0.46
2:8:241:CYS:HB2	2:8:246:TYR:CD1	2.51	0.46
10:PA:450:MET:HE2	10:PA:505:LEU:HD22	1.97	0.46
11:PB:733:MET:HE2	11:PB:733:MET:HB2	1.71	0.46
11:PB:765:GLU:H	11:PB:765:GLU:HG3	1.54	0.46
12:PC:128:ILE:O	12:PC:129:PRO:C	2.57	0.46
17:PH:2:ALA:HB2	17:PH:66:GLU:HA	1.97	0.46
22:DA:899:LYS:HE3	22:DA:899:LYS:HB2	1.82	0.46
24:DD:893:GLU:H	24:DD:893:GLU:HG3	1.44	0.46
25:DE:646:SER:OG	25:DE:647:ALA:N	2.48	0.46
26:DF:28:ILE:HD11	29:DI:55:LYS:CE	2.45	0.46
29:DI:38:GLN:HA	29:DI:41:GLU:HB2	1.97	0.46
24:Dd:860:VAL:HA	34:Dm:47:GLN:HG2	1.98	0.46
36:EB:88:ARG:HD3	36:EB:97:LEU:HD21	1.96	0.46
37:1:459:SER:HA	37:1:462:LYS:HZ2	1.80	0.46
38:2:290:PHE:HE1	38:2:295:ARG:HB3	1.81	0.46
39:3:213:LEU:HD11	39:3:245:PRO:CG	2.45	0.46
40:4:226:ARG:HD2	40:4:257:SER:HB3	1.97	0.46
40:4:300:THR:HG23	40:4:373:HIS:CB	2.43	0.46
40:4:338:PHE:CZ	42:6:79:ALA:HB2	2.51	0.46
42:6:439:ILE:HG12	42:6:464:LEU:HD23	1.97	0.46
43:7:77:VAL:HA	43:7:80:ILE:HD12	1.97	0.46
43:7:417:ILE:HG23	43:7:434:HIS:HB2	1.96	0.46
47:l:149:LEU:HD11	64:v:139:SER:HA	1.97	0.46
51:f:82:ARG:NH1	51:f:94:PRO:HB3	2.30	0.46
51:f:111:LEU:HD22	59:q:127:LEU:HD11	1.97	0.46
57:n:237:MET:HE1	59:q:45:GLN:HG2	1.96	0.46
57:n:478:MET:HE3	57:n:492:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:506:HIS:CD2	59:q:508:ASP:H	2.34	0.46
63:u:28:GLN:HG3	65:z:483:ASN:ND2	2.29	0.46
63:u:61:LEU:HD13	65:z:496:LEU:HD11	1.97	0.46
67:w:37:LEU:HD12	67:w:37:LEU:HA	1.72	0.46
67:w:41:LEU:HD11	67:w:85:MET:C	2.40	0.46
67:w:485:SER:OG	67:w:486:GLU:N	2.49	0.46
67:w:726:ASN:H	67:w:726:ASN:HD22	1.63	0.46
1:0:250:PRO:HD2	1:0:251:LEU:HD22	1.97	0.46
2:8:16:ASP:HB3	2:8:28:LYS:HB3	1.98	0.46
2:8:101:ILE:HD13	2:8:101:ILE:N	2.29	0.46
9:FB:193:LYS:HD3	24:DD:987:LYS:HB2	1.96	0.46
10:PA:118:LEU:HD23	10:PA:118:LEU:HA	1.84	0.46
10:PA:459:ASN:HB3	10:PA:469:MET:HG2	1.98	0.46
10:PA:501:MET:HE2	10:PA:501:MET:HB3	1.71	0.46
10:PA:1378:LEU:O	10:PA:1379:GLU:C	2.55	0.46
12:PC:86:ARG:H	12:PC:86:ARG:HG3	1.45	0.46
12:PC:270:ASP:O	12:PC:271:VAL:C	2.59	0.46
20:PK:77:THR:O	20:PK:78:THR:O	2.33	0.46
22:DA:857:MET:HE3	22:DA:858:ASP:H	1.81	0.46
23:DB:568:VAL:HG22	23:DB:628:ILE:HG23	1.98	0.46
27:DG:41:ASP:OD1	27:DG:41:ASP:N	2.47	0.46
37:1:136:VAL:HG13	37:1:503:THR:HG21	1.98	0.46
40:4:409:TYR:H	41:5:5:LEU:HD13	1.80	0.46
40:4:438:LYS:HG2	41:5:38:ILE:HG23	1.97	0.46
43:7:340:VAL:HA	43:7:343:ARG:HB3	1.96	0.46
49:a:99:THR:HG22	49:a:112:VAL:HG13	1.96	0.46
49:a:413:HIS:CD2	49:a:471:ASP:CB	2.91	0.46
56:k:88:LYS:CG	59:q:380:ARG:HH11	2.28	0.46
57:n:587:LEU:CD2	67:w:15:THR:CG2	2.89	0.46
59:q:103:ARG:HH11	59:q:103:ARG:HB2	1.81	0.46
59:q:166:ARG:HH11	59:q:166:ARG:HG3	1.80	0.46
61:s:152:PHE:C	61:s:154:LEU:N	2.73	0.46
63:u:4:ARG:NE	65:z:595:PRO:C	2.74	0.46
68:p:266:ARG:HH11	68:p:341:ILE:HD13	1.80	0.46
1:0:301:PHE:CE1	3:9:170:PHE:CZ	3.04	0.46
7:BA:286:ARG:CZ	7:BA:316:LEU:HD12	2.42	0.46
10:PA:436:SER:HB2	62:t:97:LYS:NZ	2.08	0.46
11:PB:43:GLN:C	11:PB:45:ASP:H	2.23	0.46
11:PB:785:TYR:CE2	11:PB:955:PRO:HD3	2.50	0.46
11:PB:994:GLY:HA2	19:PJ:50:LEU:CD2	2.46	0.46
13:PD:122:PHE:HB3	13:PD:126:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:PD:142:TYR:HD1	64:v:70:ARG:NH1	2.09	0.46
17:PH:57:ARG:O	17:PH:145:MET:HA	2.16	0.46
22:DA:847:LYS:HB3	22:DA:847:LYS:HE2	1.77	0.46
26:Df:317:LEU:HD12	26:Df:329:LEU:HD23	1.98	0.46
37:1:233:ASP:OD1	37:1:233:ASP:N	2.47	0.46
40:4:440:LEU:HD22	41:5:5:LEU:HD21	1.97	0.46
42:6:601:LYS:HG3	42:6:602:ILE:HG13	1.98	0.46
42:6:696:MET:HB3	42:6:701:LEU:HD11	1.98	0.46
57:n:141:ARG:NH2	63:u:20:CYS:HB3	2.30	0.46
57:n:229:GLU:HB3	57:n:304:GLN:NE2	2.30	0.46
57:n:387:GLU:HG3	57:n:391:LYS:HE3	1.97	0.46
57:n:523:SER:OG	57:n:583:ALA:O	2.34	0.46
57:n:802:VAL:HG22	57:n:809:ILE:HB	1.97	0.46
58:o:762:GLN:N	67:w:74:LYS:HE3	2.29	0.46
67:w:37:LEU:HD23	67:w:85:MET:HE3	1.98	0.46
1:0:80:LYS:HE2	1:0:80:LYS:HB2	1.58	0.46
2:8:37:ILE:N	2:8:37:ILE:CD1	2.79	0.46
9:FB:23:VAL:HG21	9:FB:31:TRP:CZ3	2.50	0.46
10:PA:394:VAL:HB	10:PA:444:TYR:O	2.16	0.46
10:PA:1210:TRP:CD1	10:PA:1210:TRP:N	2.81	0.46
11:PB:202:THR:O	11:PB:203:ASN:HB2	2.14	0.46
11:PB:277:GLY:O	11:PB:278:PHE:C	2.57	0.46
11:PB:1103:LEU:HG	11:PB:1107:LEU:HD13	1.97	0.46
13:PD:109:GLU:H	13:PD:109:GLU:HG3	1.53	0.46
14:PE:40:PHE:CE1	14:PE:44:PHE:CD2	3.04	0.46
22:DA:900:ASP:HB3	27:DG:154:LYS:HD2	1.97	0.46
25:DE:324:LYS:HA	25:DE:327:ASN:HB3	1.97	0.46
25:DE:476:VAL:HG11	25:DE:794:ALA:HB3	1.98	0.46
26:DF:83:LEU:HD21	26:DF:94:PHE:HB2	1.97	0.46
26:DF:92:ILE:HG13	26:DF:93:PRO:HD3	1.98	0.46
38:2:80:ARG:HD3	38:2:201:LEU:HD21	1.97	0.46
40:4:201:PHE:HA	40:4:204:LEU:HD12	1.97	0.46
42:6:296:ASP:OD1	42:6:334:ARG:N	2.49	0.46
42:6:309:ASP:HA	42:6:384:ILE:CD1	2.46	0.46
42:6:375:LYS:O	42:6:379:LYS:N	2.38	0.46
42:6:621:ASN:ND2	42:6:646:ALA:O	2.48	0.46
43:7:263:LEU:HD11	43:7:336:LEU:HD23	1.97	0.46
46:b:129:GLN:NE2	46:b:129:GLN:HA	2.31	0.46
49:a:145:LYS:HA	49:a:145:LYS:CE	2.41	0.46
49:a:160:LEU:HG	49:a:219:LEU:HD11	1.98	0.46
49:a:412:ARG:O	49:a:472:SER:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:a:421:ILE:HD11	49:a:450:PHE:CD1	2.50	0.46
50:d:40:LEU:HB3	50:d:65:VAL:HG13	1.97	0.46
50:d:45:ILE:O	54:i:76:MET:SD	2.73	0.46
54:i:109:LEU:HD21	54:i:117:GLN:HE22	1.79	0.46
55:j:20:ARG:CD	57:n:94:GLN:CA	2.39	0.46
57:n:851:ILE:HD11	57:n:911:SER:HA	1.96	0.46
59:q:113:TYR:CD1	59:q:113:TYR:C	2.93	0.46
66:x:968:LEU:HD13	66:x:986:ILE:HG13	1.98	0.46
68:p:207:CYS:HB3	68:p:242:TYR:HE2	1.79	0.46
1:0:1:MET:N	43:7:253:ARG:HH22	2.13	0.46
1:0:209:GLU:CD	1:0:209:GLU:C	2.84	0.46
1:0:283:LEU:O	1:0:284:ALA:C	2.59	0.46
5:DP:173:ASN:HB3	5:DP:251:LEU:HB2	1.97	0.46
5:DP:273:LEU:HB2	5:DP:335:PHE:CZ	2.51	0.46
10:PA:418:TYR:CD1	10:PA:426:ARG:HD3	2.51	0.46
11:PB:168:ASP:O	11:PB:169:ARG:C	2.58	0.46
12:PC:91:GLU:O	12:PC:92:GLU:HB2	2.14	0.46
17:PH:37:MET:HG2	17:PH:127:GLY:HA3	1.98	0.46
22:DA:645:LYS:HA	22:DA:645:LYS:HD2	1.77	0.46
25:DE:773:TYR:CE1	26:DF:137:SER:HB2	2.51	0.46
25:DE:774:MET:O	26:DF:142:GLN:NE2	2.49	0.46
27:DG:161:ASP:OD1	27:DG:161:ASP:N	2.48	0.46
31:Dl:106:ARG:O	31:Dl:106:ARG:CG	2.64	0.46
37:1:527:GLU:OE2	37:1:531:THR:OG1	2.34	0.46
38:2:109:THR:HG21	38:2:144:SER:H	1.81	0.46
38:2:251:ARG:HB3	38:2:310:LEU:HD13	1.98	0.46
38:2:303:VAL:HG12	38:2:304:GLU:HG2	1.98	0.46
42:6:350:GLY:O	42:6:354:ALA:N	2.49	0.46
42:6:554:ARG:HB3	42:6:647:LYS:HZ1	1.80	0.46
43:7:598:SER:HB2	43:7:604:VAL:HG21	1.97	0.46
44:c:134:LYS:HD3	47:l:46:TYR:HB2	1.96	0.46
49:a:259:ILE:O	49:a:259:ILE:CD1	2.64	0.46
50:d:126:TYR:CE1	59:q:36:MET:HB2	2.51	0.46
51:f:111:LEU:O	51:f:115:ILE:HG13	2.15	0.46
52:g:98:ARG:HG2	61:s:73:GLY:O	2.15	0.46
55:j:85:LEU:HD12	61:s:96:PHE:CE1	2.51	0.46
57:n:230:PHE:CE1	57:n:296:LEU:CB	2.98	0.46
63:u:106:ASP:O	63:u:110:ARG:HG3	2.16	0.46
70:Y:13:DC:H2"	70:Y:14:DC:C5	2.51	0.46
1:0:105:ILE:H	1:0:105:ILE:HG13	1.48	0.46
1:0:271:TYR:CE2	1:0:273:ASN:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:15:SER:O	3:9:18:GLN:HG3	2.15	0.46
9:FB:49:GLN:N	9:FB:49:GLN:CD	2.73	0.46
10:PA:408:ARG:NH2	60:r:7:THR:CG2	2.79	0.46
10:PA:965:VAL:O	10:PA:969:ILE:HG13	2.16	0.46
10:PA:983:LEU:HB3	10:PA:1048:THR:HG21	1.97	0.46
10:PA:1040:LEU:HB2	14:PE:200:ALA:O	2.16	0.46
11:PB:59:VAL:HA	11:PB:408:PHE:CE2	2.51	0.46
11:PB:743:ARG:HH21	11:PB:745:ASP:CG	2.24	0.46
15:PF:108:ARG:HH21	15:PF:123:LEU:CD2	2.29	0.46
23:DB:71:ARG:HD3	23:DB:73:TYR:CE1	2.51	0.46
23:DB:559:LYS:HB2	23:DB:559:LYS:NZ	2.31	0.46
24:Dd:1084:LEU:HB3	29:Di:99:ARG:HH21	1.81	0.46
33:Dk:150:VAL:HG22	34:Dm:82:GLN:HB3	1.98	0.46
37:1:399:ASP:HA	37:1:402:ASN:HB2	1.98	0.46
37:1:522:VAL:HA	37:1:525:ILE:HG22	1.97	0.46
40:4:280:ARG:HH12	40:4:282:TYR:HB2	1.80	0.46
40:4:330:LEU:HD12	40:4:331:PHE:HB2	1.96	0.46
40:4:425:ALA:HB2	40:4:441:MET:HE3	1.98	0.46
42:6:181:HIS:H	42:6:182:PRO:HD3	1.81	0.46
42:6:378:PHE:O	42:6:382:SER:OG	2.28	0.46
43:7:633:LEU:O	43:7:637:LEU:N	2.36	0.46
47:l:166:LEU:CD2	64:v:123:ILE:HD12	2.45	0.46
47:l:167:ILE:HD12	64:v:127:LEU:HD23	1.98	0.46
48:m:19:GLN:NE2	52:g:43:MET:HA	2.31	0.46
48:m:21:GLU:O	48:m:25:VAL:HG23	2.16	0.46
49:a:224:TYR:HE1	49:a:254:ASN:C	2.23	0.46
50:d:64:GLN:NE2	50:d:68:LEU:HD12	2.27	0.46
52:g:89:PHE:CD2	63:u:19:PHE:HE1	2.32	0.46
55:j:73:GLN:HB3	55:j:80:TYR:OH	2.16	0.46
56:k:37:LYS:HE3	56:k:37:LYS:N	2.16	0.46
57:n:238:GLY:N	57:n:243:VAL:HG21	2.31	0.46
57:n:527:THR:O	57:n:528:HIS:HB2	2.15	0.46
58:o:681:GLU:OE1	58:o:768:SER:OG	2.34	0.46
59:q:7:VAL:HG21	63:u:87:ALA:HB1	1.97	0.46
3:9:184:PRO:CB	3:9:187:LEU:HD12	2.33	0.45
8:FA:46:ARG:N	8:FA:101:ARG:O	2.39	0.45
10:PA:364:ARG:HD3	11:PB:1060:HIS:CD2	2.50	0.45
11:PB:661:VAL:O	11:PB:661:VAL:HG23	2.15	0.45
12:PC:42:VAL:HB	12:PC:178:PRO:HG3	1.98	0.45
12:PC:264:SER:C	12:PC:266:GLU:N	2.72	0.45
16:PG:38:CYS:O	16:PG:39:THR:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:PG:166:ASP:O	16:PG:167:TYR:HB2	2.16	0.45
17:PH:7:GLU:HA	17:PH:58:LEU:O	2.16	0.45
23:DB:539:ARG:HG3	41:5:31:LYS:O	2.15	0.45
26:DF:123:PRO:HD3	28:DH:35:ARG:HB2	1.98	0.45
29:DI:19:MET:HG2	29:DI:40:LEU:HG	1.98	0.45
29:Di:78:ARG:HD3	29:Di:78:ARG:HA	1.78	0.45
30:Dj:176:MET:HE1	34:Dm:75:ILE:HD11	1.97	0.45
35:EA:48:MET:HA	35:EA:51:LEU:HB2	1.98	0.45
37:1:296:LYS:HA	37:1:299:SER:HB2	1.99	0.45
38:2:279:ASN:N	38:2:298:TYR:HB3	2.31	0.45
40:4:323:LEU:O	40:4:327:LEU:N	2.48	0.45
41:5:49:LEU:O	41:5:53:LEU:N	2.43	0.45
43:7:441:SER:HB2	43:7:445:LYS:HE3	1.97	0.45
43:7:544:TYR:O	43:7:548:THR:N	2.47	0.45
48:m:93:CYS:O	48:m:97:ILE:HG22	2.16	0.45
51:f:181:LEU:HD12	57:n:270:GLN:HG3	1.98	0.45
52:g:93:LEU:HD13	55:j:106:LYS:CE	2.44	0.45
55:j:96:LYS:HZ2	61:s:80:SER:HA	1.79	0.45
56:k:37:LYS:CE	56:k:37:LYS:N	2.73	0.45
57:n:948:LYS:HD2	57:n:948:LYS:HA	1.71	0.45
58:o:752:VAL:HA	58:o:755:CYS:SG	2.56	0.45
62:t:96:VAL:HA	62:t:99:LYS:HG2	1.99	0.45
67:w:394:PRO:CB	68:p:171:PHE:CE1	2.99	0.45
68:p:24:TRP:HD1	68:p:51:LEU:HD12	1.79	0.45
1:0:284:ALA:C	1:0:286:GLY:N	2.73	0.45
8:FA:124:TYR:HD1	9:FB:22:LYS:HA	1.79	0.45
10:PA:126:ILE:O	10:PA:129:ILE:HG12	2.17	0.45
10:PA:498:GLY:HA3	11:PB:934:LYS:HE2	1.98	0.45
10:PA:784:VAL:O	10:PA:784:VAL:HG12	2.16	0.45
10:PA:883:ILE:HD12	10:PA:885:GLN:NE2	2.31	0.45
10:PA:893:GLU:HG2	14:PE:203:TYR:CD2	2.52	0.45
10:PA:952:LEU:O	10:PA:955:GLU:HB3	2.16	0.45
11:PB:59:VAL:HG12	11:PB:408:PHE:CE1	2.52	0.45
11:PB:324:ARG:HD3	11:PB:324:ARG:HA	1.61	0.45
11:PB:542:LEU:HD12	11:PB:542:LEU:HA	1.86	0.45
11:PB:750:VAL:HG12	11:PB:751:LEU:H	1.80	0.45
12:PC:101:PHE:CE2	12:PC:122:SER:HB3	2.51	0.45
13:PD:62:MET:HB3	64:v:13:THR:HG21	1.99	0.45
13:PD:103:LEU:HD21	16:PG:84:VAL:HG22	1.98	0.45
22:DA:1182:CYS:O	22:DA:1182:CYS:SG	2.75	0.45
26:DF:391:LEU:HD12	26:DF:391:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DI:19:MET:HB2	29:DI:40:LEU:HD21	1.99	0.45
25:De:633:THR:O	25:De:634:ARG:NH2	2.45	0.45
40:4:262:LEU:CD1	40:4:271:VAL:HG11	2.45	0.45
40:4:402:ARG:NH2	41:5:9:LEU:HG	2.31	0.45
43:7:71:ILE:HB	43:7:231:VAL:HG13	1.99	0.45
43:7:113:LYS:HD2	43:7:113:LYS:HA	1.72	0.45
49:a:428:THR:HB	49:a:430:LEU:CD2	2.46	0.45
49:a:518:ILE:HG22	49:a:518:ILE:O	2.17	0.45
50:d:173:ARG:H	50:d:173:ARG:HG3	1.45	0.45
51:f:57:LEU:HB3	51:f:58:GLU:H	1.50	0.45
53:h:33:LEU:HD23	53:h:33:LEU:HA	1.81	0.45
53:h:156:LYS:HA	53:h:159:ARG:NH1	2.30	0.45
53:h:187:PHE:HE2	53:h:189:LYS:HB2	1.80	0.45
55:j:121:MET:O	55:j:125:ARG:HG3	2.15	0.45
56:k:88:LYS:HZ3	59:q:303:LEU:HD22	1.80	0.45
59:q:190:LEU:HD13	59:q:190:LEU:C	2.41	0.45
60:r:1:MET:O	60:r:2:GLU:HB3	2.15	0.45
62:t:80:GLU:HB2	62:t:81:ASN:H	1.44	0.45
68:p:15:LEU:HD11	68:p:453:SER:HB2	1.98	0.45
69:X:-25:DA:H2'	69:X:-24:DA:C8	2.52	0.45
70:Y:11:DC:H2"	70:Y:12:DG:C8	2.52	0.45
3:9:102:ARG:NH1	3:9:102:ARG:CG	2.80	0.45
8:FA:45:ALA:CB	9:FB:9:LEU:HD11	2.45	0.45
9:FB:154:LYS:N	9:FB:155:PRO:HD3	2.32	0.45
10:PA:1144:LEU:HB2	10:PA:1351:ASP:C	2.42	0.45
11:PB:584:MET:O	11:PB:585:ASN:C	2.57	0.45
11:PB:789:ASN:O	11:PB:968:ASN:HB2	2.17	0.45
11:PB:1114:TYR:CD2	11:PB:1116:VAL:HG13	2.51	0.45
14:PE:47:LYS:C	14:PE:53:PRO:HD2	2.41	0.45
14:PE:110:MET:HG2	14:PE:114:ALA:HB3	1.98	0.45
17:PH:87:GLN:H	17:PH:87:GLN:HG3	1.41	0.45
18:PI:86:CYS:SG	18:PI:88:LYS:N	2.89	0.45
22:DA:505:ASN:HB3	22:DA:506:ASP:H	1.53	0.45
22:DA:1165:LEU:HB2	22:DA:1191:ILE:HG12	1.97	0.45
24:DD:956:GLN:HA	24:DD:959:ASP:HB2	1.97	0.45
25:DE:468:ASN:CG	26:DF:127:LEU:HB3	2.41	0.45
26:Df:83:LEU:HD22	29:Di:41:GLU:HG2	1.99	0.45
26:Df:330:ARG:NH1	26:Df:371:THR:O	2.48	0.45
36:EB:167:LEU:HA	36:EB:167:LEU:HD23	1.72	0.45
37:1:136:VAL:HG12	37:1:137:ILE:HG23	1.98	0.45
39:3:12:VAL:N	39:3:160:ARG:O	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:100:LEU:C	40:4:101:LEU:CD1	2.80	0.45
40:4:405:GLU:HA	41:5:47:ALA:HB1	1.96	0.45
40:4:409:TYR:N	41:5:5:LEU:HA	2.31	0.45
43:7:86:GLU:HG2	43:7:86:GLU:O	2.15	0.45
43:7:494:ILE:HA	43:7:679:PHE:HB2	1.98	0.45
51:f:52:MET:HE3	51:f:52:MET:HB3	1.84	0.45
51:f:184:LEU:HD22	57:n:299:PHE:CG	2.49	0.45
55:j:11:HIS:C	55:j:15:PHE:HD2	2.20	0.45
55:j:62:THR:HB	55:j:63:VAL:H	1.58	0.45
57:n:444:GLU:HB3	57:n:445:PRO:HD3	1.97	0.45
58:o:733:SER:HB3	58:o:766:LYS:HA	1.98	0.45
59:q:17:LYS:HB3	59:q:30:TYR:HE2	1.82	0.45
67:w:1:MET:N	67:w:1:MET:HE3	2.31	0.45
1:0:281:GLN:CD	1:0:281:GLN:N	2.73	0.45
1:0:295:ARG:CZ	3:9:165:ARG:HH21	2.25	0.45
3:9:279:ARG:HG3	3:9:279:ARG:HH21	1.81	0.45
7:BA:221:ASN:OD1	9:FB:150:THR:HG22	2.16	0.45
10:PA:800:PHE:HA	10:PA:805:ARG:O	2.16	0.45
10:PA:1231:ILE:O	10:PA:1235:ILE:HG23	2.16	0.45
11:PB:130:LYS:HB3	11:PB:142:THR:HG23	1.98	0.45
11:PB:628:VAL:CG1	11:PB:632:LYS:O	2.45	0.45
11:PB:1114:TYR:CE2	11:PB:1116:VAL:HG12	2.52	0.45
16:PG:156:ASP:OD1	16:PG:158:PHE:HD1	1.99	0.45
24:DD:893:GLU:HB2	24:DD:894:LEU:H	1.52	0.45
26:DF:424:GLN:O	26:DF:428:LEU:HG	2.16	0.45
31:DL:83:MET:CE	31:DL:86:GLN:OE1	2.64	0.45
31:DL:102:LEU:HA	31:DL:105:HIS:CD2	2.49	0.45
37:1:294:SER:O	37:1:298:ASN:ND2	2.49	0.45
42:6:418:LYS:HA	70:Y:-11:DC:OP1	2.16	0.45
43:7:326:ALA:HA	43:7:329:PHE:HB3	1.98	0.45
43:7:683:ARG:NH1	43:7:687:GLY:H	2.14	0.45
49:a:200:LEU:C	49:a:200:LEU:HD13	2.42	0.45
49:a:364:TYR:O	49:a:428:THR:CB	2.64	0.45
57:n:249:LYS:C	57:n:250:LEU:HD22	2.41	0.45
67:w:1195:ALA:O	67:w:1197:HIS:N	2.50	0.45
7:BA:284:THR:HG21	70:Y:32:DG:C5'	2.46	0.45
11:PB:309:PHE:C	11:PB:311:ILE:N	2.75	0.45
16:PG:6:SER:HA	16:PG:73:LYS:HA	1.98	0.45
22:DA:349:TRP:CH2	26:Df:282:LEU:HD11	2.52	0.45
22:DA:564:PRO:CB	23:DB:744:PHE:CD2	3.00	0.45
25:DE:700:HIS:HB3	25:DE:702:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DF:427:LEU:HD12	26:DF:427:LEU:HA	1.72	0.45
25:De:717:LEU:HD22	25:De:726:LEU:HD11	1.98	0.45
37:1:240:LYS:HA	37:1:240:LYS:HD2	1.59	0.45
38:2:58:MET:HG2	38:2:101:ILE:HB	1.98	0.45
38:2:65:VAL:HG22	38:2:170:ILE:HD12	1.99	0.45
40:4:151:TYR:HA	40:4:154:GLU:HG2	1.97	0.45
42:6:309:ASP:O	42:6:310:LEU:CD2	2.65	0.45
43:7:354:PRO:HA	43:7:416:ILE:HD12	1.97	0.45
43:7:515:ALA:HA	43:7:518:ARG:HG2	1.98	0.45
44:c:204:MET:CE	44:c:206:SER:O	2.47	0.45
48:m:106:GLN:NE2	50:d:167:TRP:CE3	2.84	0.45
50:d:121:LEU:HD12	63:u:115:LEU:HA	1.96	0.45
52:g:93:LEU:CA	55:j:106:LYS:HZ1	2.29	0.45
57:n:141:ARG:NH1	63:u:17:ASP:CA	2.80	0.45
57:n:870:GLN:NE2	57:n:874:ASP:OD2	2.48	0.45
59:q:106:LEU:C	59:q:106:LEU:CD2	2.85	0.45
62:t:110:ILE:HD12	62:t:197:PHE:HB3	1.97	0.45
63:u:96:GLU:O	63:u:99:GLU:HG3	2.17	0.45
63:u:102:THR:O	63:u:105:GLU:HG2	2.16	0.45
67:w:172:GLU:HB3	67:w:175:ALA:HB3	1.98	0.45
67:w:1204:SER:O	67:w:1208:THR:OG1	2.26	0.45
69:X:-18:DT:H2"	69:X:-17:DG:H5"	1.98	0.45
1:0:74:ILE:CG2	43:7:334:ARG:HH21	2.30	0.45
2:8:206:LEU:HD22	2:8:206:LEU:HA	1.76	0.45
3:9:207:TYR:HD2	3:9:255:MET:HE3	1.81	0.45
3:9:239:LYS:HZ2	3:9:239:LYS:N	1.87	0.45
4:DO:5:LEU:CD2	4:DO:98:CYS:SG	3.02	0.45
7:BA:179:GLU:CG	9:FB:154:LYS:NZ	2.80	0.45
10:PA:999:ARG:HE	10:PA:999:ARG:HB2	1.51	0.45
11:PB:82:PRO:HB3	11:PB:134:LYS:CA	2.46	0.45
11:PB:970:HIS:O	11:PB:973:PRO:HD2	2.16	0.45
17:PH:64:LEU:HA	17:PH:64:LEU:HD23	1.64	0.45
22:DA:496:GLU:HG3	22:DA:497:PRO:HD2	1.98	0.45
23:DB:184:ASN:N	23:DB:184:ASN:ND2	2.63	0.45
26:DF:55:LEU:HD22	26:DF:55:LEU:HA	1.72	0.45
29:DI:16:ALA:CB	29:DI:40:LEU:HD11	2.46	0.45
29:DI:23:LEU:HD13	29:DI:31:TYR:CZ	2.52	0.45
24:Dd:910:LEU:HD11	31:Dl:88:ALA:HB2	1.98	0.45
26:Df:58:MET:HE3	26:Df:64:GLN:HA	1.97	0.45
31:Dl:76:LEU:CD1	31:Dl:84:LEU:CD1	2.95	0.45
37:1:187:ASN:H	37:1:191:ASP:CB	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:224:ASP:O	38:2:228:TYR:N	2.44	0.45
40:4:28:PRO:HA	40:4:31:LEU:HG	1.98	0.45
41:5:53:LEU:HD23	41:5:56:ARG:HB3	1.96	0.45
44:c:135:ARG:NH2	45:e:92:GLU:OE1	2.49	0.45
46:b:178:LEU:HD21	47:l:78:LEU:HB3	1.98	0.45
49:a:64:THR:HG22	49:a:86:ARG:HD2	1.98	0.45
49:a:145:LYS:HD2	49:a:145:LYS:N	2.32	0.45
49:a:229:SER:HA	49:a:502:MET:HB2	1.97	0.45
50:d:63:ASN:HD22	50:d:63:ASN:HA	1.56	0.45
50:d:167:TRP:O	50:d:167:TRP:HE3	2.00	0.45
51:f:19:SER:O	51:f:22:PRO:HD2	2.16	0.45
51:f:94:PRO:C	59:q:130:VAL:HG13	2.41	0.45
51:f:185:ARG:CG	57:n:273:PHE:CZ	3.00	0.45
52:g:12:PRO:HA	52:g:13:PRO:HD3	1.84	0.45
53:h:173:PHE:HB3	60:r:197:VAL:HG12	1.99	0.45
57:n:385:LEU:HD23	57:n:407:ALA:HA	1.99	0.45
57:n:855:LEU:HD11	57:n:868:LEU:HD22	1.98	0.45
58:o:762:GLN:HB2	67:w:29:THR:HG21	1.97	0.45
59:q:127:LEU:HG	59:q:127:LEU:O	2.17	0.45
59:q:213:GLY:O	59:q:383:HIS:HA	2.17	0.45
59:q:484:TYR:CE1	59:q:636:VAL:CG1	2.99	0.45
66:x:847:PHE:HB2	66:x:899:ARG:HG2	1.97	0.45
68:p:100:ASP:OD1	68:p:100:ASP:N	2.48	0.45
68:p:146:HIS:NE2	68:p:160:SER:OG	2.49	0.45
69:X:-23:DG:OP1	69:X:-23:DG:H4'	2.17	0.45
2:8:110:THR:HB	2:8:113:HIS:CG	2.52	0.45
2:8:247:VAL:O	2:8:248:THR:C	2.58	0.45
3:9:151:ILE:H	3:9:151:ILE:HG12	1.45	0.45
3:9:177:ARG:CZ	3:9:177:ARG:CB	2.93	0.45
10:PA:663:ASP:O	10:PA:667:LEU:HG	2.16	0.45
10:PA:1054:MET:HA	10:PA:1058:PHE:HD2	1.80	0.45
10:PA:1467:GLY:C	10:PA:1469:GLY:N	2.74	0.45
11:PB:327:LYS:HB2	11:PB:328:PRO:HD2	1.99	0.45
11:PB:749:HIS:CD2	11:PB:749:HIS:N	2.85	0.45
12:PC:89:THR:OG1	62:t:201:ARG:NH2	2.48	0.45
12:PC:154:ARG:CZ	19:PJ:63:ALA:HA	2.46	0.45
13:PD:110:GLU:HB2	16:PG:167:TYR:CE1	2.51	0.45
14:PE:40:PHE:CE1	14:PE:44:PHE:HD2	2.34	0.45
14:PE:54:ARG:HD3	14:PE:54:ARG:HA	1.63	0.45
16:PG:93:ASN:HB3	16:PG:96:GLY:N	2.31	0.45
18:PI:69:ILE:H	18:PI:69:ILE:HG12	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:PK:75:VAL:O	20:PK:83:PRO:HB3	2.17	0.45
22:DA:396:LEU:HD12	22:DA:396:LEU:HA	1.82	0.45
26:DF:71:ILE:HD11	29:DI:35:VAL:CG2	2.46	0.45
35:EA:72:ILE:H	35:EA:72:ILE:HG13	1.49	0.45
37:1:307:PHE:O	37:1:311:SER:N	2.44	0.45
38:2:374:PHE:O	38:2:379:LEU:N	2.49	0.45
42:6:310:LEU:O	42:6:312:PRO:HD3	2.17	0.45
48:m:23:GLU:OE1	52:g:45:PHE:C	2.59	0.45
49:a:109:TYR:CE1	49:a:150:PHE:CZ	3.05	0.45
57:n:199:LEU:CD2	57:n:222:VAL:HG13	2.45	0.45
57:n:273:PHE:O	57:n:276:GLN:HG3	2.17	0.45
57:n:637:PHE:HD2	57:n:639:LYS:HG2	1.81	0.45
57:n:647:MET:HG2	57:n:651:ASN:ND2	2.32	0.45
59:q:118:ILE:CG2	59:q:125:MET:HG2	2.46	0.45
60:r:57:VAL:HG22	60:r:71:ARG:HG2	1.99	0.45
61:s:84:ILE:CG1	61:s:90:GLU:HG2	2.46	0.45
67:w:144:LYS:O	67:w:147:THR:OG1	2.27	0.45
2:8:24:ALA:CA	2:8:44:LYS:HB2	2.47	0.45
2:8:280:PRO:HA	2:8:283:ARG:HH12	1.81	0.45
8:FA:124:TYR:HE1	9:FB:22:LYS:CE	2.30	0.45
10:PA:376:ASP:HB3	10:PA:522:PRO:HD3	1.99	0.45
10:PA:419:ILE:O	10:PA:420:ILE:C	2.59	0.45
10:PA:588:GLY:O	10:PA:589:LYS:C	2.56	0.45
10:PA:1207:ILE:HD12	10:PA:1207:ILE:HA	1.78	0.45
11:PB:414:GLU:O	11:PB:415:VAL:C	2.58	0.45
11:PB:889:LYS:HB3	11:PB:889:LYS:HE3	1.62	0.45
11:PB:974:SER:O	11:PB:976:MET:HE2	2.17	0.45
17:PH:132:LEU:HD12	17:PH:135:PHE:HE2	1.81	0.45
23:DB:564:LEU:HB2	23:DB:581:ILE:HD13	1.97	0.45
31:DL:64:GLN:CD	31:DL:64:GLN:N	2.75	0.45
37:1:248:LYS:O	37:1:252:LYS:N	2.44	0.45
37:1:350:LYS:HG3	37:1:353:LYS:HD3	1.99	0.45
37:1:370:LYS:HA	39:3:254:ALA:HB3	1.98	0.45
38:2:64:VAL:HB	38:2:169:ILE:HA	1.99	0.45
38:2:314:SER:H	38:2:318:LEU:HD21	1.82	0.45
42:6:318:PRO:HA	42:6:321:GLU:HB2	1.99	0.45
48:m:66:TYR:CE2	52:g:38:ILE:HG23	2.51	0.45
49:a:373:CYS:HB3	49:a:439:GLN:HG2	1.99	0.45
51:f:43:ARG:H	51:f:43:ARG:HD2	1.82	0.45
65:z:529:HIS:CE1	65:z:582:LEU:HD13	2.51	0.45
67:w:10:GLU:OE1	67:w:66:PHE:CZ	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:8:15:LEU:HD23	2:8:16:ASP:HB2	1.99	0.45
3:9:104:ILE:HD12	3:9:104:ILE:HA	1.55	0.45
9:FB:175:ARG:HB3	9:FB:176:ALA:H	1.63	0.45
10:PA:637:MET:HE3	10:PA:637:MET:HB2	1.66	0.45
10:PA:1232:ALA:O	10:PA:1235:ILE:HG12	2.15	0.45
10:PA:1459:MET:HE3	10:PA:1459:MET:HB2	1.87	0.45
12:PC:264:SER:HA	12:PC:267:ILE:CG1	2.39	0.45
16:PG:59:ILE:O	16:PG:60:GLN:C	2.60	0.45
18:PI:115:THR:O	18:PI:116:ALA:C	2.59	0.45
22:DA:509:LEU:O	22:DA:510:ILE:C	2.60	0.45
26:DF:264:SER:OG	26:DF:303:GLU:HB3	2.16	0.45
26:DF:298:GLU:HA	26:DF:301:VAL:CG2	2.47	0.45
26:DF:339:GLN:H	26:DF:339:GLN:HG3	1.55	0.45
26:Df:223:TYR:CD2	26:Df:255:MET:HE1	2.52	0.45
40:4:425:ALA:CB	40:4:431:LEU:HB2	2.46	0.45
42:6:156:ILE:O	42:6:156:ILE:HG23	2.16	0.45
43:7:14:TYR:O	43:7:15:ASP:HB2	2.17	0.45
43:7:353:SER:HB2	43:7:356:ALA:HB3	1.99	0.45
43:7:683:ARG:HH12	43:7:687:GLY:H	1.63	0.45
50:d:121:LEU:HD23	50:d:121:LEU:HA	1.79	0.45
51:f:188:PHE:CB	57:n:295:CYS:SG	3.05	0.45
59:q:440:LEU:CD2	59:q:502:ILE:HD11	2.46	0.45
66:x:495:ILE:HG22	66:x:499:MET:HE2	1.99	0.45
67:w:394:PRO:C	68:p:171:PHE:HZ	2.21	0.45
67:w:673:LYS:HE2	67:w:678:ALA:HB2	1.99	0.45
67:w:770:MET:HB3	67:w:776:ILE:HD11	1.99	0.45
1:0:174:ILE:HA	1:0:177:ARG:HB2	1.98	0.45
1:0:196:LEU:HD12	1:0:196:LEU:HA	1.75	0.45
3:9:181:LEU:N	3:9:181:LEU:CD1	2.72	0.45
7:BA:45:VAL:HG23	10:PA:67:ARG:HH22	1.81	0.45
9:FB:137:LYS:HE2	9:FB:137:LYS:HB2	1.85	0.45
11:PB:82:PRO:CA	11:PB:134:LYS:HA	2.47	0.45
11:PB:601:VAL:HG23	11:PB:603:MET:SD	2.56	0.45
11:PB:721:ARG:HE	11:PB:975:ARG:HB2	1.81	0.45
11:PB:848:LEU:HD11	11:PB:865:VAL:HG22	1.99	0.45
12:PC:68:LEU:HD21	12:PC:150:ILE:HG21	1.98	0.45
20:PK:77:THR:C	20:PK:78:THR:O	2.57	0.45
21:PL:34:ILE:H	21:PL:34:ILE:HG13	1.50	0.45
22:DA:401:ASN:HD22	22:DA:401:ASN:N	2.14	0.45
22:DA:730:PHE:CD1	22:DA:730:PHE:N	2.83	0.45
23:DB:414:LEU:HB2	23:DB:523:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DF:57:PHE:HB3	26:DF:63:ARG:HH21	1.82	0.45
26:DF:104:LEU:HB2	30:DJ:217:PHE:HZ	1.71	0.45
26:DF:131:LEU:HD12	26:DF:131:LEU:HA	1.77	0.45
38:2:156:LEU:HD21	38:2:165:ARG:HB3	1.99	0.45
39:3:262:ILE:HG12	39:3:264:ILE:H	1.82	0.45
40:4:361:ALA:HA	40:4:391:ILE:HG12	1.99	0.45
49:a:413:HIS:HA	49:a:472:SER:CA	2.43	0.45
51:f:181:LEU:HD21	57:n:274:ILE:CD1	2.47	0.45
53:h:20:ALA:HB2	59:q:113:TYR:CE2	2.51	0.45
54:i:100:LEU:C	54:i:100:LEU:HD13	2.41	0.45
54:i:135:TYR:HH	63:u:125:ILE:HA	1.70	0.45
57:n:226:VAL:HG12	57:n:230:PHE:C	2.39	0.45
61:s:84:ILE:HG13	61:s:90:GLU:HG2	1.98	0.45
66:x:676:ASP:OD1	66:x:676:ASP:N	2.50	0.45
67:w:10:GLU:HB3	67:w:14:LYS:NZ	2.31	0.45
67:w:394:PRO:C	68:p:171:PHE:CZ	2.93	0.45
68:p:41:CYS:SG	68:p:42:ARG:N	2.90	0.45
2:8:47:HIS:HA	2:8:52:LYS:CG	2.44	0.44
2:8:224:ARG:HA	2:8:224:ARG:HD2	1.76	0.44
4:DO:88:ILE:HD12	4:DO:88:ILE:HA	1.69	0.44
5:DP:173:ASN:HB2	5:DP:218:LYS:NZ	2.32	0.44
6:DQ:367:PHE:CD1	6:DQ:367:PHE:C	2.95	0.44
10:PA:1121:VAL:N	10:PA:1122:PRO:HD2	2.31	0.44
10:PA:1341:VAL:HB	10:PA:1364:GLU:HG3	1.98	0.44
10:PA:1650:TYR:CD1	59:q:111:VAL:HG21	2.52	0.44
11:PB:757:PRO:HG2	11:PB:760:THR:HG22	1.99	0.44
11:PB:947:ILE:HD11	20:PK:67:LEU:HD13	1.99	0.44
16:PG:11:ILE:HD12	16:PG:26:VAL:HG12	1.98	0.44
16:PG:97:LEU:HD13	16:PG:97:LEU:HA	1.64	0.44
18:PI:32:ASN:C	18:PI:33:ARG:HG2	2.42	0.44
18:PI:82:GLU:HA	18:PI:92:LYS:O	2.17	0.44
19:PJ:13:ILE:H	19:PJ:13:ILE:HG13	1.46	0.44
29:Di:16:ALA:HB2	29:Di:40:LEU:HD11	1.99	0.44
31:Dl:83:MET:SD	31:Dl:86:GLN:OE1	2.75	0.44
37:1:495:SER:OG	37:1:496:ASN:N	2.50	0.44
40:4:443:VAL:O	41:5:6:LYS:HB3	2.17	0.44
42:6:337:VAL:HG21	42:6:484:ILE:HB	1.99	0.44
42:6:359:LYS:NZ	42:6:436:GLY:C	2.75	0.44
42:6:360:ARG:O	42:6:433:GLN:NE2	2.49	0.44
43:7:256:LEU:O	43:7:260:GLN:N	2.47	0.44
43:7:504:ILE:HD13	43:7:680:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:b:156:PRO:HD2	46:b:159:GLN:HG2	1.99	0.44
49:a:58:LEU:HD22	49:a:58:LEU:HA	1.70	0.44
49:a:177:LEU:HB2	49:a:259:ILE:HG13	1.99	0.44
49:a:340:TYR:HB2	49:a:378:LYS:HB3	1.99	0.44
49:a:400:HIS:HE1	49:a:403:ARG:HG2	1.83	0.44
54:i:108:HIS:C	54:i:109:LEU:HG	2.42	0.44
55:j:76:ASN:N	55:j:79:LEU:HD12	2.31	0.44
57:n:593:GLU:OE2	67:w:24:GLY:HA2	2.18	0.44
59:q:451:LEU:HD22	59:q:451:LEU:HA	1.85	0.44
62:t:46:TYR:HB2	62:t:63:MET:HB2	1.98	0.44
62:t:161:LEU:O	62:t:165:LEU:N	2.50	0.44
63:u:61:LEU:O	63:u:65:THR:HG23	2.16	0.44
66:x:765:VAL:HG13	66:x:812:LEU:HB2	1.99	0.44
67:w:9:PHE:HB2	67:w:66:PHE:CE2	2.46	0.44
67:w:1139:ARG:O	67:w:1140:GLU:HG3	2.17	0.44
1:0:289:SER:O	1:0:290:SER:C	2.56	0.44
2:8:279:ASN:O	2:8:280:PRO:C	2.60	0.44
8:FA:143:TRP:C	8:FA:143:TRP:CD1	2.94	0.44
9:FB:153:TYR:C	9:FB:155:PRO:HD3	2.42	0.44
10:PA:547:LYS:HB2	10:PA:679:TRP:CZ3	2.53	0.44
10:PA:1243:LEU:HD13	10:PA:1243:LEU:HA	1.79	0.44
11:PB:216:ALA:HB2	11:PB:241:ALA:O	2.17	0.44
11:PB:225:LEU:O	11:PB:226:GLU:HB3	2.16	0.44
11:PB:455:ASP:HB2	11:PB:458:LYS:HG3	1.99	0.44
11:PB:1090:GLU:H	11:PB:1090:GLU:HG2	1.52	0.44
12:PC:31:ALA:HB1	12:PC:184:PHE:HE1	1.81	0.44
16:PG:47:ALA:O	16:PG:74:ALA:HB1	2.18	0.44
28:DH:37:LEU:HD23	28:DH:37:LEU:HA	1.77	0.44
30:DJ:130:ILE:HG13	30:DJ:160:GLN:HE21	1.81	0.44
24:Dd:913:LEU:HD21	31:Dl:87:ILE:HD13	1.98	0.44
37:1:215:MET:HB3	37:1:216:THR:H	1.71	0.44
38:2:59:ARG:N	38:2:102:SER:OG	2.49	0.44
38:2:169:ILE:HD12	38:2:198:VAL:HG22	1.98	0.44
39:3:63:HIS:ND1	39:3:65:GLN:HG2	2.31	0.44
42:6:112:HIS:HD2	42:6:117:LYS:HG3	1.81	0.44
43:7:338:GLU:O	43:7:342:TRP:N	2.48	0.44
44:c:42:LYS:HB2	44:c:48:ARG:HB3	1.99	0.44
45:e:74:ARG:HD2	45:e:78:ASP:OD2	2.17	0.44
50:d:111:GLN:CD	50:d:111:GLN:C	2.86	0.44
52:g:67:LEU:HG	52:g:118:HIS:CE1	2.51	0.44
52:g:168:LEU:HD23	52:g:168:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:i:71:ASN:HA	54:i:74:LYS:HD2	1.99	0.44
56:k:60:GLU:HG3	64:v:26:ILE:CG1	2.47	0.44
56:k:101:ARG:CZ	56:k:101:ARG:CB	2.87	0.44
57:n:707:ASP:CA	58:o:684:ARG:NH2	2.80	0.44
58:o:690:LEU:HD21	59:q:605:PRO:HG2	1.98	0.44
59:q:484:TYR:CE1	59:q:636:VAL:HG12	2.52	0.44
62:t:46:TYR:HD2	62:t:63:MET:HB3	1.82	0.44
62:t:81:ASN:N	62:t:81:ASN:OD1	2.51	0.44
63:u:4:ARG:HG3	65:z:595:PRO:C	2.42	0.44
66:x:832:GLN:NE2	66:x:835:ARG:HH21	2.15	0.44
67:w:512:THR:OG1	67:w:513:ASN:ND2	2.50	0.44
69:X:-24:DA:O5'	69:X:-24:DA:C8	2.70	0.44
2:8:96:THR:HB	2:8:97:ASP:H	1.37	0.44
2:8:214:PRO:HG3	10:PA:1674:THR:HG22	1.98	0.44
3:9:36:ALA:O	3:9:37:ASN:C	2.60	0.44
4:DO:3:TYR:C	4:DO:5:LEU:N	2.74	0.44
8:FA:124:TYR:CZ	9:FB:22:LYS:HE2	2.51	0.44
10:PA:70:ARG:HH12	10:PA:77:ASN:HD22	1.65	0.44
10:PA:317:MET:HB2	10:PA:317:MET:HE3	1.71	0.44
10:PA:680:LEU:O	10:PA:684:GLY:N	2.50	0.44
10:PA:1187:ALA:O	10:PA:1190:GLN:HB3	2.17	0.44
11:PB:729:GLY:C	11:PB:731:GLN:N	2.74	0.44
22:DA:567:LEU:HD22	23:DB:745:GLN:HG3	1.99	0.44
23:DB:371:LYS:HA	23:DB:371:LYS:HD3	1.87	0.44
23:DB:987:LEU:HD12	23:DB:987:LEU:HA	1.80	0.44
25:DE:650:THR:HG22	25:DE:666:THR:HG22	1.99	0.44
26:DF:114:LEU:HD12	26:DF:114:LEU:HA	1.77	0.44
25:De:270:ASP:OD1	25:De:271:GLN:NE2	2.41	0.44
35:EA:19:LYS:HD2	35:EA:19:LYS:HA	1.59	0.44
37:1:257:MET:HE3	43:7:579:VAL:HG13	1.98	0.44
38:2:201:LEU:HA	38:2:222:ILE:HD12	1.99	0.44
39:3:268:CYS:N	39:3:273:SER:O	2.46	0.44
42:6:504:LYS:NZ	42:6:653:GLU:O	2.42	0.44
43:7:70:LEU:HD12	43:7:70:LEU:HA	1.82	0.44
47:l:157:LYS:HD3	59:q:449:ASP:OD2	2.16	0.44
48:m:71:GLN:HA	57:n:166:TYR:CE2	2.29	0.44
49:a:357:LEU:HD12	49:a:359:HIS:HB3	2.00	0.44
56:k:88:LYS:C	56:k:88:LYS:CD	2.89	0.44
57:n:865:VAL:O	57:n:869:LEU:HG	2.16	0.44
58:o:765:ASP:OD2	67:w:72:SER:HA	2.17	0.44
59:q:116:LEU:HD22	59:q:116:LEU:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:311:LEU:HG	59:q:427:LEU:HD23	2.00	0.44
59:q:457:ASP:O	59:q:634:ASN:OD1	2.36	0.44
65:z:489:TYR:HA	65:z:492:ARG:HD2	1.99	0.44
66:x:529:MET:HE3	66:x:529:MET:HB3	1.78	0.44
67:w:326:THR:HA	67:w:329:LEU:HD13	1.99	0.44
67:w:339:ILE:HD11	67:w:378:GLN:HB3	1.99	0.44
67:w:589:LEU:HA	67:w:589:LEU:HD12	1.80	0.44
68:p:40:SER:HB3	68:p:89:TRP:CD2	2.53	0.44
69:X:-19:DG:H2"	69:X:-18:DT:H71	1.97	0.44
1:0:79:LEU:O	1:0:83:ASN:HB3	2.17	0.44
1:0:287:TYR:O	1:0:288:THR:C	2.58	0.44
3:9:85:MET:HB3	3:9:85:MET:HE3	1.34	0.44
3:9:208:THR:O	3:9:212:ILE:HG13	2.18	0.44
5:DP:295:MET:HE3	5:DP:302:LEU:HD13	1.98	0.44
5:DP:299:ARG:HH22	69:X:-26:DA:H5"	1.82	0.44
7:BA:27:TYR:CE2	11:PB:1078:ARG:HB3	2.52	0.44
9:FB:11:GLY:HA3	9:FB:106:LEU:O	2.17	0.44
10:PA:373:LEU:HD23	10:PA:373:LEU:HA	1.75	0.44
10:PA:731:ASN:HD22	10:PA:731:ASN:HA	1.51	0.44
10:PA:732:THR:O	10:PA:736:THR:HG23	2.17	0.44
10:PA:1087:VAL:HG12	10:PA:1400:LEU:HD22	2.00	0.44
11:PB:657:VAL:HG12	11:PB:658:ALA:H	1.82	0.44
11:PB:1122:CYS:HB2	11:PB:1170:ARG:HH12	1.82	0.44
15:PF:108:ARG:HH21	15:PF:123:LEU:HD21	1.81	0.44
16:PG:109:SER:O	16:PG:113:ILE:HG12	2.17	0.44
25:DE:458:LEU:O	26:DF:139:GLU:HA	2.16	0.44
25:DE:613:ALA:HB3	25:DE:616:HIS:HD2	1.83	0.44
28:DH:178:LYS:HD3	28:DH:178:LYS:HA	1.82	0.44
29:DI:35:VAL:HG12	29:DI:39:MET:HE2	1.99	0.44
37:1:167:SER:OG	37:1:317:ALA:O	2.35	0.44
39:3:51:MET:HB2	39:3:55:ASN:HD21	1.83	0.44
39:3:52:ASN:HA	40:4:45:PHE:HE1	1.82	0.44
40:4:365:ILE:HA	40:4:368:LEU:HD12	1.99	0.44
42:6:73:SER:HA	42:6:145:LYS:HG3	1.98	0.44
42:6:349:VAL:O	42:6:353:ALA:N	2.40	0.44
43:7:236:ALA:HB3	43:7:456:ILE:HG13	1.98	0.44
44:c:231:TRP:CD2	59:q:469:ASP:HB2	2.52	0.44
49:a:63:GLU:HG2	54:i:77:ASP:HB3	1.99	0.44
49:a:428:THR:HB	49:a:430:LEU:HD21	1.99	0.44
49:a:501:CYS:HB2	49:a:502:MET:H	1.56	0.44
50:d:100:VAL:HG13	54:i:128:LYS:HZ2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:d:156:SER:HB3	50:d:161:VAL:HG11	1.99	0.44
51:f:181:LEU:CD2	57:n:274:ILE:CD1	2.96	0.44
52:g:126:TYR:OH	63:u:78:SER:HA	2.16	0.44
53:h:18:GLN:HB3	53:h:60:ASN:ND2	2.33	0.44
54:i:118:LEU:C	54:i:118:LEU:CD2	2.91	0.44
57:n:443:LEU:HD12	57:n:500:LEU:HD22	1.99	0.44
58:o:764:PRO:HD3	67:w:20:GLU:HG3	1.99	0.44
59:q:9:ILE:CD1	63:u:90:LEU:CD2	2.36	0.44
59:q:89:GLN:OE1	59:q:90:PRO:HD2	2.16	0.44
62:t:197:PHE:HA	62:t:200:ILE:HD11	1.99	0.44
66:x:187:SER:O	66:x:190:THR:OG1	2.35	0.44
67:w:274:LEU:O	67:w:333:HIS:NE2	2.40	0.44
67:w:1090:CYS:SG	67:w:1091:ASP:N	2.87	0.44
1:0:99:LEU:H	1:0:99:LEU:HG	1.57	0.44
2:8:75:ILE:HD12	2:8:75:ILE:HA	1.83	0.44
5:DP:207:PRO:O	5:DP:207:PRO:CD	2.65	0.44
10:PA:32:LYS:HA	10:PA:87:HIS:CD2	2.52	0.44
10:PA:405:LEU:CD1	10:PA:448:ARG:HG3	2.46	0.44
10:PA:889:LEU:HB2	14:PE:203:TYR:HE1	1.83	0.44
10:PA:1174:ALA:O	10:PA:1212:LEU:HD12	2.18	0.44
10:PA:1662:PRO:HB3	51:f:15:TRP:HE1	1.82	0.44
11:PB:51:ILE:HG23	11:PB:93:LEU:HD13	1.98	0.44
11:PB:59:VAL:HG12	11:PB:408:PHE:CZ	2.52	0.44
11:PB:285:LEU:HD12	18:PI:16:PHE:HZ	1.83	0.44
11:PB:577:HIS:CE1	11:PB:579:ASP:C	2.96	0.44
11:PB:582:GLN:O	11:PB:583:LEU:C	2.60	0.44
11:PB:627:ILE:HD12	11:PB:660:GLY:O	2.16	0.44
11:PB:737:ILE:HD12	11:PB:737:ILE:HA	1.73	0.44
12:PC:24:GLU:HG2	12:PC:228:ARG:HD3	2.00	0.44
12:PC:103:LEU:HD13	12:PC:161:LEU:HD21	1.99	0.44
14:PE:67:ASP:HB3	14:PE:70:ASP:OD1	2.17	0.44
14:PE:100:THR:HG23	14:PE:126:ILE:N	2.31	0.44
20:PK:55:GLN:OE1	20:PK:81:TYR:HB2	2.18	0.44
20:PK:70:LYS:HB2	20:PK:70:LYS:HE3	1.83	0.44
26:DF:359:PHE:HB3	26:DF:380:LEU:CD2	2.46	0.44
28:DH:59:GLU:HA	28:DH:62:THR:HG22	1.99	0.44
29:DI:32:GLU:HB3	29:DI:35:VAL:HG23	2.00	0.44
37:1:461:LEU:O	37:1:464:LEU:HB2	2.18	0.44
40:4:370:THR:HG22	40:4:373:HIS:HE2	1.83	0.44
42:6:385:ASP:OD1	42:6:385:ASP:N	2.51	0.44
42:6:509:GLU:H	42:6:687:PHE:HE1	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:7:48:LYS:H	43:7:48:LYS:HG2	1.44	0.44
44:c:70:LEU:O	46:b:60:TYR:OH	2.36	0.44
44:c:292:LEU:C	44:c:306:HIS:CE1	2.96	0.44
45:e:53:GLU:OE2	46:b:187:GLY:O	2.35	0.44
55:j:39:GLN:HG3	61:s:151:GLY:O	2.18	0.44
55:j:105:PHE:CE2	55:j:109:LEU:HD12	2.50	0.44
59:q:491:ILE:HG23	59:q:506:HIS:HE1	1.81	0.44
59:q:577:ASP:OD1	59:q:577:ASP:N	2.51	0.44
59:q:648:PRO:O	59:q:649:CYS:C	2.58	0.44
60:r:180:ASP:C	60:r:182:VAL:H	2.25	0.44
62:t:173:PRO:CD	62:t:173:PRO:O	2.65	0.44
63:u:115:LEU:HA	63:u:118:ILE:HG22	2.00	0.44
66:x:577:ALA:O	66:x:581:ILE:HG13	2.18	0.44
6:DQ:348:LYS:NZ	6:DQ:375:GLU:CD	2.76	0.44
8:FA:42:TRP:O	9:FB:13:LYS:HD3	2.17	0.44
10:PA:393:ILE:H	10:PA:393:ILE:HG12	1.32	0.44
10:PA:1312:PRO:C	10:PA:1332:GLN:HE22	2.25	0.44
11:PB:108:MET:O	11:PB:109:MET:C	2.58	0.44
11:PB:289:ILE:H	11:PB:289:ILE:HG13	1.38	0.44
11:PB:584:MET:O	11:PB:587:LEU:N	2.50	0.44
13:PD:20:LEU:HG	13:PD:93:HIS:CD2	2.53	0.44
14:PE:21:CYS:HB3	14:PE:26:TYR:HB2	1.98	0.44
14:PE:63:ALA:HA	14:PE:71:GLN:HA	2.00	0.44
17:PH:57:ARG:HE	17:PH:148:LEU:HD11	1.83	0.44
18:PI:27:LYS:HE3	18:PI:27:LYS:HB2	1.78	0.44
26:DF:370:TRP:CZ3	26:DF:420:ALA:HA	2.53	0.44
26:DF:426:LEU:C	26:DF:426:LEU:HD23	2.42	0.44
29:DI:79:ALA:HA	29:DI:83:PHE:HD2	1.83	0.44
31:DL:111:LEU:C	31:DL:114:LYS:HE3	2.43	0.44
26:Df:105:TYR:O	30:Dj:217:PHE:N	2.51	0.44
36:EB:81:ILE:HG23	36:EB:102:ILE:HG21	1.99	0.44
37:1:304:ILE:O	37:1:308:ASN:ND2	2.50	0.44
40:4:314:ARG:NH2	40:4:346:VAL:H	2.15	0.44
43:7:441:SER:O	43:7:445:LYS:N	2.32	0.44
43:7:497:ARG:HH12	43:7:711:ASP:CG	2.26	0.44
45:e:45:VAL:O	45:e:48:LEU:HG	2.18	0.44
48:m:104:HIS:CE1	57:n:169:LEU:N	2.81	0.44
50:d:89:ILE:HG21	54:i:114:GLN:HG3	1.99	0.44
50:d:111:GLN:HE22	57:n:201:HIS:CE1	2.34	0.44
51:f:136:TYR:HA	51:f:149:PHE:CB	2.47	0.44
52:g:83:MET:HE3	52:g:83:MET:C	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:i:75:CYS:HB3	54:i:88:ASN:HD22	1.81	0.44
55:j:65:LEU:HB2	55:j:67:VAL:HG23	1.99	0.44
56:k:86:SER:CB	64:v:105:LEU:HD12	2.47	0.44
57:n:659:LEU:HD11	67:w:14:LYS:HG2	1.88	0.44
58:o:691:VAL:O	59:q:607:SER:CB	2.62	0.44
66:x:420:ILE:HA	66:x:423:THR:HG22	1.99	0.44
66:x:669:ILE:HG22	66:x:673:MET:HE2	1.99	0.44
66:x:989:LEU:HD22	66:x:989:LEU:HA	1.78	0.44
67:w:1183:TRP:CH2	67:w:1185:GLY:HA3	2.52	0.44
68:p:131:ILE:HD13	68:p:183:THR:HG22	1.99	0.44
2:8:297:ASN:HB3	2:8:299:PRO:HD2	2.00	0.44
4:DO:7:ARG:NH2	4:DO:37:LEU:HB3	2.33	0.44
6:DQ:51:MET:HE2	6:DQ:51:MET:HB2	1.81	0.44
8:FA:47:LEU:HG	8:FA:98:TRP:CE3	2.53	0.44
10:PA:390:PHE:CZ	10:PA:512:ARG:HD3	2.53	0.44
10:PA:734:ARG:NH1	18:PI:104:ALA:O	2.51	0.44
10:PA:912:SER:HA	10:PA:1326:GLY:O	2.18	0.44
10:PA:1048:THR:HA	10:PA:1053:ARG:NH1	2.32	0.44
10:PA:1052:ARG:HE	10:PA:1056:GLU:HG3	1.82	0.44
10:PA:1319:LYS:HE3	10:PA:1319:LYS:HB2	1.64	0.44
13:PD:67:TYR:O	13:PD:68:THR:C	2.58	0.44
14:PE:189:GLN:O	14:PE:209:VAL:HG12	2.16	0.44
22:DA:400:GLU:HG3	22:DA:401:ASN:N	2.32	0.44
25:DE:546:VAL:CG1	25:DE:560:SER:HB2	2.48	0.44
26:DF:122:LEU:H	26:DF:122:LEU:HG	1.37	0.44
26:Df:20:LYS:HB3	26:Df:20:LYS:HE2	1.83	0.44
38:2:106:ILE:HB	38:2:118:THR:HB	1.99	0.44
42:6:66:PRO:HB3	42:6:71:HIS:HA	1.99	0.44
42:6:113:VAL:HG23	42:6:115:GLU:HG2	2.00	0.44
42:6:442:GLU:HB3	42:6:444:HIS:NE2	2.33	0.44
44:c:41:ASN:HD22	44:c:41:ASN:C	2.24	0.44
49:a:86:ARG:H	49:a:86:ARG:HG3	1.55	0.44
49:a:321:LEU:HD21	49:a:407:ILE:CG1	2.48	0.44
49:a:408:LEU:HD23	49:a:408:LEU:HA	1.84	0.44
49:a:417:TYR:OH	49:a:450:PHE:CD1	2.70	0.44
51:f:181:LEU:HD13	57:n:273:PHE:HD2	1.83	0.44
52:g:68:HIS:HB2	52:g:77:GLU:OE1	2.17	0.44
55:j:109:LEU:CD2	63:u:59:ALA:HB2	2.37	0.44
55:j:114:SER:HA	55:j:121:MET:HG3	2.00	0.44
56:k:113:GLN:HA	56:k:116:GLU:OE1	2.17	0.44
59:q:32:PRO:HB2	59:q:34:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:w:370:ASP:OD1	67:w:370:ASP:N	2.49	0.44
2:8:141:ASN:C	2:8:143:LEU:H	2.24	0.44
7:BA:177:PHE:O	7:BA:181:CYS:N	2.38	0.44
8:FA:47:LEU:HD23	9:FB:7:LEU:HD13	2.00	0.44
10:PA:1036:ASN:HB3	14:PE:202:ARG:O	2.17	0.44
16:PG:15:PRO:HB3	16:PG:18:PHE:CE2	2.52	0.44
26:DF:28:ILE:HD11	29:DI:55:LYS:NZ	2.33	0.44
29:DI:20:ALA:HB2	29:DI:36:ILE:CD1	2.44	0.44
32:Dc:24:ASP:CB	30:Dj:192:LYS:HD2	2.48	0.44
25:De:542:HIS:CE1	25:De:568:ARG:HG3	2.53	0.44
31:Dl:113:VAL:O	31:Dl:113:VAL:HG22	2.18	0.44
34:Dm:103:LEU:O	34:Dm:107:ASN:ND2	2.51	0.44
39:3:64:ILE:HD13	39:3:124:ILE:HB	1.99	0.44
39:3:147:MET:HG3	39:3:157:MET:HE1	2.00	0.44
39:3:190:LEU:HD11	39:3:212:GLY:HA2	2.00	0.44
40:4:231:VAL:HG13	40:4:232:GLU:HG3	2.00	0.44
42:6:444:HIS:HB2	42:6:472:ARG:HD3	2.00	0.44
43:7:106:GLY:HA3	43:7:174:ILE:HD12	1.99	0.44
46:b:85:ASN:ND2	58:o:641:THR:HB	2.32	0.44
47:l:91:LYS:O	47:l:94:LEU:HG	2.18	0.44
47:l:167:ILE:HD12	64:v:127:LEU:CD2	2.47	0.44
49:a:465:VAL:HG22	49:a:479:LEU:HG	1.99	0.44
50:d:167:TRP:O	50:d:167:TRP:CE3	2.70	0.44
51:f:29:VAL:HG21	51:f:79:PHE:CD1	2.53	0.44
52:g:18:ILE:HG21	52:g:21:TYR:CD2	2.53	0.44
54:i:132:LEU:HD23	54:i:132:LEU:HA	1.84	0.44
55:j:11:HIS:HB3	55:j:15:PHE:CE2	2.47	0.44
56:k:79:HIS:CD2	60:r:41:GLY:HA2	2.53	0.44
57:n:141:ARG:NH1	63:u:17:ASP:CB	2.80	0.44
66:x:255:ASN:OD1	66:x:255:ASN:N	2.47	0.44
66:x:484:LYS:HA	66:x:484:LYS:HD3	1.48	0.44
67:w:19:GLU:HA	67:w:25:MET:HG3	1.99	0.44
69:X:-35:DG:C6	69:X:-34:DC:C4	3.06	0.44
2:8:209:ARG:HG3	51:f:53:GLN:HG2	1.99	0.44
6:DQ:366:ILE:HG22	6:DQ:367:PHE:N	2.33	0.44
7:BA:123:THR:O	7:BA:127:ARG:HG2	2.17	0.44
10:PA:416:ALA:HB1	10:PA:446:VAL:HG13	1.99	0.44
10:PA:890:ARG:HA	10:PA:890:ARG:HD2	1.70	0.44
10:PA:962:ASP:O	10:PA:963:ARG:C	2.61	0.44
10:PA:1414:ILE:HG22	10:PA:1419:VAL:HG13	2.00	0.44
11:PB:230:ARG:H	11:PB:230:ARG:HE	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:400:LEU:HD23	11:PB:400:LEU:HA	1.81	0.44
11:PB:595:ASP:HB2	11:PB:596:ILE:H	1.29	0.44
14:PE:11:TRP:HB2	14:PE:40:PHE:CG	2.52	0.44
14:PE:173:ILE:O	14:PE:209:VAL:HG23	2.18	0.44
17:PH:80:ASP:H	17:PH:81:ARG:HH11	1.65	0.44
22:DA:567:LEU:HD22	23:DB:745:GLN:NE2	2.30	0.44
22:DA:854:ARG:NH2	70:Y:-26:DC:O3'	2.51	0.44
25:DE:515:LEU:C	25:DE:517:ASP:H	2.25	0.44
26:DF:243:LEU:HD12	26:DF:243:LEU:HA	1.78	0.44
31:DL:93:GLU:O	31:DL:97:THR:CG2	2.51	0.44
32:Dc:101:VAL:HG22	26:Df:127:LEU:HA	2.00	0.44
26:Df:11:ASN:OD1	26:Df:48:LYS:NZ	2.51	0.44
37:1:188:LEU:N	37:1:191:ASP:HB3	2.31	0.44
38:2:66:ASP:HB2	38:2:171:PHE:HA	2.00	0.44
38:2:107:ILE:HG12	38:2:116:LYS:HG3	2.00	0.44
42:6:339:VAL:HG13	42:6:468:ALA:HA	2.00	0.44
43:7:533:ASP:HB2	43:7:616:ARG:HD3	2.00	0.44
45:e:79:GLN:O	45:e:82:GLN:HG2	2.18	0.44
51:f:53:GLN:HB3	51:f:54:ARG:H	1.57	0.44
51:f:184:LEU:HD22	57:n:299:PHE:HB2	1.99	0.44
53:h:5:GLU:C	53:h:5:GLU:CD	2.86	0.44
56:k:33:LEU:CA	56:k:36:SER:OG	2.63	0.44
56:k:34:GLU:HB3	59:q:153:LEU:HD22	1.99	0.44
57:n:202:ARG:O	57:n:206:THR:OG1	2.31	0.44
57:n:436:PRO:HG3	57:n:458:LEU:HD21	1.99	0.44
59:q:7:VAL:CG2	63:u:90:LEU:HD11	2.45	0.44
66:x:742:TYR:HA	66:x:782:VAL:HG11	1.99	0.44
67:w:236:ALA:HB2	67:w:663:PRO:HG3	2.00	0.44
70:Y:21:DC:H2"	70:Y:22:DC:C6	2.53	0.44
1:0:295:ARG:NH2	1:0:295:ARG:HG2	2.33	0.43
2:8:141:ASN:C	2:8:143:LEU:N	2.70	0.43
3:9:98:GLU:OE2	3:9:98:GLU:CA	2.66	0.43
10:PA:355:MET:H	10:PA:355:MET:HG2	1.51	0.43
10:PA:1288:ILE:HG23	10:PA:1292:MET:HE3	1.99	0.43
10:PA:1462:GLN:O	10:PA:1463:LEU:C	2.60	0.43
13:PD:37:VAL:O	13:PD:38:HIS:C	2.59	0.43
17:PH:17:PRO:HG3	17:PH:29:HIS:CE1	2.53	0.43
18:PI:36:LEU:HD23	18:PI:47:GLU:CA	2.47	0.43
28:DH:155:ASP:N	28:DH:155:ASP:OD1	2.51	0.43
31:DL:63:LEU:O	31:DL:67:VAL:HG13	2.18	0.43
25:De:718:ARG:HD3	25:De:718:ARG:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Di:73:LEU:HD13	31:Dl:105:HIS:NE2	2.32	0.43
37:1:304:ILE:HG23	43:7:569:ILE:HG21	2.00	0.43
39:3:206:ALA:HA	39:3:209:ILE:HD12	2.00	0.43
40:4:409:TYR:H	41:5:5:LEU:HA	1.82	0.43
43:7:95:GLU:OE2	43:7:101:LYS:HD3	2.18	0.43
43:7:240:ASP:OD1	43:7:240:ASP:N	2.48	0.43
45:e:133:LEU:HD23	45:e:133:LEU:HA	1.90	0.43
46:b:178:LEU:HD13	47:l:55:LEU:HD21	1.98	0.43
50:d:42:ARG:NH2	54:i:93:LYS:N	2.66	0.43
55:j:19:ILE:CD1	55:j:45:VAL:CG2	2.71	0.43
57:n:485:ASP:N	57:n:485:ASP:OD1	2.51	0.43
57:n:909:GLN:HB2	57:n:913:HIS:O	2.18	0.43
59:q:145:GLN:NE2	64:v:45:GLU:HB3	2.33	0.43
63:u:80:GLU:O	63:u:82:THR:HG23	2.17	0.43
64:v:133:GLU:C	64:v:133:GLU:CD	2.85	0.43
1:0:287:TYR:CZ	2:8:189:MET:SD	3.11	0.43
2:8:243:LEU:HD12	2:8:244:PRO:HD3	2.00	0.43
2:8:247:VAL:O	2:8:247:VAL:HG13	2.17	0.43
7:BA:18:HIS:NE2	7:BA:37:CYS:HB3	2.33	0.43
10:PA:70:ARG:HB3	10:PA:70:ARG:HH11	1.82	0.43
10:PA:94:VAL:HG11	10:PA:311:GLN:HA	2.00	0.43
10:PA:104:MET:HE2	10:PA:104:MET:HB2	1.87	0.43
10:PA:537:ILE:CG2	10:PA:541:THR:HB	2.48	0.43
11:PB:694:THR:HB	11:PB:695:HIS:ND1	2.33	0.43
11:PB:908:MET:HE2	11:PB:920:LYS:HB2	2.00	0.43
13:PD:140:PHE:HZ	64:v:64:ARG:NH2	2.16	0.43
14:PE:208:LEU:HG	14:PE:209:VAL:H	1.80	0.43
22:DA:592:SER:OG	22:DA:695:GLY:O	2.31	0.43
25:DE:507:VAL:CB	25:DE:513:LEU:HD11	2.48	0.43
27:DG:165:GLU:HA	27:DG:168:ARG:HD2	2.00	0.43
28:DH:57:SER:N	30:DJ:197:MET:SD	2.92	0.43
32:Dc:124:ILE:HD11	26:Df:133:ALA:HB1	2.00	0.43
25:De:774:MET:HE2	25:De:774:MET:HB2	1.91	0.43
36:EB:99:LEU:HD13	36:EB:124:LEU:HD11	2.00	0.43
37:1:275:LYS:HD3	43:7:210:HIS:CE1	2.53	0.43
37:1:530:GLN:HG3	37:1:534:ASN:ND2	2.33	0.43
49:a:109:TYR:CE2	49:a:154:LEU:HD23	2.52	0.43
54:i:65:PHE:CD1	54:i:99:LYS:HD3	2.30	0.43
57:n:482:VAL:HG13	57:n:489:ILE:HD11	2.00	0.43
60:r:3:ALA:O	60:r:4:PRO:C	2.59	0.43
62:t:11:VAL:HG11	62:t:17:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:v:131:GLU:CG	64:v:135:TYR:HE2	2.31	0.43
67:w:150:ASN:O	67:w:199:TRP:NE1	2.51	0.43
67:w:427:CYS:O	67:w:431:HIS:ND1	2.40	0.43
70:Y:18:DA:N1	70:Y:19:DC:C4	2.86	0.43
1:0:162:ARG:HA	1:0:165:ILE:HD12	2.00	0.43
1:0:297:LEU:O	1:0:298:GLN:C	2.61	0.43
2:8:192:VAL:O	2:8:192:VAL:CG1	2.66	0.43
2:8:245:ASP:OD1	2:8:245:ASP:N	2.51	0.43
9:FB:169:LYS:HE3	9:FB:169:LYS:HB3	1.63	0.43
10:PA:863:ARG:HH21	10:PA:1416:ARG:NH1	2.15	0.43
10:PA:872:MET:HE3	10:PA:872:MET:HB3	1.60	0.43
10:PA:960:ARG:O	10:PA:964:GLU:HG2	2.18	0.43
11:PB:214:LYS:H	11:PB:214:LYS:HG3	1.44	0.43
11:PB:564:ALA:CB	11:PB:578:LYS:HA	2.48	0.43
11:PB:634:LEU:O	11:PB:636:LYS:HG2	2.18	0.43
12:PC:19:VAL:CG2	12:PC:241:PRO:HB2	2.39	0.43
14:PE:35:GLN:HG3	14:PE:39:GLU:HB3	2.01	0.43
22:DA:1052:ARG:O	22:DA:1052:ARG:CG	2.67	0.43
23:DB:766:LEU:HA	23:DB:807:THR:HG21	2.00	0.43
24:DD:940:VAL:HA	24:DD:943:GLN:HB3	2.00	0.43
25:DE:294:ASN:HD22	25:DE:297:MET:HG2	1.83	0.43
31:DL:69:GLU:O	31:DL:70:VAL:C	2.61	0.43
26:Df:391:LEU:HD13	26:Df:391:LEU:HA	1.73	0.43
39:3:242:ILE:HD11	40:4:78:GLU:HB3	2.00	0.43
40:4:240:LEU:C	40:4:241:SER:HG	2.26	0.43
42:6:320:GLN:O	42:6:323:SER:OG	2.27	0.43
42:6:472:ARG:NH1	42:6:473:GLU:CG	2.81	0.43
43:7:102:LEU:HB3	43:7:103:PRO:CD	2.47	0.43
48:m:116:GLN:HB3	65:z:594:LEU:CG	2.49	0.43
48:m:117:GLN:HA	65:z:594:LEU:HD11	2.00	0.43
49:a:109:TYR:HE1	49:a:150:PHE:CZ	2.36	0.43
49:a:131:ASN:ND2	49:a:131:ASN:N	2.63	0.43
50:d:44:LEU:O	50:d:44:LEU:HD23	2.18	0.43
50:d:174:ARG:HD2	50:d:174:ARG:HA	1.70	0.43
54:i:104:MET:HE3	54:i:104:MET:HB3	1.84	0.43
55:j:39:GLN:C	55:j:43:PHE:HD2	2.25	0.43
55:j:96:LYS:NZ	61:s:80:SER:CA	2.80	0.43
57:n:793:HIS:CD2	57:n:794:LEU:HG	2.53	0.43
58:o:694:ASP:HB2	58:o:705:HIS:HB2	2.00	0.43
59:q:443:ARG:NE	59:q:443:ARG:CA	2.73	0.43
62:t:109:LYS:HB3	62:t:109:LYS:HE3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:t:145:GLY:N	62:t:146:PRO:HD2	2.33	0.43
67:w:758:LYS:HA	67:w:758:LYS:HD3	1.81	0.43
2:8:269:LEU:HD13	2:8:269:LEU:C	2.42	0.43
4:DO:63:ASN:HB3	4:DO:75:VAL:O	2.19	0.43
8:FA:25:LYS:HE2	9:FB:98:GLU:HB3	2.01	0.43
10:PA:792:ASN:HB2	10:PA:796:LYS:O	2.18	0.43
10:PA:807:LEU:HD23	10:PA:807:LEU:HA	1.84	0.43
10:PA:1040:LEU:HD12	10:PA:1040:LEU:HA	1.70	0.43
10:PA:1479:LYS:HD3	10:PA:1479:LYS:HA	1.93	0.43
11:PB:225:LEU:HB3	11:PB:349:PRO:HB2	2.01	0.43
13:PD:95:PHE:HA	16:PG:1:MET:CE	2.45	0.43
25:DE:449:LYS:HG2	28:DH:144:PRO:HB2	2.01	0.43
31:DL:102:LEU:CA	31:DL:105:HIS:HD2	2.32	0.43
37:1:130:ASP:OD2	37:1:461:LEU:HD12	2.18	0.43
40:4:309:VAL:HG23	40:4:314:ARG:HA	2.01	0.43
43:7:135:HIS:CE1	43:7:139:ALA:HB3	2.54	0.43
48:m:22:LEU:HD13	52:g:43:MET:HE3	1.99	0.43
50:d:115:LYS:HE2	50:d:115:LYS:O	2.19	0.43
50:d:183:ARG:HA	52:g:15:MET:HE2	2.00	0.43
54:i:88:ASN:C	54:i:88:ASN:OD1	2.62	0.43
54:i:89:ALA:O	54:i:93:LYS:HG3	2.19	0.43
57:n:808:LEU:O	57:n:821:SER:HA	2.19	0.43
59:q:119:VAL:CG1	59:q:127:LEU:HD13	2.48	0.43
66:x:269:MET:HE2	66:x:269:MET:HB2	1.76	0.43
66:x:956:VAL:CB	66:x:968:LEU:HD11	2.48	0.43
70:Y:32:DG:H2"	70:Y:33:DC:C6	2.53	0.43
2:8:139:LYS:HB3	2:8:139:LYS:NZ	2.33	0.43
2:8:185:PHE:HE2	2:8:237:TRP:CH2	2.37	0.43
2:8:282:ALA:O	2:8:283:ARG:C	2.59	0.43
3:9:64:LEU:HD22	3:9:105:MET:HG2	2.00	0.43
5:DP:169:VAL:HG23	5:DP:169:VAL:O	2.19	0.43
6:DQ:15:ARG:HH21	6:DQ:58:GLY:HA3	1.82	0.43
6:DQ:348:LYS:HZ2	6:DQ:375:GLU:CD	2.26	0.43
10:PA:147:LEU:HD13	10:PA:147:LEU:HA	1.79	0.43
10:PA:154:CYS:HB3	10:PA:185:GLY:C	2.43	0.43
10:PA:408:ARG:HE	60:r:7:THR:HG21	1.79	0.43
11:PB:193:VAL:HG21	11:PB:482:LEU:HA	2.01	0.43
11:PB:738:THR:O	19:PJ:62:TYR:HE2	2.02	0.43
14:PE:116:GLN:O	14:PE:120:ASP:N	2.52	0.43
23:DB:653:LEU:HG	23:DB:684:ILE:HG13	2.00	0.43
26:DF:14:LEU:HD21	29:DI:19:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Dk:179:MET:HB3	33:Dk:180:PRO:HD2	2.00	0.43
31:Dl:129:PRO:HB2	34:Dm:56:ILE:HG23	2.01	0.43
35:EA:73:LYS:O	35:EA:74:CYS:C	2.62	0.43
36:EB:140:LYS:N	36:EB:141:PRO:HD2	2.34	0.43
37:1:275:LYS:HD3	43:7:210:HIS:HE1	1.83	0.43
37:1:483:THR:N	37:1:484:PRO:CD	2.81	0.43
40:4:339:PRO:HB3	42:6:52:LYS:HD3	1.99	0.43
42:6:38:VAL:HB	42:6:156:ILE:HG12	2.00	0.43
42:6:363:VAL:HB	42:6:407:ILE:HA	2.00	0.43
43:7:252:THR:HG22	43:7:254:ARG:H	1.84	0.43
43:7:309:VAL:HG13	43:7:406:LEU:HD23	2.00	0.43
45:e:73:ILE:O	45:e:77:VAL:HG13	2.18	0.43
48:m:50:ASN:HD22	52:g:26:ILE:HG13	1.83	0.43
49:a:431:LYS:HA	49:a:431:LYS:HD3	1.70	0.43
52:g:92:LEU:HD23	52:g:92:LEU:HA	1.73	0.43
52:g:140:GLU:OE2	65:z:556:GLN:HG2	2.19	0.43
53:h:149:ASN:O	53:h:153:LYS:HG2	2.19	0.43
54:i:133:GLN:O	54:i:136:LYS:HB3	2.18	0.43
56:k:17:ILE:HG12	64:v:76:MET:HE1	2.00	0.43
56:k:31:VAL:CG2	59:q:157:ALA:HB2	2.36	0.43
57:n:857:GLU:O	57:n:861:LYS:HG2	2.19	0.43
58:o:706:LEU:HG	58:o:723:LEU:HB3	1.99	0.43
67:w:273:VAL:HG21	67:w:286:MET:HE1	2.00	0.43
67:w:1135:PRO:O	67:w:1136:LEU:HB2	2.17	0.43
68:p:56:GLN:O	68:p:59:THR:OG1	2.35	0.43
2:8:169:TYR:CG	2:8:190:TYR:CZ	3.06	0.43
4:DO:56:VAL:HG23	4:DO:57:ASN:N	2.32	0.43
10:PA:96:HIS:HB2	10:PA:250:VAL:HG23	2.00	0.43
10:PA:757:GLN:H	10:PA:757:GLN:HG2	1.61	0.43
11:PB:957:THR:HG23	11:PB:961:ILE:O	2.19	0.43
11:PB:1151:MET:HB2	11:PB:1151:MET:HE2	1.64	0.43
13:PD:57:LEU:HD23	13:PD:57:LEU:HA	1.81	0.43
16:PG:117:MET:HB3	16:PG:130:THR:HG22	1.99	0.43
17:PH:5:LEU:HD12	17:PH:5:LEU:HA	1.87	0.43
23:DB:594:SER:OG	23:DB:595:LYS:N	2.51	0.43
26:Df:149:PRO:HA	26:Df:150:PRO:HD3	1.82	0.43
37:1:166:ILE:CD1	37:1:169:ALA:HB3	2.48	0.43
38:2:337:GLU:HG3	38:2:353:LYS:HE3	1.99	0.43
38:2:363:CYS:HA	38:2:388:LYS:HE2	2.01	0.43
39:3:271:CYS:SG	39:3:284:THR:OG1	2.76	0.43
40:4:42:LEU:HD11	40:4:236:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:178:LEU:O	40:4:182:ALA:N	2.51	0.43
40:4:317:ALA:C	40:4:340:ASN:O	2.61	0.43
43:7:375:CYS:O	43:7:379:LEU:N	2.39	0.43
43:7:580:ALA:O	43:7:583:LYS:HB2	2.17	0.43
44:c:180:LEU:HD12	44:c:181:SER:H	1.84	0.43
46:b:99:ILE:HD13	46:b:99:ILE:HA	1.81	0.43
48:m:105:TRP:CE2	50:d:163:ALA:HA	2.53	0.43
48:m:121:GLU:HG2	65:z:592:ASN:ND2	2.34	0.43
49:a:111:GLU:OE2	49:a:111:GLU:O	2.37	0.43
49:a:229:SER:N	49:a:502:MET:CB	2.75	0.43
49:a:357:LEU:HD22	49:a:357:LEU:HA	1.77	0.43
49:a:462:LEU:HD13	66:x:14:TRP:CD2	2.54	0.43
49:a:468:ASP:OD1	49:a:468:ASP:O	2.36	0.43
50:d:72:ARG:HE	50:d:72:ARG:HB2	1.33	0.43
51:f:94:PRO:O	59:q:130:VAL:HG13	2.18	0.43
53:h:29:PHE:HD2	59:q:102:LEU:CD1	2.26	0.43
53:h:38:GLY:C	53:h:40:LEU:H	2.25	0.43
55:j:102:MET:CG	63:u:26:LEU:HD21	2.48	0.43
56:k:104:LEU:HD23	56:k:104:LEU:HA	1.75	0.43
57:n:232:ALA:HB1	57:n:247:LEU:HD11	2.00	0.43
57:n:541:LYS:HG3	57:n:549:TYR:CZ	2.54	0.43
57:n:870:GLN:CG	58:o:655:THR:CG2	2.96	0.43
59:q:203:ILE:O	59:q:203:ILE:HG13	2.18	0.43
66:x:561:LEU:O	66:x:608:ASN:ND2	2.51	0.43
67:w:68:HIS:CD2	67:w:114:LEU:HD11	2.54	0.43
67:w:316:GLU:OE2	67:w:366:ILE:N	2.49	0.43
70:Y:8:DA:H4'	70:Y:8:DA:OP1	2.18	0.43
1:0:295:ARG:CD	1:0:295:ARG:C	2.91	0.43
10:PA:403:GLN:HE21	60:r:17:ASN:CG	2.26	0.43
10:PA:441:GLN:HE21	10:PA:441:GLN:HB3	1.67	0.43
10:PA:957:GLU:O	10:PA:958:ARG:C	2.61	0.43
11:PB:357:CYS:C	11:PB:359:THR:N	2.76	0.43
11:PB:785:TYR:CZ	11:PB:955:PRO:HD3	2.54	0.43
12:PC:262:GLN:HE21	12:PC:262:GLN:HB3	1.52	0.43
21:PL:25:GLU:H	21:PL:25:GLU:HG3	1.56	0.43
27:DG:183:ILE:H	27:DG:183:ILE:HG13	1.40	0.43
26:Df:55:LEU:HD13	29:Di:28:ILE:HG12	2.01	0.43
31:Dl:139:TYR:HD2	34:Dm:73:MET:HE3	1.83	0.43
35:EA:51:LEU:HA	35:EA:51:LEU:HD12	1.82	0.43
37:1:404:PHE:O	37:1:408:ARG:NH1	2.52	0.43
38:2:261:SER:OG	38:2:265:GLN:OE1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:l:92:LEU:HA	47:l:95:VAL:HG22	2.00	0.43
49:a:103:ILE:HG23	49:a:108:PHE:HB2	1.99	0.43
49:a:231:LEU:O	49:a:241:ILE:HB	2.19	0.43
50:d:44:LEU:HD23	50:d:44:LEU:C	2.44	0.43
50:d:133:LYS:HB2	50:d:133:LYS:HE3	1.44	0.43
52:g:81:LEU:CD1	52:g:122:LEU:HD12	2.47	0.43
54:i:94:PHE:O	54:i:94:PHE:HD1	2.01	0.43
55:j:44:ILE:O	55:j:48:LEU:HG	2.19	0.43
57:n:259:THR:HG21	57:n:311:GLN:HE21	1.84	0.43
57:n:376:PRO:HD2	57:n:377:PRO:HD3	2.01	0.43
60:r:57:VAL:HG13	60:r:69:VAL:HG13	2.00	0.43
61:s:84:ILE:H	61:s:84:ILE:HG12	1.50	0.43
66:x:543:ASP:OD1	66:x:543:ASP:N	2.48	0.43
67:w:43:ALA:O	67:w:47:PHE:HD1	2.01	0.43
67:w:381:SER:O	67:w:534:HIS:ND1	2.48	0.43
68:p:194:LYS:HG3	68:p:198:GLN:HB3	2.00	0.43
1:0:280:PRO:HB2	1:0:281:GLN:OE1	2.19	0.43
2:8:266:ASP:HA	2:8:269:LEU:CB	2.49	0.43
3:9:3:HIS:C	3:9:5:SER:H	2.26	0.43
3:9:268:GLU:CD	3:9:268:GLU:N	2.74	0.43
7:BA:128:ILE:HA	9:FB:152:ASN:HD21	1.83	0.43
7:BA:179:GLU:HG3	9:FB:154:LYS:CD	2.48	0.43
7:BA:214:PHE:HA	7:BA:217:ARG:NH1	2.34	0.43
10:PA:1068:LEU:O	10:PA:1069:LEU:C	2.61	0.43
10:PA:1261:ILE:HD12	10:PA:1261:ILE:HA	1.80	0.43
15:PF:66:LEU:HD23	15:PF:66:LEU:HA	1.51	0.43
15:PF:107:ARG:HG3	15:PF:115:TYR:HB2	1.99	0.43
17:PH:148:LEU:O	17:PH:149:ALA:C	2.62	0.43
23:DB:298:ARG:HH11	23:DB:298:ARG:HD3	1.69	0.43
24:DD:1078:LEU:HD12	31:DL:90:ASP:OD2	2.18	0.43
24:DD:1084:LEU:HB3	29:DI:99:ARG:HH21	1.84	0.43
25:DE:377:LEU:HD21	25:DE:422:PRO:HG2	2.00	0.43
26:DF:28:ILE:HG13	29:DI:55:LYS:HD3	2.00	0.43
26:DF:50:ILE:O	26:DF:54:ALA:N	2.47	0.43
37:1:312:ALA:O	37:1:316:ALA:N	2.45	0.43
37:1:335:MET:O	37:1:337:GLY:N	2.51	0.43
38:2:318:LEU:H	38:2:318:LEU:HG	1.61	0.43
42:6:316:LEU:HD22	42:6:348:LEU:HD13	2.01	0.43
43:7:144:ALA:HB2	43:7:387:GLU:CD	2.44	0.43
43:7:250:ASN:HB2	43:7:432:ILE:HD11	2.00	0.43
43:7:536:VAL:HG22	43:7:596:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:b:64:ILE:HD13	46:b:64:ILE:HA	1.79	0.43
48:m:70:PRO:C	57:n:166:TYR:OH	2.62	0.43
50:d:45:ILE:CG1	54:i:73:ILE:CA	2.69	0.43
51:f:181:LEU:HD13	57:n:273:PHE:CD2	2.54	0.43
57:n:231:GLU:CB	57:n:253:LEU:CD2	2.96	0.43
58:o:625:VAL:HG23	58:o:634:PHE:HZ	1.84	0.43
58:o:715:LEU:CA	66:x:25:ILE:HG12	2.48	0.43
59:q:19:VAL:HG22	59:q:22:VAL:HG22	2.01	0.43
60:r:47:GLU:H	60:r:47:GLU:CD	2.26	0.43
61:s:84:ILE:HG22	61:s:93:TYR:CD2	2.53	0.43
63:u:28:GLN:CD	63:u:28:GLN:C	2.86	0.43
64:v:82:LEU:HA	64:v:82:LEU:HD23	1.75	0.43
67:w:470:ASN:N	67:w:470:ASN:OD1	2.52	0.43
68:p:145:LEU:HD22	68:p:359:LEU:HD21	2.00	0.43
2:8:17:PHE:C	2:8:17:PHE:CD1	2.96	0.43
2:8:71:HIS:HB3	2:8:74:ILE:HG13	2.00	0.43
2:8:274:GLY:O	2:8:275:LEU:C	2.61	0.43
6:DQ:351:PHE:CD1	6:DQ:351:PHE:N	2.87	0.43
7:BA:182:ALA:HB2	9:FB:153:TYR:O	2.18	0.43
8:FA:124:TYR:CE1	9:FB:22:LYS:CE	3.02	0.43
9:FB:51:ARG:CG	9:FB:52:THR:N	2.82	0.43
10:PA:192:ARG:O	10:PA:198:LEU:HA	2.19	0.43
10:PA:200:ALA:O	10:PA:213:LYS:HA	2.19	0.43
10:PA:331:LYS:HE3	10:PA:331:LYS:HB3	1.39	0.43
10:PA:1102:MET:CB	10:PA:1120:GLY:HA2	2.45	0.43
10:PA:1661:SER:O	52:g:11:LEU:HA	2.19	0.43
11:PB:34:PHE:CZ	11:PB:528:LEU:HB3	2.51	0.43
11:PB:953:ASP:HB2	11:PB:1032:PHE:CE1	2.54	0.43
14:PE:105:VAL:HG13	14:PE:135:LEU:HD12	2.00	0.43
15:PF:79:VAL:HB	15:PF:83:LEU:HD21	2.00	0.43
18:PI:69:ILE:O	18:PI:72:VAL:HG23	2.18	0.43
18:PI:72:VAL:O	18:PI:73:SER:C	2.60	0.43
21:PL:21:GLU:HB2	21:PL:41:TYR:CD1	2.53	0.43
23:DB:639:LYS:NZ	23:DB:641:GLU:OE2	2.43	0.43
25:DE:784:HIS:HB3	25:DE:792:LEU:HB2	2.00	0.43
28:DH:132:LYS:HA	28:DH:132:LYS:HD2	1.69	0.43
37:1:487:GLU:HA	37:1:490:VAL:HG12	2.00	0.43
39:3:98:ASP:HA	39:3:102:GLU:HB2	2.01	0.43
39:3:179:ASN:OD1	39:3:179:ASN:N	2.52	0.43
42:6:665:GLN:HA	42:6:670:MET:HE3	2.01	0.43
43:7:95:GLU:HG3	43:7:101:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:7:186:ARG:HB3	43:7:187:GLN:H	1.73	0.43
43:7:469:LYS:HD3	43:7:640:LEU:HD22	2.00	0.43
43:7:638:GLU:HA	43:7:641:ARG:HB2	2.01	0.43
43:7:672:THR:O	43:7:672:THR:HG22	2.18	0.43
48:m:116:GLN:HG2	65:z:595:PRO:CD	2.45	0.43
49:a:163:LEU:HD23	49:a:163:LEU:HA	1.88	0.43
49:a:455:GLN:CD	66:x:11:LEU:HD23	2.43	0.43
50:d:64:GLN:NE2	50:d:68:LEU:CD1	2.82	0.43
51:f:127:GLN:HE22	64:v:62:HIS:HD2	1.66	0.43
53:h:183:ALA:O	53:h:187:PHE:CD1	2.72	0.43
56:k:103:LYS:HA	56:k:103:LYS:HD3	1.70	0.43
58:o:759:ARG:O	58:o:762:GLN:HG3	2.19	0.43
59:q:437:HIS:O	59:q:437:HIS:CD2	2.71	0.43
59:q:633:ARG:NH2	59:q:633:ARG:CG	2.78	0.43
64:v:26:ILE:HD13	64:v:26:ILE:HA	1.70	0.43
66:x:177:LEU:HD23	66:x:177:LEU:HA	1.86	0.43
67:w:237:ILE:HG21	67:w:285:ASN:HB3	2.01	0.43
67:w:253:LYS:HD2	67:w:253:LYS:HA	1.80	0.43
2:8:162:PHE:CD1	2:8:162:PHE:N	2.86	0.43
5:DP:171:THR:HG21	69:X:-24:DA:O4'	2.18	0.43
5:DP:303:LEU:H	5:DP:303:LEU:HG	1.69	0.43
10:PA:1049:LEU:HD21	10:PA:1068:LEU:HD21	2.01	0.43
10:PA:1134:PRO:HG2	10:PA:1137:PRO:CB	2.49	0.43
10:PA:1170:THR:HA	10:PA:1216:LEU:HD23	2.00	0.43
10:PA:1242:ASP:O	10:PA:1262:MET:N	2.52	0.43
11:PB:286:GLU:H	11:PB:286:GLU:HG3	1.65	0.43
11:PB:767:LEU:H	11:PB:767:LEU:HG	1.66	0.43
11:PB:788:TYR:CZ	20:PK:66:PRO:HG3	2.53	0.43
12:PC:5:ASN:OD1	12:PC:5:ASN:N	2.52	0.43
14:PE:175:ALA:O	14:PE:180:ALA:HB3	2.19	0.43
15:PF:94:MET:HE3	15:PF:94:MET:HB2	1.72	0.43
15:PF:110:LEU:HB3	15:PF:111:PRO:HD2	2.01	0.43
22:DA:475:LEU:HD22	22:DA:475:LEU:HA	1.88	0.43
22:DA:690:LEU:HD22	22:DA:747:LEU:HD22	1.99	0.43
22:DA:727:THR:HG23	22:DA:727:THR:O	2.19	0.43
23:DB:831:GLU:OE1	23:DB:835:ARG:NH2	2.52	0.43
24:DD:937:ALA:HB2	29:DI:128:ARG:NH1	2.34	0.43
25:DE:460:SER:HB3	26:DF:135:TRP:CZ3	2.54	0.43
25:DE:754:THR:OG1	25:DE:755:ALA:N	2.43	0.43
26:DF:238:LYS:HB2	26:DF:238:LYS:HE2	1.93	0.43
31:DL:128:ILE:O	31:DL:128:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:254:PHE:HB2	39:3:263:GLU:HA	2.01	0.43
39:3:242:ILE:HG12	40:4:75:VAL:HG13	2.00	0.43
42:6:418:LYS:HB3	42:6:419:ARG:H	1.57	0.43
42:6:441:ASP:HA	42:6:466:LEU:HB2	2.01	0.43
42:6:472:ARG:CG	42:6:473:GLU:N	2.81	0.43
42:6:586:GLN:HA	42:6:589:ARG:HD2	2.01	0.43
43:7:320:PRO:O	43:7:322:SER:N	2.50	0.43
43:7:655:ASP:HA	43:7:658:ARG:HG2	2.00	0.43
44:c:245:HIS:HD2	44:c:295:THR:O	2.02	0.43
49:a:412:ARG:O	49:a:472:SER:HB2	2.18	0.43
50:d:156:SER:CB	50:d:161:VAL:CG1	2.96	0.43
51:f:127:GLN:NE2	64:v:62:HIS:HD2	2.17	0.43
53:h:23:LYS:NZ	53:h:23:LYS:CB	2.73	0.43
53:h:130:ARG:O	53:h:131:ILE:C	2.61	0.43
56:k:30:THR:HA	56:k:33:LEU:HD12	2.01	0.43
56:k:101:ARG:NH1	56:k:101:ARG:CG	2.73	0.43
57:n:509:ILE:HD11	57:n:516:SER:HB2	2.00	0.43
59:q:20:HIS:HB3	59:q:31:LEU:HB2	2.01	0.43
59:q:412:ALA:HB2	62:t:86:ILE:HG21	2.01	0.43
60:r:125:MET:HB3	60:r:125:MET:HE3	1.82	0.43
60:r:196:LEU:HD23	60:r:196:LEU:HA	1.77	0.43
63:u:81:SER:HB3	63:u:85:LEU:HG	1.99	0.43
1:0:21:LEU:HA	1:0:31:CYS:HA	2.00	0.42
1:0:203:ASP:O	1:0:207:GLN:HG2	2.18	0.42
1:0:264:GLU:HB2	1:0:269:LEU:HB2	2.01	0.42
3:9:85:MET:HE3	3:9:85:MET:C	2.44	0.42
7:BA:260:MET:HG3	7:BA:313:LEU:HD21	2.01	0.42
10:PA:392:GLU:O	10:PA:393:ILE:C	2.60	0.42
10:PA:866:LYS:O	10:PA:869:GLU:HB2	2.19	0.42
10:PA:1210:TRP:CZ3	18:PI:28:GLU:HB3	2.53	0.42
11:PB:547:GLU:H	11:PB:547:GLU:HG3	1.56	0.42
14:PE:12:LYS:O	14:PE:13:ILE:C	2.59	0.42
14:PE:100:THR:HG22	14:PE:101:ARG:HD2	2.01	0.42
16:PG:30:LEU:HD22	16:PG:72:TYR:CE2	2.54	0.42
22:DA:1007:LEU:HD22	22:DA:1012:VAL:HG21	2.01	0.42
28:DH:61:LEU:HD11	30:DJ:200:LEU:HD21	2.01	0.42
31:DL:62:LYS:HD3	31:DL:62:LYS:C	2.44	0.42
25:De:667:GLY:O	25:De:692:ARG:NH2	2.52	0.42
26:Df:320:ARG:HH11	26:Df:320:ARG:HB2	1.83	0.42
26:Df:393:LEU:HD23	26:Df:393:LEU:HA	1.86	0.42
34:Dm:68:MET:HE3	34:Dm:68:MET:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:EA:36:ILE:HA	35:EA:39:ARG:HD3	2.01	0.42
35:EA:39:ARG:H	35:EA:39:ARG:HG3	1.61	0.42
35:EA:67:LYS:HA	35:EA:67:LYS:HD3	1.38	0.42
36:EB:146:ARG:HB3	36:EB:173:GLU:HB3	2.00	0.42
38:2:173:SER:HB3	38:2:203:ALA:HB3	2.00	0.42
40:4:394:TRP:HE3	40:4:397:GLU:HB2	1.83	0.42
42:6:51:THR:OG1	42:6:52:LYS:N	2.49	0.42
42:6:582:GLY:HA2	42:6:610:VAL:HG21	2.01	0.42
43:7:233:PHE:HE2	43:7:454:VAL:HB	1.84	0.42
44:c:114:SER:O	44:c:117:LEU:HG	2.19	0.42
44:c:307:ASP:N	44:c:307:ASP:OD1	2.52	0.42
56:k:19:ARG:HG3	56:k:58:HIS:CD2	2.53	0.42
57:n:168:ARG:HD3	57:n:168:ARG:HA	1.77	0.42
57:n:237:MET:HB2	57:n:246:ARG:HD2	2.00	0.42
59:q:146:LEU:HD22	59:q:150:LYS:HG3	2.00	0.42
59:q:166:ARG:CG	59:q:166:ARG:NH1	2.79	0.42
62:t:134:SER:O	62:t:134:SER:OG	2.37	0.42
66:x:47:LEU:HD23	66:x:47:LEU:HA	1.82	0.42
66:x:61:LEU:HD23	66:x:61:LEU:HA	1.88	0.42
67:w:107:LEU:HD22	67:w:118:THR:HG21	2.01	0.42
70:Y:37:DC:H2"	70:Y:38:DT:C6	2.54	0.42
2:8:143:LEU:C	2:8:143:LEU:CD2	2.80	0.42
2:8:160:LYS:HG2	2:8:167:ARG:HH22	1.84	0.42
2:8:266:ASP:HA	2:8:269:LEU:HB2	2.01	0.42
5:DP:174:LEU:HA	5:DP:249:LYS:O	2.19	0.42
6:DQ:19:GLU:OE1	6:DQ:19:GLU:HA	2.20	0.42
10:PA:273:GLN:H	10:PA:273:GLN:HG3	1.61	0.42
10:PA:1218:ARG:O	10:PA:1222:THR:N	2.41	0.42
10:PA:1474:LEU:HD11	15:PF:107:ARG:CZ	2.49	0.42
11:PB:506:TRP:HZ2	11:PB:677:MET:HE1	1.83	0.42
11:PB:628:VAL:HG11	11:PB:683:GLN:HE22	1.84	0.42
11:PB:747:LEU:HD23	11:PB:810:PHE:CE1	2.54	0.42
14:PE:78:GLU:H	14:PE:78:GLU:CD	2.26	0.42
17:PH:10:PHE:CE2	17:PH:32:SER:HB3	2.53	0.42
25:DE:747:LEU:N	25:DE:747:LEU:HD13	2.34	0.42
26:DF:349:ASN:O	26:DF:350:ASN:C	2.62	0.42
28:DH:127:GLN:N	28:DH:128:PRO:HD2	2.34	0.42
24:Dd:1078:LEU:HD21	31:Dl:90:ASP:OD2	2.19	0.42
37:1:413:ALA:HA	37:1:416:PRO:HG3	2.01	0.42
37:1:535:LYS:HA	37:1:538:THR:HG22	2.00	0.42
40:4:28:PRO:O	40:4:32:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:656:ASN:OD1	42:6:656:ASN:N	2.47	0.42
45:e:132:HIS:CE1	47:l:163:LEU:HD11	2.54	0.42
49:a:107:MET:O	49:a:107:MET:SD	2.76	0.42
49:a:378:LYS:O	49:a:379:ASP:HB2	2.18	0.42
62:t:78:LEU:CD1	62:t:84:CYS:HB3	2.46	0.42
66:x:101:MET:HE1	66:x:131:LEU:HD11	2.01	0.42
67:w:727:TRP:HB2	67:w:732:LEU:HD13	2.02	0.42
67:w:952:LEU:HA	67:w:952:LEU:HD23	1.80	0.42
68:p:216:ALA:HA	68:p:229:ALA:O	2.19	0.42
70:Y:12:DG:N3	70:Y:12:DG:H2'	2.34	0.42
1:0:254:GLU:CD	1:0:254:GLU:O	2.62	0.42
2:8:164:SER:N	2:8:165:PRO:HD2	2.34	0.42
8:FA:121:ASN:O	9:FB:25:LYS:CE	2.66	0.42
11:PB:269:ILE:O	11:PB:270:ILE:C	2.61	0.42
11:PB:701:SER:HB2	11:PB:1001:PRO:HG2	2.00	0.42
11:PB:1125:MET:H	11:PB:1125:MET:HG2	1.54	0.42
12:PC:93:PHE:O	12:PC:94:CYS:HB3	2.18	0.42
16:PG:149:GLY:HA3	16:PG:160:ILE:HD12	2.01	0.42
19:PJ:30:THR:O	19:PJ:33:ASP:N	2.53	0.42
23:DB:539:ARG:HB2	23:DB:539:ARG:HH11	1.84	0.42
25:De:332:ILE:HA	25:De:336:HIS:HD2	1.84	0.42
26:Df:317:LEU:HG	26:Df:330:ARG:HE	1.83	0.42
35:EA:11:PRO:HD2	35:EA:14:LEU:H	1.84	0.42
37:1:203:VAL:HA	37:1:206:LYS:HD2	2.01	0.42
40:4:316:TYR:CZ	40:4:371:ARG:HD3	2.53	0.42
42:6:117:LYS:HE3	42:6:117:LYS:HB2	1.89	0.42
42:6:168:LEU:HD13	42:6:174:ARG:HD3	2.01	0.42
43:7:112:ARG:HD2	43:7:112:ARG:N	2.34	0.42
43:7:710:VAL:O	43:7:714:VAL:N	2.49	0.42
45:e:49:GLU:CD	46:b:186:THR:CG2	2.88	0.42
49:a:109:TYR:C	49:a:109:TYR:CD1	2.97	0.42
49:a:441:GLU:HG2	49:a:453:SER:OG	2.19	0.42
49:a:457:PRO:HB3	49:a:512:ARG:HD2	2.00	0.42
50:d:187:LEU:HB3	50:d:188:GLY:H	1.74	0.42
52:g:89:PHE:CE2	63:u:19:PHE:HD1	2.37	0.42
53:h:113:PRO:HB2	53:h:117:VAL:CG2	2.50	0.42
54:i:140:MET:HG3	54:i:141:PHE:N	2.34	0.42
56:k:109:ARG:NH1	56:k:109:ARG:HB2	2.34	0.42
59:q:569:ILE:HG22	59:q:582:VAL:HB	2.01	0.42
60:r:18:MET:SD	60:r:176:PRO:HA	2.60	0.42
60:r:141:MET:HA	60:r:173:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:t:79:PHE:C	62:t:80:GLU:HG3	2.44	0.42
62:t:85:LEU:HD23	62:t:85:LEU:HA	1.77	0.42
62:t:197:PHE:O	62:t:200:ILE:HG12	2.20	0.42
66:x:68:ILE:HD11	66:x:78:VAL:HG11	2.01	0.42
67:w:547:VAL:HG13	67:w:559:LEU:HD11	2.00	0.42
68:p:273:ARG:HD2	68:p:273:ARG:HA	1.83	0.42
2:8:67:GLN:HE22	3:9:157:HIS:HA	1.83	0.42
2:8:135:HIS:CD2	2:8:137:ASP:H	2.35	0.42
3:9:182:GLU:O	3:9:182:GLU:OE2	2.37	0.42
10:PA:216:LEU:HD22	10:PA:216:LEU:HA	1.90	0.42
10:PA:286:ILE:O	10:PA:289:GLN:HG3	2.18	0.42
10:PA:890:ARG:O	10:PA:891:TYR:C	2.62	0.42
11:PB:908:MET:HE2	11:PB:908:MET:HB3	1.41	0.42
12:PC:258:ASP:OD1	62:t:134:SER:HA	2.19	0.42
14:PE:19:GLN:O	14:PE:20:LEU:C	2.62	0.42
20:PK:49:GLN:O	20:PK:50:LEU:C	2.58	0.42
24:DD:890:GLY:HA3	31:DL:104:ARG:NH2	2.32	0.42
29:DI:23:LEU:HD22	29:DI:28:ILE:HD12	2.01	0.42
32:Dc:21:LEU:HD11	32:Dc:23:TRP:CD1	2.54	0.42
32:Dc:94:HIS:CD2	26:Df:122:LEU:HD22	2.54	0.42
30:Dj:149:PRO:O	30:Dj:153:ARG:NH1	2.46	0.42
35:EA:70:LYS:HE2	35:EA:70:LYS:HB2	1.34	0.42
40:4:58:ARG:O	40:4:62:LEU:N	2.52	0.42
40:4:185:MET:HG2	40:4:196:ILE:HD13	2.01	0.42
42:6:375:LYS:HE2	42:6:391:ARG:HH11	1.83	0.42
42:6:448:ALA:HA	42:6:451:PHE:HB2	2.02	0.42
44:c:296:TRP:HE1	44:c:298:ASP:HA	1.85	0.42
46:b:157:TYR:N	46:b:158:PRO:HD2	2.35	0.42
49:a:72:THR:HB	49:a:73:SER:H	1.63	0.42
49:a:305:LEU:HD22	49:a:305:LEU:HA	1.82	0.42
49:a:437:LEU:HD22	49:a:437:LEU:HA	1.67	0.42
55:j:17:GLU:HG2	55:j:20:ARG:HE	1.85	0.42
57:n:647:MET:HG2	57:n:651:ASN:HD21	1.85	0.42
59:q:102:LEU:HA	59:q:102:LEU:HD23	1.80	0.42
62:t:89:THR:C	62:t:91:PHE:N	2.74	0.42
63:u:15:LEU:CD1	63:u:18:GLN:OE1	2.67	0.42
2:8:13:GLU:OE2	2:8:15:LEU:HB2	2.19	0.42
3:9:107:THR:O	3:9:108:CYS:C	2.58	0.42
5:DP:268:ILE:HD12	5:DP:304:ILE:HG23	2.00	0.42
5:DP:283:TYR:HB2	5:DP:291:LEU:HD12	2.00	0.42
6:DQ:323:GLU:HG3	6:DQ:325:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BA:158:ALA:HA	7:BA:186:ILE:HG13	2.02	0.42
9:FB:25:LYS:O	9:FB:29:GLN:N	2.45	0.42
10:PA:21:VAL:HA	11:PB:1170:ARG:O	2.20	0.42
10:PA:377:GLN:HA	10:PA:473:ARG:O	2.20	0.42
10:PA:697:LYS:O	10:PA:700:GLN:HG3	2.19	0.42
10:PA:1434:GLU:O	10:PA:1438:VAL:HG22	2.19	0.42
11:PB:140:LEU:HD12	11:PB:140:LEU:HA	1.73	0.42
11:PB:1038:THR:HA	12:PC:195:THR:HA	2.01	0.42
16:PG:51:ILE:HG23	16:PG:72:TYR:CZ	2.55	0.42
17:PH:28:LEU:HD11	17:PH:50:VAL:HG11	2.01	0.42
17:PH:64:LEU:C	17:PH:84:ARG:HB3	2.45	0.42
22:DA:925:ASP:OD1	22:DA:925:ASP:N	2.52	0.42
23:DB:431:LEU:H	23:DB:431:LEU:CD2	2.32	0.42
26:DF:138:ILE:HG13	28:DH:159:TYR:CE2	2.46	0.42
28:DH:137:GLY:O	28:DH:138:GLN:C	2.62	0.42
42:6:58:ALA:HB1	42:6:75:PRO:HG3	2.00	0.42
42:6:92:VAL:HB	42:6:94:LYS:NZ	2.34	0.42
42:6:581:TYR:O	42:6:589:ARG:NH2	2.43	0.42
43:7:207:TYR:HD2	43:7:211:TYR:HB3	1.84	0.42
43:7:482:THR:O	43:7:695:ARG:NE	2.50	0.42
44:c:16:GLN:HB3	44:c:73:LEU:HD21	2.01	0.42
53:h:19:VAL:CG2	59:q:112:LEU:HD23	2.45	0.42
53:h:77:ILE:HD12	59:q:126:THR:HG21	1.97	0.42
54:i:65:PHE:CE1	54:i:99:LYS:HA	2.54	0.42
54:i:112:GLU:H	54:i:112:GLU:HG3	1.44	0.42
58:o:741:TRP:CZ3	66:x:107:ARG:HG2	2.54	0.42
62:t:21:VAL:HG22	62:t:138:ILE:HD11	2.01	0.42
64:v:39:THR:C	64:v:41:LYS:N	2.76	0.42
64:v:131:GLU:O	64:v:135:TYR:CD2	2.66	0.42
67:w:1046:ASP:N	67:w:1046:ASP:OD1	2.52	0.42
68:p:398:SER:O	68:p:400:GLN:N	2.51	0.42
69:X:-35:DG:H1	70:Y:36:DC:N4	2.18	0.42
1:0:255:THR:OG1	1:0:256:TYR:N	2.53	0.42
1:0:290:SER:O	1:0:291:LEU:C	2.63	0.42
2:8:235:GLU:O	2:8:236:GLN:C	2.63	0.42
2:8:279:ASN:C	2:8:281:CYS:N	2.74	0.42
7:BA:178:LYS:CB	9:FB:154:LYS:HB3	2.41	0.42
9:FB:27:LEU:HD11	9:FB:58:LEU:HD21	2.02	0.42
10:PA:191:ILE:HG22	10:PA:198:LEU:HB2	2.00	0.42
10:PA:238:MET:HE2	10:PA:238:MET:HB3	1.85	0.42
10:PA:489:THR:O	10:PA:493:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:516:GLN:O	10:PA:520:MET:HG3	2.19	0.42
12:PC:114:HIS:HB3	12:PC:149:LEU:HD11	2.00	0.42
14:PE:55:ARG:HB3	14:PE:55:ARG:HE	1.66	0.42
23:DB:839:MET:HE1	23:DB:843:LEU:HD13	2.00	0.42
25:De:378:LYS:HZ3	25:De:378:LYS:HG2	1.60	0.42
26:Df:447:ALA:CB	26:Df:456:GLY:HA3	2.49	0.42
29:Di:45:ARG:HG3	30:Dj:212:LYS:HB3	2.01	0.42
35:EA:31:ALA:HA	35:EA:34:LEU:HD12	2.00	0.42
37:1:187:ASN:CB	37:1:191:ASP:HB2	2.39	0.42
42:6:95:TYR:O	42:6:99:PHE:N	2.52	0.42
42:6:415:HIS:CD2	70:Y:-12:DT:C5'	2.88	0.42
42:6:547:LEU:HA	42:6:550:PHE:HB3	2.01	0.42
43:7:640:LEU:HG	43:7:647:ARG:HG3	2.02	0.42
45:e:99:ARG:HB2	47:l:34:CYS:SG	2.60	0.42
50:d:156:SER:HB2	50:d:161:VAL:HG11	2.01	0.42
52:g:124:ASN:HA	52:g:127:ARG:HD3	2.01	0.42
53:h:183:ALA:O	53:h:187:PHE:CE1	2.72	0.42
55:j:105:PHE:CD1	63:u:55:ALA:HB1	2.52	0.42
56:k:71:THR:HG21	64:v:15:LEU:HB2	2.02	0.42
56:k:106:ASP:HA	56:k:109:ARG:HE	1.85	0.42
58:o:715:LEU:HD13	66:x:21:TYR:O	2.20	0.42
58:o:763:LEU:HD11	58:o:775:THR:HG21	2.01	0.42
59:q:152:SER:HB2	64:v:58:ASN:CB	2.50	0.42
62:t:1:MET:HG2	62:t:186:PRO:HD3	2.01	0.42
62:t:122:PHE:CE2	62:t:156:LEU:HD11	2.55	0.42
66:x:269:MET:O	66:x:273:MET:HG2	2.19	0.42
66:x:591:ALA:HB1	66:x:597:LEU:HD23	2.00	0.42
66:x:821:TYR:HE2	66:x:946:PHE:HE2	1.67	0.42
67:w:10:GLU:OE1	67:w:10:GLU:N	2.53	0.42
1:0:187:LEU:HD12	42:6:185:ILE:HD13	2.02	0.42
3:9:175:LYS:CE	3:9:175:LYS:CA	2.86	0.42
5:DP:299:ARG:HH22	69:X:-26:DA:C5'	2.32	0.42
7:BA:18:HIS:CE1	7:BA:36:GLU:HG2	2.54	0.42
7:BA:27:TYR:HB3	7:BA:28:ARG:CZ	2.50	0.42
7:BA:179:GLU:HG3	9:FB:154:LYS:HD2	2.02	0.42
9:FB:158:ASN:HD22	9:FB:158:ASN:N	2.18	0.42
10:PA:382:ARG:NE	10:PA:478:PRO:HA	2.35	0.42
10:PA:787:VAL:HG12	10:PA:789:GLY:H	1.83	0.42
10:PA:860:ILE:HG22	10:PA:864:LEU:HD22	2.01	0.42
10:PA:878:THR:HA	10:PA:889:LEU:O	2.19	0.42
11:PB:475:PHE:CE2	11:PB:768:ARG:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:839:GLY:O	11:PB:840:MET:C	2.62	0.42
11:PB:986:GLN:OE1	11:PB:1011:ILE:HG21	2.18	0.42
11:PB:1114:TYR:HD2	11:PB:1116:VAL:CG1	2.32	0.42
11:PB:1142:ASN:ND2	11:PB:1145:GLN:HB2	2.26	0.42
16:PG:31:PHE:HA	16:PG:48:VAL:HG11	2.01	0.42
18:PI:121:HIS:CD2	18:PI:123:TRP:HB3	2.54	0.42
19:PJ:22:LEU:HD23	19:PJ:22:LEU:HA	1.72	0.42
23:DB:176:HIS:HE1	23:DB:310:ASP:H	1.68	0.42
29:DI:35:VAL:CG1	29:DI:39:MET:HE2	2.50	0.42
29:DI:81:GLN:HE21	29:DI:81:GLN:HB2	1.49	0.42
25:De:690:ASP:OD1	25:De:690:ASP:N	2.53	0.42
26:Df:402:ARG:HH22	26:Df:403:ILE:HD12	1.85	0.42
37:1:304:ILE:HA	43:7:569:ILE:HD13	2.01	0.42
37:1:400:ILE:HG21	39:3:122:SER:HB3	2.01	0.42
40:4:109:ILE:HG12	40:4:115:ARG:HH22	1.85	0.42
40:4:184:LEU:HA	40:4:199:ALA:HB3	2.02	0.42
40:4:360:THR:HB	40:4:363:GLN:HB2	2.01	0.42
42:6:74:ARG:HB3	42:6:87:GLU:CD	2.45	0.42
42:6:109:ARG:HA	42:6:109:ARG:HD3	1.77	0.42
42:6:305:ASP:OD1	42:6:305:ASP:N	2.52	0.42
43:7:497:ARG:HG2	43:7:709:THR:HA	2.01	0.42
43:7:543:GLN:O	43:7:547:SER:N	2.43	0.42
49:a:420:LEU:HD22	49:a:504:ILE:CG1	2.49	0.42
50:d:42:ARG:HH22	54:i:93:LYS:CG	2.32	0.42
50:d:45:ILE:HG12	54:i:73:ILE:CB	2.49	0.42
50:d:156:SER:CA	50:d:161:VAL:CG1	2.95	0.42
51:f:177:VAL:HG13	57:n:266:VAL:CG2	2.49	0.42
52:g:112:LEU:CA	61:s:69:ARG:HH22	2.32	0.42
57:n:587:LEU:CD1	67:w:15:THR:HG22	2.48	0.42
58:o:772:LEU:HA	58:o:775:THR:HG22	2.02	0.42
59:q:36:MET:SD	59:q:37:SER:N	2.92	0.42
65:z:529:HIS:NE2	65:z:580:ILE:HG21	2.34	0.42
66:x:53:GLY:O	66:x:90:ARG:NH1	2.51	0.42
69:X:-19:DG:C8	69:X:-18:DT:H73	2.54	0.42
69:X:-16:DG:H2"	69:X:-15:DG:H8	1.85	0.42
2:8:200:GLY:HA3	2:8:276:PHE:HE1	1.84	0.42
2:8:250:LYS:HB3	2:8:252:PHE:CZ	2.55	0.42
3:9:201:THR:C	3:9:203:ALA:N	2.78	0.42
6:DQ:369:LYS:HE2	6:DQ:369:LYS:HB3	1.71	0.42
7:BA:47:ASP:HA	11:PB:1075:MET:HE1	2.02	0.42
7:BA:118:PHE:HA	7:BA:121:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:FB:170:LYS:HE3	9:FB:170:LYS:HB3	1.54	0.42
9:FB:217:LEU:O	9:FB:220:ILE:HG13	2.20	0.42
10:PA:436:SER:CB	62:t:97:LYS:CD	2.98	0.42
10:PA:793:VAL:HG12	10:PA:798:ILE:HD13	2.02	0.42
10:PA:797:ARG:O	10:PA:798:ILE:C	2.62	0.42
11:PB:407:MET:HE2	11:PB:407:MET:HB2	1.66	0.42
11:PB:840:MET:HE3	11:PB:840:MET:HB3	1.69	0.42
11:PB:1000:THR:O	11:PB:1001:PRO:C	2.63	0.42
11:PB:1158:LEU:HD12	11:PB:1158:LEU:HA	1.89	0.42
16:PG:114:PRO:HA	16:PG:164:MET:SD	2.60	0.42
16:PG:146:LYS:HZ3	16:PG:148:VAL:HG12	1.84	0.42
17:PH:26:SER:HB2	17:PH:45:ILE:HD13	2.02	0.42
26:DF:404:ARG:HD3	26:DF:404:ARG:HA	1.87	0.42
35:EA:11:PRO:HB2	35:EA:12:ALA:H	1.72	0.42
35:EA:23:ARG:HE	35:EA:23:ARG:HB2	1.57	0.42
37:1:268:ASP:OD1	43:7:77:VAL:N	2.42	0.42
38:2:175:THR:HG23	43:7:592:ARG:HA	2.01	0.42
41:5:17:LYS:NZ	41:5:42:HIS:H	2.17	0.42
42:6:706:LYS:O	42:6:710:GLN:N	2.48	0.42
44:c:286:LYS:HE2	44:c:286:LYS:HB2	1.86	0.42
47:l:166:LEU:HD22	64:v:123:ILE:HD12	2.01	0.42
52:g:112:LEU:N	61:s:69:ARG:NH2	2.68	0.42
53:h:116:GLU:O	53:h:120:GLN:HG2	2.20	0.42
55:j:45:VAL:O	55:j:49:GLN:HG3	2.20	0.42
57:n:528:HIS:CE1	67:w:39:SER:HB3	2.55	0.42
57:n:751:ASN:OD1	57:n:752:LEU:N	2.52	0.42
59:q:348:SER:OG	59:q:350:ASN:OD1	2.37	0.42
59:q:523:ASP:HA	59:q:563:ILE:HD12	2.02	0.42
62:t:15:LYS:HB3	62:t:15:LYS:HE2	1.68	0.42
62:t:23:LEU:HA	62:t:23:LEU:HD22	1.84	0.42
66:x:466:ARG:NH2	66:x:512:ILE:O	2.53	0.42
67:w:442:LYS:HB3	67:w:442:LYS:HE2	1.88	0.42
2:8:37:ILE:H	2:8:37:ILE:CD1	2.32	0.42
2:8:102:ILE:O	2:8:102:ILE:CG2	2.67	0.42
2:8:267:ASP:HB2	2:8:294:TYR:HB2	2.01	0.42
9:FB:18:VAL:HG13	9:FB:108:GLY:HA3	2.01	0.42
10:PA:875:TYR:HA	10:PA:1083:PRO:HB3	2.01	0.42
10:PA:1042:ASN:HB3	10:PA:1046:ARG:HH22	1.84	0.42
11:PB:592:ARG:NE	11:PB:627:ILE:HD13	2.34	0.42
11:PB:988:LYS:HD2	11:PB:1015:LEU:HD11	2.01	0.42
14:PE:137:ILE:H	14:PE:137:ILE:HG13	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:PE:148:HIS:CE1	14:PE:179:VAL:HG11	2.55	0.42
16:PG:78:ARG:HG2	16:PG:80:PHE:HD2	1.84	0.42
22:DA:1169:ARG:CZ	22:DA:1181:ARG:HH11	2.32	0.42
23:DB:219:ASP:OD1	23:DB:219:ASP:N	2.52	0.42
23:DB:496:MET:HE3	23:DB:496:MET:HB2	1.84	0.42
23:DB:859:ARG:HA	23:DB:859:ARG:HD2	1.80	0.42
25:DE:589:TRP:HH2	26:DF:57:PHE:CE1	2.37	0.42
26:DF:320:ARG:H	26:DF:320:ARG:HG3	1.52	0.42
28:DH:87:GLN:HA	28:DH:88:PRO:HD3	1.82	0.42
26:Df:26:MET:HE3	26:Df:26:MET:HB3	1.77	0.42
26:Df:244:GLN:O	26:Df:248:THR:OG1	2.34	0.42
31:Dl:80:VAL:O	31:Dl:84:LEU:HG	2.19	0.42
38:2:16:GLU:OE2	42:6:101:VAL:HG11	2.19	0.42
40:4:27:SER:HB2	40:4:30:VAL:HG23	2.01	0.42
40:4:241:SER:C	40:4:242:PHE:CD1	2.98	0.42
40:4:364:ILE:HG21	40:4:387:ILE:HG23	2.01	0.42
42:6:71:HIS:CE1	42:6:95:TYR:HE2	2.38	0.42
43:7:70:LEU:HB3	43:7:204:VAL:HG22	2.02	0.42
43:7:198:SER:O	43:7:202:ALA:HB2	2.20	0.42
48:m:26:GLN:NE2	52:g:45:PHE:HD2	2.08	0.42
49:a:168:LYS:HE3	49:a:168:LYS:HB3	1.48	0.42
49:a:367:LEU:CD1	49:a:509:ARG:NH1	2.82	0.42
51:f:111:LEU:HD22	59:q:127:LEU:CD1	2.49	0.42
53:h:29:PHE:HD2	59:q:102:LEU:HD13	1.85	0.42
53:h:151:LEU:HG	64:v:37:ILE:HB	2.01	0.42
56:k:35:LEU:HD22	59:q:154:ALA:HB2	2.02	0.42
56:k:64:SER:HB2	56:k:68:ARG:NH2	2.35	0.42
57:n:382:ASP:O	57:n:386:VAL:HG22	2.20	0.42
57:n:435:LEU:HG	59:q:325:ILE:HD11	2.01	0.42
58:o:787:ALA:HB1	66:x:21:TYR:OH	2.18	0.42
62:t:204:GLN:CA	62:t:204:GLN:HE21	2.33	0.42
67:w:397:LYS:HB2	68:p:171:PHE:HE2	1.81	0.42
67:w:1221:ILE:HD12	67:w:1221:ILE:HA	1.90	0.42
4:DO:36:VAL:HG13	6:DQ:25:VAL:HG11	2.01	0.42
7:BA:259:TYR:HD1	7:BA:274:ILE:HD12	1.85	0.42
10:PA:244:ARG:HB3	10:PA:246:GLU:CD	2.45	0.42
10:PA:404:GLU:O	10:PA:405:LEU:C	2.61	0.42
10:PA:489:THR:HG21	10:PA:496:PHE:CZ	2.54	0.42
10:PA:1343:LEU:O	10:PA:1344:MET:C	2.60	0.42
11:PB:565:THR:CB	11:PB:610:ARG:HB3	2.50	0.42
11:PB:829:PHE:HE1	11:PB:869:LYS:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:PG:125:PRO:O	16:PG:126:PRO:C	2.61	0.42
17:PH:117:SER:HA	17:PH:122:LEU:HD23	2.02	0.42
26:DF:26:MET:HE2	29:DI:48:THR:HG22	2.02	0.42
28:DH:65:LEU:HD11	30:DJ:159:ALA:HB1	2.01	0.42
30:DJ:172:GLN:H	30:DJ:172:GLN:HG3	1.54	0.42
30:DJ:177:LYS:HB3	30:DJ:177:LYS:HE3	1.80	0.42
32:Dc:77:LEU:HD12	30:Dj:116:LEU:CD2	2.45	0.42
26:Df:432:ALA:HB1	26:Df:462:GLN:CB	2.50	0.42
33:Dk:179:MET:HB3	33:Dk:180:PRO:CD	2.49	0.42
37:1:398:GLN:HG3	37:1:402:ASN:HD21	1.85	0.42
38:2:360:CYS:HB3	38:2:364:GLN:H	1.85	0.42
40:4:245:LEU:HG	40:4:280:ARG:NE	2.27	0.42
40:4:245:LEU:HG	40:4:280:ARG:HB2	2.01	0.42
42:6:62:ARG:HG3	42:6:74:ARG:H	1.85	0.42
42:6:337:VAL:HG22	42:6:465:GLY:H	1.85	0.42
43:7:108:ALA:HA	43:7:206:VAL:O	2.20	0.42
43:7:420:PRO:HA	43:7:431:PRO:HA	2.02	0.42
44:c:291:GLY:O	44:c:306:HIS:HE1	2.03	0.42
49:a:221:ASN:HB3	49:a:254:ASN:ND2	2.35	0.42
53:h:74:GLN:CG	59:q:129:PRO:HB3	2.49	0.42
55:j:90:ALA:O	55:j:94:GLN:HG3	2.19	0.42
56:k:8:ASN:OD1	56:k:8:ASN:N	2.52	0.42
57:n:203:LEU:CD1	57:n:215:LEU:CD1	2.74	0.42
57:n:512:LEU:HD21	59:q:565:ASN:HD22	1.84	0.42
59:q:475:VAL:HG22	59:q:495:LEU:HB2	2.01	0.42
62:t:91:PHE:O	62:t:95:MET:HG2	2.20	0.42
66:x:794:ASP:HB3	66:x:797:LYS:HB2	2.02	0.42
67:w:297:CYS:HA	67:w:298:PRO:HD3	1.89	0.42
68:p:182:VAL:HG21	68:p:228:VAL:HG21	2.02	0.42
2:8:207:LEU:O	51:f:52:MET:HE1	2.20	0.41
3:9:3:HIS:C	3:9:5:SER:N	2.77	0.41
3:9:43:ASN:O	3:9:43:ASN:CG	2.62	0.41
3:9:52:GLU:HB3	3:9:273:LEU:CD1	2.42	0.41
5:DP:288:PHE:HE2	5:DP:305:PHE:HE1	1.68	0.41
5:DP:329:TYR:N	5:DP:330:PRO:HD2	2.35	0.41
7:BA:127:ARG:HH21	7:BA:127:ARG:HG2	1.78	0.41
7:BA:216:SER:HA	7:BA:229:GLN:NE2	2.35	0.41
8:FA:37:VAL:HG11	8:FA:42:TRP:CZ2	2.55	0.41
10:PA:436:SER:HB2	62:t:97:LYS:CD	2.50	0.41
10:PA:606:HIS:ND1	10:PA:641:CYS:HB3	2.35	0.41
10:PA:712:ASP:O	10:PA:713:VAL:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:775:LYS:HG2	11:PB:970:HIS:O	2.20	0.41
11:PB:108:MET:CE	11:PB:118:LEU:HB3	2.51	0.41
11:PB:153:PRO:HB3	11:PB:187:ILE:HD11	2.01	0.41
11:PB:423:ILE:HD12	11:PB:423:ILE:HA	1.72	0.41
11:PB:494:LYS:HA	11:PB:494:LYS:HD3	1.78	0.41
11:PB:712:PRO:HG2	11:PB:939:HIS:HE1	1.85	0.41
11:PB:816:GLU:HB2	11:PB:867:ILE:HD13	2.02	0.41
11:PB:847:LYS:O	11:PB:848:LEU:C	2.61	0.41
11:PB:1151:MET:HE3	11:PB:1151:MET:HB3	1.79	0.41
14:PE:54:ARG:C	14:PE:56:THR:H	2.28	0.41
14:PE:148:HIS:ND1	14:PE:179:VAL:HG11	2.35	0.41
23:DB:159:LEU:HD12	23:DB:177:VAL:CG1	2.51	0.41
23:DB:490:SER:O	23:DB:491:HIS:C	2.62	0.41
24:DD:940:VAL:HG12	25:DE:574:THR:HG21	2.01	0.41
25:DE:489:PHE:CZ	26:DF:129:VAL:HG11	2.55	0.41
26:DF:335:ARG:HE	26:DF:382:GLU:HB2	1.85	0.41
25:De:636:HIS:CD2	25:De:638:ASN:H	2.36	0.41
37:1:287:PRO:HG3	43:7:628:THR:HA	2.01	0.41
38:2:64:VAL:HB	38:2:169:ILE:HG12	2.02	0.41
38:2:85:LEU:HA	38:2:88:LEU:HD12	2.02	0.41
44:c:113:TRP:CZ2	46:b:175:HIS:CD2	3.06	0.41
45:e:129:VAL:CG1	56:k:114:MET:HE2	2.48	0.41
49:a:337:ALA:CB	49:a:338:PRO:CD	2.89	0.41
49:a:351:ASP:O	49:a:351:ASP:CG	2.63	0.41
50:d:45:ILE:HG22	54:i:76:MET:HB2	1.77	0.41
51:f:114:VAL:O	51:f:118:ARG:HG2	2.20	0.41
57:n:554:MET:HE3	57:n:554:MET:HB2	1.88	0.41
57:n:586:LEU:HD23	57:n:587:LEU:HD22	2.02	0.41
57:n:793:HIS:HD2	57:n:794:LEU:HG	1.85	0.41
59:q:487:ILE:HG21	59:q:543:VAL:HG21	2.00	0.41
62:t:61:LYS:HB2	62:t:62:LEU:H	1.69	0.41
64:v:35:GLU:OE2	64:v:64:ARG:NH2	2.53	0.41
67:w:18:ILE:HD13	67:w:18:ILE:C	2.45	0.41
67:w:37:LEU:O	67:w:41:LEU:HD13	2.19	0.41
67:w:916:ASP:OD1	67:w:916:ASP:N	2.53	0.41
67:w:1291:MET:H	67:w:1291:MET:HG2	1.64	0.41
2:8:185:PHE:HE2	2:8:237:TRP:HH2	1.68	0.41
5:DP:264:VAL:HG23	5:DP:266:PHE:H	1.84	0.41
5:DP:269:ARG:O	5:DP:335:PHE:HB3	2.20	0.41
8:FA:53:ASN:HB2	8:FA:96:GLN:OE1	2.19	0.41
9:FB:145:LEU:HB2	11:PB:94:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:344:LYS:HB3	10:PA:345:GLY:H	1.34	0.41
10:PA:403:GLN:NE2	60:r:17:ASN:OD1	2.47	0.41
10:PA:406:VAL:HG23	10:PA:429:LEU:CD1	2.50	0.41
10:PA:986:MET:O	10:PA:987:ILE:C	2.60	0.41
11:PB:403:LEU:HD12	11:PB:403:LEU:HA	1.70	0.41
14:PE:58:LEU:HB2	14:PE:76:PHE:CD1	2.54	0.41
18:PI:15:ARG:C	18:PI:24:LEU:HD12	2.46	0.41
22:DA:996:ARG:HH22	22:DA:1023:TRP:HA	1.84	0.41
25:DE:292:LYS:HA	25:DE:298:LEU:HD11	2.01	0.41
25:DE:369:LYS:HD3	25:DE:369:LYS:HA	1.74	0.41
25:DE:468:ASN:CG	26:DF:127:LEU:CB	2.94	0.41
26:Df:219:GLU:H	26:Df:219:GLU:CD	2.21	0.41
38:2:345:CYS:HB3	38:2:349:GLN:H	1.85	0.41
38:2:354:ASP:HB3	38:2:356:HIS:HD2	1.85	0.41
39:3:142:CYS:SG	39:3:143:TYR:N	2.93	0.41
39:3:193:ALA:O	39:3:215:LEU:N	2.53	0.41
39:3:227:LEU:HD12	39:3:231:PHE:HB2	2.01	0.41
40:4:18:ASN:OD1	40:4:19:LEU:N	2.52	0.41
40:4:255:SER:H	40:4:258:LEU:HB3	1.84	0.41
42:6:112:HIS:CD2	42:6:117:LYS:HA	2.55	0.41
42:6:122:SER:HB3	42:6:123:LEU:H	1.66	0.41
42:6:338:ILE:HG23	42:6:489:TYR:HB3	2.02	0.41
42:6:538:PRO:O	42:6:542:ARG:N	2.45	0.41
43:7:189:TRP:O	43:7:190:CYS:HB2	2.19	0.41
46:b:116:LEU:HD23	46:b:116:LEU:HA	1.80	0.41
48:m:17:ARG:HG2	52:g:21:TYR:CE1	2.56	0.41
49:a:374:TYR:CE2	49:a:440:PHE:CD2	3.04	0.41
50:d:96:LEU:HD12	50:d:96:LEU:HA	1.81	0.41
51:f:57:LEU:HD13	51:f:57:LEU:HA	1.78	0.41
52:g:83:MET:CA	52:g:83:MET:CE	2.98	0.41
53:h:102:HIS:H	53:h:102:HIS:HD2	1.58	0.41
57:n:573:VAL:HG21	57:n:583:ALA:HB1	2.02	0.41
57:n:676:ASP:OD2	59:q:581:SER:HB2	2.20	0.41
57:n:707:ASP:OD1	57:n:708:CYS:N	2.53	0.41
58:o:715:LEU:HD23	66:x:25:ILE:HD11	2.02	0.41
66:x:443:LEU:HD11	66:x:495:ILE:HD12	2.01	0.41
67:w:389:LEU:HA	67:w:392:PHE:HD2	1.84	0.41
67:w:684:ASN:HD22	67:w:723:THR:HG21	1.85	0.41
1:0:288:THR:O	1:0:289:SER:C	2.62	0.41
3:9:288:ASN:ND2	3:9:288:ASN:O	2.53	0.41
7:BA:178:LYS:HB3	9:FB:154:LYS:CB	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BA:286:ARG:NH1	7:BA:316:LEU:CD1	2.68	0.41
9:FB:23:VAL:HG13	9:FB:27:LEU:HD23	2.01	0.41
9:FB:123:ASN:HB3	9:FB:124:TYR:H	1.62	0.41
10:PA:23:PHE:CE1	11:PB:1169:PRO:HB3	2.55	0.41
10:PA:61:ARG:HG2	10:PA:72:GLN:HB2	2.00	0.41
10:PA:191:ILE:H	10:PA:191:ILE:HG12	1.51	0.41
10:PA:229:SER:O	10:PA:232:GLU:HG2	2.19	0.41
10:PA:341:GLN:O	10:PA:344:LYS:HB2	2.19	0.41
10:PA:696:SER:O	10:PA:697:LYS:C	2.62	0.41
10:PA:1205:ALA:O	10:PA:1206:ARG:HB2	2.20	0.41
10:PA:1442:ALA:HA	10:PA:1447:GLU:OE1	2.21	0.41
11:PB:826:GLU:O	11:PB:871:VAL:HA	2.20	0.41
11:PB:989:VAL:HG22	11:PB:1015:LEU:HB2	2.02	0.41
13:PD:80:ILE:HD13	13:PD:80:ILE:HA	1.86	0.41
15:PF:88:ASP:O	15:PF:89:PRO:C	2.63	0.41
17:PH:93:TYR:CG	17:PH:94:GLY:N	2.88	0.41
18:PI:42:CYS:SG	18:PI:43:ASP:N	2.94	0.41
20:PK:109:ILE:O	20:PK:110:LYS:C	2.64	0.41
22:DA:825:ILE:HD12	22:DA:830:ILE:HD11	2.01	0.41
22:DA:1021:SER:O	22:DA:1022:ARG:C	2.63	0.41
23:DB:158:GLY:CA	23:DB:188:PHE:HB3	2.49	0.41
23:DB:431:LEU:CD2	23:DB:431:LEU:N	2.82	0.41
26:DF:85:GLY:O	26:DF:86:PHE:HB3	2.20	0.41
26:DF:332:PHE:HA	26:DF:335:ARG:HD3	2.02	0.41
30:DJ:171:LEU:HD12	30:DJ:171:LEU:HA	1.84	0.41
31:DL:120:LEU:O	31:DL:125:ASN:N	2.52	0.41
25:De:504:LEU:HD22	25:De:575:PHE:HZ	1.85	0.41
31:Dl:59:THR:O	31:Dl:59:THR:OG1	2.36	0.41
37:1:461:LEU:HD21	37:1:504:LYS:HE3	2.03	0.41
39:3:165:LYS:HB3	39:3:195:VAL:HA	2.01	0.41
39:3:181:ILE:O	39:3:185:GLN:N	2.46	0.41
40:4:17:ARG:O	40:4:21:GLU:N	2.50	0.41
43:7:259:CYS:HA	43:7:262:ASN:ND2	2.35	0.41
44:c:245:HIS:CD2	44:c:295:THR:O	2.72	0.41
49:a:384:ASP:N	49:a:384:ASP:OD1	2.52	0.41
49:a:462:LEU:CD1	66:x:14:TRP:CD2	3.04	0.41
52:g:74:HIS:ND1	52:g:125:GLU:HB3	2.35	0.41
53:h:72:ARG:HH11	59:q:134:ALA:CB	2.32	0.41
56:k:87:ARG:NH1	56:k:87:ARG:CG	2.73	0.41
59:q:31:LEU:N	59:q:32:PRO:CD	2.82	0.41
59:q:375:LEU:CD2	59:q:431:ILE:CG1	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:r:19:MET:CE	60:r:177:ALA:HB1	2.39	0.41
63:u:4:ARG:HE	65:z:595:PRO:CA	2.33	0.41
64:v:35:GLU:HB3	64:v:64:ARG:HD2	2.02	0.41
65:z:485:ILE:H	65:z:485:ILE:HG13	1.67	0.41
66:x:273:MET:HE1	66:x:818:LEU:HB2	2.01	0.41
67:w:1183:TRP:HE1	67:w:1190:LEU:HD13	1.85	0.41
1:0:301:PHE:CE1	3:9:170:PHE:CE1	3.08	0.41
2:8:57:ARG:HE	2:8:57:ARG:HB2	1.63	0.41
2:8:151:LEU:C	2:8:151:LEU:CD2	2.93	0.41
2:8:261:PHE:CZ	2:8:272:ILE:HG21	2.55	0.41
2:8:276:PHE:N	2:8:276:PHE:CD1	2.87	0.41
2:8:293:LYS:HA	2:8:293:LYS:HD3	1.92	0.41
3:9:140:LEU:HD22	3:9:140:LEU:HA	1.74	0.41
3:9:186:ILE:H	3:9:186:ILE:CD1	2.05	0.41
7:BA:18:HIS:CE1	7:BA:36:GLU:CG	3.03	0.41
7:BA:280:VAL:C	70:Y:33:DC:OP2	2.63	0.41
10:PA:1098:PRO:HB2	10:PA:1386:ILE:CG2	2.51	0.41
10:PA:1177:TYR:HD2	10:PA:1210:TRP:CE3	2.38	0.41
11:PB:593:GLN:HE21	11:PB:593:GLN:HB2	1.51	0.41
11:PB:924:ARG:HH11	12:PC:62:GLU:HG3	1.84	0.41
12:PC:10:ARG:O	12:PC:11:ILE:C	2.62	0.41
12:PC:48:ASP:HB3	12:PC:166:LYS:HG3	2.03	0.41
15:PF:91:LEU:HD13	15:PF:91:LEU:HA	1.72	0.41
16:PG:49:THR:HG22	16:PG:73:LYS:O	2.20	0.41
17:PH:82:PRO:O	17:PH:83:SER:C	2.61	0.41
23:DB:669:LEU:HD23	23:DB:669:LEU:HA	1.92	0.41
26:DF:45:TYR:O	26:DF:49:GLU:N	2.46	0.41
26:Df:428:LEU:HD13	26:Df:458:LEU:CB	2.50	0.41
37:1:404:PHE:CZ	39:3:116:LYS:HG3	2.55	0.41
39:3:144:ILE:O	39:3:148:ASN:N	2.39	0.41
40:4:412:PHE:CE1	41:5:5:LEU:HD22	2.54	0.41
43:7:383:LEU:HD12	43:7:386:LEU:HD12	2.02	0.41
48:m:84:PHE:HB2	57:n:178:ILE:HD11	2.01	0.41
49:a:87:GLN:HE21	49:a:87:GLN:HB2	1.64	0.41
49:a:407:ILE:HD13	49:a:407:ILE:N	2.34	0.41
51:f:181:LEU:HD21	57:n:274:ILE:HG13	2.02	0.41
53:h:68:THR:HB	53:h:69:PRO:HD2	2.03	0.41
57:n:529:PRO:HG2	67:w:35:THR:HB	2.02	0.41
57:n:567:LYS:HG2	57:n:592:LYS:NZ	2.35	0.41
59:q:146:LEU:HD23	59:q:146:LEU:HA	1.86	0.41
59:q:160:LEU:HD23	59:q:160:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:q:613:ASN:O	59:q:616:SER:OG	2.37	0.41
60:r:148:ILE:H	60:r:148:ILE:HG13	1.65	0.41
64:v:45:GLU:CD	64:v:45:GLU:C	2.88	0.41
66:x:183:LEU:HD21	66:x:974:SER:HB3	2.03	0.41
67:w:10:GLU:HB3	67:w:14:LYS:CE	2.50	0.41
67:w:363:ARG:HD2	67:w:365:LEU:HD11	2.01	0.41
68:p:286:LEU:HD13	68:p:286:LEU:HA	1.92	0.41
68:p:444:VAL:HG22	68:p:452:LEU:HD11	2.02	0.41
2:8:110:THR:HB	2:8:113:HIS:ND1	2.35	0.41
3:9:27:ASN:OD1	3:9:27:ASN:C	2.63	0.41
7:BA:283:VAL:O	7:BA:287:GLN:HG2	2.20	0.41
7:BA:289:TYR:HA	7:BA:292:ILE:HG12	2.02	0.41
8:FA:48:GLU:CG	9:FB:5:GLY:HA3	2.50	0.41
10:PA:54:LEU:H	10:PA:54:LEU:HD12	1.85	0.41
10:PA:104:MET:H	10:PA:104:MET:HG3	1.65	0.41
10:PA:1054:MET:HE2	10:PA:1054:MET:HB2	1.66	0.41
10:PA:1176:TYR:CD1	18:PI:52:CYS:CB	3.03	0.41
10:PA:1183:SER:O	10:PA:1184:THR:C	2.63	0.41
11:PB:514:THR:HG23	11:PB:723:THR:HG21	2.01	0.41
11:PB:761:THR:HG23	11:PB:1001:PRO:HD3	2.01	0.41
12:PC:21:PHE:CD1	12:PC:21:PHE:N	2.89	0.41
12:PC:116:THR:HB	12:PC:147:ASP:HB3	2.02	0.41
12:PC:181:GLY:HA3	19:PJ:42:ARG:HH12	1.85	0.41
13:PD:37:VAL:HG12	13:PD:41:LEU:HG	2.03	0.41
14:PE:173:ILE:HG13	14:PE:177:ASP:OD2	2.20	0.41
15:PF:50:LYS:HB3	15:PF:50:LYS:HE2	1.69	0.41
18:PI:32:ASN:O	18:PI:33:ARG:C	2.64	0.41
22:DA:954:ALA:HA	27:DG:149:ARG:HH22	1.85	0.41
23:DB:100:GLN:O	23:DB:101:ARG:NH1	2.46	0.41
23:DB:562:GLY:O	23:DB:581:ILE:HG12	2.19	0.41
23:DB:713:TRP:NE1	23:DB:716:PRO:O	2.50	0.41
23:DB:749:LEU:HA	23:DB:752:THR:HG22	2.03	0.41
25:DE:452:ARG:O	25:DE:453:LEU:C	2.63	0.41
25:DE:645:GLY:N	25:DE:675:LEU:HD11	2.34	0.41
26:DF:209:LYS:CB	26:DF:210:PRO:HD2	2.51	0.41
27:DG:74:MET:HE1	27:DG:136:ILE:HD12	2.02	0.41
31:DL:61:LYS:HZ3	31:DL:61:LYS:C	2.22	0.41
36:EB:167:LEU:HG	36:EB:200:ILE:HB	2.01	0.41
37:1:125:PHE:O	37:1:129:LYS:N	2.52	0.41
37:1:497:LEU:HD21	37:1:501:GLN:NE2	2.35	0.41
39:3:224:LEU:O	39:3:228:LEU:CG	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:130:SER:C	40:4:131:ASP:CG	2.89	0.41
40:4:251:VAL:HA	40:4:254:MET:HB3	2.03	0.41
40:4:313:TYR:HA	40:4:345:GLN:HB3	2.02	0.41
40:4:328:ILE:C	40:4:331:PHE:H	2.28	0.41
43:7:233:PHE:HB2	43:7:456:ILE:HA	2.02	0.41
43:7:523:LEU:C	43:7:523:LEU:CD1	2.93	0.41
44:c:281:CYS:HB3	44:c:284:CYS:C	2.46	0.41
47:l:148:LYS:HE3	47:l:148:LYS:HB3	1.95	0.41
48:m:34:LEU:HD23	48:m:34:LEU:HA	1.95	0.41
49:a:463:VAL:HG11	49:a:488:ILE:HD12	2.02	0.41
50:d:149:ILE:HG22	52:g:56:ILE:HG12	2.01	0.41
52:g:175:LEU:HD21	54:i:132:LEU:CD1	2.43	0.41
55:j:65:LEU:C	55:j:67:VAL:N	2.77	0.41
56:k:63:LEU:HD12	56:k:63:LEU:HA	1.89	0.41
57:n:237:MET:CE	59:q:45:GLN:HG2	2.48	0.41
57:n:237:MET:HE2	59:q:45:GLN:CG	2.51	0.41
57:n:552:VAL:HG22	57:n:568:TYR:HD1	1.86	0.41
58:o:729:TYR:C	58:o:731:ALA:H	2.28	0.41
65:z:543:LEU:HD12	65:z:543:LEU:HA	1.88	0.41
67:w:247:THR:O	67:w:247:THR:OG1	2.39	0.41
67:w:356:LEU:HD21	67:w:372:LEU:HD11	2.02	0.41
69:X:-36:DG:N2	70:Y:36:DC:C4	2.89	0.41
69:X:3:DT:H3	70:Y:-3:DA:H61	1.68	0.41
70:Y:36:DC:H2”	70:Y:37:DC:C6	2.56	0.41
2:8:141:ASN:O	2:8:143:LEU:N	2.53	0.41
3:9:25:ASP:OD1	3:9:25:ASP:C	2.63	0.41
7:BA:189:LYS:HD2	69:X:-30:DT:C5’	2.28	0.41
10:PA:76:GLY:O	10:PA:77:ASN:C	2.62	0.41
10:PA:152:ASN:HB2	10:PA:190:ARG:NH1	2.36	0.41
10:PA:1228:MET:HE2	10:PA:1250:ASP:HB2	2.02	0.41
11:PB:97:THR:HG23	11:PB:106:SER:H	1.86	0.41
11:PB:379:ARG:H	11:PB:379:ARG:HG2	1.50	0.41
11:PB:797:ASN:O	11:PB:801:VAL:HG13	2.21	0.41
16:PG:131:MET:HG3	16:PG:132:ASP:N	2.36	0.41
17:PH:39:LEU:C	17:PH:40:ILE:HG12	2.45	0.41
22:DA:797:LYS:HB3	22:DA:797:LYS:HE2	1.90	0.41
24:DD:925:ASN:HD22	24:DD:925:ASN:HA	1.71	0.41
26:DF:40:THR:HA	26:DF:43:VAL:HG12	2.03	0.41
28:DH:117:MET:HB3	28:DH:118:VAL:H	1.74	0.41
36:EB:189:ILE:H	36:EB:189:ILE:HG13	1.64	0.41
37:1:472:LEU:HD21	37:1:496:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2:146:TYR:N	38:2:178:ASP:OD2	2.51	0.41
38:2:362:VAL:HG12	38:2:388:LYS:HE3	2.02	0.41
42:6:62:ARG:HH11	42:6:75:PRO:CG	2.33	0.41
42:6:74:ARG:O	42:6:95:TYR:OH	2.35	0.41
42:6:317:ARG:HB2	42:6:319:TYR:CE1	2.55	0.41
43:7:601:ARG:NH2	43:7:624:PRO:O	2.54	0.41
43:7:610:PHE:HB2	43:7:667:ALA:HA	2.03	0.41
49:a:317:PHE:CD1	49:a:317:PHE:C	2.98	0.41
49:a:348:LEU:HD12	49:a:348:LEU:HA	1.73	0.41
49:a:454:PHE:HE1	49:a:465:VAL:HG23	1.84	0.41
49:a:498:VAL:CG2	49:a:507:THR:HG22	2.51	0.41
50:d:108:GLN:HE22	57:n:205:THR:HA	1.85	0.41
50:d:121:LEU:CD1	63:u:115:LEU:HD12	2.51	0.41
51:f:16:VAL:CG1	51:f:104:VAL:HA	2.50	0.41
52:g:83:MET:CE	52:g:83:MET:HA	2.37	0.41
52:g:161:ILE:CG2	54:i:140:MET:SD	3.01	0.41
57:n:310:SER:O	57:n:313:LEU:HG	2.21	0.41
57:n:311:GLN:O	57:n:315:LEU:HG	2.20	0.41
57:n:794:LEU:HA	57:n:797:PHE:HB3	2.03	0.41
62:t:3:VAL:HG22	62:t:150:ALA:CB	2.50	0.41
66:x:717:LYS:HB2	66:x:717:LYS:HE3	1.87	0.41
1:0:184:LEU:HA	1:0:187:LEU:HD23	2.03	0.41
1:0:259:HIS:ND1	1:0:259:HIS:N	2.68	0.41
2:8:56:ASN:HD22	2:8:56:ASN:HA	1.67	0.41
4:DO:88:ILE:CD1	6:DQ:361:ASN:HB2	2.51	0.41
10:PA:436:SER:CA	62:t:97:LYS:HZ2	2.18	0.41
10:PA:713:VAL:HG11	10:PA:817:PRO:HD3	2.02	0.41
10:PA:864:LEU:O	10:PA:865:ILE:C	2.64	0.41
10:PA:913:ASN:CG	10:PA:1326:GLY:HA3	2.46	0.41
10:PA:1062:GLY:O	10:PA:1063:GLU:C	2.64	0.41
10:PA:1167:ARG:HE	10:PA:1167:ARG:HB3	1.44	0.41
11:PB:385:ARG:HE	11:PB:385:ARG:HB3	1.64	0.41
11:PB:1000:THR:HG22	11:PB:1003:ASN:HB2	2.01	0.41
11:PB:1068:GLN:HG3	11:PB:1073:GLN:O	2.21	0.41
13:PD:55:GLN:O	13:PD:56:GLU:C	2.63	0.41
22:DA:500:LEU:H	22:DA:500:LEU:HG	1.42	0.41
23:DB:203:LYS:HZ3	23:DB:235:HIS:HB3	1.86	0.41
23:DB:539:ARG:CD	41:5:32:LYS:HA	2.50	0.41
23:DB:835:ARG:CZ	28:DH:184:ARG:HH11	2.33	0.41
25:DE:306:VAL:HA	25:DE:338:TYR:HB3	2.03	0.41
25:DE:359:LEU:HD12	25:DE:359:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DE:564:ASP:OD1	25:DE:564:ASP:N	2.51	0.41
25:DE:651:VAL:HG21	25:DE:686:THR:HG21	2.01	0.41
26:DF:211:ARG:HG2	26:DF:211:ARG:HH11	1.85	0.41
35:EA:22:ILE:HA	35:EA:25:PHE:HB2	2.02	0.41
39:3:22:TRP:CD2	39:3:34:LEU:HD13	2.56	0.41
39:3:157:MET:HB2	39:3:157:MET:HE3	1.88	0.41
42:6:94:LYS:HG2	42:6:94:LYS:H	1.69	0.41
43:7:488:VAL:O	43:7:488:VAL:HG12	2.21	0.41
43:7:626:VAL:HG12	43:7:628:THR:H	1.86	0.41
44:c:311:GLN:NE2	57:n:715:ARG:HH12	2.18	0.41
49:a:462:LEU:HD23	66:x:11:LEU:HD11	0.50	0.41
50:d:115:LYS:O	50:d:115:LYS:HD3	2.20	0.41
50:d:152:ALA:HB1	57:n:152:PHE:O	2.21	0.41
51:f:50:VAL:HG11	51:f:56:THR:HB	2.03	0.41
51:f:114:VAL:HG12	51:f:115:ILE:N	2.36	0.41
52:g:119:VAL:O	52:g:123:ILE:HG23	2.20	0.41
52:g:140:GLU:HG2	63:u:93:LEU:HD21	2.01	0.41
56:k:31:VAL:HG23	59:q:157:ALA:CB	2.36	0.41
57:n:199:LEU:HD13	57:n:222:VAL:CG1	2.50	0.41
57:n:199:LEU:CD1	57:n:222:VAL:HG13	2.49	0.41
57:n:289:LEU:HD22	57:n:289:LEU:HA	1.54	0.41
57:n:553:GLU:OE2	57:n:569:TYR:OH	2.37	0.41
57:n:713:GLN:O	57:n:719:THR:HB	2.20	0.41
59:q:142:GLN:CD	59:q:142:GLN:N	2.78	0.41
59:q:290:HIS:CE1	59:q:294:LYS:NZ	2.82	0.41
64:v:116:LEU:HD23	64:v:116:LEU:HA	1.70	0.41
68:p:35:LEU:HD22	68:p:49:MET:HA	2.01	0.41
69:X:-33:DG:H2"	69:X:-32:DC:C6	2.56	0.41
69:X:-21:DG:H1	70:Y:21:DC:N4	2.16	0.41
1:0:145:GLU:HB2	53:h:3:ARG:NH1	2.35	0.41
1:0:254:GLU:OE2	1:0:254:GLU:N	2.29	0.41
1:0:295:ARG:O	1:0:296:ALA:C	2.61	0.41
5:DP:312:LEU:HD12	5:DP:312:LEU:N	2.35	0.41
6:DQ:11:PRO:O	6:DQ:15:ARG:HG2	2.21	0.41
10:PA:58:MET:O	10:PA:59:ASP:C	2.63	0.41
10:PA:267:GLN:HE22	11:PB:892:CYS:HA	1.85	0.41
10:PA:400:ASP:N	10:PA:400:ASP:OD1	2.53	0.41
10:PA:514:GLU:OE2	11:PB:1099:ALA:HB1	2.21	0.41
10:PA:602:CYS:SG	10:PA:604:ARG:HG2	2.61	0.41
10:PA:680:LEU:HD12	10:PA:680:LEU:HA	1.85	0.41
10:PA:1005:HIS:O	10:PA:1006:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PA:1184:THR:O	10:PA:1185:VAL:C	2.62	0.41
10:PA:1395:TYR:HA	10:PA:1398:LEU:HD12	2.03	0.41
11:PB:269:ILE:O	11:PB:272:VAL:HG12	2.20	0.41
11:PB:1084:LEU:H	11:PB:1084:LEU:HG	1.43	0.41
13:PD:137:LYS:CG	53:h:55:GLN:HB2	2.44	0.41
14:PE:16:THR:O	14:PE:17:ILE:C	2.62	0.41
17:PH:94:GLY:HA3	17:PH:118:TYR:HD1	1.83	0.41
18:PI:64:GLU:O	18:PI:65:LEU:C	2.64	0.41
22:DA:620:LEU:HD11	22:DA:766:ARG:HD3	2.02	0.41
22:DA:710:LYS:HD2	22:DA:710:LYS:HA	1.88	0.41
23:DB:77:ILE:HG12	23:DB:146:ILE:HG23	2.03	0.41
23:DB:417:ILE:HD13	23:DB:417:ILE:HA	1.94	0.41
23:DB:464:ILE:HG12	23:DB:513:LYS:HE2	2.03	0.41
24:DD:953:ILE:HG13	25:DE:518:LYS:HB2	2.03	0.41
26:DF:426:LEU:O	26:DF:429:LYS:HG2	2.21	0.41
28:DH:50:PHE:CD1	28:DH:50:PHE:N	2.88	0.41
28:DH:197:THR:HB	26:Df:238:LYS:HG2	2.02	0.41
29:DI:21:GLN:HE22	29:DI:24:LYS:HE2	1.84	0.41
24:Dd:1060:LEU:HD11	31:Dl:83:MET:HG3	2.02	0.41
36:EB:129:LYS:O	36:EB:140:LYS:HB2	2.21	0.41
38:2:27:SER:OG	38:2:28:GLY:N	2.53	0.41
38:2:162:HIS:HA	38:2:246:GLU:HB3	2.03	0.41
39:3:11:LEU:HB2	39:3:48:HIS:CE1	2.56	0.41
40:4:212:LEU:HD23	40:4:268:PHE:HD1	1.85	0.41
40:4:304:PRO:HG2	40:4:305:GLY:H	1.86	0.41
42:6:390:CYS:HB3	42:6:392:PHE:CE2	2.56	0.41
42:6:435:TRP:HD1	42:6:460:ALA:HA	1.85	0.41
43:7:275:GLU:OE1	43:7:279:GLN:NE2	2.54	0.41
48:m:116:GLN:CG	65:z:595:PRO:HD2	2.43	0.41
50:d:42:ARG:HH21	54:i:93:LYS:N	2.18	0.41
50:d:66:LEU:HD23	50:d:66:LEU:HA	1.89	0.41
55:j:17:GLU:HA	55:j:20:ARG:NE	2.36	0.41
55:j:110:ILE:HG21	55:j:128:ARG:HH21	1.81	0.41
56:k:33:LEU:HG	56:k:33:LEU:H	1.68	0.41
57:n:220:GLY:C	57:n:221:ARG:HG3	2.46	0.41
57:n:379:PRO:HB3	57:n:411:GLN:HE22	1.86	0.41
59:q:36:MET:O	59:q:39:ASN:N	2.54	0.41
59:q:633:ARG:CZ	59:q:633:ARG:CB	2.86	0.41
59:q:633:ARG:HD2	59:q:637:TYR:HE2	1.85	0.41
60:r:101:LEU:HD23	60:r:101:LEU:HA	1.79	0.41
63:u:11:ALA:C	63:u:69:ILE:HD11	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:v:115:LYS:HA	64:v:115:LYS:HD3	1.46	0.41
66:x:169:LEU:HD13	66:x:169:LEU:HA	1.91	0.41
66:x:305:TRP:O	66:x:309:THR:HG23	2.21	0.41
67:w:51:LEU:HB3	67:w:52:SER:H	1.80	0.41
67:w:213:ARG:HA	67:w:213:ARG:HD3	1.95	0.41
67:w:844:ASN:HA	67:w:847:ILE:HG22	2.02	0.41
70:Y:31:DG:H2"	70:Y:32:DG:H8	1.85	0.41
1:0:1:MET:H2	43:7:253:ARG:HH22	1.69	0.41
2:8:20:GLU:CD	2:8:20:GLU:N	2.79	0.41
2:8:48:ARG:HA	2:8:48:ARG:HD3	1.77	0.41
2:8:109:LEU:H	2:8:109:LEU:HG	1.43	0.41
3:9:111:LEU:O	3:9:115:VAL:HG12	2.21	0.41
3:9:145:GLU:H	3:9:145:GLU:HG2	1.51	0.41
4:DO:65:TYR:CD1	5:DP:191:GLU:HG2	2.46	0.41
7:BA:127:ARG:CG	7:BA:127:ARG:NH2	2.61	0.41
8:FA:176:ILE:O	8:FA:176:ILE:CG2	2.69	0.41
9:FB:123:ASN:H	9:FB:126:ARG:NH1	2.19	0.41
10:PA:70:ARG:H	10:PA:70:ARG:HG2	1.74	0.41
10:PA:236:LEU:HA	10:PA:236:LEU:HD12	1.75	0.41
10:PA:362:SER:HB2	11:PB:1084:LEU:HD12	2.02	0.41
10:PA:514:GLU:O	10:PA:515:ILE:C	2.62	0.41
10:PA:1034:GLN:HG3	10:PA:1035:GLU:N	2.35	0.41
10:PA:1309:MET:HG2	10:PA:1334:TRP:CE3	2.56	0.41
11:PB:68:GLN:CA	11:PB:83:ARG:HA	2.51	0.41
11:PB:275:ALA:O	11:PB:276:LEU:C	2.64	0.41
11:PB:590:LEU:O	11:PB:591:ARG:C	2.63	0.41
11:PB:834:ARG:HA	11:PB:840:MET:HG3	2.03	0.41
11:PB:856:PRO:HA	11:PB:904:VAL:CG2	2.51	0.41
12:PC:199:LYS:HB2	12:PC:202:GLU:OE1	2.20	0.41
14:PE:95:GLN:HA	14:PE:125:TYR:CZ	2.56	0.41
16:PG:116:GLU:HB2	16:PG:131:MET:HG2	2.02	0.41
17:PH:7:GLU:HG2	17:PH:8:ASP:N	2.36	0.41
17:PH:17:PRO:HG3	17:PH:29:HIS:NE2	2.36	0.41
17:PH:64:LEU:HD21	17:PH:144:LEU:HD21	2.03	0.41
20:PK:50:LEU:HD13	20:PK:75:VAL:HG22	2.03	0.41
22:DA:345:PRO:O	22:DA:346:ALA:HB3	2.21	0.41
25:DE:257:GLU:HG3	25:DE:286:THR:HB	2.02	0.41
25:DE:506:SER:HB2	25:DE:537:LYS:HZ1	1.84	0.41
26:DF:104:LEU:CB	30:DJ:217:PHE:HE2	2.12	0.41
26:DF:277:ALA:O	26:DF:278:LEU:C	2.64	0.41
26:DF:278:LEU:HD23	26:DF:278:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DF:392:ILE:O	26:DF:392:ILE:CG2	2.69	0.41
28:DH:33:ARG:HG2	30:DJ:134:VAL:HG13	2.02	0.41
33:Dk:130:PRO:HD3	34:Dm:35:GLU:HG2	2.02	0.41
33:Dk:165:VAL:O	33:Dk:169:ALA:N	2.47	0.41
37:1:349:VAL:HB	38:2:54:ARG:NH2	2.35	0.41
37:1:486:LEU:HD12	37:1:489:LYS:HE3	2.03	0.41
38:2:54:ARG:HB3	38:2:55:LEU:H	1.51	0.41
38:2:322:TYR:CZ	38:2:326:PHE:HB3	2.56	0.41
38:2:345:CYS:H	38:2:349:GLN:HA	1.86	0.41
40:4:306:PHE:CD2	40:4:375:VAL:HA	2.55	0.41
40:4:431:LEU:HA	40:4:442:VAL:HG13	2.03	0.41
42:6:133:THR:OG1	42:6:158:LEU:HB2	2.21	0.41
42:6:279:GLU:O	42:6:283:ARG:NE	2.51	0.41
42:6:562:ALA:HB3	42:6:568:LEU:HD22	2.02	0.41
43:7:105:LEU:HD21	43:7:198:SER:HB2	2.03	0.41
43:7:262:ASN:HA	43:7:265:THR:CB	2.50	0.41
43:7:523:LEU:HD12	43:7:523:LEU:O	2.21	0.41
45:e:133:LEU:HD12	56:k:115:LEU:CD1	2.51	0.41
46:b:101:ARG:NH2	57:n:944:PHE:CD2	2.89	0.41
48:m:21:GLU:OE1	52:g:36:PRO:HG3	2.21	0.41
48:m:59:LYS:CE	48:m:77:GLU:OE2	2.64	0.41
49:a:106:ASP:HA	49:a:127:HIS:HB3	2.03	0.41
49:a:229:SER:CA	49:a:502:MET:HB2	2.50	0.41
49:a:361:MET:HE2	49:a:378:LYS:HG2	2.03	0.41
49:a:402:GLY:O	49:a:405:PRO:HD2	2.20	0.41
49:a:445:LEU:N	49:a:445:LEU:HD23	2.36	0.41
50:d:99:GLU:HG2	50:d:103:ARG:NH1	2.36	0.41
50:d:126:TYR:CD1	50:d:126:TYR:C	2.98	0.41
53:h:32:LYS:NZ	53:h:40:LEU:HD11	2.36	0.41
53:h:50:ALA:O	53:h:51:LEU:C	2.62	0.41
53:h:80:VAL:HG23	59:q:124:PHE:HD1	1.86	0.41
53:h:173:PHE:CZ	60:r:198:HIS:HB2	2.56	0.41
55:j:58:LEU:C	55:j:59:HIS:CG	2.98	0.41
57:n:394:HIS:CD2	57:n:399:LYS:HD2	2.56	0.41
57:n:524:ASN:C	57:n:526:SER:H	2.29	0.41
57:n:678:PHE:CE1	59:q:583:ARG:HB2	2.55	0.41
57:n:689:PRO:O	57:n:690:CYS:HB2	2.21	0.41
57:n:731:LEU:HD12	57:n:800:VAL:HG11	2.03	0.41
59:q:183:PHE:CE2	59:q:226:LYS:NZ	2.89	0.41
60:r:94:GLY:H	60:r:98:ARG:HE	1.68	0.41
62:t:6:VAL:CG2	62:t:141:GLU:HB2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:u:18:GLN:OE1	63:u:62:ILE:HA	2.21	0.41
63:u:64:ARG:HG3	65:z:585:HIS:NE2	2.33	0.41
66:x:7:LYS:HB3	66:x:49:GLN:HE22	1.85	0.41
67:w:301:GLU:HG3	67:w:347:ALA:HB1	2.03	0.41
1:0:272:LEU:HD22	1:0:272:LEU:HA	1.78	0.41
5:DP:179:ASP:OD1	5:DP:179:ASP:C	2.62	0.41
5:DP:326:GLU:OE1	5:DP:326:GLU:HA	2.21	0.41
6:DQ:360:LEU:C	6:DQ:362:GLY:N	2.79	0.41
8:FA:24:LYS:HB3	8:FA:24:LYS:HE2	1.64	0.41
10:PA:123:ASN:HB3	10:PA:125:LYS:HG3	2.02	0.41
10:PA:129:ILE:HB	10:PA:143:HIS:CD2	2.56	0.41
11:PB:634:LEU:HD23	11:PB:634:LEU:HA	1.71	0.41
11:PB:665:ILE:HD11	11:PB:695:HIS:CE1	2.56	0.41
12:PC:117:SER:O	12:PC:118:ARG:C	2.59	0.41
12:PC:189:ASP:O	12:PC:191:ALA:N	2.52	0.41
12:PC:268:GLN:HE21	12:PC:268:GLN:HB2	1.68	0.41
13:PD:63:LYS:HE2	13:PD:63:LYS:HB2	1.91	0.41
14:PE:58:LEU:H	14:PE:58:LEU:HG	1.57	0.41
14:PE:84:ILE:CG2	14:PE:114:ALA:HA	2.49	0.41
16:PG:57:GLY:HA2	16:PG:67:LEU:O	2.20	0.41
18:PI:14:ILE:HG21	18:PI:16:PHE:CZ	2.56	0.41
20:PK:38:GLU:HB3	20:PK:39:ASP:H	1.72	0.41
22:DA:415:ILE:H	22:DA:415:ILE:HG13	1.56	0.41
23:DB:68:LYS:HE2	23:DB:68:LYS:HB3	1.98	0.41
26:DF:14:LEU:HD23	26:DF:14:LEU:HA	1.71	0.41
37:1:281:TYR:O	37:1:285:SER:OG	2.29	0.41
38:2:354:ASP:HB3	38:2:356:HIS:CD2	2.56	0.41
39:3:70:LEU:HB3	39:3:111:ILE:HD12	2.03	0.41
40:4:23:LEU:HG	40:4:31:LEU:HD22	2.02	0.41
40:4:385:PRO:HD2	40:4:386:THR:HG22	2.03	0.41
40:4:407:VAL:HG22	40:4:408:LEU:H	1.86	0.41
41:5:5:LEU:HD11	41:5:35:ILE:CD1	2.51	0.41
42:6:48:GLU:HB3	42:6:52:LYS:H	1.86	0.41
43:7:94:TYR:HA	43:7:97:GLN:HB2	2.02	0.41
43:7:170:LEU:HA	43:7:171:PRO:HD2	1.97	0.41
47:l:160:MET:CE	64:v:134:TYR:CD2	3.04	0.41
50:d:42:ARG:CZ	54:i:96:GLU:CD	2.94	0.41
50:d:79:LEU:HD12	50:d:79:LEU:HA	1.76	0.41
50:d:109:GLN:HA	50:d:112:LYS:NZ	2.32	0.41
51:f:190:PRO:HA	57:n:281:ARG:CG	2.51	0.41
52:g:28:GLU:OE2	52:g:30:LEU:CA	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:29:PHE:CD2	59:q:102:LEU:HD13	2.54	0.41
53:h:151:LEU:CG	64:v:37:ILE:HB	2.50	0.41
57:n:470:LEU:HD12	57:n:470:LEU:HA	1.93	0.41
57:n:524:ASN:O	57:n:525:TYR:HB3	2.21	0.41
61:s:157:GLY:O	61:s:158:PRO:C	2.63	0.41
67:w:8:ILE:HD11	67:w:47:PHE:CZ	2.56	0.41
1:0:73:GLU:HG2	1:0:74:ILE:N	2.35	0.40
1:0:148:GLU:OE1	53:h:3:ARG:CG	2.68	0.40
1:0:159:GLU:HA	1:0:162:ARG:HG2	2.02	0.40
3:9:186:ILE:HG12	3:9:187:LEU:H	1.86	0.40
3:9:239:LYS:N	3:9:239:LYS:HE3	2.36	0.40
3:9:285:LEU:O	3:9:286:ALA:HB3	2.21	0.40
6:DQ:329:PHE:O	6:DQ:329:PHE:HD1	2.04	0.40
7:BA:248:ARG:HH11	7:BA:284:THR:CG2	2.34	0.40
8:FA:173:HIS:HB3	22:DA:1008:ARG:NH2	2.35	0.40
9:FB:175:ARG:HA	9:FB:175:ARG:HD3	1.87	0.40
10:PA:436:SER:O	62:t:97:LYS:NZ	2.43	0.40
10:PA:525:ILE:O	10:PA:533:PRO:HA	2.21	0.40
10:PA:708:LYS:HA	10:PA:708:LYS:HD3	1.88	0.40
10:PA:1214:VAL:CG2	10:PA:1259:ILE:HD11	2.51	0.40
10:PA:1215:GLU:OE1	10:PA:1256:VAL:HG23	2.21	0.40
10:PA:1217:ASP:O	10:PA:1221:MET:HG2	2.22	0.40
10:PA:1452:LYS:HB2	10:PA:1452:LYS:HE3	1.76	0.40
10:PA:1796:SER:CB	59:q:24:LEU:HD22	2.47	0.40
11:PB:643:LEU:O	11:PB:646:ARG:HG3	2.21	0.40
12:PC:151:VAL:HG22	12:PC:152:LYS:O	2.21	0.40
19:PJ:25:LEU:HD23	19:PJ:29:TYR:O	2.21	0.40
22:DA:485:ILE:HD12	22:DA:485:ILE:HA	1.74	0.40
22:DA:725:CYS:SG	22:DA:734:LEU:HD12	2.61	0.40
24:DD:940:VAL:C	29:DI:123:THR:HB	2.46	0.40
24:DD:943:GLN:N	25:DE:510:ALA:HB2	2.36	0.40
27:DG:128:LYS:HE3	27:DG:128:LYS:HB3	1.99	0.40
29:DI:55:LYS:HA	29:DI:58:SER:HB2	2.03	0.40
31:DL:61:LYS:HA	31:DL:61:LYS:HD2	1.55	0.40
33:Dk:182:LEU:HD23	33:Dk:182:LEU:HA	1.84	0.40
38:2:27:SER:HA	38:2:31:LYS:HG2	2.02	0.40
38:2:156:LEU:HD23	38:2:194:ILE:HD12	2.04	0.40
39:3:12:VAL:HA	39:3:58:ALA:HB3	2.02	0.40
39:3:234:ASP:C	39:3:236:ASP:N	2.79	0.40
40:4:11:ARG:HG3	40:4:11:ARG:O	2.21	0.40
40:4:215:PHE:O	40:4:219:TYR:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:106:PRO:HB3	42:6:119:THR:HG21	2.03	0.40
43:7:307:ASN:ND2	43:7:310:LEU:HA	2.36	0.40
44:c:214:VAL:HG22	44:c:243:THR:HG23	2.03	0.40
49:a:161:TYR:C	49:a:163:LEU:H	2.27	0.40
49:a:463:VAL:HG11	49:a:488:ILE:CD1	2.51	0.40
52:g:44:MET:HE3	52:g:44:MET:HB3	1.91	0.40
53:h:151:LEU:HD11	64:v:37:ILE:C	2.45	0.40
55:j:85:LEU:O	55:j:89:LEU:HG	2.20	0.40
57:n:279:GLN:O	57:n:282:LEU:HG	2.21	0.40
57:n:297:HIS:HA	57:n:300:CYS:SG	2.61	0.40
57:n:528:HIS:NE2	67:w:39:SER:HB3	2.37	0.40
57:n:740:GLY:O	57:n:742:SER:N	2.53	0.40
57:n:743:ARG:HB3	57:n:805:TYR:CE2	2.56	0.40
57:n:903:CYS:HB3	57:n:904:PHE:H	1.67	0.40
58:o:715:LEU:HD22	66:x:21:TYR:HD1	1.87	0.40
61:s:80:SER:O	61:s:83:LEU:CD2	2.69	0.40
62:t:39:PHE:O	62:t:39:PHE:CG	2.71	0.40
63:u:80:GLU:CB	65:z:563:VAL:HG22	2.49	0.40
66:x:131:LEU:O	66:x:134:CYS:SG	2.79	0.40
66:x:956:VAL:HG21	66:x:985:ALA:HB1	2.03	0.40
67:w:11:GLU:O	67:w:15:THR:N	2.54	0.40
67:w:51:LEU:HD12	67:w:51:LEU:HA	1.90	0.40
67:w:707:ILE:HG23	67:w:713:LYS:HD3	2.03	0.40
70:Y:18:DA:C6	70:Y:19:DC:C4	3.09	0.40
1:0:148:GLU:CD	53:h:3:ARG:HB2	2.42	0.40
2:8:141:ASN:OD1	2:8:141:ASN:N	2.53	0.40
2:8:195:ASP:O	2:8:199:VAL:HG23	2.22	0.40
3:9:129:LEU:HD13	3:9:129:LEU:HA	1.92	0.40
3:9:203:ALA:O	3:9:204:TYR:C	2.63	0.40
3:9:243:THR:O	3:9:244:CYS:C	2.65	0.40
4:DO:6:TYR:CZ	4:DO:48:LEU:CD1	3.05	0.40
5:DP:193:ASN:HD22	5:DP:194:PRO:HD2	1.86	0.40
6:DQ:50:LEU:H	6:DQ:50:LEU:HG	1.70	0.40
10:PA:459:ASN:HA	10:PA:468:SER:O	2.21	0.40
10:PA:792:ASN:H	10:PA:792:ASN:HD22	1.68	0.40
10:PA:897:ALA:HB2	10:PA:1081:ALA:HA	2.02	0.40
11:PB:99:TRP:CZ3	11:PB:105:PRO:CB	2.98	0.40
11:PB:112:GLU:O	11:PB:113:ALA:C	2.62	0.40
11:PB:130:LYS:O	11:PB:141:GLN:HA	2.22	0.40
11:PB:473:LEU:HD22	11:PB:473:LEU:HA	1.85	0.40
11:PB:834:ARG:NH2	11:PB:840:MET:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:PD:48:ASN:HD22	13:PD:57:LEU:HD11	1.86	0.40
18:PI:17:CYS:HB3	18:PI:21:ASN:H	1.85	0.40
22:DA:1166:LYS:HD2	22:DA:1168:TYR:HE1	1.86	0.40
23:DB:560:TYR:CE2	23:DB:581:ILE:HD11	2.57	0.40
23:DB:684:ILE:HD13	23:DB:684:ILE:HA	1.94	0.40
26:DF:298:GLU:HA	26:DF:301:VAL:HG23	2.04	0.40
26:DF:374:TYR:CE1	26:DF:422:HIS:HB3	2.56	0.40
28:DH:50:PHE:CE1	30:DJ:195:LEU:HD13	2.56	0.40
25:De:504:LEU:HD23	25:De:504:LEU:HA	1.90	0.40
26:Df:254:GLN:O	26:Df:254:GLN:HG3	2.21	0.40
37:1:397:SER:HA	37:1:400:ILE:HD12	2.03	0.40
42:6:62:ARG:CZ	42:6:77:TRP:CH2	3.04	0.40
43:7:20:GLU:O	43:7:21:GLN:C	2.62	0.40
45:e:136:LEU:HD11	56:k:107:VAL:CG1	2.50	0.40
46:b:71:LEU:HD23	46:b:71:LEU:HA	1.88	0.40
46:b:164:ILE:O	46:b:168:ILE:HG12	2.21	0.40
48:m:116:GLN:CG	65:z:595:PRO:CD	2.99	0.40
48:m:124:GLN:NE2	65:z:590:ARG:HB2	2.35	0.40
49:a:211:LEU:HD11	49:a:220:MET:SD	2.61	0.40
51:f:181:LEU:CD1	57:n:270:GLN:HA	2.50	0.40
52:g:11:LEU:HA	52:g:11:LEU:HD13	1.80	0.40
53:h:18:GLN:HB3	53:h:60:ASN:HD21	1.86	0.40
53:h:191:LEU:HD23	53:h:191:LEU:HA	1.89	0.40
55:j:11:HIS:C	55:j:15:PHE:CD2	2.91	0.40
56:k:37:LYS:H	56:k:37:LYS:CD	2.27	0.40
57:n:138:SER:O	57:n:141:ARG:HG2	2.21	0.40
57:n:936:ILE:N	57:n:1197:GLY:O	2.49	0.40
58:o:689:PHE:CG	58:o:773:LEU:HD13	2.57	0.40
66:x:289:CYS:SG	66:x:313:ILE:HG13	2.61	0.40
66:x:671:GLU:HG2	66:x:687:PHE:CD1	2.56	0.40
1:0:126:GLN:HG2	1:0:127:LYS:HG2	2.03	0.40
1:0:268:ARG:H	1:0:268:ARG:HD3	1.87	0.40
3:9:85:MET:O	3:9:86:TYR:C	2.65	0.40
3:9:181:LEU:HD22	3:9:181:LEU:C	2.46	0.40
3:9:239:LYS:H	3:9:239:LYS:CE	2.33	0.40
7:BA:281:ALA:CB	70:Y:33:DC:C6	3.00	0.40
10:PA:265:VAL:HG22	10:PA:268:GLY:H	1.86	0.40
10:PA:421:ARG:NH2	10:PA:427:ILE:HD11	2.37	0.40
10:PA:551:ARG:HH12	17:PH:27:ARG:HH21	1.70	0.40
10:PA:811:ILE:HG23	11:PB:689:TYR:CE2	2.53	0.40
10:PA:1426:PRO:O	10:PA:1430:CYS:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:41:ARG:HE	11:PB:41:ARG:HA	1.86	0.40
11:PB:327:LYS:O	11:PB:328:PRO:C	2.65	0.40
12:PC:211:LEU:HD23	12:PC:211:LEU:HA	1.79	0.40
13:PD:115:ILE:C	13:PD:117:SER:N	2.78	0.40
14:PE:75:PHE:O	14:PE:77:PRO:HD3	2.22	0.40
23:DB:218:GLY:HA2	23:DB:238:LEU:HD13	2.03	0.40
23:DB:267:HIS:HB3	23:DB:277:LEU:HD11	2.03	0.40
23:DB:463:ARG:HD2	23:DB:515:ILE:HG22	2.03	0.40
23:DB:544:LEU:HD22	23:DB:625:LEU:HD22	2.02	0.40
26:DF:433:PRO:O	26:DF:437:LYS:N	2.33	0.40
29:DI:19:MET:CE	29:DI:40:LEU:HD23	2.51	0.40
26:Df:217:SER:H	26:Df:220:GLN:HE21	1.70	0.40
37:1:351:ARG:HG2	38:2:54:ARG:HG3	2.04	0.40
37:1:469:GLY:HA2	37:1:472:LEU:HD12	2.04	0.40
40:4:394:TRP:CE3	40:4:397:GLU:HB2	2.55	0.40
42:6:160:THR:HG21	42:6:291:LEU:HD22	2.03	0.40
42:6:186:GLN:H	42:6:186:GLN:HG3	1.59	0.40
42:6:363:VAL:O	42:6:408:SER:N	2.37	0.40
42:6:365:GLY:N	42:6:408:SER:O	2.40	0.40
42:6:442:GLU:HA	42:6:467:THR:HA	2.03	0.40
43:7:64:PRO:HB2	43:7:65:LEU:H	1.58	0.40
46:b:181:CYS:SG	47:l:82:LEU:CD2	3.10	0.40
48:m:56:LEU:CD2	48:m:80:GLN:HE21	2.23	0.40
50:d:181:GLU:HA	52:g:47:ASN:HD21	1.85	0.40
52:g:93:LEU:HB3	55:j:106:LYS:HD3	2.03	0.40
53:h:137:GLN:OE1	53:h:137:GLN:HA	2.20	0.40
54:i:110:SER:CB	54:i:111:PRO:CD	3.00	0.40
66:x:420:ILE:HA	66:x:420:ILE:HD13	1.91	0.40
66:x:901:LEU:HD23	66:x:901:LEU:HA	1.91	0.40
67:w:711:TRP:CD1	67:w:711:TRP:H	2.39	0.40
70:Y:3:DG:H2"	70:Y:4:DA:OP2	2.21	0.40
1:0:284:ALA:C	1:0:286:GLY:H	2.28	0.40
5:DP:173:ASN:CB	5:DP:218:LYS:NZ	2.84	0.40
5:DP:220:VAL:HG22	69:X:-24:DA:C2'	2.25	0.40
10:PA:1171:ALA:N	10:PA:1216:LEU:HA	2.36	0.40
10:PA:1184:THR:HG21	10:PA:1190:GLN:CD	2.46	0.40
10:PA:1405:MET:HB3	10:PA:1405:MET:HE3	1.86	0.40
10:PA:1482:TYR:O	10:PA:1483:GLY:C	2.64	0.40
11:PB:47:PHE:CE2	11:PB:51:ILE:HD11	2.56	0.40
11:PB:224:CYS:O	11:PB:350:HIS:HB3	2.21	0.40
11:PB:730:LYS:HE2	11:PB:730:LYS:HB3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:PB:787:GLY:C	11:PB:789:ASN:H	2.29	0.40
11:PB:1063:ALA:O	11:PB:1064:ARG:C	2.65	0.40
11:PB:1122:CYS:SG	11:PB:1140:CYS:SG	3.12	0.40
12:PC:6:GLN:N	12:PC:6:GLN:CD	2.70	0.40
12:PC:29:ALA:O	12:PC:30:VAL:C	2.60	0.40
12:PC:252:LEU:HB3	20:PK:98:LEU:HD13	2.03	0.40
16:PG:131:MET:HG3	16:PG:132:ASP:H	1.85	0.40
16:PG:158:PHE:CD2	35:EA:142:ASN:HB2	2.56	0.40
17:PH:24:ARG:H	17:PH:24:ARG:HG2	1.43	0.40
18:PI:34:ILE:HD13	18:PI:34:ILE:HA	1.83	0.40
18:PI:96:PHE:HD2	18:PI:110:LEU:HD21	1.84	0.40
20:PK:90:ALA:O	20:PK:91:ILE:C	2.61	0.40
22:DA:567:LEU:HA	23:DB:745:GLN:HE21	1.84	0.40
22:DA:797:LYS:HD3	70:Y:-16:DG:OP1	2.22	0.40
26:Df:104:LEU:HD22	30:Dj:216:TYR:HB2	2.02	0.40
37:1:235:LEU:HD12	37:1:236:ASN:HB2	2.03	0.40
39:3:223:LEU:O	39:3:223:LEU:HG	2.21	0.40
42:6:109:ARG:HH22	42:6:471:VAL:HG23	1.86	0.40
42:6:472:ARG:NH1	42:6:473:GLU:HG2	2.36	0.40
42:6:563:ASP:HA	42:6:627:SER:HB2	2.02	0.40
43:7:18:TYR:O	43:7:19:PRO:C	2.65	0.40
43:7:52:LEU:HD23	43:7:52:LEU:HA	1.93	0.40
43:7:268:LYS:HB3	43:7:272:ARG:HH21	1.87	0.40
43:7:651:PHE:O	43:7:654:PHE:N	2.54	0.40
44:c:210:ASP:OD2	59:q:465:SER:OG	2.34	0.40
45:e:49:GLU:CG	46:b:186:THR:HG21	2.51	0.40
49:a:364:TYR:HE1	49:a:437:LEU:HD11	1.87	0.40
49:a:424:CYS:CA	49:a:505:PRO:HG3	2.48	0.40
50:d:128:ALA:CB	63:u:108:VAL:CG2	2.86	0.40
50:d:164:PRO:CD	50:d:167:TRP:HB2	2.45	0.40
52:g:95:ILE:HG21	52:g:105:ARG:HB2	2.02	0.40
53:h:109:LEU:HD23	53:h:109:LEU:HA	1.93	0.40
56:k:88:LYS:HZ3	59:q:303:LEU:CD2	2.35	0.40
56:k:106:ASP:HA	56:k:109:ARG:NE	2.36	0.40
57:n:838:VAL:O	57:n:838:VAL:HG23	2.21	0.40
59:q:139:GLN:C	59:q:139:GLN:CD	2.89	0.40
60:r:68:PHE:CZ	62:t:98:LEU:HG	2.57	0.40
63:u:82:THR:H	63:u:86:GLN:HE21	1.69	0.40
64:v:41:LYS:HE2	64:v:41:LYS:HB3	1.79	0.40
66:x:491:LEU:O	66:x:495:ILE:HG12	2.22	0.40
67:w:80:TYR:CD1	67:w:121:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:p:388:ASP:N	68:p:388:ASP:OD1	2.52	0.40
70:Y:35:DC:C2	70:Y:36:DC:H5	2.38	0.40
1:0:210:MET:O	1:0:211:GLN:C	2.64	0.40
1:0:287:TYR:CG	2:8:189:MET:HG2	2.56	0.40
1:0:294:HIS:O	1:0:295:ARG:C	2.62	0.40
2:8:134:LEU:O	2:8:159:ALA:HB1	2.22	0.40
2:8:148:ASN:N	2:8:148:ASN:OD1	2.53	0.40
7:BA:18:HIS:CE1	7:BA:36:GLU:HB2	2.57	0.40
9:FB:229:HIS:CE1	70:Y:13:DC:H1'	2.55	0.40
10:PA:565:MET:HE1	20:PK:74:ARG:H	1.85	0.40
10:PA:778:LYS:HD3	10:PA:778:LYS:HA	1.89	0.40
10:PA:1486:ILE:N	10:PA:1487:PRO:HD2	2.29	0.40
11:PB:788:TYR:OH	20:PK:66:PRO:HD2	2.21	0.40
11:PB:1037:ILE:HG22	11:PB:1039:SER:O	2.21	0.40
13:PD:77:ARG:O	13:PD:78:GLU:C	2.61	0.40
13:PD:90:LYS:O	13:PD:91:LYS:C	2.62	0.40
13:PD:104:CYS:O	13:PD:104:CYS:SG	2.79	0.40
18:PI:16:PHE:O	18:PI:17:CYS:C	2.63	0.40
22:DA:939:ILE:HG22	22:DA:943:LYS:NZ	2.37	0.40
23:DB:159:LEU:HD23	23:DB:159:LEU:N	2.37	0.40
26:DF:105:TYR:O	30:DJ:217:PHE:CD1	2.70	0.40
28:DH:194:MET:HE2	28:DH:194:MET:HB2	1.85	0.40
31:DL:82:GLU:O	31:DL:86:GLN:HG3	2.22	0.40
31:DL:120:LEU:HD23	31:DL:126:MET:HG3	2.03	0.40
25:De:298:LEU:HD12	25:De:298:LEU:HA	1.98	0.40
25:De:721:ARG:HD3	25:De:721:ARG:HA	1.92	0.40
26:Df:83:LEU:HD11	29:Di:42:PHE:HB2	2.03	0.40
26:Df:216:LEU:HD21	26:Df:254:GLN:O	2.21	0.40
38:2:368:CYS:SG	38:2:371:CYS:N	2.95	0.40
41:5:46:ILE:HG22	41:5:48:GLU:HG3	2.04	0.40
42:6:377:GLN:HB3	42:6:381:TRP:CE3	2.57	0.40
43:7:240:ASP:OD2	43:7:658:ARG:NH2	2.53	0.40
43:7:699:GLU:HB2	43:7:700:HIS:CE1	2.56	0.40
44:c:294:PRO:CB	44:c:304:ALA:CB	2.95	0.40
49:a:211:LEU:HD12	49:a:212:THR:N	2.37	0.40
51:f:34:SER:C	51:f:36:ARG:N	2.78	0.40
51:f:77:ILE:HG13	51:f:78:LEU:N	2.37	0.40
52:g:48:GLN:N	52:g:48:GLN:CD	2.78	0.40
57:n:172:CYS:HG	59:q:20:HIS:C	2.18	0.40
57:n:853:HIS:O	57:n:857:GLU:HG2	2.21	0.40
57:n:944:PHE:O	57:n:945:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:o:749:LEU:HA	58:o:752:VAL:HG22	2.04	0.40
62:t:125:LYS:HB2	62:t:125:LYS:HE2	1.52	0.40
66:x:472:ASN:O	66:x:476:THR:HG23	2.22	0.40
67:w:2:GLU:N	67:w:2:GLU:CD	2.80	0.40
67:w:1167:ARG:HD3	67:w:1167:ARG:HA	1.90	0.40
68:p:313:LYS:HB3	68:p:337:LEU:HD23	2.04	0.40
69:X:-31:DC:H2'	69:X:-30:DT:C6	2.56	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	0	304/309 (98%)	242 (80%)	51 (17%)	11 (4%)	2 23
2	8	297/346 (86%)	266 (90%)	20 (7%)	11 (4%)	2 22
3	9	285/323 (88%)	268 (94%)	14 (5%)	3 (1%)	11 44
4	DO	95/109 (87%)	83 (87%)	11 (12%)	1 (1%)	11 44
5	DP	175/339 (52%)	166 (95%)	7 (4%)	2 (1%)	11 44
6	DQ	118/307 (38%)	105 (89%)	8 (7%)	5 (4%)	2 20
7	BA	251/316 (79%)	237 (94%)	10 (4%)	4 (2%)	7 38
8	FA	130/517 (25%)	117 (90%)	12 (9%)	1 (1%)	16 52
9	FB	218/249 (88%)	200 (92%)	13 (6%)	5 (2%)	5 31
10	PA	1461/1970 (74%)	1363 (93%)	81 (6%)	17 (1%)	10 43
11	PB	1128/1174 (96%)	1029 (91%)	83 (7%)	16 (1%)	9 39
12	PC	253/275 (92%)	229 (90%)	18 (7%)	6 (2%)	4 30
13	PD	127/142 (89%)	123 (97%)	3 (2%)	1 (1%)	16 52
14	PE	207/210 (99%)	201 (97%)	5 (2%)	1 (0%)	24 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	PF	77/127 (61%)	72 (94%)	3 (4%)	2 (3%)	4 28
16	PG	169/172 (98%)	159 (94%)	8 (5%)	2 (1%)	10 43
17	PH	146/150 (97%)	129 (88%)	16 (11%)	1 (1%)	18 55
18	PI	112/125 (90%)	102 (91%)	8 (7%)	2 (2%)	6 35
19	PJ	62/67 (92%)	59 (95%)	2 (3%)	1 (2%)	7 38
20	PK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	14 49
21	PL	42/58 (72%)	38 (90%)	3 (7%)	1 (2%)	4 30
22	DA	582/1872 (31%)	539 (93%)	33 (6%)	10 (2%)	7 36
23	DB	959/1199 (80%)	912 (95%)	47 (5%)	0	100 100
24	DD	153/1085 (14%)	144 (94%)	6 (4%)	3 (2%)	6 33
24	Dd	154/1085 (14%)	150 (97%)	4 (3%)	0	100 100
25	DE	540/800 (68%)	500 (93%)	36 (7%)	4 (1%)	18 55
25	De	531/800 (66%)	484 (91%)	47 (9%)	0	100 100
26	DF	404/677 (60%)	369 (91%)	29 (7%)	6 (2%)	8 39
26	Df	399/677 (59%)	371 (93%)	27 (7%)	1 (0%)	36 70
27	DG	139/349 (40%)	135 (97%)	4 (3%)	0	100 100
28	DH	207/310 (67%)	183 (88%)	20 (10%)	4 (2%)	6 34
29	DI	118/264 (45%)	103 (87%)	14 (12%)	1 (1%)	16 52
29	Di	119/264 (45%)	115 (97%)	4 (3%)	0	100 100
30	DJ	86/218 (39%)	82 (95%)	4 (5%)	0	100 100
30	Dj	91/218 (42%)	89 (98%)	2 (2%)	0	100 100
31	DL	73/161 (45%)	65 (89%)	5 (7%)	3 (4%)	2 21
31	Dl	105/161 (65%)	101 (96%)	4 (4%)	0	100 100
32	Dc	125/929 (14%)	116 (93%)	9 (7%)	0	100 100
33	Dk	96/211 (46%)	91 (95%)	5 (5%)	0	100 100
34	Dm	85/124 (68%)	79 (93%)	6 (7%)	0	100 100
35	EA	175/439 (40%)	160 (91%)	12 (7%)	3 (2%)	7 36
36	EB	170/291 (58%)	160 (94%)	6 (4%)	4 (2%)	4 30
37	1	431/548 (79%)	350 (81%)	73 (17%)	8 (2%)	6 34
38	2	383/395 (97%)	311 (81%)	72 (19%)	0	100 100
39	3	293/308 (95%)	238 (81%)	51 (17%)	4 (1%)	9 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	4	455/462 (98%)	374 (82%)	70 (15%)	11 (2%)	4	30
41	5	64/71 (90%)	57 (89%)	6 (9%)	1 (2%)	7	38
42	6	648/782 (83%)	514 (79%)	123 (19%)	11 (2%)	7	36
43	7	730/760 (96%)	600 (82%)	112 (15%)	18 (2%)	4	29
44	c	255/311 (82%)	235 (92%)	17 (7%)	3 (1%)	10	43
45	e	98/178 (55%)	92 (94%)	4 (4%)	2 (2%)	6	33
46	b	111/200 (56%)	109 (98%)	1 (1%)	1 (1%)	14	49
47	l	120/178 (67%)	115 (96%)	5 (4%)	0	100	100
48	m	110/131 (84%)	106 (96%)	4 (4%)	0	100	100
49	a	457/1581 (29%)	421 (92%)	31 (7%)	5 (1%)	11	44
50	d	154/270 (57%)	143 (93%)	9 (6%)	2 (1%)	9	41
51	f	163/246 (66%)	145 (89%)	13 (8%)	5 (3%)	3	25
52	g	164/233 (70%)	150 (92%)	11 (7%)	3 (2%)	6	35
53	h	188/268 (70%)	163 (87%)	15 (8%)	10 (5%)	1	18
54	i	69/146 (47%)	65 (94%)	2 (3%)	2 (3%)	3	26
55	j	120/135 (89%)	107 (89%)	9 (8%)	4 (3%)	3	24
56	k	110/117 (94%)	98 (89%)	10 (9%)	2 (2%)	6	35
57	n	980/1454 (67%)	876 (89%)	83 (8%)	21 (2%)	5	32
58	o	152/788 (19%)	138 (91%)	13 (9%)	1 (1%)	18	55
59	q	543/651 (83%)	476 (88%)	53 (10%)	14 (3%)	4	28
60	r	204/208 (98%)	190 (93%)	10 (5%)	4 (2%)	6	33
61	s	75/244 (31%)	64 (85%)	7 (9%)	4 (5%)	1	18
62	t	189/212 (89%)	168 (89%)	17 (9%)	4 (2%)	5	32
63	u	103/144 (72%)	99 (96%)	0	4 (4%)	2	21
64	v	132/200 (66%)	117 (89%)	9 (7%)	6 (4%)	2	20
65	z	93/600 (16%)	84 (90%)	6 (6%)	3 (3%)	3	25
66	x	876/989 (89%)	824 (94%)	50 (6%)	2 (0%)	43	75
67	w	1332/1368 (97%)	1266 (95%)	62 (5%)	4 (0%)	36	70
68	p	400/841 (48%)	366 (92%)	33 (8%)	1 (0%)	36	70
All	All	21285/34555 (62%)	19303 (91%)	1689 (8%)	293 (1%)	11	39

All (293) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	214	LYS
1	0	220	PRO
1	0	237	PRO
10	PA	539	GLN
10	PA	980	PRO
10	PA	1666	PRO
11	PB	630	LYS
12	PC	228	ARG
19	PJ	28	GLU
20	PK	39	ASP
22	DA	466	SER
22	DA	498	PRO
22	DA	1000	LEU
22	DA	1034	THR
24	DD	876	ALA
25	DE	452	ARG
25	DE	509	GLN
26	DF	68	THR
26	DF	69	SER
26	DF	350	ASN
26	DF	442	PRO
28	DH	141	PRO
31	DL	73	ASN
35	EA	123	ASN
36	EB	172	GLU
37	1	191	ASP
40	4	340	ASN
40	4	402	ARG
42	6	267	THR
43	7	19	PRO
43	7	64	PRO
43	7	153	PRO
43	7	671	LYS
44	c	283	ARG
44	c	293	PRO
44	c	294	PRO
50	d	187	LEU
51	f	145	TYR
51	f	148	HIS
53	h	100	PHE
53	h	130	ARG
53	h	167	ARG
53	h	168	PRO

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Mol	Chain	Res	Type
55	j	29	PHE
55	j	61	ILE
57	n	150	PRO
57	n	154	ILE
57	n	363	GLU
57	n	1196	PRO
57	n	1255	PRO
57	n	1266	THR
57	n	1326	PRO
59	q	131	SER
59	q	288	SER
59	q	393	PRO
59	q	398	ALA
59	q	399	PRO
62	t	173	PRO
63	u	81	SER
64	v	91	PHE
66	x	566	GLU
67	w	51	LEU
1	0	233	ILE
1	0	234	SER
2	8	96	THR
2	8	192	VAL
2	8	236	GLN
2	8	239	ASP
2	8	310	PRO
6	DQ	57	ASP
6	DQ	320	VAL
10	PA	538	VAL
10	PA	1645	PRO
10	PA	1663	SER
11	PB	226	GLU
11	PB	310	VAL
11	PB	673	VAL
11	PB	806	PHE
12	PC	41	GLU
13	PD	75	LYS
14	PE	201	GLY
15	PF	76	CYS
16	PG	16	ARG
22	DA	495	LEU
22	DA	510	ILE

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Mol	Chain	Res	Type
24	DD	893	GLU
24	DD	898	VAL
28	DH	129	VAL
29	DI	83	PHE
31	DL	111	LEU
31	DL	114	LYS
36	EB	134	ASP
37	1	163	ASP
37	1	187	ASN
37	1	192	ILE
37	1	201	PRO
37	1	336	ASP
37	1	418	LEU
40	4	301	VAL
42	6	92	VAL
43	7	15	ASP
43	7	148	HIS
43	7	704	ALA
43	7	739	LEU
45	e	146	ILE
49	a	164	PRO
49	a	334	PRO
49	a	430	LEU
53	h	37	TYR
53	h	131	ILE
54	i	108	HIS
54	i	138	LEU
55	j	78	GLN
57	n	169	LEU
57	n	254	VAL
57	n	920	ASN
57	n	957	PRO
57	n	1351	PRO
59	q	395	PRO
59	q	419	ASN
62	t	99	LYS
64	v	40	ALA
64	v	41	LYS
64	v	42	ILE
64	v	139	SER
67	w	32	ASP
67	w	1196	CYS

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Mol	Chain	Res	Type
1	0	289	SER
2	8	106	SER
2	8	277	LEU
3	9	237	MET
5	DP	207	PRO
6	DQ	319	ASP
9	FB	136	SER
9	FB	172	ASP
10	PA	921	ARG
10	PA	1134	PRO
10	PA	1206	ARG
10	PA	1486	ILE
11	PB	308	ALA
11	PB	973	PRO
12	PC	185	GLU
16	PG	80	PHE
22	DA	1037	ALA
36	EB	212	VAL
37	1	148	ASN
39	3	244	PRO
40	4	242	PHE
40	4	339	PRO
40	4	411	GLN
41	5	6	LYS
42	6	289	TYR
42	6	397	LYS
49	a	487	LEU
50	d	170	GLY
52	g	39	LYS
52	g	41	SER
53	h	159	ARG
55	j	60	ASP
57	n	1206	PRO
58	o	709	LYS
59	q	91	SER
59	q	420	SER
59	q	458	PRO
60	r	156	ASN
61	s	77	LEU
61	s	158	PRO
64	v	38	LYS
66	x	564	SER

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Mol	Chain	Res	Type
67	w	1203	MET
68	p	249	VAL
1	0	198	LEU
2	8	264	ALA
3	9	286	ALA
4	DO	84	VAL
7	BA	28	ARG
7	BA	46	ILE
7	BA	47	ASP
9	FB	38	GLY
9	FB	140	ARG
10	PA	195	GLY
10	PA	270	ALA
10	PA	300	ALA
10	PA	622	SER
11	PB	19	PRO
11	PB	730	LYS
12	PC	92	GLU
22	DA	1036	GLN
25	DE	482	SER
26	DF	321	PRO
35	EA	54	PHE
35	EA	56	ARG
36	EB	225	VAL
39	3	235	GLN
39	3	248	HIS
40	4	241	SER
40	4	384	PRO
40	4	413	LEU
42	6	114	HIS
42	6	266	GLN
43	7	66	GLU
43	7	113	LYS
43	7	487	ARG
43	7	670	GLY
45	e	147	ASN
46	b	100	GLN
49	a	208	VAL
57	n	165	SER
57	n	265	LEU
57	n	1355	PRO
59	q	127	LEU

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Mol	Chain	Res	Type
59	q	134	ALA
60	r	113	ASN
61	s	155	HIS
62	t	172	ALA
65	z	533	PRO
1	0	89	PHE
1	0	225	THR
1	0	265	MET
3	9	16	GLU
8	FA	24	LYS
10	PA	821	GLY
10	PA	884	ASN
11	PB	328	PRO
11	PB	428	ASP
11	PB	978	ILE
17	PH	69	THR
18	PI	53	ILE
22	DA	1038	ARG
26	DF	440	PRO
28	DH	138	GLN
40	4	304	PRO
42	6	418	LYS
42	6	434	GLU
43	7	111	SER
43	7	172	ALA
43	7	740	SER
51	f	53	GLN
51	f	55	LEU
51	f	143	LYS
52	g	74	HIS
56	k	79	HIS
56	k	81	GLY
57	n	264	ALA
57	n	524	ASN
57	n	1343	PRO
61	s	153	ARG
62	t	129	VAL
63	u	82	THR
63	u	83	ALA
65	z	540	LEU
2	8	82	GLY
2	8	212	PHE

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Mol	Chain	Res	Type
5	DP	298	PRO
6	DQ	312	GLU
7	BA	19	PRO
11	PB	1079	SER
12	PC	60	HIS
22	DA	1040	GLY
28	DH	137	GLY
26	Df	411	VAL
39	3	69	PHE
42	6	181	HIS
42	6	417	THR
43	7	190	CYS
53	h	187	PHE
57	n	164	GLY
59	q	89	GLN
59	q	647	SER
25	DE	472	GLY
40	4	138	PRO
60	r	94	GLY
60	r	153	VAL
65	z	537	PRO
9	FB	173	GLY
11	PB	779	ILE
53	h	188	GLY
57	n	528	HIS
63	u	77	PRO
1	0	193	PRO
2	8	186	GLY
6	DQ	313	PRO
10	PA	1648	PRO
21	PL	34	ILE
43	7	204	VAL
53	h	99	VAL
15	PF	113	GLY
42	6	109	ARG
43	7	320	PRO
11	PB	330	VAL
11	PB	858	VAL
12	PC	94	CYS
18	PI	26	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	0	209/283 (74%)	171 (82%)	38 (18%)	2 11
2	8	259/299 (87%)	180 (70%)	79 (30%)	0 2
3	9	252/296 (85%)	173 (69%)	79 (31%)	0 2
4	DO	84/98 (86%)	68 (81%)	16 (19%)	1 10
5	DP	153/293 (52%)	141 (92%)	12 (8%)	11 34
6	DQ	111/269 (41%)	93 (84%)	18 (16%)	2 13
7	BA	214/268 (80%)	198 (92%)	16 (8%)	12 35
8	FA	117/448 (26%)	109 (93%)	8 (7%)	14 39
9	FB	196/218 (90%)	159 (81%)	37 (19%)	1 10
10	PA	1305/1748 (75%)	1045 (80%)	260 (20%)	1 9
11	PB	993/1027 (97%)	800 (81%)	193 (19%)	1 9
12	PC	234/252 (93%)	194 (83%)	40 (17%)	2 12
13	PD	108/126 (86%)	87 (81%)	21 (19%)	1 9
14	PE	191/192 (100%)	151 (79%)	40 (21%)	1 7
15	PF	69/111 (62%)	53 (77%)	16 (23%)	1 5
16	PG	147/153 (96%)	111 (76%)	36 (24%)	1 5
17	PH	129/131 (98%)	105 (81%)	24 (19%)	1 10
18	PI	103/112 (92%)	78 (76%)	25 (24%)	1 5
19	PJ	53/56 (95%)	42 (79%)	11 (21%)	1 7
20	PK	106/106 (100%)	88 (83%)	18 (17%)	2 12
21	PL	41/55 (74%)	29 (71%)	12 (29%)	0 3
22	DA	532/1665 (32%)	482 (91%)	50 (9%)	8 28
23	DB	876/1083 (81%)	859 (98%)	17 (2%)	50 67
24	DD	144/815 (18%)	126 (88%)	18 (12%)	4 20
24	Dd	146/815 (18%)	146 (100%)	0	100 100
25	DE	478/657 (73%)	460 (96%)	18 (4%)	29 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	De	475/657 (72%)	474 (100%)	1 (0%)	87 87
26	DF	324/574 (56%)	260 (80%)	64 (20%)	1 9
26	Df	322/574 (56%)	300 (93%)	22 (7%)	14 39
27	DG	133/322 (41%)	124 (93%)	9 (7%)	14 39
28	DH	181/270 (67%)	156 (86%)	25 (14%)	3 17
29	DI	106/235 (45%)	90 (85%)	16 (15%)	3 15
29	Di	107/235 (46%)	107 (100%)	0	100 100
30	DJ	79/154 (51%)	68 (86%)	11 (14%)	3 17
30	Dj	83/154 (54%)	83 (100%)	0	100 100
31	DL	70/141 (50%)	59 (84%)	11 (16%)	2 14
31	Dl	98/141 (70%)	98 (100%)	0	100 100
32	Dc	113/833 (14%)	111 (98%)	2 (2%)	51 68
33	Dk	87/182 (48%)	87 (100%)	0	100 100
34	Dm	80/106 (76%)	79 (99%)	1 (1%)	61 72
35	EA	163/373 (44%)	126 (77%)	37 (23%)	1 6
36	EB	155/261 (59%)	143 (92%)	12 (8%)	12 34
37	1	384/484 (79%)	367 (96%)	17 (4%)	25 48
38	2	342/352 (97%)	335 (98%)	7 (2%)	48 66
39	3	259/272 (95%)	255 (98%)	4 (2%)	57 71
40	4	394/399 (99%)	376 (95%)	18 (5%)	24 47
41	5	59/64 (92%)	54 (92%)	5 (8%)	10 32
42	6	576/688 (84%)	552 (96%)	24 (4%)	26 49
43	7	630/664 (95%)	595 (94%)	35 (6%)	19 43
44	c	231/280 (82%)	218 (94%)	13 (6%)	19 43
45	e	94/152 (62%)	94 (100%)	0	100 100
46	b	102/163 (63%)	92 (90%)	10 (10%)	7 27
47	l	116/155 (75%)	116 (100%)	0	100 100
48	m	102/115 (89%)	102 (100%)	0	100 100
49	a	393/1391 (28%)	313 (80%)	80 (20%)	1 8
50	d	139/230 (60%)	93 (67%)	46 (33%)	0 2
51	f	144/223 (65%)	123 (85%)	21 (15%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	g	157/216 (73%)	131 (83%)	26 (17%)	2 13
53	h	161/225 (72%)	129 (80%)	32 (20%)	1 9
54	i	71/133 (53%)	62 (87%)	9 (13%)	4 19
55	j	113/124 (91%)	109 (96%)	4 (4%)	32 54
56	k	94/98 (96%)	44 (47%)	50 (53%)	0 0
57	n	689/1272 (54%)	662 (96%)	27 (4%)	28 51
58	o	141/697 (20%)	138 (98%)	3 (2%)	47 66
59	q	461/577 (80%)	385 (84%)	76 (16%)	2 13
60	r	180/183 (98%)	148 (82%)	32 (18%)	2 12
61	s	31/208 (15%)	28 (90%)	3 (10%)	8 27
62	t	166/178 (93%)	124 (75%)	42 (25%)	0 4
63	u	78/119 (66%)	73 (94%)	5 (6%)	16 40
64	v	122/173 (70%)	77 (63%)	45 (37%)	0 1
65	z	89/512 (17%)	75 (84%)	14 (16%)	2 14
66	x	787/864 (91%)	770 (98%)	17 (2%)	45 65
67	w	1202/1232 (98%)	1184 (98%)	18 (2%)	57 71
68	p	353/736 (48%)	346 (98%)	7 (2%)	48 66
All	All	18686/29967 (62%)	16683 (89%)	2003 (11%)	8 24

All (2003) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	6	CYS
1	0	9	CYS
1	0	31	CYS
1	0	34	CYS
1	0	73	GLU
1	0	75	ARG
1	0	80	LYS
1	0	83	ASN
1	0	84	LYS
1	0	85	ARG
1	0	87	GLU
1	0	92	LEU
1	0	93	ARG
1	0	95	TYR

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Mol	Chain	Res	Type
1	0	99	LEU
1	0	100	GLU
1	0	103	GLU
1	0	104	GLU
1	0	105	ILE
1	0	180	LYS
1	0	184	LEU
1	0	187	LEU
1	0	190	SER
1	0	196	LEU
1	0	251	LEU
1	0	252	GLN
1	0	254	GLU
1	0	263	LEU
1	0	268	ARG
1	0	272	LEU
1	0	275	VAL
1	0	276	ARG
1	0	287	TYR
1	0	288	THR
1	0	293	CYS
1	0	295	ARG
1	0	304	LEU
1	0	305	PHE
2	8	13	GLU
2	8	15	LEU
2	8	20	GLU
2	8	23	PHE
2	8	30	ARG
2	8	32	LYS
2	8	33	ASN
2	8	34	THR
2	8	36	GLN
2	8	37	ILE
2	8	38	VAL
2	8	45	LEU
2	8	47	HIS
2	8	48	ARG
2	8	52	LYS
2	8	55	ILE
2	8	56	ASN
2	8	57	ARG

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Mol	Chain	Res	Type
2	8	58	THR
2	8	60	LEU
2	8	63	ILE
2	8	64	LYS
2	8	66	LEU
2	8	67	GLN
2	8	69	LEU
2	8	74	ILE
2	8	75	ILE
2	8	83	HIS
2	8	84	LYS
2	8	86	ASN
2	8	88	SER
2	8	96	THR
2	8	101	ILE
2	8	102	ILE
2	8	107	LEU
2	8	108	VAL
2	8	109	LEU
2	8	110	THR
2	8	115	LYS
2	8	125	LEU
2	8	131	HIS
2	8	132	TRP
2	8	139	LYS
2	8	141	ASN
2	8	143	LEU
2	8	153	LEU
2	8	160	LYS
2	8	162	PHE
2	8	164	SER
2	8	169	TYR
2	8	170	THR
2	8	174	VAL
2	8	178	TYR
2	8	189	MET
2	8	205	GLU
2	8	206	LEU
2	8	209	ARG
2	8	210	VAL
2	8	213	LEU
2	8	223	THR

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Mol	Chain	Res	Type
2	8	225	ILE
2	8	237	TRP
2	8	241	CYS
2	8	245	ASP
2	8	249	PHE
2	8	257	LEU
2	8	258	HIS
2	8	259	HIS
2	8	260	ILE
2	8	261	PHE
2	8	267	ASP
2	8	268	LEU
2	8	272	ILE
2	8	276	PHE
2	8	280	PRO
2	8	284	ILE
2	8	285	THR
2	8	288	GLN
2	8	292	MET
3	9	3	HIS
3	9	7	GLN
3	9	8	LYS
3	9	10	HIS
3	9	11	TRP
3	9	12	THR
3	9	14	SER
3	9	15	SER
3	9	21	ARG
3	9	28	ARG
3	9	32	CYS
3	9	33	LYS
3	9	37	ASN
3	9	41	LEU
3	9	44	ASP
3	9	55	THR
3	9	56	LEU
3	9	60	TYR
3	9	65	LEU
3	9	84	CYS
3	9	85	MET
3	9	92	LEU
3	9	93	ASN

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Mol	Chain	Res	Type
3	9	94	ASN
3	9	96	VAL
3	9	97	MET
3	9	98	GLU
3	9	102	ARG
3	9	104	ILE
3	9	106	LEU
3	9	107	THR
3	9	108	CYS
3	9	111	LEU
3	9	113	CYS
3	9	114	LYS
3	9	115	VAL
3	9	129	LEU
3	9	134	LEU
3	9	136	GLN
3	9	140	LEU
3	9	141	GLU
3	9	143	ILE
3	9	145	GLU
3	9	148	LEU
3	9	149	LEU
3	9	150	LEU
3	9	151	ILE
3	9	153	GLN
3	9	154	LEU
3	9	158	LEU
3	9	160	VAL
3	9	165	ARG
3	9	166	PRO
3	9	171	LEU
3	9	172	ILE
3	9	174	LEU
3	9	175	LYS
3	9	180	ILE
3	9	181	LEU
3	9	182	GLU
3	9	186	ILE
3	9	189	LYS
3	9	192	ASP
3	9	200	LEU
3	9	208	THR

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Mol	Chain	Res	Type
3	9	211	GLN
3	9	226	ILE
3	9	227	THR
3	9	229	GLU
3	9	231	TYR
3	9	232	LEU
3	9	239	LYS
3	9	245	LEU
3	9	252	MET
3	9	262	TYR
3	9	266	ARG
3	9	277	LEU
3	9	279	ARG
3	9	288	ASN
4	DO	24	GLN
4	DO	27	GLN
4	DO	29	THR
4	DO	32	LEU
4	DO	34	LEU
4	DO	56	VAL
4	DO	57	ASN
4	DO	59	ARG
4	DO	76	LEU
4	DO	79	VAL
4	DO	80	GLU
4	DO	84	VAL
4	DO	87	LEU
4	DO	88	ILE
4	DO	89	LYS
4	DO	90	VAL
5	DP	172	VAL
5	DP	209	THR
5	DP	221	CYS
5	DP	268	ILE
5	DP	274	VAL
5	DP	278	GLN
5	DP	300	ILE
5	DP	301	VAL
5	DP	303	LEU
5	DP	306	VAL
5	DP	317	VAL
5	DP	328	ILE

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Mol	Chain	Res	Type
6	DQ	13	LEU
6	DQ	22	ILE
6	DQ	27	ASP
6	DQ	34	VAL
6	DQ	36	GLU
6	DQ	37	GLN
6	DQ	38	VAL
6	DQ	40	MET
6	DQ	49	LYS
6	DQ	50	LEU
6	DQ	57	ASP
6	DQ	63	GLU
6	DQ	320	VAL
6	DQ	321	SER
6	DQ	322	ASP
6	DQ	333	ASN
6	DQ	360	LEU
6	DQ	364	ASP
7	BA	15	CYS
7	BA	16	PRO
7	BA	18	HIS
7	BA	24	VAL
7	BA	28	ARG
7	BA	36	GLU
7	BA	39	LEU
7	BA	41	VAL
7	BA	45	VAL
7	BA	120	GLU
7	BA	127	ARG
7	BA	128	ILE
7	BA	206	VAL
7	BA	313	LEU
7	BA	315	GLN
7	BA	316	LEU
8	FA	8	SER
8	FA	9	GLN
8	FA	12	THR
8	FA	20	LYS
8	FA	22	THR
8	FA	24	LYS
8	FA	25	LYS
8	FA	29	MET

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Mol	Chain	Res	Type
9	FB	39	GLU
9	FB	42	LYS
9	FB	43	LEU
9	FB	55	SER
9	FB	57	THR
9	FB	85	LEU
9	FB	91	GLN
9	FB	92	THR
9	FB	94	THR
9	FB	98	GLU
9	FB	121	SER
9	FB	122	GLU
9	FB	123	ASN
9	FB	126	ARG
9	FB	129	ARG
9	FB	137	LYS
9	FB	139	VAL
9	FB	140	ARG
9	FB	141	LEU
9	FB	158	ASN
9	FB	160	GLN
9	FB	164	GLU
9	FB	166	GLU
9	FB	167	ARG
9	FB	168	LYS
9	FB	169	LYS
9	FB	170	LYS
9	FB	174	LYS
9	FB	175	ARG
9	FB	179	ASP
9	FB	180	LYS
9	FB	182	HIS
9	FB	189	SER
9	FB	207	LYS
9	FB	211	VAL
9	FB	219	GLU
9	FB	225	VAL
10	PA	25	VAL
10	PA	48	GLU
10	PA	51	ARG
10	PA	66	GLU
10	PA	70	ARG

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Mol	Chain	Res	Type
10	PA	71	CYS
10	PA	77	ASN
10	PA	84	HIS
10	PA	87	HIS
10	PA	88	ILE
10	PA	101	VAL
10	PA	104	MET
10	PA	119	VAL
10	PA	125	LYS
10	PA	130	LEU
10	PA	134	LYS
10	PA	136	GLN
10	PA	138	LYS
10	PA	140	ARG
10	PA	143	HIS
10	PA	147	LEU
10	PA	149	LYS
10	PA	151	LYS
10	PA	188	GLN
10	PA	191	ILE
10	PA	193	ARG
10	PA	198	LEU
10	PA	215	LEU
10	PA	216	LEU
10	PA	221	VAL
10	PA	228	ILE
10	PA	229	SER
10	PA	233	CYS
10	PA	236	LEU
10	PA	252	VAL
10	PA	253	LEU
10	PA	255	VAL
10	PA	258	LEU
10	PA	259	SER
10	PA	264	VAL
10	PA	265	VAL
10	PA	277	THR
10	PA	278	HIS
10	PA	284	VAL
10	PA	286	ILE
10	PA	309	LEU
10	PA	316	THR

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Mol	Chain	Res	Type
10	PA	321	GLU
10	PA	325	LEU
10	PA	329	MET
10	PA	331	LYS
10	PA	334	ARG
10	PA	336	LEU
10	PA	343	LEU
10	PA	347	GLU
10	PA	350	VAL
10	PA	355	MET
10	PA	357	LYS
10	PA	364	ARG
10	PA	366	VAL
10	PA	378	VAL
10	PA	389	THR
10	PA	393	ILE
10	PA	394	VAL
10	PA	395	THR
10	PA	396	PRO
10	PA	399	ILE
10	PA	406	VAL
10	PA	417	LYS
10	PA	421	ARG
10	PA	423	ASN
10	PA	434	LYS
10	PA	437	ASP
10	PA	438	LEU
10	PA	439	HIS
10	PA	446	VAL
10	PA	455	ILE
10	PA	460	ARG
10	PA	461	GLN
10	PA	463	THR
10	PA	474	VAL
10	PA	476	ILE
10	PA	481	THR
10	PA	495	ASP
10	PA	499	ASP
10	PA	503	LEU
10	PA	506	PRO
10	PA	507	GLN
10	PA	509	LEU

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Mol	Chain	Res	Type
10	PA	517	GLU
10	PA	520	MET
10	PA	521	VAL
10	PA	541	THR
10	PA	542	LEU
10	PA	545	VAL
10	PA	547	LYS
10	PA	556	GLU
10	PA	562	ASN
10	PA	565	MET
10	PA	567	LEU
10	PA	574	VAL
10	PA	580	LEU
10	PA	583	ARG
10	PA	593	SER
10	PA	612	ASP
10	PA	614	ASP
10	PA	625	ASP
10	PA	631	GLU
10	PA	634	GLU
10	PA	645	LEU
10	PA	668	PHE
10	PA	676	ILE
10	PA	686	THR
10	PA	687	ILE
10	PA	695	ASP
10	PA	699	TYR
10	PA	705	THR
10	PA	715	GLU
10	PA	721	HIS
10	PA	729	PRO
10	PA	731	ASN
10	PA	738	GLU
10	PA	754	SER
10	PA	755	SER
10	PA	757	GLN
10	PA	762	GLU
10	PA	785	ILE
10	PA	792	ASN
10	PA	793	VAL
10	PA	806	THR
10	PA	811	ILE

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Mol	Chain	Res	Type
10	PA	847	LEU
10	PA	849	ASP
10	PA	852	VAL
10	PA	853	LYS
10	PA	861	GLN
10	PA	864	LEU
10	PA	865	ILE
10	PA	867	SER
10	PA	871	VAL
10	PA	872	MET
10	PA	878	THR
10	PA	882	SER
10	PA	883	ILE
10	PA	888	GLN
10	PA	899	GLU
10	PA	900	SER
10	PA	906	LEU
10	PA	908	THR
10	PA	912	SER
10	PA	920	PHE
10	PA	924	TYR
10	PA	932	ARG
10	PA	934	LEU
10	PA	937	ASP
10	PA	938	LEU
10	PA	947	HIS
10	PA	972	THR
10	PA	974	ASP
10	PA	977	VAL
10	PA	978	VAL
10	PA	981	CYS
10	PA	983	LEU
10	PA	986	MET
10	PA	992	LYS
10	PA	993	ILE
10	PA	999	ARG
10	PA	1007	ILE
10	PA	1010	VAL
10	PA	1018	LYS
10	PA	1021	VAL
10	PA	1023	VAL
10	PA	1030	SER

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Mol	Chain	Res	Type
10	PA	1032	GLN
10	PA	1034	GLN
10	PA	1040	LEU
10	PA	1042	ASN
10	PA	1048	THR
10	PA	1049	LEU
10	PA	1054	MET
10	PA	1060	LEU
10	PA	1074	SER
10	PA	1087	VAL
10	PA	1093	GLN
10	PA	1103	THR
10	PA	1107	PHE
10	PA	1115	LYS
10	PA	1118	THR
10	PA	1124	LEU
10	PA	1128	ILE
10	PA	1135	LYS
10	PA	1139	LEU
10	PA	1140	THR
10	PA	1150	ASP
10	PA	1158	LEU
10	PA	1170	THR
10	PA	1173	THR
10	PA	1182	GLN
10	PA	1188	GLU
10	PA	1193	VAL
10	PA	1195	VAL
10	PA	1198	GLU
10	PA	1199	MET
10	PA	1201	ASP
10	PA	1207	ILE
10	PA	1210	TRP
10	PA	1211	LEU
10	PA	1233	GLU
10	PA	1243	LEU
10	PA	1244	ASN
10	PA	1248	ASN
10	PA	1254	LYS
10	PA	1255	LEU
10	PA	1256	VAL
10	PA	1259	ILE

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Mol	Chain	Res	Type
10	PA	1260	ARG
10	PA	1261	ILE
10	PA	1287	CYS
10	PA	1292	MET
10	PA	1293	LEU
10	PA	1296	MET
10	PA	1304	ILE
10	PA	1319	LYS
10	PA	1327	GLU
10	PA	1338	THR
10	PA	1341	VAL
10	PA	1344	MET
10	PA	1345	ARG
10	PA	1349	GLU
10	PA	1362	ILE
10	PA	1368	VAL
10	PA	1375	ARG
10	PA	1378	LEU
10	PA	1379	GLU
10	PA	1385	VAL
10	PA	1386	ILE
10	PA	1388	PHE
10	PA	1389	ASP
10	PA	1391	SER
10	PA	1402	CYS
10	PA	1403	ASP
10	PA	1407	CYS
10	PA	1417	HIS
10	PA	1419	VAL
10	PA	1429	LYS
10	PA	1432	PHE
10	PA	1434	GLU
10	PA	1435	THR
10	PA	1451	MET
10	PA	1454	VAL
10	PA	1463	LEU
10	PA	1480	CYS
10	PA	1486	ILE
10	PA	1487	PRO
10	PA	1643	TYR
10	PA	1646	THR
10	PA	1647	SER

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Mol	Chain	Res	Type
10	PA	1663	SER
10	PA	1678	TYR
10	PA	1794	SER
11	PB	18	THR
11	PB	28	ILE
11	PB	29	VAL
11	PB	39	LEU
11	PB	40	VAL
11	PB	42	GLN
11	PB	43	GLN
11	PB	52	GLN
11	PB	53	MET
11	PB	55	VAL
11	PB	83	ARG
11	PB	87	LYS
11	PB	91	ILE
11	PB	97	THR
11	PB	99	TRP
11	PB	100	GLU
11	PB	101	ARG
11	PB	102	ASP
11	PB	118	LEU
11	PB	128	ILE
11	PB	131	THR
11	PB	132	VAL
11	PB	133	ILE
11	PB	134	LYS
11	PB	140	LEU
11	PB	141	GLN
11	PB	142	THR
11	PB	146	LYS
11	PB	147	THR
11	PB	149	ILE
11	PB	155	MET
11	PB	162	LEU
11	PB	167	THR
11	PB	195	ILE
11	PB	204	THR
11	PB	214	LYS
11	PB	225	LEU
11	PB	230	ARG
11	PB	233	SER

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Mol	Chain	Res	Type
11	PB	235	ILE
11	PB	264	LYS
11	PB	265	GLN
11	PB	273	PHE
11	PB	281	ASP
11	PB	282	ARG
11	PB	285	LEU
11	PB	286	GLU
11	PB	287	HIS
11	PB	289	ILE
11	PB	297	MET
11	PB	304	SER
11	PB	316	VAL
11	PB	318	LEU
11	PB	324	ARG
11	PB	327	LYS
11	PB	330	VAL
11	PB	331	THR
11	PB	348	LEU
11	PB	351	VAL
11	PB	353	VAL
11	PB	356	PHE
11	PB	379	ARG
11	PB	388	TYR
11	PB	403	LEU
11	PB	407	MET
11	PB	420	GLN
11	PB	423	ILE
11	PB	432	GLU
11	PB	433	LEU
11	PB	440	ILE
11	PB	448	LEU
11	PB	458	LYS
11	PB	473	LEU
11	PB	482	LEU
11	PB	487	SER
11	PB	489	ILE
11	PB	495	LEU
11	PB	501	LEU
11	PB	508	MET
11	PB	514	THR
11	PB	520	VAL

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Mol	Chain	Res	Type
11	PB	523	VAL
11	PB	524	LYS
11	PB	525	ASN
11	PB	536	SER
11	PB	539	SER
11	PB	541	ILE
11	PB	542	LEU
11	PB	545	LEU
11	PB	546	GLU
11	PB	547	GLU
11	PB	553	LEU
11	PB	554	GLU
11	PB	555	GLU
11	PB	566	LYS
11	PB	568	PHE
11	PB	572	CYS
11	PB	574	VAL
11	PB	576	ILE
11	PB	579	ASP
11	PB	592	ARG
11	PB	593	GLN
11	PB	595	ASP
11	PB	596	ILE
11	PB	597	ILE
11	PB	598	VAL
11	PB	613	ARG
11	PB	627	ILE
11	PB	634	LEU
11	PB	643	LEU
11	PB	645	GLU
11	PB	648	TYR
11	PB	656	LEU
11	PB	662	VAL
11	PB	665	ILE
11	PB	667	THR
11	PB	678	THR
11	PB	686	GLU
11	PB	687	VAL
11	PB	694	THR
11	PB	696	CYS
11	PB	698	ILE
11	PB	706	VAL

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Mol	Chain	Res	Type
11	PB	707	CYS
11	PB	733	MET
11	PB	738	THR
11	PB	742	VAL
11	PB	745	ASP
11	PB	746	THR
11	PB	749	HIS
11	PB	751	LEU
11	PB	756	LYS
11	PB	767	LEU
11	PB	768	ARG
11	PB	780	VAL
11	PB	784	SER
11	PB	795	ILE
11	PB	809	VAL
11	PB	829	PHE
11	PB	834	ARG
11	PB	837	CYS
11	PB	840	MET
11	PB	841	ARG
11	PB	842	HIS
11	PB	847	LYS
11	PB	854	ILE
11	PB	865	VAL
11	PB	866	ILE
11	PB	870	THR
11	PB	873	LEU
11	PB	888	THR
11	PB	889	LYS
11	PB	890	ARG
11	PB	896	LEU
11	PB	897	ARG
11	PB	898	THR
11	PB	901	THR
11	PB	904	VAL
11	PB	906	GLN
11	PB	908	MET
11	PB	918	PHE
11	PB	922	ARG
11	PB	923	VAL
11	PB	959	GLU
11	PB	965	ILE

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Mol	Chain	Res	Type
11	PB	966	ILE
11	PB	967	ILE
11	PB	976	MET
11	PB	978	ILE
11	PB	983	GLU
11	PB	996	ILE
11	PB	998	ASP
11	PB	1000	THR
11	PB	1002	PHE
11	PB	1006	VAL
11	PB	1007	ASN
11	PB	1008	VAL
11	PB	1022	LEU
11	PB	1026	GLU
11	PB	1027	VAL
11	PB	1048	TYR
11	PB	1052	LYS
11	PB	1068	GLN
11	PB	1070	LEU
11	PB	1073	GLN
11	PB	1080	ARG
11	PB	1084	LEU
11	PB	1090	GLU
11	PB	1101	GLN
11	PB	1125	MET
11	PB	1133	HIS
11	PB	1138	ARG
11	PB	1151	MET
12	PC	5	ASN
12	PC	6	GLN
12	PC	9	VAL
12	PC	11	ILE
12	PC	17	GLU
12	PC	21	PHE
12	PC	39	ILE
12	PC	44	ILE
12	PC	60	HIS
12	PC	64	ILE
12	PC	75	SER
12	PC	79	VAL
12	PC	80	ASP
12	PC	86	ARG

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Mol	Chain	Res	Type
12	PC	88	CYS
12	PC	94	CYS
12	PC	109	GLU
12	PC	110	ASP
12	PC	112	THR
12	PC	118	ARG
12	PC	128	ILE
12	PC	131	THR
12	PC	148	ILE
12	PC	159	LEU
12	PC	169	PHE
12	PC	172	GLU
12	PC	179	THR
12	PC	193	ARG
12	PC	195	THR
12	PC	201	GLU
12	PC	202	GLU
12	PC	204	PRO
12	PC	211	LEU
12	PC	223	ASN
12	PC	227	GLU
12	PC	243	THR
12	PC	247	SER
12	PC	250	SER
12	PC	259	LEU
12	PC	266	GLU
13	PD	19	GLN
13	PD	20	LEU
13	PD	32	LEU
13	PD	33	LEU
13	PD	45	LYS
13	PD	50	SER
13	PD	76	ASN
13	PD	82	SER
13	PD	96	GLU
13	PD	99	CYS
13	PD	107	THR
13	PD	109	GLU
13	PD	115	ILE
13	PD	117	SER
13	PD	118	LEU
13	PD	119	GLU

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Mol	Chain	Res	Type
13	PD	121	ARG
13	PD	124	ASP
13	PD	131	LEU
13	PD	135	GLN
13	PD	141	GLN
14	PE	3	ASP
14	PE	5	GLU
14	PE	17	ILE
14	PE	21	CYS
14	PE	47	LYS
14	PE	54	ARG
14	PE	57	ASP
14	PE	58	LEU
14	PE	60	VAL
14	PE	62	VAL
14	PE	64	HIS
14	PE	78	GLU
14	PE	81	LYS
14	PE	84	ILE
14	PE	87	ILE
14	PE	92	GLN
14	PE	95	GLN
14	PE	96	GLU
14	PE	99	ILE
14	PE	100	THR
14	PE	104	ILE
14	PE	108	GLN
14	PE	111	THR
14	PE	119	VAL
14	PE	120	ASP
14	PE	127	LEU
14	PE	137	ILE
14	PE	145	VAL
14	PE	153	LYS
14	PE	168	ASN
14	PE	178	PRO
14	PE	179	VAL
14	PE	191	VAL
14	PE	195	ARG
14	PE	198	GLU
14	PE	199	THR
14	PE	205	THR

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Mol	Chain	Res	Type
14	PE	208	LEU
14	PE	209	VAL
14	PE	210	GLN
15	PF	53	THR
15	PF	59	LYS
15	PF	66	LEU
15	PF	71	LEU
15	PF	73	ILE
15	PF	75	MET
15	PF	81	VAL
15	PF	82	GLU
15	PF	83	LEU
15	PF	86	GLU
15	PF	90	LEU
15	PF	91	LEU
15	PF	97	LEU
15	PF	101	LYS
15	PF	105	ILE
15	PF	106	ILE
16	PG	1	MET
16	PG	6	SER
16	PG	7	LEU
16	PG	10	GLU
16	PG	13	LEU
16	PG	30	LEU
16	PG	34	VAL
16	PG	38	CYS
16	PG	39	THR
16	PG	46	ILE
16	PG	48	VAL
16	PG	49	THR
16	PG	53	ASN
16	PG	59	ILE
16	PG	60	GLN
16	PG	63	ARG
16	PG	80	PHE
16	PG	84	VAL
16	PG	88	VAL
16	PG	90	THR
16	PG	97	LEU
16	PG	101	ILE
16	PG	105	SER

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Mol	Chain	Res	Type
16	PG	106	CYS
16	PG	113	ILE
16	PG	116	GLU
16	PG	118	GLU
16	PG	132	ASP
16	PG	136	VAL
16	PG	143	ILE
16	PG	145	LEU
16	PG	150	THR
16	PG	152	VAL
16	PG	158	PHE
16	PG	164	MET
16	PG	168	LEU
17	PH	4	ILE
17	PH	5	LEU
17	PH	15	ILE
17	PH	24	ARG
17	PH	33	GLU
17	PH	40	ILE
17	PH	43	VAL
17	PH	45	ILE
17	PH	50	VAL
17	PH	59	VAL
17	PH	64	LEU
17	PH	66	GLU
17	PH	70	LEU
17	PH	72	ASP
17	PH	76	ASN
17	PH	81	ARG
17	PH	87	GLN
17	PH	96	VAL
17	PH	102	ASP
17	PH	105	SER
17	PH	132	LEU
17	PH	133	HIS
17	PH	136	GLU
17	PH	141	VAL
18	PI	12	VAL
18	PI	14	ILE
18	PI	27	LYS
18	PI	28	GLU
18	PI	32	ASN

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Mol	Chain	Res	Type
18	PI	33	ARG
18	PI	34	ILE
18	PI	35	LEU
18	PI	42	CYS
18	PI	45	GLN
18	PI	53	ILE
18	PI	61	GLU
18	PI	62	VAL
18	PI	69	ILE
18	PI	72	VAL
18	PI	75	ASP
18	PI	77	THR
18	PI	81	THR
18	PI	83	ASP
18	PI	88	LYS
18	PI	92	LYS
18	PI	93	GLU
18	PI	95	VAL
18	PI	99	SER
18	PI	113	VAL
19	PJ	1	MET
19	PJ	6	ARG
19	PJ	7	CYS
19	PJ	10	CYS
19	PJ	13	ILE
19	PJ	14	VAL
19	PJ	22	LEU
19	PJ	28	GLU
19	PJ	30	THR
19	PJ	48	MET
19	PJ	53	VAL
20	PK	11	LEU
20	PK	12	LEU
20	PK	14	GLU
20	PK	17	LYS
20	PK	38	GLU
20	PK	40	HIS
20	PK	41	THR
20	PK	42	LEU
20	PK	45	ILE
20	PK	81	TYR
20	PK	92	THR

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Mol	Chain	Res	Type
20	PK	94	LEU
20	PK	101	LEU
20	PK	109	ILE
20	PK	111	ASP
20	PK	112	LYS
20	PK	114	GLU
20	PK	116	ILE
21	PL	18	ILE
21	PL	23	HIS
21	PL	25	GLU
21	PL	28	ILE
21	PL	34	ILE
21	PL	37	ARG
21	PL	39	CYS
21	PL	44	MET
21	PL	47	LYS
21	PL	51	ARG
21	PL	52	LEU
21	PL	56	ASP
22	DA	348	LEU
22	DA	353	LEU
22	DA	396	LEU
22	DA	397	LEU
22	DA	400	GLU
22	DA	401	ASN
22	DA	403	LEU
22	DA	404	MET
22	DA	405	VAL
22	DA	408	LEU
22	DA	414	ILE
22	DA	415	ILE
22	DA	416	TRP
22	DA	470	ILE
22	DA	475	LEU
22	DA	480	TRP
22	DA	482	ASP
22	DA	485	ILE
22	DA	486	TRP
22	DA	487	ASP
22	DA	491	MET
22	DA	493	ARG
22	DA	494	LEU

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Mol	Chain	Res	Type
22	DA	496	GLU
22	DA	500	LEU
22	DA	501	THR
22	DA	502	LEU
22	DA	507	GLU
22	DA	510	ILE
22	DA	573	TYR
22	DA	639	LEU
22	DA	661	GLU
22	DA	667	THR
22	DA	711	ASP
22	DA	727	THR
22	DA	730	PHE
22	DA	828	GLU
22	DA	925	ASP
22	DA	943	LYS
22	DA	970	ASN
22	DA	992	ASP
22	DA	997	ARG
22	DA	1020	LEU
22	DA	1025	VAL
22	DA	1029	VAL
22	DA	1039	SER
22	DA	1052	ARG
22	DA	1165	LEU
22	DA	1169	ARG
22	DA	1203	GLU
23	DB	21	GLU
23	DB	71	ARG
23	DB	140	GLU
23	DB	184	ASN
23	DB	262	MET
23	DB	266	THR
23	DB	293	GLU
23	DB	431	LEU
23	DB	539	ARG
23	DB	559	LYS
23	DB	603	LYS
23	DB	640	VAL
23	DB	746	SER
23	DB	771	VAL
23	DB	818	THR

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Mol	Chain	Res	Type
23	DB	942	SER
23	DB	945	CYS
24	DD	893	GLU
24	DD	894	LEU
24	DD	897	ASP
24	DD	899	VAL
24	DD	913	LEU
24	DD	917	ILE
24	DD	919	GLU
24	DD	924	LYS
24	DD	931	ASP
24	DD	933	ARG
24	DD	935	GLU
24	DD	940	VAL
24	DD	944	LEU
24	DD	950	LEU
24	DD	965	ILE
24	DD	966	LEU
24	DD	1005	ASN
24	DD	1006	LEU
25	DE	431	GLU
25	DE	432	LEU
25	DE	433	LYS
25	DE	446	GLU
25	DE	449	LYS
25	DE	450	ARG
25	DE	451	VAL
25	DE	471	GLN
25	DE	479	THR
25	DE	481	ASP
25	DE	508	LYS
25	DE	509	GLN
25	DE	519	GLU
25	DE	521	ASP
25	DE	523	VAL
25	DE	745	GLU
25	DE	746	ASP
25	DE	747	LEU
26	DF	14	LEU
26	DF	39	LEU
26	DF	55	LEU
26	DF	60	MET

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Mol	Chain	Res	Type
26	DF	62	LYS
26	DF	63	ARG
26	DF	65	LYS
26	DF	66	LEU
26	DF	110	LYS
26	DF	114	LEU
26	DF	115	SER
26	DF	116	ASP
26	DF	117	ILE
26	DF	118	ILE
26	DF	122	LEU
26	DF	131	LEU
26	DF	132	LYS
26	DF	207	ARG
26	DF	208	LEU
26	DF	209	LYS
26	DF	211	ARG
26	DF	218	VAL
26	DF	238	LYS
26	DF	239	ARG
26	DF	243	LEU
26	DF	245	SER
26	DF	246	ILE
26	DF	261	THR
26	DF	269	VAL
26	DF	271	VAL
26	DF	280	ILE
26	DF	295	LEU
26	DF	299	LYS
26	DF	301	VAL
26	DF	304	LEU
26	DF	305	ILE
26	DF	308	VAL
26	DF	309	MET
26	DF	312	ILE
26	DF	313	VAL
26	DF	315	ARG
26	DF	316	GLN
26	DF	317	LEU
26	DF	318	CYS
26	DF	319	LEU
26	DF	320	ARG

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Mol	Chain	Res	Type
26	DF	323	VAL
26	DF	327	TRP
26	DF	330	ARG
26	DF	339	GLN
26	DF	342	LYS
26	DF	345	SER
26	DF	346	THR
26	DF	348	THR
26	DF	351	ILE
26	DF	368	THR
26	DF	391	LEU
26	DF	396	LEU
26	DF	406	VAL
26	DF	411	VAL
26	DF	412	LEU
26	DF	413	SER
26	DF	416	ASP
26	DF	427	LEU
27	DG	41	ASP
27	DG	129	LYS
27	DG	131	ILE
27	DG	143	VAL
27	DG	161	ASP
27	DG	180	ARG
27	DG	181	TRP
27	DG	182	GLU
27	DG	183	ILE
28	DH	34	ARG
28	DH	35	ARG
28	DH	37	LEU
28	DH	38	GLN
28	DH	42	SER
28	DH	43	SER
28	DH	50	PHE
28	DH	104	VAL
28	DH	106	THR
28	DH	107	LEU
28	DH	113	ARG
28	DH	116	ARG
28	DH	117	MET
28	DH	118	VAL
28	DH	119	ILE

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Mol	Chain	Res	Type
28	DH	120	THR
28	DH	132	LYS
28	DH	155	ASP
28	DH	159	TYR
28	DH	160	ILE
28	DH	161	LYS
28	DH	162	THR
28	DH	164	THR
28	DH	167	GLU
28	DH	169	VAL
29	DI	31	TYR
29	DI	32	GLU
29	DI	35	VAL
29	DI	62	LYS
29	DI	63	LYS
29	DI	65	THR
29	DI	67	ASP
29	DI	69	ASP
29	DI	70	ASP
29	DI	81	GLN
29	DI	84	THR
29	DI	107	ILE
29	DI	108	LYS
29	DI	111	SER
29	DI	129	LEU
29	DI	130	LYS
30	DJ	125	ASP
30	DJ	127	THR
30	DJ	129	THR
30	DJ	130	ILE
30	DJ	151	ILE
30	DJ	155	ILE
30	DJ	172	GLN
30	DJ	175	LYS
30	DJ	177	LYS
30	DJ	192	LYS
30	DJ	193	TYR
31	DL	56	GLN
31	DL	59	THR
31	DL	60	LYS
31	DL	61	LYS
31	DL	62	LYS

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Mol	Chain	Res	Type
31	DL	63	LEU
31	DL	64	GLN
31	DL	107	LYS
31	DL	110	THR
31	DL	111	LEU
31	DL	128	ILE
32	Dc	24	ASP
32	Dc	106	VAL
25	De	546	VAL
26	Df	214	HIS
26	Df	253	TYR
26	Df	261	THR
26	Df	272	VAL
26	Df	299	LYS
26	Df	301	VAL
26	Df	302	HIS
26	Df	305	ILE
26	Df	309	MET
26	Df	313	VAL
26	Df	314	SER
26	Df	322	ASP
26	Df	323	VAL
26	Df	326	HIS
26	Df	356	THR
26	Df	366	GLU
26	Df	383	LEU
26	Df	387	VAL
26	Df	388	ILE
26	Df	389	LYS
26	Df	391	LEU
26	Df	421	ASP
34	Dm	31	LEU
35	EA	15	LYS
35	EA	19	LYS
35	EA	21	VAL
35	EA	22	ILE
35	EA	23	ARG
35	EA	28	ILE
35	EA	32	LEU
35	EA	38	ILE
35	EA	39	ARG
35	EA	40	ASN

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Mol	Chain	Res	Type
35	EA	43	VAL
35	EA	44	LYS
35	EA	46	GLU
35	EA	48	MET
35	EA	50	GLU
35	EA	51	LEU
35	EA	56	ARG
35	EA	57	LYS
35	EA	60	ARG
35	EA	65	ASN
35	EA	67	LYS
35	EA	70	LYS
35	EA	72	ILE
35	EA	73	LYS
35	EA	75	ARG
35	EA	77	ARG
35	EA	100	VAL
35	EA	109	HIS
35	EA	111	ARG
35	EA	112	ARG
35	EA	139	LEU
35	EA	143	GLN
35	EA	145	PHE
35	EA	158	HIS
35	EA	161	VAL
35	EA	162	GLU
35	EA	187	ILE
36	EB	84	TYR
36	EB	97	LEU
36	EB	102	ILE
36	EB	132	VAL
36	EB	140	LYS
36	EB	159	ASP
36	EB	160	GLN
36	EB	167	LEU
36	EB	171	ILE
36	EB	209	GLN
36	EB	223	VAL
36	EB	224	THR
37	1	188	LEU
37	1	189	THR
37	1	191	ASP

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Mol	Chain	Res	Type
37	1	204	LYS
37	1	206	LYS
37	1	207	TYR
37	1	215	MET
37	1	216	THR
37	1	217	GLU
37	1	218	LYS
37	1	222	THR
37	1	223	ARG
37	1	237	THR
37	1	239	SER
37	1	240	LYS
37	1	242	LEU
37	1	461	LEU
38	2	18	THR
38	2	20	GLU
38	2	21	ILE
38	2	22	LEU
38	2	54	ARG
38	2	194	ILE
38	2	318	LEU
39	3	74	LYS
39	3	132	LEU
39	3	195	VAL
39	3	224	LEU
40	4	14	LEU
40	4	56	VAL
40	4	105	LEU
40	4	145	VAL
40	4	262	LEU
40	4	290	LEU
40	4	386	THR
40	4	387	ILE
40	4	388	THR
40	4	391	ILE
40	4	398	ARG
40	4	408	LEU
40	4	413	LEU
40	4	431	LEU
40	4	432	VAL
40	4	441	MET
40	4	442	VAL

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Mol	Chain	Res	Type
40	4	451	VAL
41	5	2	VAL
41	5	8	VAL
41	5	9	LEU
41	5	35	ILE
41	5	38	ILE
42	6	107	VAL
42	6	123	LEU
42	6	136	ILE
42	6	140	LEU
42	6	141	ARG
42	6	154	GLN
42	6	170	LEU
42	6	183	ASP
42	6	184	VAL
42	6	185	ILE
42	6	186	GLN
42	6	188	LEU
42	6	194	ILE
42	6	195	ARG
42	6	196	GLU
42	6	267	THR
42	6	270	PHE
42	6	271	GLU
42	6	272	VAL
42	6	416	THR
42	6	418	LYS
42	6	419	ARG
42	6	420	SER
42	6	580	ILE
43	7	17	ILE
43	7	19	PRO
43	7	48	LYS
43	7	60	GLN
43	7	77	VAL
43	7	112	ARG
43	7	113	LYS
43	7	120	GLU
43	7	174	ILE
43	7	178	ASP
43	7	180	LEU
43	7	181	LYS

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Mol	Chain	Res	Type
43	7	185	ARG
43	7	186	ARG
43	7	187	GLN
43	7	190	CYS
43	7	194	LEU
43	7	203	ASN
43	7	296	SER
43	7	299	ARG
43	7	300	GLU
43	7	301	THR
43	7	302	ASP
43	7	304	HIS
43	7	309	VAL
43	7	487	ARG
43	7	488	VAL
43	7	557	ILE
43	7	668	ILE
43	7	671	LYS
43	7	697	ILE
43	7	705	ASN
43	7	728	PHE
43	7	741	LEU
43	7	742	GLU
44	c	36	LYS
44	c	44	THR
44	c	45	LEU
44	c	72	ARG
44	c	73	LEU
44	c	77	VAL
44	c	274	ILE
44	c	275	LYS
44	c	276	LEU
44	c	283	ARG
44	c	284	CYS
44	c	300	ARG
44	c	301	THR
46	b	57	VAL
46	b	74	LEU
46	b	82	LEU
46	b	92	GLN
46	b	99	ILE
46	b	103	ASP

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Mol	Chain	Res	Type
46	b	122	LEU
46	b	126	CYS
46	b	127	LEU
46	b	132	ASP
49	a	58	LEU
49	a	61	CYS
49	a	62	LEU
49	a	64	THR
49	a	66	GLN
49	a	67	LYS
49	a	69	LEU
49	a	70	LYS
49	a	71	VAL
49	a	72	THR
49	a	74	LEU
49	a	77	MET
49	a	78	THR
49	a	80	ARG
49	a	82	GLU
49	a	83	SER
49	a	86	ARG
49	a	87	GLN
49	a	93	HIS
49	a	106	ASP
49	a	107	MET
49	a	108	PHE
49	a	109	TYR
49	a	111	GLU
49	a	128	HIS
49	a	131	ASN
49	a	133	VAL
49	a	135	CYS
49	a	145	LYS
49	a	148	ASP
49	a	160	LEU
49	a	162	ASN
49	a	167	ASN
49	a	168	LYS
49	a	173	MET
49	a	201	ASP
49	a	214	ARG
49	a	226	VAL

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Mol	Chain	Res	Type
49	a	232	LEU
49	a	246	ASN
49	a	253	MET
49	a	254	ASN
49	a	258	THR
49	a	259	ILE
49	a	267	LYS
49	a	278	HIS
49	a	297	VAL
49	a	305	LEU
49	a	309	GLN
49	a	324	CYS
49	a	325	THR
49	a	327	ILE
49	a	329	LEU
49	a	332	THR
49	a	333	GLN
49	a	335	THR
49	a	339	LEU
49	a	348	LEU
49	a	357	LEU
49	a	367	LEU
49	a	373	CYS
49	a	376	LEU
49	a	384	ASP
49	a	388	LEU
49	a	391	THR
49	a	400	HIS
49	a	421	ILE
49	a	430	LEU
49	a	432	GLU
49	a	433	ASP
49	a	437	LEU
49	a	438	LEU
49	a	443	CYS
49	a	467	MET
49	a	479	LEU
49	a	481	LYS
49	a	501	CYS
49	a	504	ILE
49	a	509	ARG
49	a	514	LYS

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Mol	Chain	Res	Type
50	d	28	GLU
50	d	30	LEU
50	d	51	SER
50	d	62	GLU
50	d	63	ASN
50	d	64	GLN
50	d	66	LEU
50	d	67	GLU
50	d	69	LEU
50	d	70	ILE
50	d	71	HIS
50	d	72	ARG
50	d	73	ASP
50	d	78	GLU
50	d	79	LEU
50	d	80	MET
50	d	81	LYS
50	d	82	LEU
50	d	85	ASN
50	d	92	GLU
50	d	93	MET
50	d	98	LYS
50	d	101	GLU
50	d	106	ASP
50	d	107	ILE
50	d	108	GLN
50	d	110	LEU
50	d	114	LEU
50	d	115	LYS
50	d	116	GLU
50	d	119	GLN
50	d	121	LEU
50	d	126	TYR
50	d	127	GLN
50	d	129	LYS
50	d	130	GLU
50	d	131	LYS
50	d	132	LEU
50	d	133	LYS
50	d	135	ILE
50	d	173	ARG
50	d	181	GLU

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Mol	Chain	Res	Type
50	d	184	SER
50	d	186	LEU
50	d	187	LEU
50	d	189	GLN
51	f	16	VAL
51	f	19	SER
51	f	20	TRP
51	f	24	LEU
51	f	30	LEU
51	f	41	TYR
51	f	48	GLU
51	f	49	VAL
51	f	50	VAL
51	f	51	LYS
51	f	52	MET
51	f	53	GLN
51	f	56	THR
51	f	57	LEU
51	f	60	LEU
51	f	64	VAL
51	f	66	ILE
51	f	114	VAL
51	f	117	SER
51	f	120	LEU
51	f	137	CYS
52	g	11	LEU
52	g	15	MET
52	g	18	ILE
52	g	20	GLU
52	g	26	ILE
52	g	27	GLN
52	g	28	GLU
52	g	39	LYS
52	g	45	PHE
52	g	54	LEU
52	g	55	ILE
52	g	64	ILE
52	g	72	PHE
52	g	74	HIS
52	g	83	MET
52	g	92	LEU
52	g	95	ILE

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Mol	Chain	Res	Type
52	g	119	VAL
52	g	126	TYR
52	g	132	ARG
52	g	137	VAL
52	g	143	LYS
52	g	154	GLN
52	g	159	ARG
52	g	166	ASN
52	g	171	LEU
53	h	7	GLN
53	h	15	LEU
53	h	16	LEU
53	h	17	SER
53	h	18	GLN
53	h	19	VAL
53	h	22	LEU
53	h	23	LYS
53	h	30	ILE
53	h	32	LYS
53	h	33	LEU
53	h	34	GLU
53	h	37	TYR
53	h	39	ARG
53	h	40	LEU
53	h	49	PHE
53	h	66	GLU
53	h	100	PHE
53	h	101	SER
53	h	102	HIS
53	h	110	ARG
53	h	111	THR
53	h	112	LYS
53	h	117	VAL
53	h	130	ARG
53	h	131	ILE
53	h	143	LEU
53	h	170	LYS
53	h	185	VAL
53	h	187	PHE
53	h	189	LYS
53	h	192	SER
54	i	86	ASP

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Mol	Chain	Res	Type
54	i	87	LEU
54	i	88	ASN
54	i	90	LEU
54	i	95	GLN
54	i	100	LEU
54	i	112	GLU
54	i	122	ARG
54	i	136	LYS
55	j	51	ILE
55	j	52	ASP
55	j	53	LYS
55	j	62	THR
56	k	8	ASN
56	k	10	ARG
56	k	11	LEU
56	k	12	ARG
56	k	14	LEU
56	k	15	GLU
56	k	18	GLU
56	k	19	ARG
56	k	21	ILE
56	k	25	LEU
56	k	26	GLN
56	k	32	ILE
56	k	33	LEU
56	k	34	GLU
56	k	35	LEU
56	k	36	SER
56	k	37	LYS
56	k	40	THR
56	k	42	GLU
56	k	43	ARG
56	k	44	LEU
56	k	45	LEU
56	k	48	GLN
56	k	53	THR
56	k	56	VAL
56	k	57	GLN
56	k	58	HIS
56	k	60	GLU
56	k	64	SER
56	k	67	ILE

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Mol	Chain	Res	Type
56	k	70	LEU
56	k	75	THR
56	k	82	SER
56	k	83	SER
56	k	86	SER
56	k	87	ARG
56	k	88	LYS
56	k	90	CYS
56	k	91	GLN
56	k	92	MET
56	k	94	LEU
56	k	96	ARG
56	k	97	VAL
56	k	101	ARG
56	k	102	LEU
56	k	103	LYS
56	k	104	LEU
56	k	107	VAL
56	k	109	ARG
56	k	114	MET
57	n	149	LEU
57	n	154	ILE
57	n	159	ASP
57	n	166	TYR
57	n	168	ARG
57	n	169	LEU
57	n	212	LEU
57	n	229	GLU
57	n	252	ILE
57	n	253	LEU
57	n	254	VAL
57	n	255	GLU
57	n	261	ASP
57	n	265	LEU
57	n	266	VAL
57	n	267	HIS
57	n	283	PHE
57	n	286	GLU
57	n	287	LYS
57	n	289	LEU
57	n	363	GLU
57	n	371	GLN

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Mol	Chain	Res	Type
57	n	528	HIS
57	n	959	LEU
57	n	960	LYS
57	n	961	THR
57	n	965	MET
58	o	715	LEU
58	o	717	SER
58	o	721	LEU
59	q	7	VAL
59	q	16	GLU
59	q	19	VAL
59	q	22	VAL
59	q	28	GLU
59	q	29	THR
59	q	31	LEU
59	q	34	LEU
59	q	36	MET
59	q	91	SER
59	q	92	LEU
59	q	93	TRP
59	q	95	TRP
59	q	98	VAL
59	q	100	ASN
59	q	103	ARG
59	q	107	THR
59	q	109	MET
59	q	110	CYS
59	q	111	VAL
59	q	112	LEU
59	q	115	VAL
59	q	116	LEU
59	q	118	ILE
59	q	120	ARG
59	q	122	LYS
59	q	123	LYS
59	q	124	PHE
59	q	125	MET
59	q	128	ASP
59	q	130	VAL
59	q	131	SER
59	q	132	GLN
59	q	133	ASP

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Mol	Chain	Res	Type
59	q	135	LEU
59	q	138	LYS
59	q	139	GLN
59	q	143	THR
59	q	144	LEU
59	q	145	GLN
59	q	146	LEU
59	q	147	ILE
59	q	149	LYS
59	q	153	LEU
59	q	159	ILE
59	q	161	LEU
59	q	165	GLU
59	q	166	ARG
59	q	168	THR
59	q	169	LYS
59	q	171	VAL
59	q	172	THR
59	q	184	ASN
59	q	185	SER
59	q	187	LEU
59	q	188	LEU
59	q	428	LEU
59	q	430	LYS
59	q	431	ILE
59	q	432	ILE
59	q	434	GLN
59	q	438	ILE
59	q	440	LEU
59	q	441	ARG
59	q	442	SER
59	q	443	ARG
59	q	447	THR
59	q	448	ILE
59	q	451	LEU
59	q	544	MET
59	q	629	LYS
59	q	631	GLU
59	q	633	ARG
59	q	646	LEU
59	q	647	SER
59	q	650	LEU

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Mol	Chain	Res	Type
60	r	6	VAL
60	r	7	THR
60	r	9	MET
60	r	11	VAL
60	r	12	THR
60	r	16	ILE
60	r	17	ASN
60	r	18	MET
60	r	32	LEU
60	r	35	LEU
60	r	42	LEU
60	r	47	GLU
60	r	53	ASP
60	r	56	MET
60	r	60	LEU
60	r	85	LEU
60	r	88	LEU
60	r	93	MET
60	r	101	LEU
60	r	107	ASP
60	r	124	ARG
60	r	143	ILE
60	r	152	LEU
60	r	156	ASN
60	r	168	LEU
60	r	179	GLN
60	r	187	LYS
60	r	197	VAL
60	r	200	GLU
60	r	201	LYS
60	r	202	ILE
60	r	206	ARG
61	s	65	PHE
61	s	84	ILE
61	s	89	LEU
62	t	1	MET
62	t	9	MET
62	t	16	SER
62	t	17	VAL
62	t	21	VAL
62	t	23	LEU
62	t	24	LEU

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Mol	Chain	Res	Type
62	t	28	LEU
62	t	34	GLU
62	t	43	CYS
62	t	47	HIS
62	t	61	LYS
62	t	62	LEU
62	t	66	MET
62	t	67	HIS
62	t	70	GLU
62	t	78	LEU
62	t	79	PHE
62	t	80	GLU
62	t	81	ASN
62	t	84	CYS
62	t	85	LEU
62	t	98	LEU
62	t	99	LYS
62	t	101	PHE
62	t	103	GLN
62	t	106	LYS
62	t	109	LYS
62	t	110	ILE
62	t	124	VAL
62	t	138	ILE
62	t	148	VAL
62	t	149	VAL
62	t	156	LEU
62	t	162	GLN
62	t	173	PRO
62	t	179	ARG
62	t	183	VAL
62	t	193	TYR
62	t	196	LEU
62	t	200	ILE
62	t	204	GLN
63	u	20	CYS
63	u	26	LEU
63	u	27	GLN
63	u	76	LEU
63	u	80	GLU
64	v	14	LEU
64	v	15	LEU

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Mol	Chain	Res	Type
64	v	22	LEU
64	v	26	ILE
64	v	37	ILE
64	v	38	LYS
64	v	39	THR
64	v	41	LYS
64	v	43	GLU
64	v	45	GLU
64	v	47	GLN
64	v	50	ARG
64	v	52	THR
64	v	55	GLU
64	v	56	GLN
64	v	58	ASN
64	v	60	GLU
64	v	61	MET
64	v	62	HIS
64	v	63	VAL
64	v	69	VAL
64	v	81	ASP
64	v	82	LEU
64	v	86	LEU
64	v	87	ILE
64	v	98	ILE
64	v	103	GLN
64	v	105	LEU
64	v	108	LEU
64	v	110	GLU
64	v	112	CYS
64	v	114	ARG
64	v	115	LYS
64	v	116	LEU
64	v	117	ILE
64	v	118	THR
64	v	119	LEU
64	v	120	ARG
64	v	123	ILE
64	v	125	ILE
64	v	130	LEU
64	v	131	GLU
64	v	132	GLU
64	v	133	GLU

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Mol	Chain	Res	Type
64	v	138	SER
65	z	492	ARG
65	z	528	LEU
65	z	530	VAL
65	z	540	LEU
65	z	551	ASP
65	z	564	ASN
65	z	567	GLN
65	z	572	ASN
65	z	579	CYS
65	z	582	LEU
65	z	585	HIS
65	z	591	LEU
65	z	593	ILE
65	z	599	LEU
66	x	4	VAL
66	x	11	LEU
66	x	118	ILE
66	x	239	THR
66	x	359	CYS
66	x	477	TYR
66	x	482	SER
66	x	484	LYS
66	x	564	SER
66	x	565	SER
66	x	686	LYS
66	x	802	MET
66	x	897	LEU
66	x	959	SER
66	x	965	LYS
66	x	966	VAL
66	x	989	LEU
67	w	1	MET
67	w	2	GLU
67	w	7	SER
67	w	10	GLU
67	w	11	GLU
67	w	12	VAL
67	w	17	VAL
67	w	18	ILE
67	w	36	LYS
67	w	37	LEU

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Mol	Chain	Res	Type
67	w	41	LEU
67	w	51	LEU
67	w	171	LEU
67	w	205	VAL
67	w	723	THR
67	w	726	ASN
67	w	1130	VAL
67	w	1134	GLN
68	p	162	VAL
68	p	170	LEU
68	p	228	VAL
68	p	249	VAL
68	p	252	LYS
68	p	289	ASP
68	p	401	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (476) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	156	GLN
1	0	160	GLN
1	0	200	GLN
1	0	249	GLN
1	0	298	GLN
2	8	22	GLN
2	8	56	ASN
2	8	67	GLN
2	8	83	HIS
2	8	86	ASN
2	8	135	HIS
2	8	166	ASN
2	8	171	HIS
2	8	221	GLN
3	9	7	GLN
3	9	10	HIS
3	9	37	ASN
3	9	100	HIS
3	9	211	GLN
3	9	275	GLN
3	9	288	ASN
4	DO	8	ASN
4	DO	13	ASN

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Mol	Chain	Res	Type
4	DO	31	GLN
4	DO	39	GLN
4	DO	54	ASN
4	DO	57	ASN
4	DO	70	ASN
5	DP	173	ASN
5	DP	278	GLN
6	DQ	60	HIS
6	DQ	352	HIS
7	BA	17	ASN
7	BA	129	ASN
7	BA	156	ASN
7	BA	229	GLN
8	FA	10	ASN
8	FA	152	HIS
8	FA	172	ASN
9	FB	14	GLN
9	FB	86	GLN
9	FB	91	GLN
9	FB	152	ASN
9	FB	158	ASN
9	FB	229	HIS
9	FB	231	ASN
10	PA	22	GLN
10	PA	77	ASN
10	PA	87	HIS
10	PA	123	ASN
10	PA	267	GLN
10	PA	353	ASN
10	PA	403	GLN
10	PA	410	ASN
10	PA	441	GLN
10	PA	472	HIS
10	PA	504	HIS
10	PA	507	GLN
10	PA	531	ASN
10	PA	601	ASN
10	PA	632	ASN
10	PA	671	ASN
10	PA	703	GLN
10	PA	721	HIS
10	PA	731	ASN

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Mol	Chain	Res	Type
10	PA	739	ASN
10	PA	742	ASN
10	PA	780	ASN
10	PA	791	GLN
10	PA	792	ASN
10	PA	1044	HIS
10	PA	1101	GLN
10	PA	1163	HIS
10	PA	1180	ASN
10	PA	1332	GLN
10	PA	1462	GLN
11	PB	43	GLN
11	PB	139	GLN
11	PB	143	GLN
11	PB	144	HIS
11	PB	197	GLN
11	PB	227	ASN
11	PB	245	GLN
11	PB	265	GLN
11	PB	370	HIS
11	PB	430	ASN
11	PB	452	ASN
11	PB	468	GLN
11	PB	471	ASN
11	PB	486	ASN
11	PB	570	ASN
11	PB	577	HIS
11	PB	585	ASN
11	PB	593	GLN
11	PB	639	HIS
11	PB	650	ASN
11	PB	716	HIS
11	PB	717	ASN
11	PB	749	HIS
11	PB	906	GLN
11	PB	913	GLN
11	PB	941	GLN
11	PB	1009	GLN
11	PB	1021	HIS
11	PB	1030	ASN
11	PB	1094	GLN
11	PB	1142	ASN

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Mol	Chain	Res	Type
12	PC	6	GLN
12	PC	83	GLN
12	PC	114	HIS
12	PC	157	GLN
12	PC	177	ASN
12	PC	262	GLN
12	PC	268	GLN
13	PD	34	ASN
13	PD	38	HIS
13	PD	47	GLN
13	PD	48	ASN
13	PD	89	GLN
13	PD	129	GLN
13	PD	135	GLN
14	PE	92	GLN
14	PE	95	GLN
14	PE	107	GLN
14	PE	108	GLN
14	PE	116	GLN
14	PE	133	GLN
14	PE	210	GLN
16	PG	139	GLN
17	PH	29	HIS
17	PH	126	GLN
18	PI	22	ASN
18	PI	91	HIS
19	PJ	26	GLN
20	PK	2	ASN
20	PK	29	ASN
20	PK	40	HIS
22	DA	401	ASN
22	DA	409	HIS
22	DA	569	ASN
22	DA	630	GLN
22	DA	693	GLN
22	DA	702	ASN
22	DA	802	HIS
22	DA	896	GLN
22	DA	1058	HIS
23	DB	30	HIS
23	DB	36	ASN
23	DB	123	ASN

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Mol	Chain	Res	Type
23	DB	176	HIS
23	DB	183	GLN
23	DB	235	HIS
23	DB	272	GLN
23	DB	348	GLN
23	DB	432	HIS
23	DB	439	HIS
23	DB	450	GLN
23	DB	509	ASN
23	DB	577	HIS
23	DB	644	GLN
23	DB	652	GLN
23	DB	662	GLN
23	DB	663	GLN
23	DB	745	GLN
23	DB	750	GLN
23	DB	813	ASN
23	DB	864	ASN
23	DB	908	GLN
23	DB	912	ASN
23	DB	963	HIS
24	DD	922	GLN
24	DD	952	GLN
24	DD	1053	GLN
24	DD	1075	HIS
25	DE	268	HIS
25	DE	326	ASN
25	DE	327	ASN
25	DE	351	GLN
25	DE	468	ASN
25	DE	471	GLN
25	DE	585	ASN
25	DE	616	HIS
25	DE	640	ASN
25	DE	733	ASN
26	DF	244	GLN
26	DF	270	ASN
26	DF	273	GLN
26	DF	275	ASN
26	DF	326	HIS
26	DF	343	HIS
26	DF	349	ASN

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Mol	Chain	Res	Type
27	DG	10	HIS
27	DG	48	HIS
27	DG	142	ASN
28	DH	145	HIS
29	DI	21	GLN
29	DI	38	GLN
29	DI	81	GLN
29	DI	98	GLN
30	DJ	160	GLN
30	DJ	173	HIS
31	DL	105	HIS
31	DL	117	GLN
32	Dc	27	GLN
32	Dc	50	HIS
24	Dd	912	ASN
25	De	223	HIS
25	De	256	HIS
25	De	258	ASN
25	De	320	HIS
25	De	368	ASN
25	De	424	GLN
25	De	638	ASN
25	De	660	ASN
25	De	733	ASN
26	Df	30	GLN
26	Df	37	GLN
26	Df	64	GLN
26	Df	119	ASN
26	Df	134	HIS
26	Df	325	ASN
30	Dj	210	ASN
33	Dk	186	HIS
33	Dk	202	ASN
33	Dk	205	HIS
31	Dl	73	ASN
31	Dl	105	HIS
34	Dm	107	ASN
35	EA	65	ASN
35	EA	109	HIS
35	EA	198	ASN
36	EB	95	HIS
36	EB	193	ASN

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Mol	Chain	Res	Type
36	EB	204	ASN
36	EB	209	GLN
37	1	126	GLN
37	1	187	ASN
37	1	210	ASN
37	1	298	ASN
37	1	300	ASN
37	1	328	GLN
37	1	384	HIS
37	1	393	GLN
37	1	402	ASN
37	1	447	GLN
37	1	450	ASN
37	1	501	GLN
37	1	534	ASN
38	2	49	HIS
38	2	98	GLN
38	2	99	ASN
38	2	123	ASN
38	2	234	HIS
38	2	275	HIS
38	2	323	HIS
38	2	324	HIS
38	2	340	ASN
38	2	365	ASN
39	3	92	ASN
39	3	148	ASN
39	3	235	GLN
39	3	237	GLN
40	4	54	ASN
40	4	64	GLN
40	4	117	ASN
40	4	202	GLN
40	4	260	ASN
40	4	289	ASN
40	4	363	GLN
40	4	458	GLN
41	5	36	GLN
41	5	64	ASN
42	6	64	GLN
42	6	190	GLN
42	6	307	ASN

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Mol	Chain	Res	Type
42	6	320	GLN
42	6	330	ASN
42	6	497	GLN
42	6	665	GLN
43	7	21	GLN
43	7	118	HIS
43	7	135	HIS
43	7	164	HIS
43	7	176	ASN
43	7	210	HIS
43	7	241	ASN
43	7	304	HIS
43	7	307	ASN
43	7	347	GLN
43	7	430	ASN
43	7	522	ASN
44	c	10	ASN
44	c	41	ASN
44	c	237	GLN
44	c	245	HIS
44	c	306	HIS
44	c	311	GLN
45	e	97	GLN
45	e	105	GLN
45	e	132	HIS
46	b	66	GLN
46	b	129	GLN
46	b	136	HIS
47	l	72	GLN
47	l	102	ASN
48	m	26	GLN
48	m	35	ASN
48	m	50	ASN
48	m	80	GLN
48	m	100	GLN
48	m	106	GLN
48	m	116	GLN
49	a	56	GLN
49	a	57	HIS
49	a	66	GLN
49	a	87	GLN
49	a	131	ASN

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Mol	Chain	Res	Type
49	a	146	ASN
49	a	221	ASN
49	a	254	ASN
49	a	333	GLN
49	a	359	HIS
49	a	399	GLN
49	a	413	HIS
49	a	459	ASN
50	d	63	ASN
50	d	64	GLN
50	d	71	HIS
50	d	85	ASN
50	d	90	HIS
50	d	91	HIS
50	d	94	GLN
50	d	111	GLN
50	d	113	GLN
50	d	119	GLN
50	d	127	GLN
50	d	189	GLN
51	f	72	HIS
51	f	84	GLN
51	f	87	GLN
51	f	127	GLN
51	f	140	HIS
52	g	47	ASN
52	g	50	GLN
52	g	74	HIS
52	g	88	ASN
52	g	120	HIS
52	g	124	ASN
53	h	18	GLN
53	h	60	ASN
53	h	102	HIS
53	h	123	GLN
53	h	169	ASN
54	i	70	HIS
54	i	85	GLN
54	i	108	HIS
54	i	113	GLN
54	i	117	GLN
55	j	11	HIS

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Mol	Chain	Res	Type
55	j	38	ASN
56	k	41	ASN
56	k	66	GLN
56	k	77	GLN
56	k	79	HIS
56	k	91	GLN
57	n	267	HIS
57	n	304	GLN
57	n	311	GLN
57	n	330	HIS
57	n	410	HIS
57	n	411	GLN
57	n	494	GLN
57	n	507	GLN
57	n	532	ASN
57	n	590	GLN
57	n	668	HIS
57	n	669	GLN
57	n	672	GLN
57	n	698	GLN
57	n	716	ASN
57	n	841	ASN
57	n	848	HIS
57	n	880	ASN
57	n	883	ASN
58	o	701	ASN
59	q	39	ASN
59	q	139	GLN
59	q	142	GLN
59	q	262	GLN
59	q	290	HIS
59	q	292	GLN
59	q	340	GLN
59	q	367	HIS
59	q	374	ASN
59	q	434	GLN
59	q	437	HIS
59	q	461	GLN
59	q	463	HIS
59	q	492	GLN
59	q	496	ASN
59	q	506	HIS

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Mol	Chain	Res	Type
59	q	532	HIS
59	q	533	GLN
59	q	539	GLN
59	q	547	GLN
59	q	595	GLN
59	q	626	GLN
59	q	634	ASN
60	r	156	ASN
61	s	82	ASN
62	t	8	GLN
62	t	18	GLN
62	t	103	GLN
62	t	178	ASN
62	t	180	HIS
63	u	7	GLN
63	u	18	GLN
63	u	21	ASN
63	u	86	GLN
63	u	97	ASN
64	v	16	GLN
64	v	32	ASN
64	v	62	HIS
64	v	103	GLN
65	z	483	ASN
65	z	527	GLN
65	z	549	GLN
65	z	567	GLN
65	z	585	HIS
65	z	592	ASN
66	x	8	GLN
66	x	49	GLN
66	x	111	HIS
66	x	214	GLN
66	x	217	GLN
66	x	335	ASN
66	x	361	ASN
66	x	380	ASN
66	x	402	ASN
66	x	404	GLN
66	x	472	ASN
66	x	544	HIS
66	x	737	HIS

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Mol	Chain	Res	Type
66	x	799	HIS
67	w	46	GLN
67	w	113	GLN
67	w	239	ASN
67	w	295	GLN
67	w	357	HIS
67	w	358	GLN
67	w	378	GLN
67	w	421	HIS
67	w	433	ASN
67	w	438	ASN
67	w	513	ASN
67	w	596	HIS
67	w	616	GLN
67	w	618	HIS
67	w	638	GLN
67	w	726	ASN
67	w	822	HIS
67	w	841	GLN
67	w	851	ASN
67	w	874	HIS
67	w	923	ASN
67	w	972	HIS
67	w	1037	ASN
67	w	1040	GLN
67	w	1059	ASN
67	w	1124	ASN
67	w	1320	ASN
68	p	63	HIS
68	p	225	ASN
68	p	272	ASN
68	p	400	GLN
68	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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
73	SF4	7	801	43	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
73	SF4	7	801	43	-	-	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.

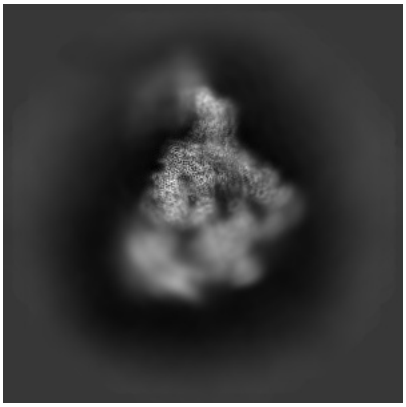
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31204. These allow visual inspection of the internal detail of the map and identification of artifacts.

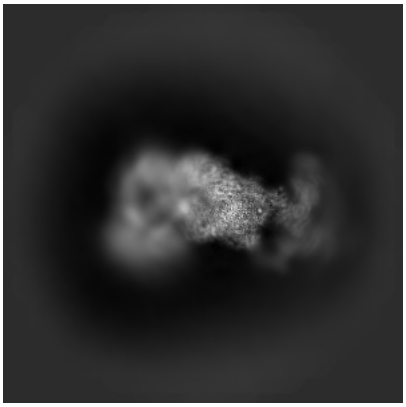
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

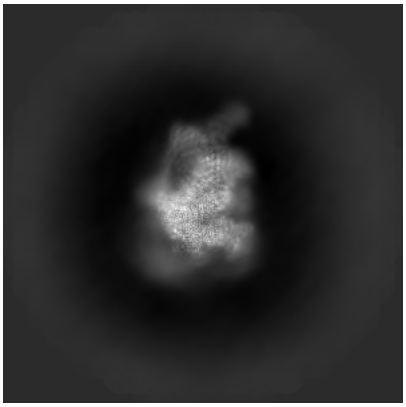
6.1.1 Primary map



X



Y

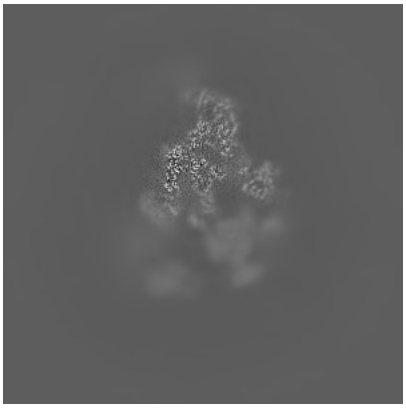


Z

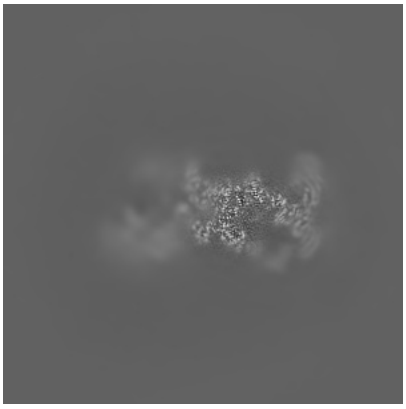
The images above show the map projected in three orthogonal directions.

6.2 Central slices

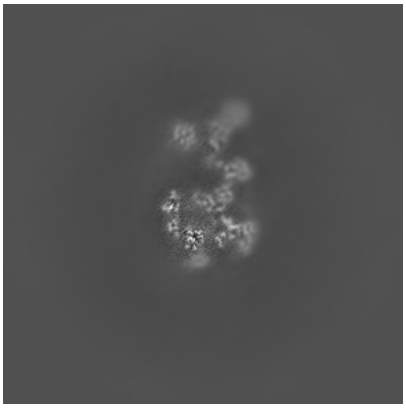
6.2.1 Primary map



X Index: 256



Y Index: 256

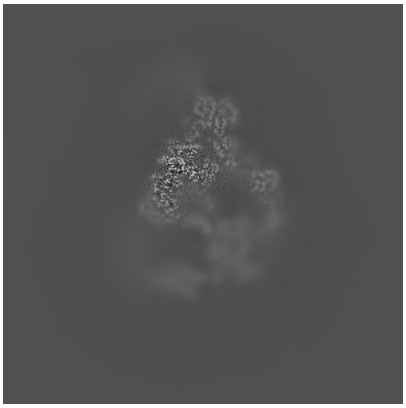


Z Index: 256

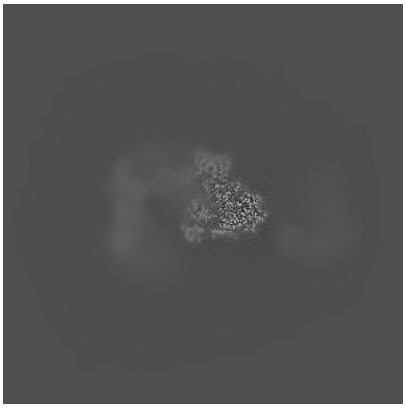
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

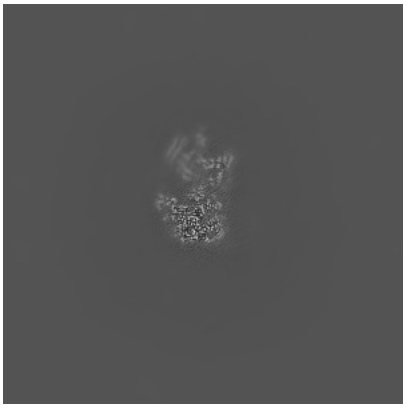
6.3.1 Primary map



X Index: 245



Y Index: 219

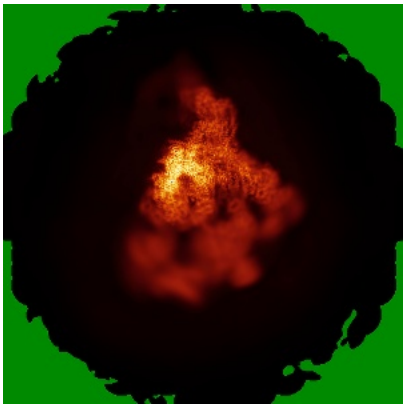


Z Index: 301

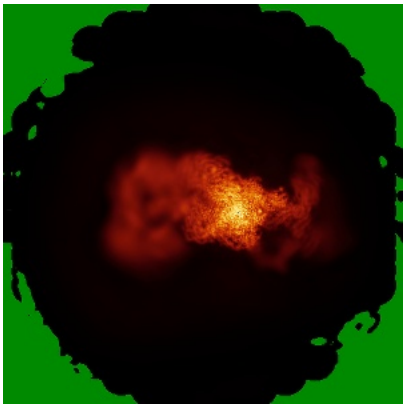
The images above show the largest variance slices of the map in three orthogonal directions.

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

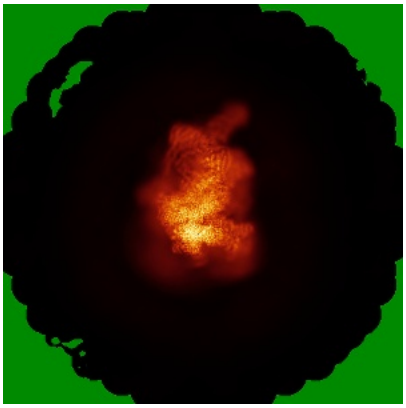
6.4.1 Primary map



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)

This section was not generated.

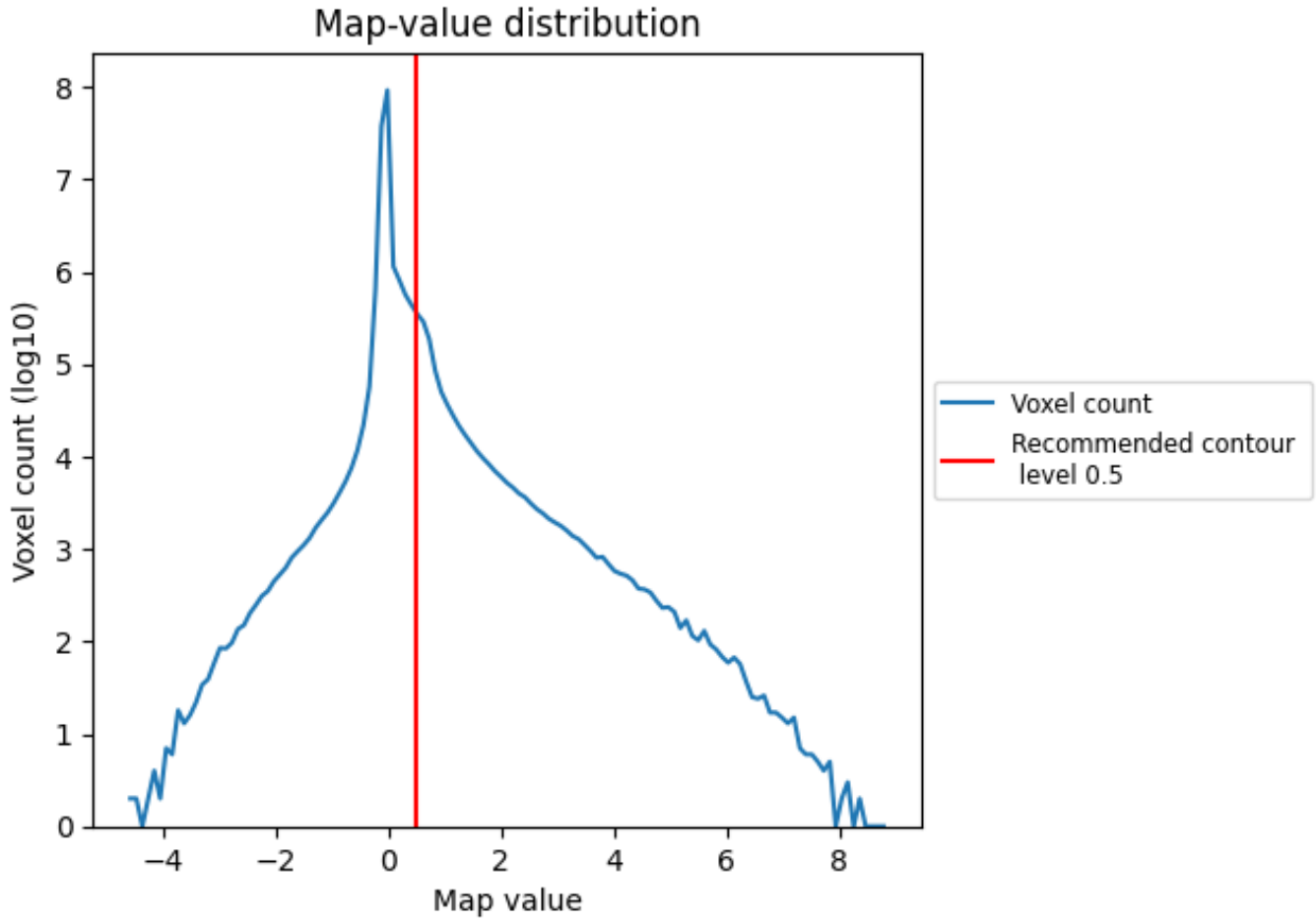
6.6 Mask visualisation (i)

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

7 Map analysis

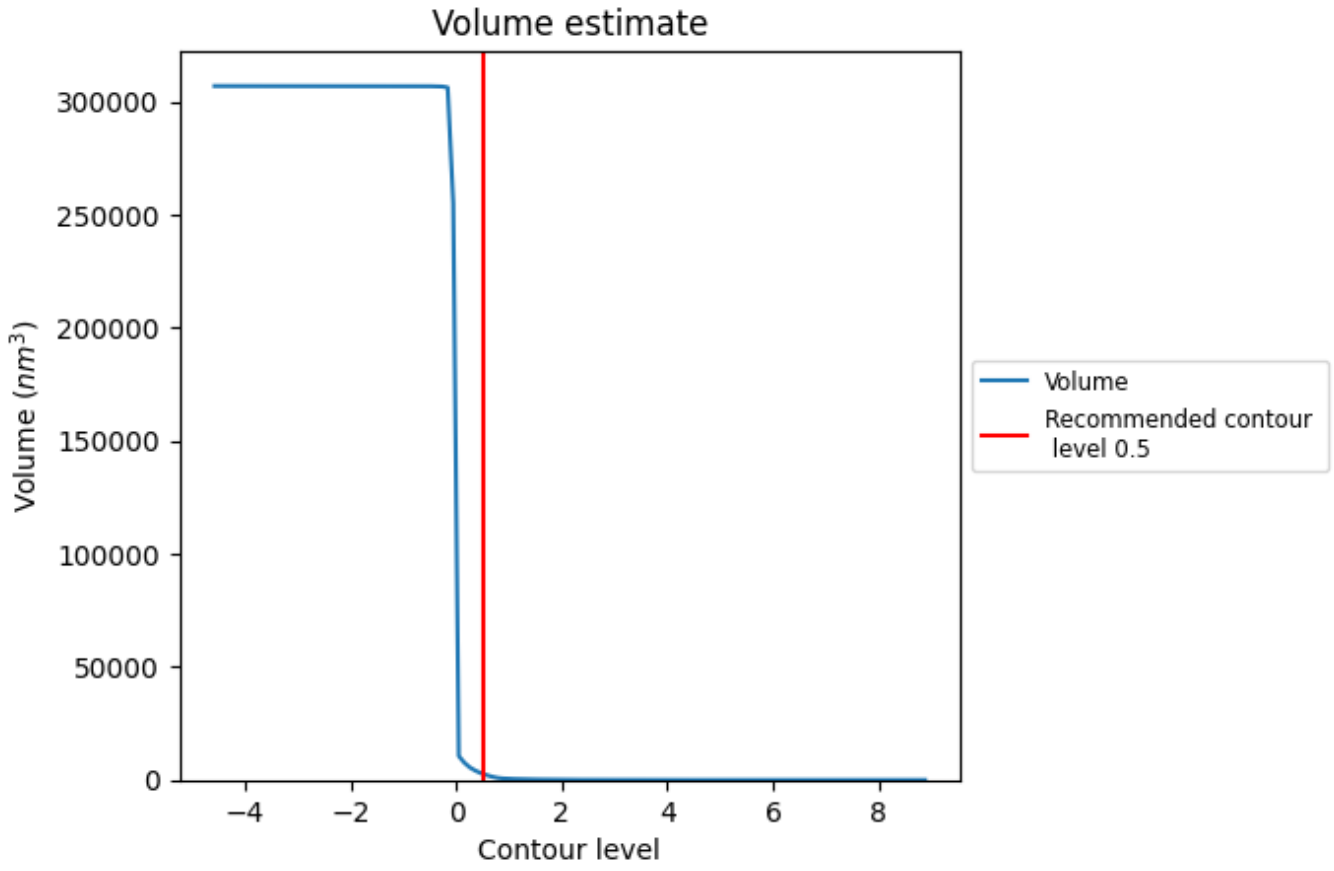
This section contains the results of statistical analysis of the map.

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.

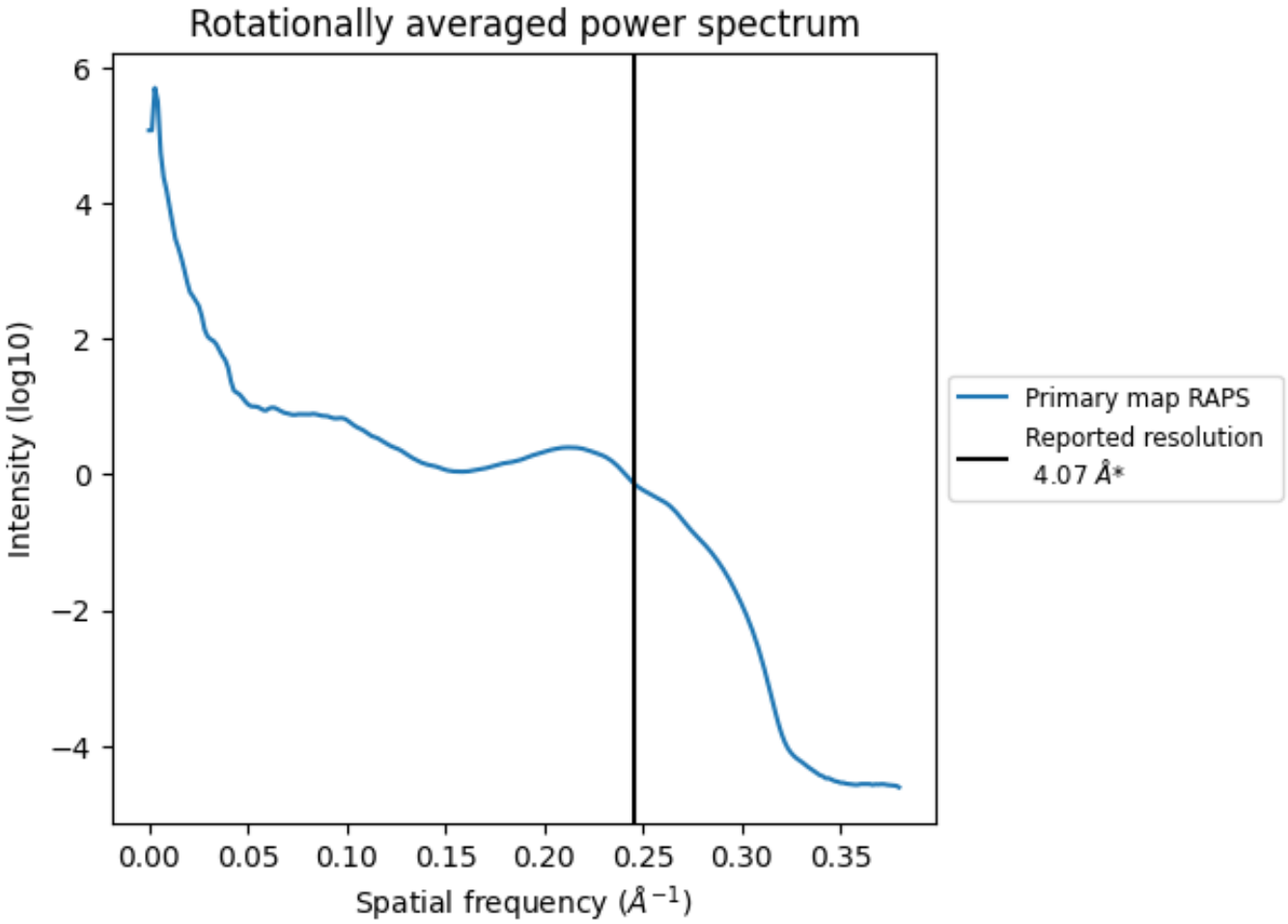
7.2 Volume estimate



The volume at the recommended contour level is 2784 nm^3; this corresponds to an approximate mass of 2515 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 0.246 Å^{-1}

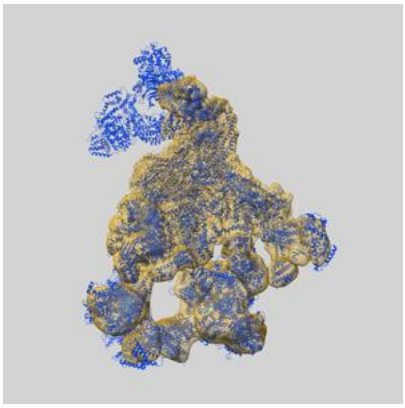
8 Fourier-Shell correlation

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

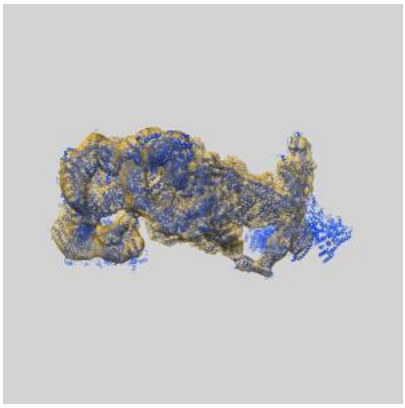
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31204 and PDB model 7ENA. Per-residue inclusion information can be found in section 3 on page 18.

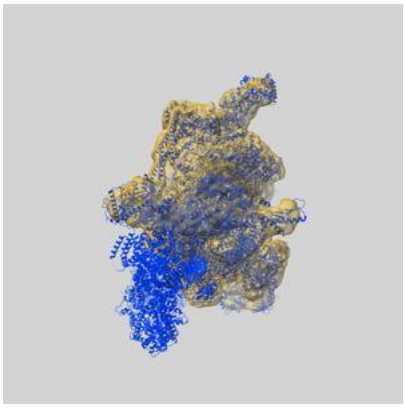
9.1 Map-model overlay



X



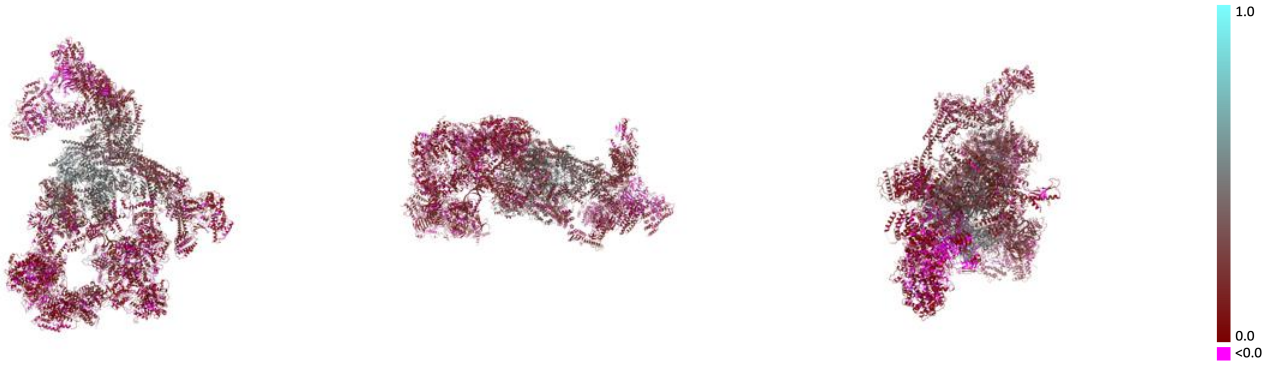
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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



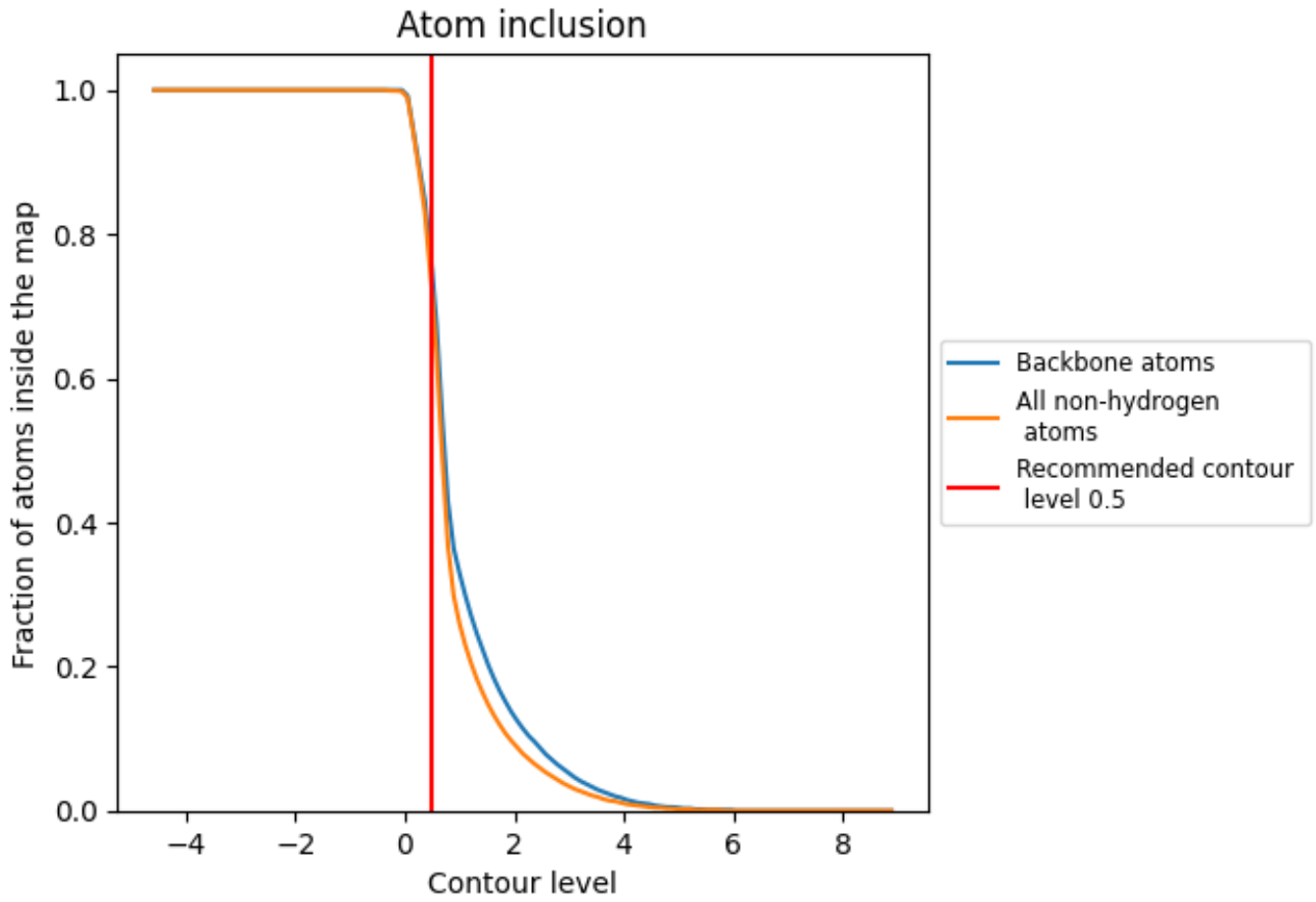
X Y Z

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

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7170	0.1680
0	0.7760	0.1210
1	0.6320	0.0350
2	0.8070	0.0600
3	0.9160	0.0610
4	0.7590	0.0700
5	0.8320	0.0600
6	0.8640	0.0830
7	0.9110	0.1070
8	0.8330	0.1070
9	0.6160	0.0680
BA	0.9210	0.2770
DA	0.8310	0.0650
DB	0.8880	0.0600
DD	0.7420	0.0830
DE	0.8120	0.0650
DF	0.7670	0.0520
DG	0.8530	0.0550
DH	0.8340	0.0500
DI	0.8170	0.0540
DJ	0.8740	0.0580
DL	0.5260	0.0640
DO	0.9130	0.1060
DP	0.9510	0.1750
DQ	0.7990	0.1050
Dc	0.0000	0.0350
Dd	0.0000	0.0350
De	0.0040	0.0330
Df	0.4390	0.0530
Di	0.0000	0.0290
Dj	0.0000	0.0260
Dk	0.0000	0.0420
Dl	0.0000	0.0460
Dm	0.0000	0.0440
EA	0.9470	0.1860

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Chain	Atom inclusion	Q-score
EB	0.9150	0.1040
FA	0.8960	0.0700
FB	0.8840	0.1080
PA	0.9540	0.4180
PB	0.9500	0.4520
PC	0.9630	0.4890
PD	0.9350	0.4060
PE	0.9720	0.3600
PF	0.9770	0.5210
PG	0.9610	0.4380
PH	0.9610	0.4530
PI	0.9710	0.3540
PJ	0.9740	0.5150
PK	0.9360	0.4430
PL	0.9580	0.4470
X	0.9510	0.1560
Y	0.9660	0.1760
a	0.5990	0.0940
b	0.7900	0.1460
c	0.8980	0.2830
d	0.9100	0.1440
e	0.8860	0.1890
f	0.9330	0.2460
g	0.9520	0.1380
h	0.8910	0.2730
i	0.9110	0.1540
j	0.9320	0.1050
k	0.9320	0.2870
l	0.9220	0.1950
m	0.9190	0.1730
n	0.8870	0.1890
o	0.9030	0.1670
p	0.0000	-0.0140
q	0.9170	0.3040
r	0.9260	0.3830
s	0.9400	0.1130
t	0.8860	0.3610
u	0.9390	0.1550
v	0.9140	0.3410
w	0.0420	0.0510
x	0.1950	0.0640
z	0.8980	0.1220